

– Electronic Supplementary Information –

Electrophilic Reactivities of Cyclic Enones and α,β -Unsaturated Lactones

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Additional Tables and Figures

Table S1. Calculated pyramidalization Δ in the transition states of the reactions of **7** with the cyclohexenones **2a**, **2b**, and **2c**.

Electrophile	Pyramidalization Δ (in Å) ^[a]	
	<i>cis</i> -TS	<i>trans</i> -TS
2a	0.220 (2a_sy_c_1_ts1) ^[b]	0.218 (2a_sy_tr_4_ts1) ^[b]
2b	0.243 (2b_sy_c_6_ts1) ^[b]	0.239 (2b_sy_tr_2_ts1) ^[b]
2c	0.288 (2c_sy_c_1_ts1) ^[b]	0.302 (2c_sy_tr_2_ts1_rot1) ^[b]

[a] Pyramidalization Δ describes the distance of the attacked C-atom of the electrophile from the plane defined by the three surrounding atoms (for visualization see Figures 8 in the main text). [b] For geometries, see section 'Geometries of Optimized Structures'.

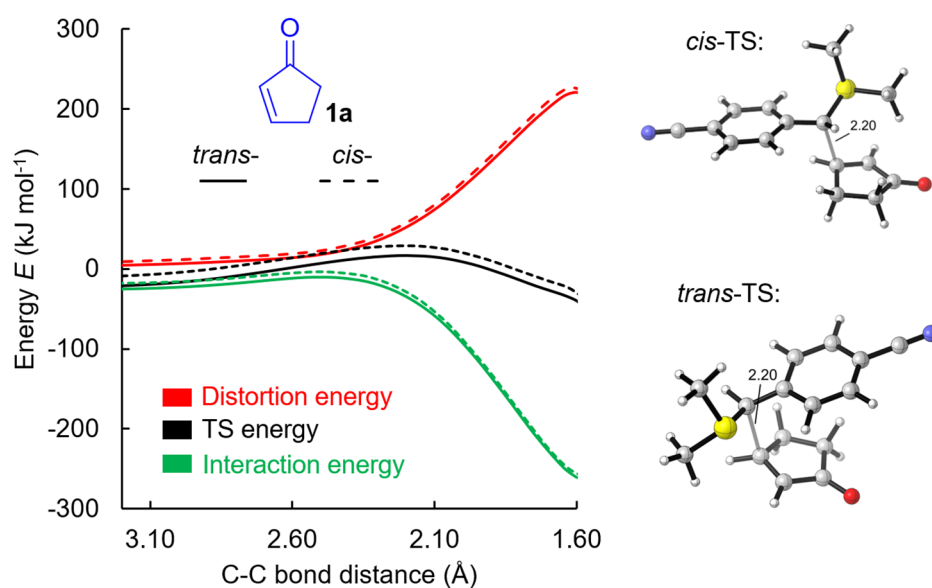


Figure S1. Distortion-interaction analysis (DIA) of the lowest energy conformers for the *cis*- and *trans*-transition state of the reaction of **7** with **1a**. DIA indicates that both distortion and interaction contribute to slightly favor the *trans*-TS.

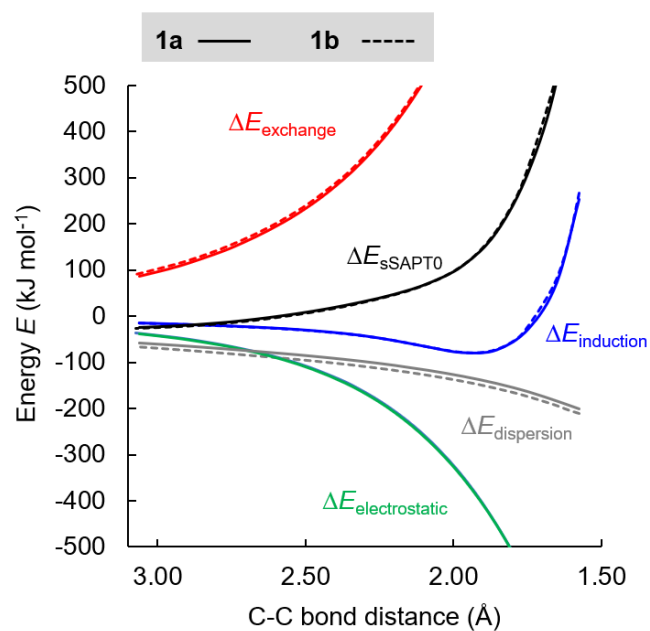


Figure S2. SAPT analysis of the reaction of **7** with **1a** and **1b** (both via *trans*-TS!) at the sSAPT0/jun-cc-pVDZ level of theory in the gas-phase. As indicated by the overlay of the black lines, the computation does not reveal a notable difference in the interaction energies.

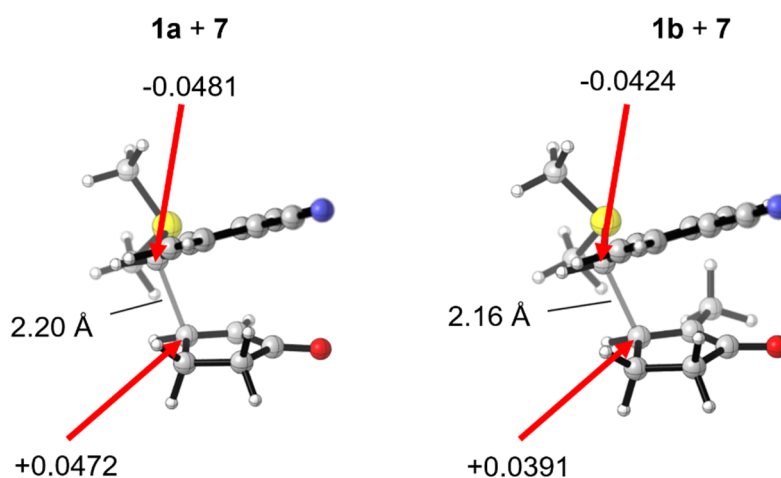


Figure S3. Hirshfeld atomic charge analysis for the reaction centers in the *trans*-transition states of the reactions of **7** with **1a** and **1b**.

General

Dry DMSO (stored over molecular sieves) was used without further purification as purchased from Acros Organics for both product studies and kinetic measurements. Electrophiles **1-5** (purchased from Sigma-Aldrich, ABCR or TCI) were purified by distillation and stored under an atmosphere of dry argon.

For thin-layer chromatography, silica gel plates with F-254 fluorescence indicator (Merck) were used. Purification by flash column chromatography was performed using Merck silica gel 60 (0.040–0.063 mm) with freshly distilled solvents.

Melting points were acquired using Büchi Melting Point B-560 devices and are not corrected.

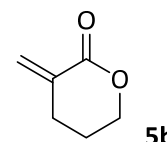
Nuclear magnetic resonance (NMR) spectra were recorded on 400 or 600 MHz spectrometers. The following abbreviations and their combinations are used in the analysis of NMR spectra: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br s = broad singlet. NMR signals were assigned based on information from additional 2D NMR experiments (COSY, gHSQC, gHMBC, NOESY). Chemical shifts are given in ppm. Internal reference was set to the residual solvent signals ($\delta_{\text{H}} = 7.26$ ppm, $\delta_{\text{C}} = 77.16$ ppm for CDCl_3 and $\delta_{\text{H}} = 2.50$ ppm, $\delta_{\text{C}} = 39.52$ ppm for $\text{DMSO}-d_6$).⁵¹ The ^{13}C NMR spectra were recorded under broad-band proton-decoupling.

Infrared (IR) spectra were recorded on a Perkin Elmer Spectrum BX-59343 instrument with a Smiths Detection DuraSamplIR II Diamond ATR sensor in the range 4500–600 cm^{-1} as a film for liquids or neat for solids.

High resolution (HRMS) mass spectra were recorded on a Finnigan MAT 90, a Finnigan MAT 95, a Thermo Finnigan LTQ FT Ultra Fourier Transform ion cyclotron resonance or a Q Exactive GC Orbitrap GC/MS. For ionization of the samples, either electron-impact ionization (EI) or electrospray ionization (ESI) was applied.

Kinetic measurements of fast reactions ($\tau_{1/2} < 120$ s) were performed by employing stopped-flow UV/Vis photometry on Applied Photophysics SX.20 systems. The temperature (20.0 ± 0.2 °C) was maintained constant by using circulating bath cryostats. Slower reactions were studied by conventional UV/Vis measurements which were carried out using a J&M TIDAS diode array spectrophotometer, which was controlled by TIDASDAQ3 (v3) software and connected to a Hellma 661.502-QX quartz Suprasil immersion probe (light path $d = 5$ mm) via fiber optic cables and standard SMA connectors. All solutions were prepared by using dry DMSO and were kept under a nitrogen atmosphere.

3-Methylenetetrahydro-2H-pyran-2-one (5b).⁵² A solution of δ -valerolactone (1.71 g, 17.1 mmol) and diethyl oxalate (5.13 g, 35.1 mmol, 2 equiv) in THF (100 mL) was added dropwise to a suspension of NaH (1.13 g, 28.2 mmol, 1.65 equiv, 60% dispersion in mineral oil) in THF (100 mL) at 0 °C under argon atmosphere. After addition of EtOH (4.50 mL), the mixture was stirred for 4 h at room temperature. Upon cooling to 0 °C, a solution of K_2CO_3 (9.60 g, 69.5 mmol, 4 equiv) in water (14.1 mL) and formaldehyde (6.99 g, 86.2 mmol, 5 equiv, 37 wt. % in water) were added. After stirring for 30 min at 0 °C, the mixture was diluted with brine (50 mL) and the phases were separated. The aqueous phase was extracted with diethyl ether (3 \times 30 mL) and the combined organic phases were washed with brine (2 \times 50 mL), dried over MgSO_4 and concentrated under reduced pressure. Purification by column chromatography (hexane/EtOAc 5:1) yielded **5b** as colorless oil (1.44 g, 75%). The analytical data obtained are in agreement with those reported in the literature.⁵²



^1H NMR (400 MHz, CDCl_3) $\delta = 6.31\text{--}6.29$ (m, 1 H), 5.48–5.46 (m, 1 H), 4.30–4.27 (m, 2 H), 2.60–2.56 (m, 2 H), 1.89–1.83 (m, 2 H); ^{13}C NMR (101 MHz, CDCl_3) $\delta = 165.4, 134.2, 128.0, 69.7, 28.0, 23.1$.

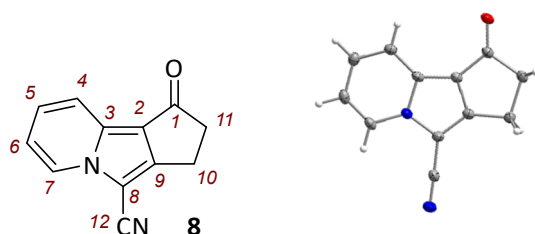
Product Studies

Reactions of the Michael Acceptors 1-5 with Pyridinium Ylides 6

General procedure (GP1) for the reactions of pyridinium ylides 6 with Michael acceptors: A flame-dried Schlenk flask under nitrogen was charged with the pyridinium salt (1 equiv) and Na₂CO₃ (1 equiv). Under stirring, a solution of the cyclic Michael acceptor (2 equiv) in DMSO (0.2 M) was added, causing the formation of an orange solution. After stirring for 1 h at room temperature, chloranil (2 equiv) was added. Stirring the reaction mixture was continued until TLC indicated disappearance of the oxidant (usually within 1 h). Aqueous 2 M HCl was added and the reaction extracted with chloroform (3 x). The combined organic layers were washed twice with aq. 2 M NaOH followed by brine. Then the organic phase was dried over Na₂SO₄ and concentrated under reduced pressure. Purification by column chromatography yielded the indolizines as crystalline solids.

1-Oxo-2,3-dihydro-1*H*-cyclopenta[*a*]indolizine-4-carbonitrile (**8**) (RM436)

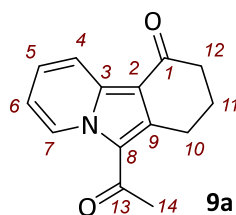
According to GP1: From cyclopentenone (**1a**, 36.2 mg, 0.441 mmol) and the pyridinium salt **6b**·HBr (43.9 mg, 0.221 mmol), **8** was obtained as colorless solid (7.6 mg, 18%) after column chromatography (50% EtOAc in pentane, silica). Slow evaporation of a CDCl₃ solution gave crystals suitable for single crystal X-ray diffraction experiments.



R_f (50% EtOAc in pentane, silica, UV) = 0.36; **Mp** 180-191 °C; ¹H NMR (400 MHz, CDCl₃) δ = 8.38 (dt, *J* = 7.0 Hz, 1.1 Hz, 1 H, 7-H), 8.01 (dt, *J* = 8.8 Hz, 1.2 Hz, 1 H, 4-H), 7.42 (ddd, *J* = 8.8 Hz, 7.0 Hz, 1.1 Hz, 1 H, 5-H), 7.14 (td, *J* = 6.9 Hz, 1.3 Hz, 1 H, 6-H), 3.25–3.22 (m, 2 H, 10-H), 3.00–2.98 (m, 2 H, 11-H); ¹³C NMR (151 MHz, CDCl₃) δ = 196.4 (C_q, C-1), 156.1 (C_q, C-9), 131.6 (C_q, C-3), 127.3 (CH, C-5), 126.7 (CH, C-7), 119.6 (CH, C-4), 119.1 (C_q, C-2), 116.1 (CH, C-6), 112.5 (C_q, C-12), 91.8 (C_q, C-8), 41.7 (CH₂, C-11), 20.8 (CH₂, C-10); **IR** (ATR, neat): 3085, 2926, 2208, 1686, 1633, 1542, 1499, 1402, 1236, 1084, 756 cm⁻¹; **HRMS** (ESI): Calcd *m/z* for C₁₂H₉N₂O⁺ [M+H⁺]: 197.0709; Found: 197.0710.

6-Acetyl-8,9-dihydropyrido[2,1-*a*]isoindol-10(7*H*)-one (**9a**) (RM516)

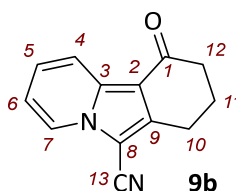
According to GP1: From cyclohexenone (**2a**, 29.2 mg, 0.304 mmol) and pyridinium salt **6a**·HCl (26.0 mg, 0.152 mmol), **9a** was obtained as colorless solid (32.2 mg, 93%) after column chromatography (50% EtOAc in pentane, silica).



R_f (50% EtOAc in pentane, silica, UV) = 0.30; **Mp** 179-181 °C (turns black at 170 °C); **¹H NMR** (400 MHz, CDCl₃) δ = 10.06 (dt, *J* = 7.1 Hz, 1.1 Hz, 1 H, 7-H), 8.51 (dt, *J* = 8.7 Hz, 1.3 Hz, 1 H, 4-H), 7.47 (ddd, *J* = 8.6 Hz, 6.9 Hz, 1.2 Hz, 1 H, 5-H), 7.06 (td, *J* = 7.0 Hz, 1.5 Hz, 1 H, 6-H), 3.22 (t, *J* = 6.2 Hz, 2 H, 10-H), 2.61 (t, *J* = 6.4 Hz, 2 H, 12-H) superimposed with 2.60 (s, 3 H, 14-H), 2.26 (p, *J* = 6.4 Hz, 2 H, 11-H); **¹³C NMR** (101 MHz, CDCl₃) δ = 194.1 (C_q, C-1), 188.1 (C_q, C-13), 142.2 (C_q, C-9), 137.8 (C_q, C-3), 129.5 (CH, C-7), 129.0 (CH, C-5), 120.8 (C_q, C-8), 119.4 (CH, C-4), 116.1 (CH, C-6), 112.3 (C_q, C-2), 38.5 (CH₂, C-12), 30.9 (CH₃, C-14), 25.3 (CH₂, C-10), 24.5 (CH₂, C-11); **IR** (ATR, neat): 2950, 2920, 2850, 1648, 1604, 1502, 1485, 1451, 1401, 1365, 1177, 1142, 1119, 1082, 1031, 1017, 978, 909, 845, 776, 759, 754, 653 cm⁻¹; **HRMS** (EI): Calcd *m/z* for [C₁₄H₁₃NO₂⁺] [M⁺]: 227.0941; Found: 227.0940.

10-Oxo-7,8,9,10-tetrahydropyrido[2,1-*a*]isoindole-6-carbonitrile (**9b**) (RM290)

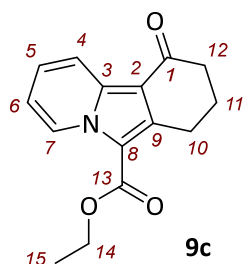
According to *GP1*: From cyclohexenone (**2a**, 40.0 mg, 0.416 mmol) and pyridinium salt **6b**·HBr (41.5 mg, 0.208 mmol), **9b** was obtained as colorless solid (31.5 mg, 72%) after column chromatography (50% EtOAc in pentane, silica).



R_f (50% EtOAc in pentane, silica, UV) = 0.40; **Mp** 145-146 °C; **¹H NMR** (400 MHz, CDCl₃) δ = 8.35 (dd, *J* = 8.8 Hz, 1.6 Hz, 1 H, 4-H), 8.30 (dd, *J* = 6.8 Hz, 1.5 Hz, 1 H, 7-H), 7.38 (ddd, *J* = 8.9 Hz, 6.9 Hz, 1.0 Hz, 1 H, 5-H), 7.06 (td, *J* = 6.9 Hz, 1.6 Hz, 1 H, 6-H), 3.01 (t, *J* = 6.2 Hz, 2 H, 10-H), 2.59 (dd, *J* = 6.9 Hz, 5.8 Hz, 2 H, 12-H), 2.24–2.17 (m 2 H, 11-H); **¹³C NMR** (101 MHz, CDCl₃) δ = 193.0 (C_q, C-1), 143.7 (C_q, C-9), 136.3 (C_q, C-3), 127.6 (CH, C-5), 125.7 (CH, C-7), 120.5 (CH, C-4), 115.8 (CH, C-6), 112.6 (C_q, C-13), 111.5 (C_q, C-2), 94.1 (C_q, C-8), 38.9 (CH₂, C-12), 24.3 (CH₂, C-11), 22.0 (CH₂, C-10); **IR** (ATR, neat): 2919, 2202, 1655, 1633, 1501, 1395, 1178, 1160, 1099, 957, 843, 752, 739 cm⁻¹; **HRMS** (EI): Calcd *m/z* for [C₁₃H₁₀N₂O⁺] [M⁺]: 210.0788; Found: 210.0789.

Ethyl 10-oxo-7,8,9,10-tetrahydropyrido[2,1-*a*]isoindole-6-carboxylate (**9c**) (RM517)

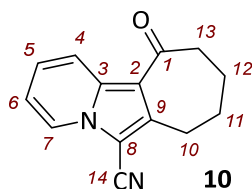
According to *GP1*: From cyclohexenone (**2a**, 30.1 mg, 0.313 mmol) and pyridinium salt **6c**·HBr (38.5 mg, 0.156 mmol), **9c** was obtained as pale orange solid (35.9 mg, 89%) after column chromatography (30% EtOAc in pentane, silica). The NMR spectroscopic data for **9c** agree with those reported by Tamura and co-workers.^{S3}



R_f (50% EtOAc in pentane, silica, UV) = 0.55; **Mp** 147–150 °C (ref. **S3**: mp 151–152 °C, from light petroleum (bp 60–80 °C)); **¹H NMR** (400 MHz, CDCl₃) δ = 9.59 (dt, *J* = 7.1 Hz, 1.1 Hz, 1 H, 7-H), 8.43 (dt, *J* = 8.8 Hz, 1.3 Hz, 1 H, 4-H), 7.37 (ddd, *J* = 8.8 Hz, 6.9 Hz, 1.2 Hz, 1 H, 5-H), 7.01 (td, *J* = 7.0 Hz, 1.5 Hz, 1 H, 6-H), 4.41 (q, *J* = 7.1 Hz, 2 H, 14-H), 3.21 (t, *J* = 6.2 Hz, 2 H, 10-H), 2.58 (dd, *J* = 7.2 Hz, 5.7 Hz, 2 H, 12-H), 2.18 (p, *J* = 6.3 Hz, 2 H, 11-H), 1.43 (t, *J* = 7.1 Hz, 3 H, 15-H); **¹³C NMR** (101 MHz, CDCl₃) δ = 194.3 (C_q, C-1), 162.1 (C_q, C-13), 142.6 (C_q, C-9), 137.4 (C_q, C-3), 128.3 (CH, C-7), 127.3 (CH, C-5), 119.6 (CH, C-4), 115.3 (CH, C-6), 111.8 (C_q, C-2), 111.4 (C_q, C-8), 60.3 (CH₂, C-14), 39.0 (CH₂, C-12), 24.4 (CH₂, C-11), 24.1 (CH₂, C-10), 14.7 (CH₃, C-15); **IR** (ATR, neat): 2954, 2921, 2850, 1679, 1644, 1626, 1506, 1496, 1411, 1387, 1338, 1211, 1178, 1148, 1139, 1088, 1045, 1024, 781, 768 cm⁻¹; **HRMS** (EI): Calcd *m/z* for [C₁₅H₁₅NO₃⁺] [M⁺]: 257.1046; Found: 257.1046.

11-Oxo-8,9,10,11-tetrahydro-7H-cyclohepta[a]indolizine-6-carbonitrile (**10**) (RM563)

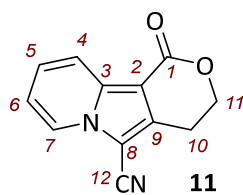
According to *GP1*: From cycloheptenone **3** (45.1 mg, 0.409 mmol) and pyridinium salt **6b**·HBr (40.7 mg, 0.204 mmol), **10** was obtained as colorless solid (39.2 mg, 86%) after column chromatography (30% EtOAc in pentane, silica).



R_f (50% EtOAc in pentane, silica, UV) = 0.45; **Mp** 127–128 °C; **¹H NMR** (400 MHz, CDCl₃) δ = 8.50 (dt, *J* = 9.0 Hz, 1.2 Hz, 1 H, 4-H), 8.27 (dt, *J* = 6.8 Hz, 1.1 Hz, 1 H, 7-H), 7.36 (ddd, *J* = 9.0 Hz, 6.9 Hz, 1.1 Hz, 1 H, 6-H), 7.04 (td, *J* = 6.9 Hz, 1.3 Hz, 1 H, 5-H), 3.13–3.10 (m, 2 H, 10-H), 2.79–2.76 (m, 2 H, 13-H), 2.04–1.92 (m, 4 H, 11-H and 12-H); **¹³C NMR** (101 MHz, CDCl₃) δ = 197.3 (C_q, C-1), 142.2 (C_q, C-9), 138.3 (C_q, C-3), 127.3 (CH, C-6), 125.4 (CH, C-7), 120.8 (CH, C-4), 115.6 (CH, C-5), 114.2 (C_q, C-2), 112.9 (C_q, C-14), 96.2 (C_q, C-8), 42.3 (CH₂, C-13), 25.03 and 25.02 (2 × CH₂, C-10 and C-11), 21.8 (CH₂, C-12); **IR** (ATR, neat): 2921, 2849, 2200, 1631, 1613, 1488, 1380, 1222, 1102, 918, 909, 801, 752, 739 cm⁻¹; **HRMS** (EI): Calcd *m/z* for [C₁₄H₁₂N₂O⁺] [M⁺]: 224.0944; Found: 224.0941.

1-Oxo-3,4-dihydro-1H-pyrano[3,4-a]indolizine-5-carbonitrile (**11**) (RM438)

According to *GP1*: From **5a** (35.1 mg, 0.358 mmol) and pyridinium salt **6b**·HBr (35.6 mg, 0.179 mmol), **11** was obtained as colorless solid (29.6 mg, 78%) after column chromatography (50% EtOAc in pentane, silica).

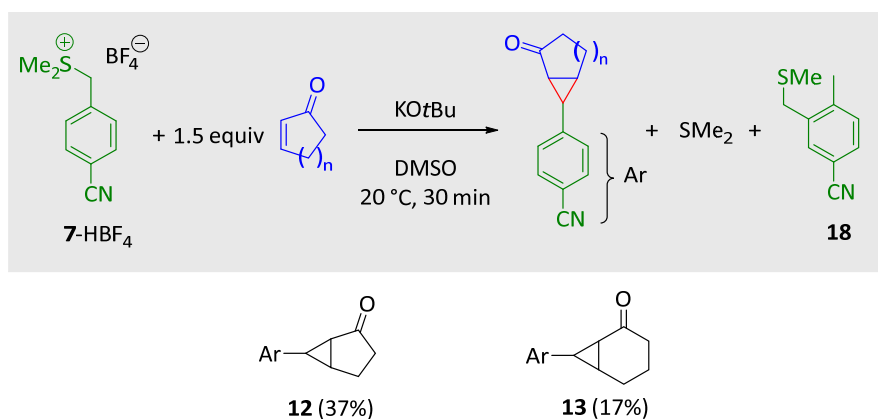


R_f (50% EtOAc in pentane, silica, UV) = 0.40; **Mp** 265-266 °C; **¹H NMR** (599 MHz, CDCl₃) δ = 8.36 (dt, *J* = 6.9 Hz, 1.1 Hz, 1 H, 7-H), 8.24 (dt, *J* = 8.9 Hz, 1.2 Hz, 1 H, 4-H), 7.43 (ddd, *J* = 8.9 Hz, 6.9 Hz, 1.1 Hz, 1 H, 5-H), 7.12 (td, *J* = 6.9 Hz, 1.3 Hz, 1 H, 6-H), 4.61 (dd, *J* = 6.3 Hz, 5.9 Hz, 1 H, 11-H), 3.18 (dd, *J* = 6.4 Hz, 5.8 Hz, 1 H, 10-H); **¹³C NMR** (151 MHz, CDCl₃) δ = 161.9 (C_q, C-1), 138.2 (C_q, C-9), 137.7 (C_q, C-3), 127.6 (CH, C-5), 126.1 (CH, C-7), 119.9 (CH, C-4), 116.0 (CH, C-6), 112.0 (C_q, C-12), 101.6 (C_q, C-2), 93.6 (C_q, C-8), 67.9 (CH₂, C-11), 21.7 (CH₂, C-10); **IR** (ATR, neat): 2923, 2850, 2203, 1699, 1633, 1502, 1462, 1400, 1307, 1257, 1201, 1157, 1085, 1066, 1040, 966, 787, 778, 752 cm⁻¹. **HRMS** (EI): Calcd *m/z* for [C₁₂H₈N₂O₂]⁺ [M⁺]: 212.0580; Found: 212.0581.

Reactions of the Michael Acceptors 1-5 with the Sulfonium Ylide 7

Initial Experiments

Product studies of simple Michael acceptors with sulfonium ylide **7** were performed at an ylide concentration of 0.15 M using the ylide in excess over the enone (0.66 equiv).^{S4} However, cyclopropanations of cyclopentenone (**1a**) and cyclohexenone (**2a**) were inefficient with this protocol owing to a partial consumption of **7** by a concomitant rearrangement to the sulfide **18**.



Reaction of cyclopentenone (**1a**) with **7**

(RM445)

In a flame dried Schlenk-flask cyclopentenone **1a** (41.1 mg, 0.50 mmol) and the sulfonium salt (**7**·HBF₄, 199 mg, 0.75 mmol) were dissolved in DMSO (5 mL). A solution of potassium *tert*-butoxide in DMSO (84.2 mg, 0.75 mmol in 2 mL) was added dropwise within 5 min. After stirring of the orange reaction mixture for another 5 min, saturated aq. NH₄Cl was added (20 mL), and the mixture was extracted with CH₂Cl₂ (3×), washed with brine, dried over Na₂SO₄, and concentrated. Purification by column chromatography (silica gel, 10 to 50% EtOAc in pentane) yielded two main fractions: (a) the rearrangement product **18** of the sulfonium ylide (48.5 mg, 37%) and (b) the cyclopropane **12** as a mixture of diastereomers (36.6 mg, 37%).

The sulfide **18** crystallized readily and its structure was characterized by single-crystal X-ray diffraction (analytics, see below).

Reaction of cyclohexenone (**2a**) with **7**

(RM446)

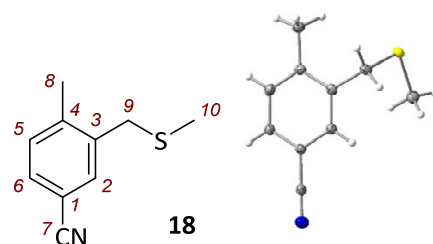
Under analogous conditions as for the reaction of **1a** (RM445), the reaction of cyclohexenone **2a** (48.1 mg, 0.50 mmol) with **7**·HBF₄ yielded the sulfide **18** (57.6 mg, 43%) and the cyclopropane **13** (18.3 mg, 17%) after column chromatography (silica gel, 10 to 40% EtOAc in pentane).

4-Methyl-3-((methylthio)methyl)benzonitrile (**18**)

(RM445)

In the reaction of the sulfonium ylide **7** with cyclopentenone (**1a**) described above (RM445), the sulfonium ylide concomitantly rearranged to the sulfide **18**. The sulfide **18**^{S5} was isolated as major by-product (48.5 mg, 37%) and fully characterized. For reported ¹H NMR chemical shift of **18** in *d*₆-DMSO, see ref [S5b](#).

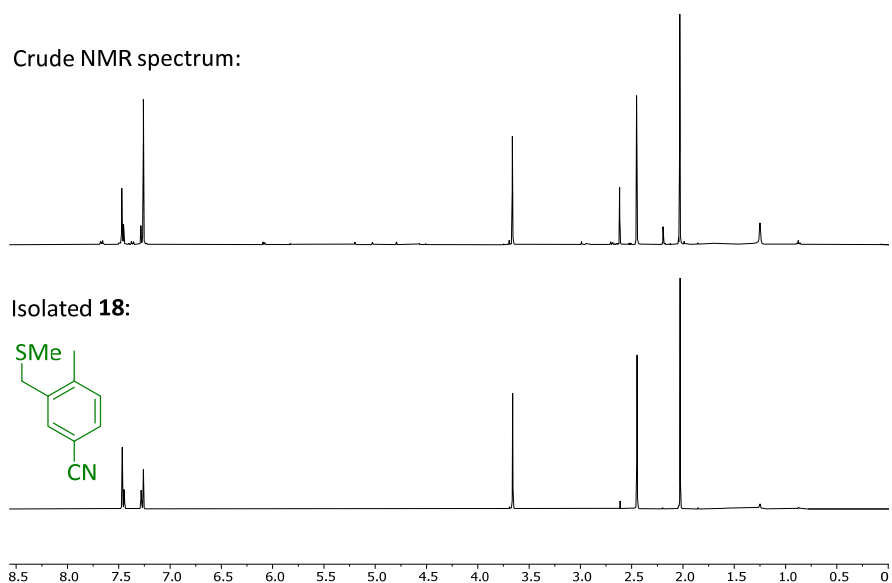
Crystalline **18** was obtained over night by slow crystallization of the neat sample obtained after column chromatography.



R_f (10% EtOAc in pentane, silica, UV) = 0.67; **Mp** 66-67 °C (ref. [S5a](#): mp 57–58 °C, from methanol); **¹H NMR** (400 MHz, CDCl₃) δ = 7.47–7.44 (m, 2 H, 2-H and 6-H), 7.28–7.26 (m, 1 H, 5-H), 3.66 (s, 2 H, 9-H), 2.45 (s, 3 H, 8-H), 2.03 (s, 3 H, 10-H); **f**; **¹³C NMR** (101 MHz, CDCl₃) δ = 142.8 (C_q, C-3), 137.6 (C_q, C-4), 132.8 (CH, C-2), 131.6 (CH, C-5), 131.0 (CH, C-6), 119.1 (C_q, C-7), 109.7 (C_q, C-1), 35.9 (CH₂, C-9), 19.7 (CH₃, C-8), 15.4 (CH₃, C-10); **IR** (ATR, neat): 2953, 2917, 2852, 2222, 1603, 1497, 1435, 1104, 1029, 982, 960, 908, 822 cm⁻¹; **HRMS** (EI): Calcd *m/z* for [C₁₀H₁₁NS⁺] [M⁺]: 177.0607; Found: 177.0598.

Rearrangement of **7** (to **18**) in DMSO solution

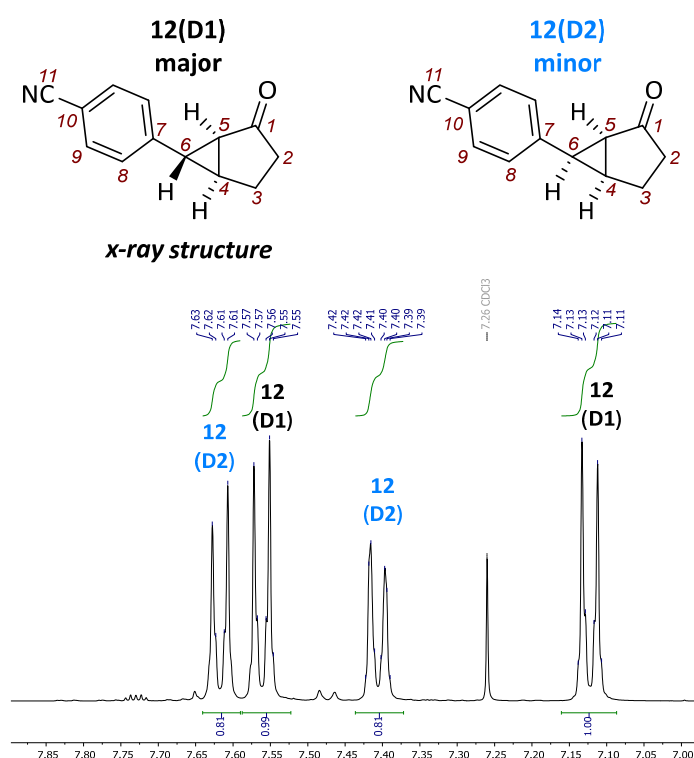
In a flame dried Schlenk-flask the sulfonium salt **7**·HBF₄ (100 mg, 0.377 mmol) was dissolved in DMSO (3 mL). A solution of KO^tBu in DMSO (42.3 mg, 0.377 mmol in 1.5 mL) was added dropwise within 5 min, which yielded a dark-green solution. After stirring for another 20 min, saturated aq. NH₄Cl was added (20 mL), and the mixture was extracted with dichloromethane (3 ×), washed with brine, dried over Na₂SO₄ and concentrated to yield a dark yellow solid (60.3 mg) which almost entirely consisted of the rearrangement product **18**.



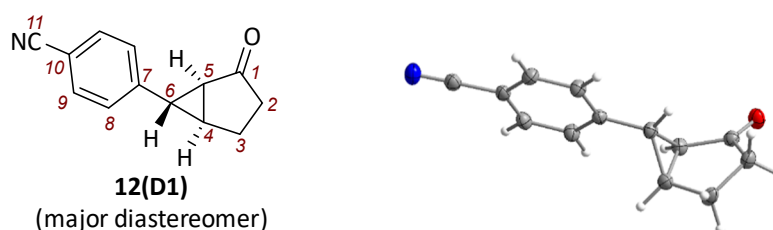
4-(2-Oxobicyclo[3.1.0]hexan-6-yl)benzonitrile (**12**)
(RNH389)

To a mixture of cyclopentenone **1a** (287 mg, 3.50 mmol) and the sulfonium salt **7**·HBF₄ (186 mg, 0.700 mmol) in DMSO (26 mL) was added KOtBu (78.6 mg, 0.700 mmol) in DMSO (30 mL). After stirring for 5 min, saturated aq. NH₄Cl was added (20 mL), and the mixture was extracted with dichloromethane (3 ×). The combined extracts were washed with brine, dried over Na₂SO₄ and concentrated. At this stage, the diastereomeric ratio of the products was determined by ¹H NMR spectroscopy (see spectrum below). After column chromatography (30 to 60% EtOAc in pentane, silica) **12** was isolated as a yellowish oil (mixture of diastereomers, 116 mg, 84%; **12(D1)/12(D2)** = 1.00/0.81).

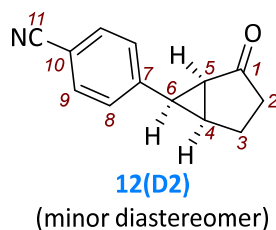
Aromatic part of the ¹H NMR spectrum after aqueous workup and extraction:



While standing for elongated time at room temperature, the major diastereomer **12(D1)** partially crystallized in an aggregate of colorless needles, leaving an oil, in which the minor diastereomer **12(D2)** was significantly enriched.



Analytical data for **12(D1)**. *R_f* (30% EtOAc in pentane, silica, UV) = 0.40; *Mp* 99-103 °C; ¹H NMR (400 MHz, CDCl₃) δ = 7.58–7.55 (m, 2 H, 9-H), 7.14–7.11 (m, 2 H, 8-H), 2.43–2.40 (m, 1 H, 4-H), 2.37 (dd, *J* = 3.8 Hz, 2.8 Hz, 1 H, 6-H), 2.35–2.16 (m, 4 H, 2-H₂, 3-H₂), 2.10 (dd, *J* = 5.4 Hz, 2.7 Hz, 1 H, 5-H); ¹³C NMR (101 MHz, CDCl₃) δ = 212.2 (C_q, C-1), 144.9 (C_q, C-7), 132.5 (CH, C-9), 126.6 (CH, C-8), 118.8 (C_q, C-11), 110.5 (C_q, C-10), 39.4 (CH, C-5), 32.3 (CH₂, C-2), 31.4 (CH, C-4), 30.3 (CH, C-6), 23.4 (CH₂, C-3); IR (ATR, neat): 2943, 2223, 1714, 1605, 1505, 1185, 1177, 1042, 878, 851, 842, 825, 799 cm⁻¹; HRMS (EI⁺): Calcd *m/z* for [C₁₃H₁₁NO⁺] [M⁺]: 197.0835; Found: 197.0834.

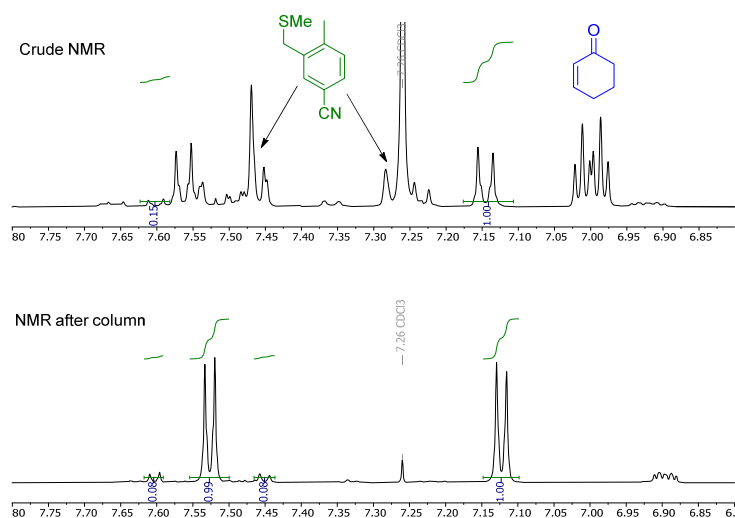


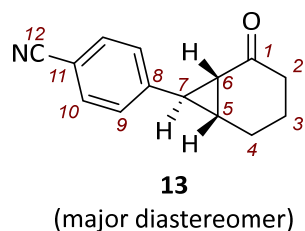
Analytical data for 12(D2). Oil, NMR spectroscopic analytics for a **12(D2)**-enriched mixture which contains additional contaminations. R_f (30% EtOAc in pentane, silica, UV) = 0.40; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ = 7.64–7.61 (m, 2 H, 9- $\text{H}^{\text{D}2}$), 7.58–7.55 (m, 2 H, 9- $\text{H}^{\text{D}1}$), 7.43–7.39 (m, 2 H, 8- $\text{H}^{\text{D}2}$), 7.14–7.11 (m, 2 H, 8- $\text{H}^{\text{D}1}$), 2.79 (t, J = 8.8 Hz, 1 H, 6- $\text{H}^{\text{D}2}$), 2.48 (dt, J = 8.2 Hz, 5.6 Hz, 1 H, 4- $\text{H}^{\text{D}2}$), 2.43–2.40 (m, 1 H, 4- $\text{H}^{\text{D}1}$), 2.37–2.17 (m, 5 H + 2 $\text{H}^{\text{D}2}$, 2- $\text{H}_2^{\text{D}1}$ 3- $\text{H}_2^{\text{D}1}$ 6- H^{D} ; 3- $\text{H}^{\text{D}2}$ and 5- $\text{H}^{\text{D}2}$), 2.10 (dd, J = 5.4 Hz, 2.7 Hz, 1 H, 5- $\text{H}^{\text{D}1}$), 1.99–1.84 (m, 2 H, 2- $\text{H}^{\text{D}2}$ and 3- $\text{H}^{\text{D}2}$), 0.91–0.80 (m, 1 H, 2- $\text{H}^{\text{D}2}$); $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ = 213.9 (C_q , C-1 $^{\text{D}2}$), 212.2 (C_q , C-1 $^{\text{D}1}$), 144.9 (C_q , C-7 $^{\text{D}1}$), 141.0 (C_q , C-7 $^{\text{D}2}$), 132.7 (CH, C-9 $^{\text{D}2}$), 132.5 (CH, C-9 $^{\text{D}1}$), 130.6 (CH, C-8 $^{\text{D}2}$), 126.6 (CH, C-8 $^{\text{D}1}$), 118.8 (C_q , C-11 $^{\text{D}1}$), 118.7 (C_q , C-11 $^{\text{D}2}$), 111.4 (C_q , C-10 $^{\text{D}2}$), 110.5 (C_q , C-10 $^{\text{D}1}$), 39.4 (CH, C-5 $^{\text{D}1}$), 35.1 (CH_2 , C-2 $^{\text{D}2}$), 33.8 (CH, C-5 $^{\text{D}2}$), 32.3 (CH_2 , C-2 $^{\text{D}1}$), 31.4 (CH, C-4 $^{\text{D}1}$), 30.3 (CH, C-6 $^{\text{D}1}$), 28.7 (CH, C-6 $^{\text{D}2}$), 27.7 (CH, C-4 $^{\text{D}2}$), 23.4 (CH_2 , C-3 $^{\text{D}1}$), 20.2 (CH_2 , C-3 $^{\text{D}2}$).

4-(2-Oxobicyclo[4.1.0]heptan-7-yl)benzonitrile (**13**) (RNH503)

A solution of cyclohexenone **2a** (674 mg, 7.00 mmol) and the sulfonium salt **7**· HBF_4 (186 mg, 0.700 mmol) in DMSO (26 mL) was mixed with a solution of KOtBu (78.6 mg, 0.700 mmol) in DMSO (30 mL). After stirring for 5 min, saturated aq. NH_4Cl was added (20 mL), and the mixture was extracted with dichloromethane (3 \times). The combined extracts were washed with brine, dried over Na_2SO_4 and concentrated. At this stage, the diastereomeric ratio of the products was determined by $^1\text{H NMR}$ spectroscopy (see spectrum below). After column chromatography (30% EtOAc in pentane, silica) **13** was isolated as a colorless oil (mixture of diastereomers, 55.1 mg, 37%).

A diastereomeric ratio of d.r. = 1:0.15 was determined from the $^1\text{H NMR}$ spectrum of the crude material after aq workup. After column chromatography d.r. changed to 1:0.08. Only the resonances for the major diastereomer are reported. Further unassigned resonances originate mainly from the minor diastereomer.



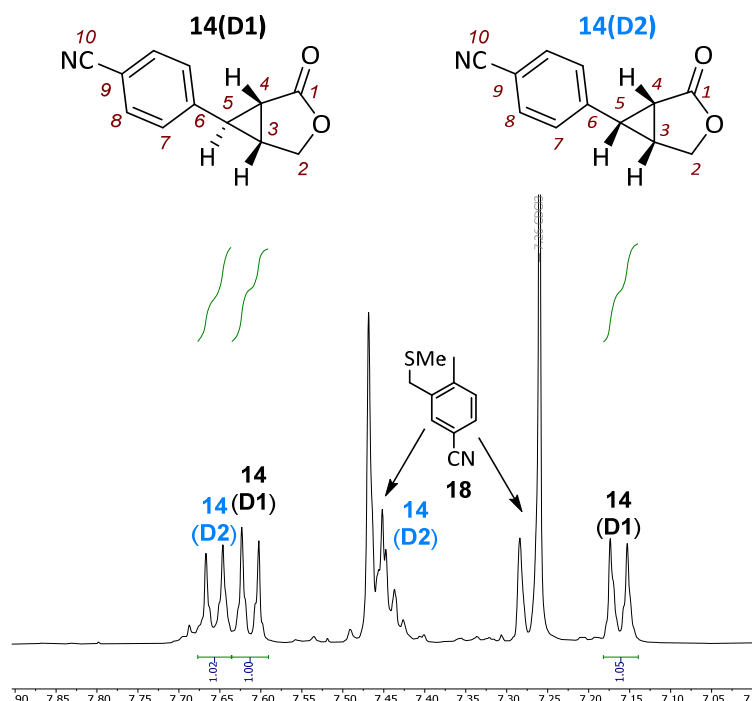


R_f (30% EtOAc in pentane, silica, UV) = 0.30; **¹H NMR** (599 MHz, CDCl₃) δ = 7.57–7.55 (m, 2 H, 10-H), 7.16–7.13 (m, 2 H, 9-H), 2.65 (t, *J* = 4.6 Hz, 1 H, 7-H), 2.43–2.38 (m, 1 H, 2-H), 2.21–2.00 (m, 5 H, 2-H', 6-H, 5-H, 3-H₂), 1.86–1.75 (m, 2 H, 4-H₂); **¹³C NMR** (151 MHz, CDCl₃) δ = 205.6 (C_q, C-1), 145.7 (C_q, C-8), 132.5 (CH, C-10), 126.8 (CH, C-9), 118.9 (C_q, C-12), 110.3 (C_q, C-11), 37.4 (CH, C-6), 37.1 (CH₂, C-2), 27.5 (CH, C-7), 27.4 (CH, C-5), 21.3 (CH₂, C-3), 18.6 (CH₂, C-4); the relative stereochemistry was assigned based on additional data from NOESY experiments; **HRMS** (EI⁺): Calcd *m/z* for [C₁₄H₁₃NO⁺] [M⁺]: 211.0992; Found: 211.0991.

4-(2-Oxo-3-oxabicyclo[3.1.0]hexan-6-yl)benzimidazole (14) (RNH394)

A solution of furanone **4a** (589 mg, 7.00 mmol) and the sulfonium salt **7**·HBF₄ (186 mg, 0.702 mmol) in DMSO (26 mL) was mixed with a solution of KOtBu (78.6 mg, 0.700 mmol) in DMSO (30 mL). Aq workup (as described for **12**, RNH389) followed by column chromatography (30 to 60% EtOAc in pentane, silica) and preparative TLC (80% EtOAc in pentane) furnished two diastereomers of **14** (total: 29.3 mg, 21%).

The ¹H NMR spectrum of the crude material after extraction and removal of solvents indicates a diastereomeric ratio d.r. ≈ 1:1.



Analytical data for **14(D1)**. Yield: 22.2 mg (after column chromatography but still containing minor impurities); **R_f** (30% EtOAc in pentane, silica, UV) = 0.23; **Mp** 117–118 °C; **¹H NMR** (400 MHz, CDCl₃) δ = 7.62–7.60 (m, 2 H, 8-H), 7.18–7.15 (m, 2 H, 7-H), 4.50 (dd, *J* = 9.7 Hz, 4.7 Hz, 1 H, 2-H), 4.44 (d, *J* = 9.7 Hz, 1 H, 2-H'), 2.62–2.55 (m, 1 H, 3-H), 2.41 (dd, *J* = 6.2 Hz, 2.8 Hz, 1 H, 4-H), 2.35 (t, *J* = 3.3 Hz, 1 H, 5-

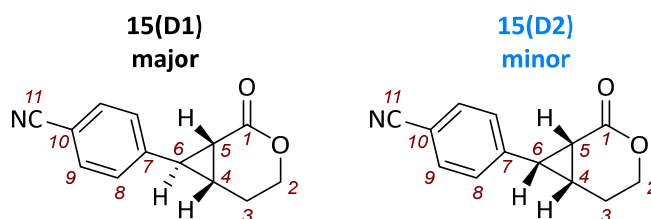
H); ^{13}C NMR (101 MHz, CDCl_3) δ = 174.1 (C_q , C-1), 142.9 (C_q , C-6), 132.7 (CH, C-8), 126.7 (CH, C-7), 118.6 (C_q , C-10), 111.2 (C_q , C-9), 69.7 (CH_2 , C-2), 29.1 (CH, C-5), 28.1 (CH, C-4), 27.0 (CH, C-3); HRMS (EI $^+$): Calcd m/z for $[\text{C}_{12}\text{H}_8\text{NO}_2]^+$ $[\text{M}-\text{H}^+]$: 198.0550; Found: 198.0549.

Analytical data for **14(D2)**. Yield: 7.1 mg (after preparative TLC); R_f (30% EtOAc in pentane, silica, UV) = 0.11; Mp 86 °C; ^1H NMR (400 MHz, CDCl_3) δ = 7.66–7.64 (m, 2 H, 8-H), 7.46–7.43 (m, 2 H, 7-H), 4.41 (dt, J = 10.1 Hz, 2.6 Hz, 1 H, 2-H), 3.99 (d, J = 10.1 Hz, 1 H, 2-H'), 2.81 (t, J = 8.4 Hz, 1 H, 5-H), 2.68–2.65 (m, 2 H, 3-H and 4-H); ^{13}C NMR (101 MHz, CDCl_3) δ = 174.2 (C_q , C-1), 138.1 (C_q , C-6), 132.9 (CH, C-8), 130.5 (CH, C-7), 118.6 (C_q , C-10), 112.1 (C_q , C-9), 65.8 (CH_2 , C-2), 26.0 (CH, C-5), 24.0 (CH, C-3 or C-4), 23.8 (CH, C-3 or C-4); IR (ATR, neat): 2915, 2228, 1760, 1609, 1365, 1175, 1065, 1035, 982, 844 cm^{-1} ; HRMS (EI $^+$): Calcd m/z for $[\text{C}_{12}\text{H}_8\text{NO}_2]^+$ $[\text{M}-\text{H}^+]$: 198.0550; Found: 198.0550.

4-(2-Oxo-3-oxabicyclo[4.1.0]heptan-7-yl)benzotrile (15) (RM447, RNH399)

A solution of pyranone **5a** (687 mg, 7.00 mmol) and the sulfonium salt **7**· HBF_4 (186 mg, 0.700 mmol) in DMSO (26 mL) was mixed with a solution of KOtBu (78.5 mg, 0.700 mmol) in DMSO (30 mL). Aq workup (as described for **12**, RNH389) followed by column chromatography (10 to 50% EtOAc in pentane, silica) yielded **15** as a colorless oil (mixture of diastereomers, 31.1 mg, 21%).

Due to superimposed resonances in the crude ^1H NMR spectrum, the diastereomeric ratio was determined after column chromatography to be d.r. = 1.7:1.0.



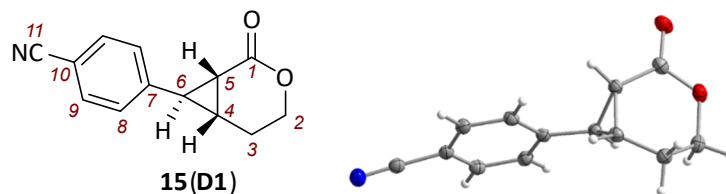
One of the two diastereomers was separately isolated from an independent experiment (RM447, see below), which facilitates the assignment of the NMR resonances.

^1H NMR (400 MHz, CDCl_3) δ = 7.64–7.62 (m, 2 H, 9- $\text{H}^{\text{D}2}$), 7.61–7.58 (m, 2 H, 9- $\text{H}^{\text{D}1}$), 7.46–7.43 (m, 2 H, 8- $\text{H}^{\text{D}2}$), 7.20–7.18 (m, 2 H, 8- $\text{H}^{\text{D}1}$), 4.41–4.35 (m, 1 H, 2- $\text{H}^{\text{D}1}$), 4.26 (td, J = 12.6 Hz, 3.6 Hz, 1 H, 2- $\text{H}'^{\text{D}1}$), 3.96 (ddd, J = 12.0 Hz, 6.6 Hz, 3.3 Hz, 1 H, 2- $\text{H}^{\text{D}2}$), 3.02 (ddd, J = 12.0 Hz, 11.1 Hz, 4.5 Hz, 1 H, 2- $\text{H}'^{\text{D}2}$), 2.94 (t, J = 4.4 Hz, 1 H, 6- $\text{H}^{\text{D}1}$), 2.78 (t, J = 9.2 Hz, 1 H, 6- $\text{H}^{\text{D}2}$), 2.36 (dd, J = 9.7 Hz, 7.8 Hz, 1 H, 5- $\text{H}^{\text{D}2}$), 2.33–2.25 (m, 1 H, 3- $\text{H}^{\text{D}1}$ and 1 H, 3- $\text{H}^{\text{D}2}$), 2.21 (dd, J = 8.9 Hz, 3.9 Hz, 1 H, 5- $\text{H}^{\text{D}1}$), 2.19–2.08 (m, 2 H, 3- $\text{H}'^{\text{D}1}$ and 4- $\text{H}^{\text{D}1}$), 1.96–1.90 (m, 1 H, 3- $\text{H}'^{\text{D}2}$); ^{13}C NMR (101 MHz, CDCl_3) δ = 170.0 (C_q , C-1 $^{\text{D}2}$), 168.5 (C_q , C-1 $^{\text{D}1}$), 143.9 (C_q , C-10 $^{\text{D}1}$), 141.3 (C_q , C-10 $^{\text{D}2}$), 133.0 (CH, C-9 $^{\text{D}2}$), 132.6 (CH, C-9 $^{\text{D}1}$), 129.9 (CH, C-8 $^{\text{D}2}$), 127.0 (CH, C-8 $^{\text{D}1}$), 118.6 (C_q , C-11 $^{\text{D}1}$), 118.5 (C_q , C-11 $^{\text{D}2}$), 111.8 (C_q , C-10 $^{\text{D}2}$), 111.0 (C_q , C-10 $^{\text{D}1}$), 65.9 (CH_2 , C-2 $^{\text{D}2}$), 64.6 (CH_2 , C-2 $^{\text{D}1}$), 28.1 (CH, C-5 $^{\text{D}2}$), 27.2 (CH, C-5 $^{\text{D}1}$), 24.8 (CH, C-6 $^{\text{D}1}$), 24.4 (CH, C-4 $^{\text{D}1}$), 20.4 (CH_2 , C-3 $^{\text{D}1}$), 19.6 (CH, C-4 $^{\text{D}2}$), 19.1 (CH_2 , C-3 $^{\text{D}2}$), 18.8 (CH, C-6 $^{\text{D}2}$).

4-((1R,6R,7R)-2-Oxo-3-oxabicyclo[4.1.0]heptan-7-yl)benzotrile **15(D1)** (and enantiomer) (RM447)

The diastereomer **15(D1)** was also isolated from a reaction of **5a** with **7** under non-optimized reaction conditions: From pyranone **5a** (49.1 mg, 0.500 mmol), the sulfonium salt **7**· HBF_4 (199 mg, 0.751 mmol)

and KOtBu (84.2 mg), a single diastereomer of **15** was obtained as colorless solid (7.1 mg, 7%) after aq workup (as described for **12**, RNH389), column chromatography (10 to 50% EtOAc in pentane, silica) and subsequent preparative TLC (50% EtOAc in pentane). Assignments of NMR signals are based on additional gHSQC and gHMBC experiments. Slow evaporation of a CDCl₃ solution gave crystals suitable for single crystal X-ray analysis.

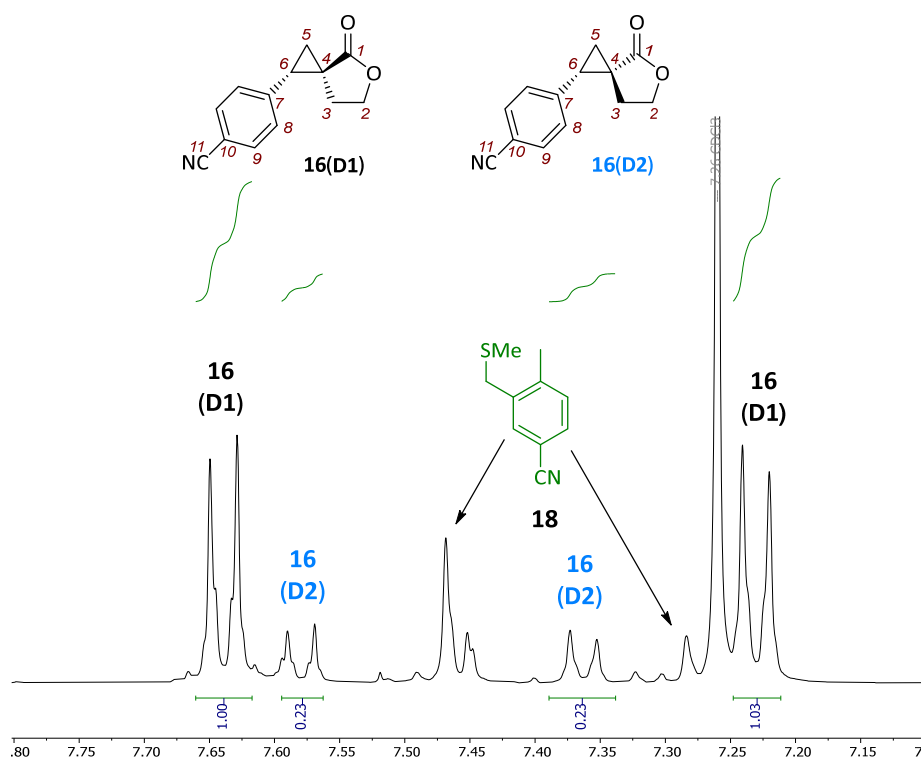


R_f (40% EtOAc in pentane, silica, UV) = 0.43; **¹H NMR** (400 MHz, CDCl₃) δ = 7.62–7.59 (m, 2 H, 9-H), 7.21–7.18 (m, 2 H, 8-H), 4.39 (ddt, *J* = 12.2 Hz, 6.2 Hz, 1.4 Hz, 1 H, 2-H), 4.27 (td, *J* = 12.7 Hz, 3.5 Hz, 1 H, 2-H'), 2.95–2.93 (m, 1 H, 6-H), 2.35–2.26 (m, 1 H, 3-H), 2.24–2.21 (m, 1 H, 5-H), 2.19–2.13 (m, 2 H, 4-H, 3-H'); **¹³C NMR** (101 MHz, CDCl₃) δ = 168.5 (C_q, C-1), 143.9 (C_q, C-10), 132.7 (CH, C-9), 127.0 (CH, C-8), 118.6 (C_q, C-11), 111.1 (C_q, C-10), 64.6 (CH₂, C-2), 27.2 (CH, C-5), 24.9 (CH, C-6), 24.4 (CH, C-4), 20.4 (CH₂, C-3); **HRMS** (EI⁺): Calcd *m/z* for [C₁₃H₁₁NO₂⁺] [*M*⁺]: 213.0784; Found: 213.0788.

4-(4-Oxo-5-oxaspiro[2.4]heptan-1-yl)benzonitrile (**16**) (RNH382, RM444)

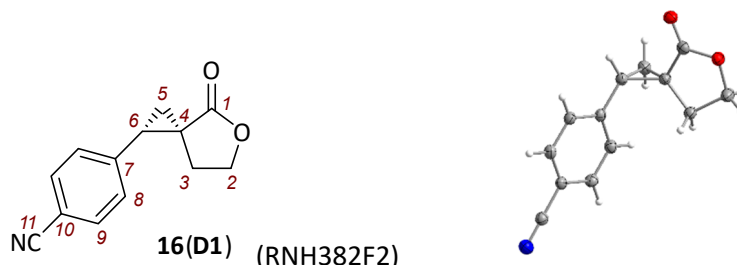
A solution of methylene furanone **4b** (99.9 mg, 1.02 mmol) and the sulfonium salt **7**·HBF₄ (180 mg, 0.679 mmol) in DMSO (5 mL) was mixed with a solution of KOtBu (76.2 mg, 0.679 mmol) in DMSO (2 mL). Aq workup (as described for **12**, RNH389) followed by column chromatography (10 to 50% EtOAc in pentane, silica) furnished **16** (two diastereomers, 67 mg, 46%).

The diastereomeric ratio was determined as **16(D1)/16(D2)** = 1.00/0.23 from the ¹H NMR spectrum of the crude material after aqueous workup.

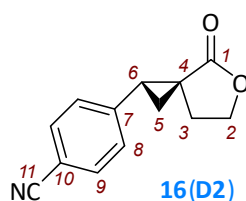


Slow evaporation of a CDCl_3 solution of **16(D1)** in a separate experiment (RNH444) gave crystals suitable for single crystal X-ray diffraction that allowed for an unambiguous assignment of the relative stereochemistry.

4-((1S,3S)-4-Oxo-5-oxaspiro[2.4]heptan-1-yl)benzonitrile (and enantiomer)



R_f (40% EtOAc in pentane, silica, UV) = 0.43; **Mp** 126–127 °C; **¹H NMR** (400 MHz, CDCl_3) δ = 7.65–7.62 (m, 2 H, 9-H), 7.25–7.22 (m, 2 H, 8-H), 4.43 (td, J = 8.9 Hz, 6.1 Hz, 1 H, 2-H), 4.30 (td, J = 9.0 Hz, 6.2 Hz, 1 H, 2-H'), 2.79 (dd, J = 9.3 Hz, 7.1 Hz, 1 H, 6-H), 2.18 (ddd, J = 13.0 Hz, 8.8 Hz, 6.2 Hz, 1 H, 3-H), 1.92–1.85 (m, 1 H, 3-H', superimposed with resonances of 5-H), 1.88 (dd, J = 9.3 Hz, 5.2 Hz, 1 H, 5-H, superimposed with resonances of 3-H'), 1.50 (dd, J = 7.1 Hz, 5.3 Hz, 1 H, 5-H'); **¹³C NMR** (101 MHz, CDCl_3) δ = 178.6 (C_q , C-1), 142.1 (C_q , C-7), 132.6 (CH, C-9), 128.8 (CH, C-8), 118.7 (C_q , C-11), 111.2 (C_q , C-10), 65.9 (CH_2 , C-2), 30.6 (CH, C-6), 28.4 (C_q , C-4), 25.4 (CH_2 , C-3), 19.2 (CH_2 , C-5); **IR** (ATR, neat): 3010, 2913, 2223, 1754, 1607, 1508, 1388, 1374, 1226, 1200, 1132, 1118, 1024, 1017, 996, 854, 833, 744, 737 cm^{-1} ; **HRMS** (EI⁺): Calcd m/z for $[\text{C}_{13}\text{H}_{11}\text{NO}_2]^+$ [M^{++}]: 213.0784; Found: 213.0793.

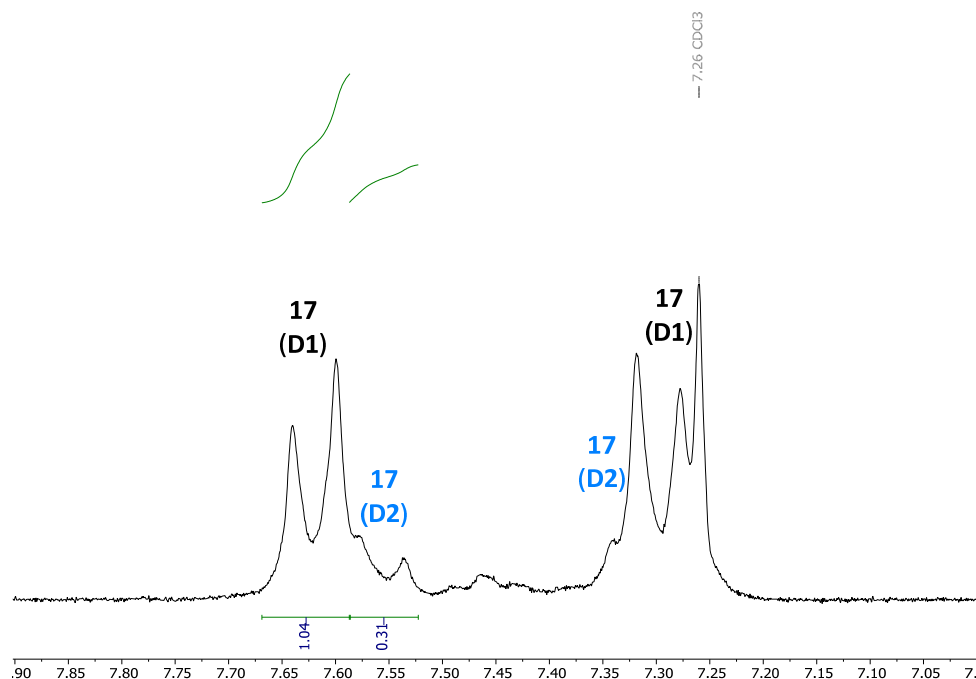


Analytical data for **16(D2)**. **R_f** (40% EtOAc in pentane, silica, UV) = 0.23; **Mp** 112–114 °C; **¹H NMR** (400 MHz, CDCl_3) δ = 7.59–7.56 (m, 2 H, 9-H), 7.38–7.35 (m, 2 H, 8-H), 4.48 (td, J = 9.0 Hz, 3.3 Hz, 1 H, 2-H), 4.41 (td, J = 9.2 Hz, 7.5 Hz, 1 H, 2-H'), 2.67–2.60 (m, 2 H, 3-H and 6-H), 2.34 (ddd, J = 12.9 Hz, 7.5 Hz, 3.3 Hz, 1 H, 3-H'), 1.95 (dd, J = 7.7 Hz, 5.5 Hz, 1 H, 5-H), 1.63 (dd, J = 8.8 Hz, 5.5 Hz, 1 H, 5-H'); **¹³C NMR** (101 MHz, CDCl_3) δ = 175.5 (C_q , C-1), 141.0 (C_q , C-7), 132.0 (CH, C-9), 129.8 (CH, C-8), 119.0 (C_q , C-11), 111.0 (C_q , C-10), 65.7 (CH_2 , C-2), 34.1 (CH, C-6), 31.8 (CH_2 , C-3), 28.6 (C_q , C-4), 17.9 (CH_2 , C-5); **IR** (ATR, neat): 2922, 2853, 2226, 1749, 1606, 1382, 1372, 1274, 1256, 1192, 1123, 1106, 1027, 1015, 999, 860, 851, 843, 760, 708 cm^{-1} ; **HRMS** (EI⁺): Calcd m/z for $[\text{C}_{13}\text{H}_{11}\text{NO}_2]^+$ [M^{++}]: 213.0784; Found: 213.0782.

4-(4-Oxo-5-oxaspiro[2.5]octan-1-yl)benzonitrile (**17**) (RNH142)

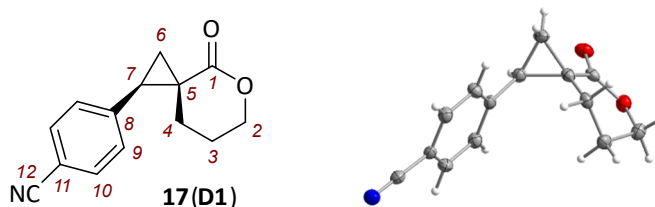
A solution of methylene pyranone **5b** (105.3 mg, 0.939) and the sulfonium salt **7**· HBF_4 (166 mg, 0.626 mmol) in DMSO (5 mL) was mixed with a solution of $\text{KO}t\text{Bu}$ (70.3 mg, 0.626 mmol) in DMSO (2 mL). Aq workup (as described for **12**, RNH389) followed by column chromatography (5 to 30% EtOAc in pentane, silica) furnished **17** (two diastereomers, in total: 98.1 mg, 69%).

The ^1H NMR spectrum of the crude material after extraction and removal of solvents indicates a diastereomeric ratio d.r. \approx 1:0.31.

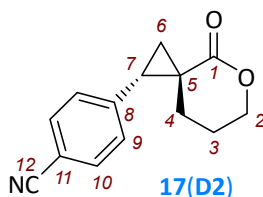


Slow evaporation of a CDCl_3 solution gave crystals suitable for single crystal X-ray diffraction that allowed for an unambiguous assignment of the stereochemistry of the diastereomers.

4-((1R,3S)-4-Oxo-5-oxaspiro[2.5]octan-1-yl)benzotrile (and enantiomer)



Yield: 79.8 mg as colorless oil which slowly crystallized. R_f (20% EtOAc in pentane, silica, UV) = 0.26; **Mp** 106–107 °C; ^1H NMR (400 MHz, CDCl_3) δ = 7.63–7.60 (m, 2 H, 10-H), 7.32–7.29 (m, 2 H, 9-H), 4.46–4.36 (m, 2 H, 2-H₂), 3.03 (dd, J = 9.1 Hz, 7.3 Hz, 1 H, 7-H), 1.96 (dd, J = 9.1 Hz, 4.8 Hz, 1 H, 6-H), 1.91–1.82 (m, 1 H, 3-H), 1.78–1.69 (m, 1 H, 3-H'), 1.57–1.50 (m, 1 H, 4-H), 1.37–1.28 (m, 1 H, 4-H') 1.29 (dd, J = 7.3 Hz, 4.9 Hz, 1 H, 6'-H); ^{13}C NMR (101 MHz, CDCl_3) δ = 173.5 (C_q, C-1), 141.8 (C_q, C-8), 132.3 (CH, C-10), 129.9 (CH, C-9), 118.7 (C_q, C-12), 111.1 (C_q, C-11), 70.4 (CH₂, C-2), 33.7 (CH, C-7), 26.7 (C_q, C-5), 25.0 (CH₂, C-4), 23.1 (CH₂, C-3), 21.8 (CH₂, C-6); **IR** (ATR, neat): 2954, 2925, 2226, 1711, 1608, 1401, 1298, 1259, 1145, 1006, 850 cm^{-1} ; **HRMS** (EI): Calcd m/z for [$\text{C}_{14}\text{H}_{13}\text{NO}_2$]⁺ [M^{*+}]: 227.0941; Found: 227.0934.

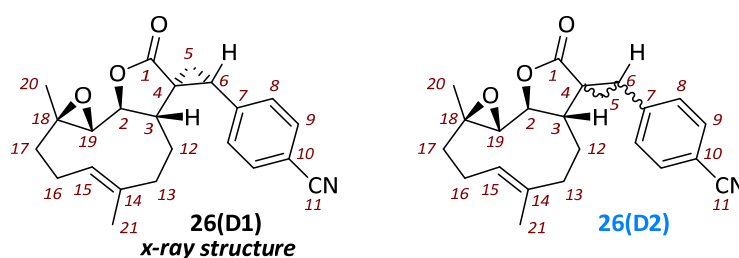


Analytical data for **17(D2)**. Yield: 18.3 mg as colorless crystalline solid. R_f (20% EtOAc in pentane, silica, UV): 0.18; **Mp** 136–137 °C; ^1H NMR (400 MHz, CDCl_3) δ = 7.58–7.55 (m, 2 H, 10-H), 7.35–7.32 (m, 2 H,

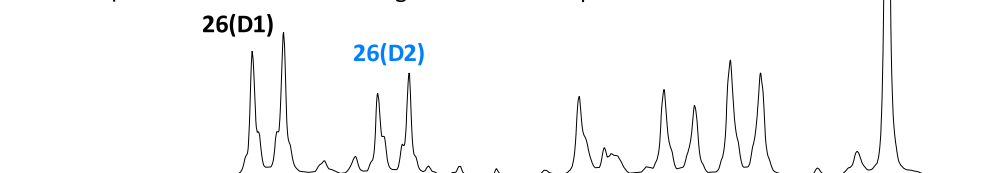
9-H), 4.40–4.36 (m, 2 H, 2-H₂), 2.39 (t, *J* = 8.1 Hz, 1 H, 7-H), 2.27 (ddd, *J* = 13.9 Hz, 9.4 Hz, 5.1 Hz, 1 H, 4-H), 2.17 (dd, *J* = 7.6 Hz, 5.3 Hz, 1 H, 6-H), 2.16–2.00 (m, 2 H, 3-H₂), 1.71 (dt, *J* = 13.6, 5.4 Hz, 1 H, 4-H'), 1.34 (dd, *J* = 8.6, 5.3 Hz, 1 H, 6-H'); ¹³C NMR (101 MHz, CDCl₃) δ = 169.7 (C_q, C-1), 141.5 (C_q, C-8), 132.0 (CH, C-9), 129.9 (CH, C-10), 119.0 (C_q, C-12), 110.8 (C_q, C-11), 69.8 (CH₂, C-2), 37.3 (CH, C-7), 31.4 (CH₂, C-4), 30.5 (C_q, C-5), 23.4 (CH₂, C-3), 19.2 (CH₂, C-6); IR (ATR, neat): 2923, 2853, 2225, 1715, 1608, 1401, 1350, 1276, 1138, 1067, 1017, 845, 728 cm⁻¹; HRMS (EI⁺): Calcd *m/z* for [C₁₄H₁₃NO₂⁺] [M⁺]: 227.0941; Found: 227.0934.

Cyclopropanation of Parthenolide (RNH378)

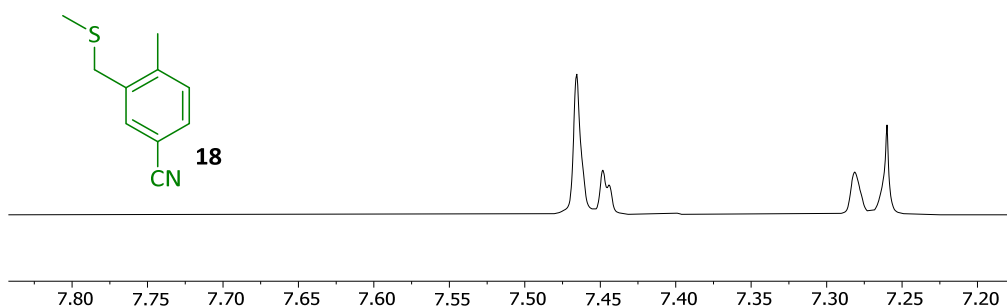
A solution of parthenolide **22** (100 mg, 0.40 mmol) and the sulfonium salt **7**·HBF₄ (107 mg, 0.40 mmol) in DMSO (5 mL) was mixed with a solution of KO^tBu (45.2 mg, 0.40 mmol) in DMSO (2 mL). Aq workup (as described for **12**, RNH389) followed by preparative TLC (30% EtOAc in pentane, silica) delivered a mixture of the two major diastereomers (d.r. = 1:0.85, from the ¹H NMR spectrum, see below). Subsequent crystallization through slow diffusion of diethyl ether into a CDCl₃ solution yielded **26** (21.2 mg, 14%).

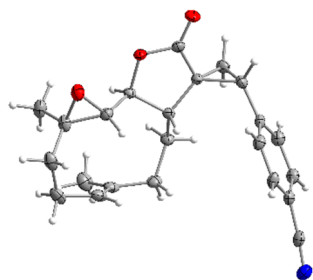


¹H NMR spectrum of the aromatic region of the crude product:



¹H NMR spectrum of the isolated mixture of diastereoisomers (d.r. = 1 : 0.85):





X-ray crystal structure of **26(D1)** arbitrarily taken from the diastereomeric mixture of crystalline material.

Due to superimposed resonances in the NMR spectra, we were not able to assign the stereochemistry of **26(D2)**.

R_f (30% EtOAc in pentane, silica, UV) = 0.29; **Mp** 209-210 °C; **¹H NMR** (400 MHz, CDCl₃) δ = 7.67 (d, *J* = 8.3 Hz, 2 H, 9-H^{D1}), 7.58 (d, *J* = 8.3 Hz, 2 H, 9-H^{D2}), 7.40 (d, *J* = 8.1 Hz, 2 H, 8-H^{D2}), 7.36 (d, *J* = 8.1 Hz, 2 H, 8-H^{D1}), 5.22 (d, *J* = 11.1 Hz, 1 H, 15-H^{D2}), 4.94 (d, *J* = 11.1 Hz, 1 H, 15-H^{D1}), 3.98–3.92 (m, 1 H, 2-H^{D1} and 1 H, 2-H^{D2}), 2.91 (dd, *J* = 9.3 Hz, 7.2 Hz, 1 H, 6-H^{D1}), 2.85 (d, *J* = 8.7 Hz, 1 H, 19-H^{D2}), 2.72 (d, *J* = 8.8 Hz, 1 H, 19-H^{D1}), 2.65 (t, *J* = 9.5 Hz, 1 H, 3-H^{D2}), 2.46–2.26 (m, 1 H, 16-H^{D1} and 3 H, 6-H^{D2}, 13-H^{D2}, 16-H^{D2}), 2.21–2.08 (m, 2 H, 16-H^{D1}, 17-H^{D1} and 3 H, 13-H^{D2}, 16-H^{D2}, 17-H^{D2}), 2.02 (t, *J* = 8.7 Hz, 1 H, 3-H^{D1}), 1.73–1.55 (m, 6 H, 5-H^{D1}, 13-H^{D1}, 21-H^{D1} and 6 H, 5-H^{D2}, 12-H^{D2}, 21-H^{D2}), 1.37–1.17 (m, 5 H, 12-H^{D1}, 17-H^{D1}, 20-H^{D1} and 5 H, 12-H^{D2}, 17-H^{D2}, 20-H^{D2}), 0.98–0.86 (m, 2 H, 12-H^{D1}, 13-H^{D1}); **¹³C NMR** (101 MHz, CDCl₃) δ = 177.6 (C_q, C-1^{D1}), 174.9 (C_q, C-1^{D2}), 140.6 (C_q, C-7^{D1}), 140.5 (C_q, C-7^{D2}), 134.3 (C_q, C-14^{D2}), 134.2 (C_q, C-14^{D1}), 132.6 (CH, C-9^{D1}), 131.8 (CH, C-9^{D2}), 130.2 (CH, C-8^{D1}), 130.1 (CH, C-8^{D2}), 126.0 (CH, C-15^{D2}), 125.1 (CH, C-15^{D1}), 119.1 (C_q, C-11^{D2}), 118.6 (C_q, C-11^{D1}), 111.4 (C_q, C-10^{D1}), 110.8 (C_q, C-10^{D2}), 83.0 (CH, C-2^{D1}), 81.9 (CH, C-2^{D2}), 66.8 (CH, C-19^{D1}), 66.5 (CH, C-19^{D2}), 61.8 (C_q, C-18^{D2}), 61.7 (C_q, C-18^{D1}), 47.3 (CH, C-3^{D2}), 43.5 (CH, C-3^{D1}), 41.2 (CH₂, C-13^{D2}), 40.0 (CH₂, C-13^{D1}), 36.6 (CH₂, C-17^{D2}), 36.4 (CH₂, C-17^{D1}), 31.4 (C_q, C-4^{D1}), 31.0 (C_q, C-4^{D2}), 28.9 (CH₂, C-12^{D1}), 28.2 (CH, C-6^{D1}), 27.7 (CH, C-6^{D2}), 26.9 (CH₂, C-12^{D2}), 24.3 (CH₂, C-16^{D2}), 24.1 (CH₂, C-16^{D1}), 17.4 (CH₃, C-20^{D2}), 17.3 (CH₃, C-20^{D1}), 17.1 (CH₃, C-21^{D1}), 17.0 (CH₂, C-5^{D2}), 16.9 (CH₃, C-21^{D2}), 15.9 (CH₂, C-5^{D1}); **HRMS** (EI⁺): Calcd *m/z* for [C₂₃H₂₅NO₃⁺] [M⁺]: 363.1829; Found: 363.1832.

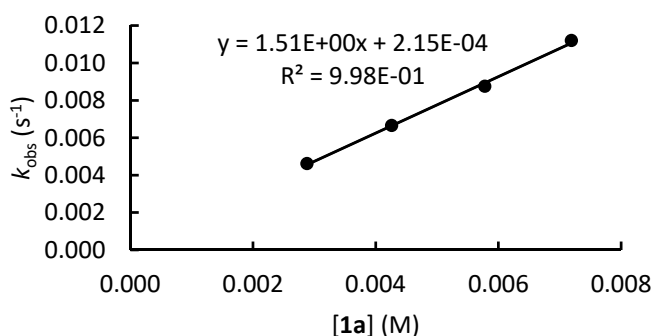
Kinetics with Reference Nucleophiles

Reactions of cyclopentenone (**1a**) with reference nucleophiles

1a + **6a** (from **6a**·HCl + 1 equiv KOTBu) in DMSO (conventional UV/Vis, detection at 427 nm) RM1005

[6a] ₀ , M	[1a] ₀ , M	<i>k</i> _{obs} , s ⁻¹
1.00 × 10 ⁻⁴	2.88 × 10 ⁻³	4.62 × 10 ⁻³
1.00 × 10 ⁻⁴	4.26 × 10 ⁻³	6.66 × 10 ⁻³
1.00 × 10 ⁻⁴	5.78 × 10 ⁻³	8.75 × 10 ⁻³
1.00 × 10 ⁻⁴	7.19 × 10 ⁻³	1.12 × 10 ⁻²

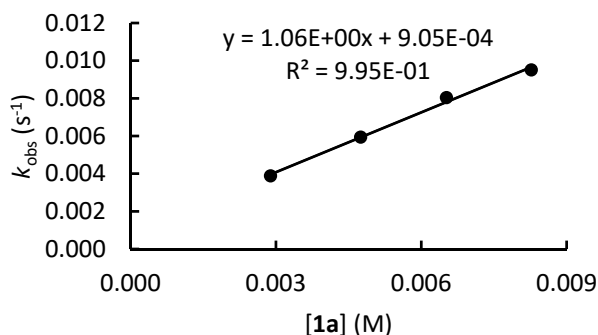
$$k_2 = 1.51 \pm 0.05 \text{ M}^{-1} \text{ s}^{-1}$$



1a + **7** (from **7**·HBF₄ + 1 equiv KOTBu) in DMSO (conventional UV/Vis, detection at 378 nm) RM1005

[7] ₀ , M	[1a] ₀ , M	<i>k</i> _{obs} , s ⁻¹
1.00 × 10 ⁻⁴	2.89 × 10 ⁻³	3.89 × 10 ⁻³
1.00 × 10 ⁻⁴	4.75 × 10 ⁻³	5.94 × 10 ⁻³
1.00 × 10 ⁻⁴	6.52 × 10 ⁻³	8.04 × 10 ⁻³
1.00 × 10 ⁻⁴	8.27 × 10 ⁻³	9.51 × 10 ⁻³

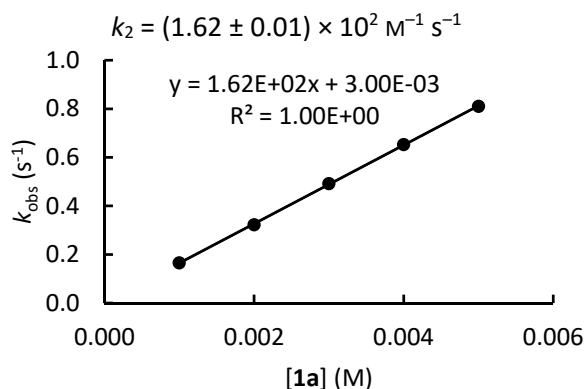
$$k_2 = 1.06 \pm 0.05 \text{ M}^{-1} \text{ s}^{-1}$$



1a + **6c** (from **6c**·HBr + 1 equiv KOTBu) in DMSO (sequential mixing stopped-flow, detection at 425 nm)

RM1005

[6c] ₀ , M	[1a] ₀ , M	<i>k</i> _{obs} , s ⁻¹					average
		1	2	3	4		
1.00 × 10 ⁻⁴	1.00 × 10 ⁻³	1.66 × 10 ⁻¹	1.66 × 10 ⁻¹	1.65 × 10 ⁻¹	1.66 × 10 ⁻¹	1.66 × 10 ⁻¹	
1.00 × 10 ⁻⁴	2.00 × 10 ⁻³	3.22 × 10 ⁻¹	3.28 × 10 ⁻¹	3.19 × 10 ⁻¹	3.22 × 10 ⁻¹	3.23 × 10 ⁻¹	
1.00 × 10 ⁻⁴	3.00 × 10 ⁻³	4.91 × 10 ⁻¹	4.94 × 10 ⁻¹	4.93 × 10 ⁻¹	4.89 × 10 ⁻¹	4.92 × 10 ⁻¹	
1.00 × 10 ⁻⁴	4.00 × 10 ⁻³	6.47 × 10 ⁻¹	6.59 × 10 ⁻¹	6.54 × 10 ⁻¹	6.52 × 10 ⁻¹	6.53 × 10 ⁻¹	
1.00 × 10 ⁻⁴	5.00 × 10 ⁻³	8.05 × 10 ⁻¹	8.06 × 10 ⁻¹	8.16 × 10 ⁻¹	8.18 × 10 ⁻¹	8.11 × 10 ⁻¹	

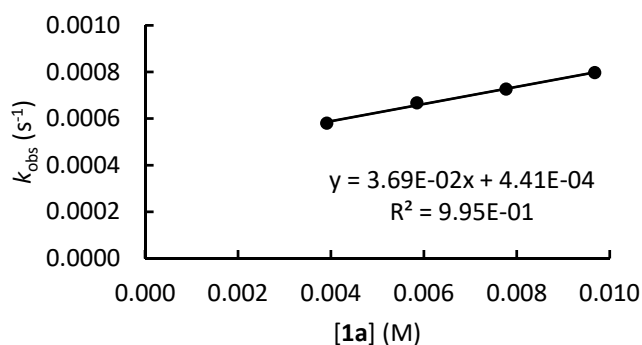


Reactions of 2-methylcyclopentenone (**1b**) with reference nucleophiles

1b + **6a** (from **6a**·HCl + 1 equiv KOTBu) in DMSO (conventional UV/Vis, detection at 427 nm) RM885

[6a] ₀ , M	[1b] ₀ , M	<i>k</i> _{obs} , s ⁻¹
1.00 × 10 ⁻⁴	3.91 × 10 ⁻³	5.80 × 10 ⁻⁴
1.00 × 10 ⁻⁴	5.85 × 10 ⁻³	6.67 × 10 ⁻⁴
1.00 × 10 ⁻⁴	7.77 × 10 ⁻³	7.26 × 10 ⁻⁴
1.00 × 10 ⁻⁴	9.68 × 10 ⁻³	7.97 × 10 ⁻⁴

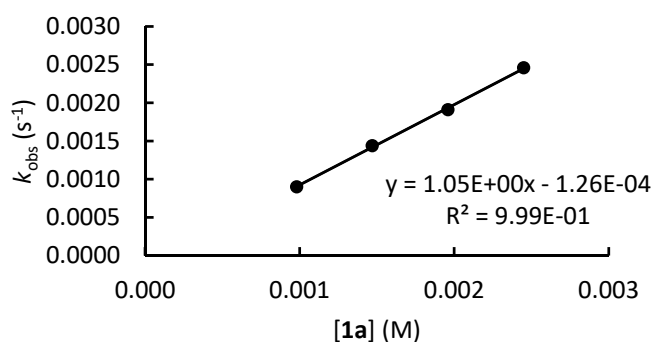
$$k_2 = (3.69 \pm 0.19) \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$$



1b + **7** (from **7**·HBF₄ + 1 equiv KOTBu) in DMSO (conventional UV/Vis, detection at 378 nm) RM892

[7] ₀ , M	[1b] ₀ , M	<i>k</i> _{obs} , s ⁻¹
1.00 × 10 ⁻⁴	9.81 × 10 ⁻⁴	9.00 × 10 ⁻⁴
1.00 × 10 ⁻⁴	1.47 × 10 ⁻³	1.44 × 10 ⁻³
1.00 × 10 ⁻⁴	1.96 × 10 ⁻³	1.91 × 10 ⁻³
1.00 × 10 ⁻⁴	2.45 × 10 ⁻³	2.46 × 10 ⁻³

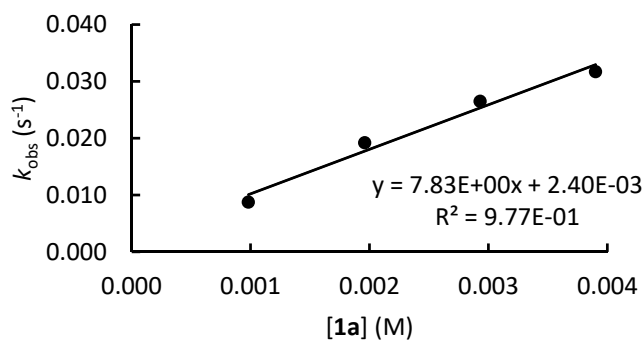
$$k_2 = 1.05 \pm 0.02 \text{ M}^{-1} \text{ s}^{-1}$$



1b + **6c** (from **6c**·HBr + 1 equiv KOTBu) in DMSO (conventional UV/Vis, detection at 425 nm) RM902

[6c] ₀ , M	[1b] ₀ , M	<i>k</i> _{obs} , s ⁻¹
1.00 × 10 ⁻⁴	9.82 × 10 ⁻⁴	8.75 × 10 ⁻³
1.00 × 10 ⁻⁴	1.96 × 10 ⁻³	1.92 × 10 ⁻²
1.00 × 10 ⁻⁴	2.93 × 10 ⁻³	2.65 × 10 ⁻²
1.00 × 10 ⁻⁴	3.90 × 10 ⁻³	3.17 × 10 ⁻²

$$k_2 = 7.83 \pm 0.85 \text{ M}^{-1} \text{ s}^{-1}$$

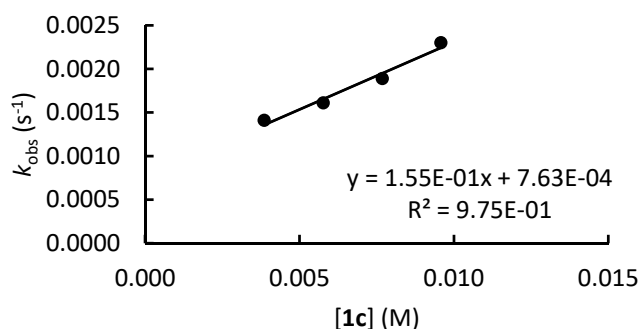


Reactions of 3-methylcyclopentenone (1c) with reference nucleophiles

1c + 6c (from 6c·HBr + 1 equiv KOTBu) in DMSO (conventional UV/Vis, detection at 425 nm) RM1022

[6c] ₀ , M	[1c] ₀ , M	k _{obs} , s ⁻¹
1.00 × 10 ⁻⁴	3.86 × 10 ⁻³	1.41 × 10 ⁻³
1.00 × 10 ⁻⁴	5.77 × 10 ⁻³	1.61 × 10 ⁻³
1.00 × 10 ⁻⁴	7.68 × 10 ⁻³	1.89 × 10 ⁻³
1.00 × 10 ⁻⁴	9.58 × 10 ⁻³	2.30 × 10 ⁻³

$$k_2 = (1.55 \pm 0.18) \times 10^{-1} \text{ M}^{-1} \text{ s}^{-1}$$

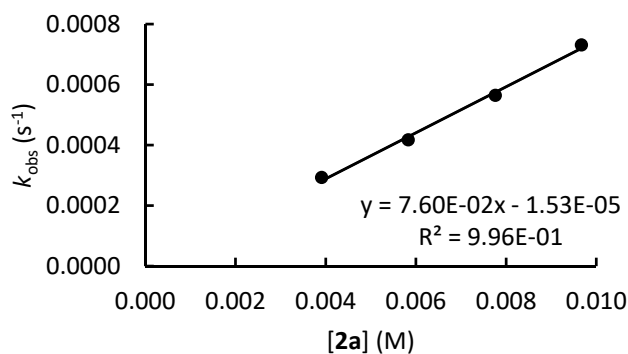


Reactions of cyclohexenone (2a) with reference nucleophiles

2a + 6a (from 6a·HCl + 1 equiv KOTBu) in DMSO (conventional UV/Vis, detection at 427 nm) RM488

[6a] ₀ , M	[2a] ₀ , M	k _{obs} , s ⁻¹
1.00 × 10 ⁻⁴	3.91 × 10 ⁻³	2.93 × 10 ⁻⁴
1.00 × 10 ⁻⁴	5.83 × 10 ⁻³	4.17 × 10 ⁻⁴
1.00 × 10 ⁻⁴	7.76 × 10 ⁻³	5.64 × 10 ⁻⁴
1.00 × 10 ⁻⁴	9.67 × 10 ⁻³	7.31 × 10 ⁻⁴

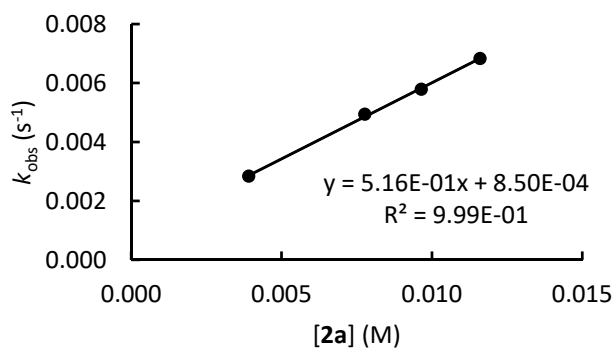
$$k_2 = (7.60 \pm 0.36) \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$$



2a + 7 (from 7·HBF₄ + 1 equiv KOTBu) in DMSO (conventional UV/Vis, detection at 378 nm) RM497

[7] ₀ , M	[2a] ₀ , M	k _{obs} , s ⁻¹
1.00 × 10 ⁻⁴	3.91 × 10 ⁻³	2.84 × 10 ⁻³
1.00 × 10 ⁻⁴	7.77 × 10 ⁻³	4.94 × 10 ⁻³
1.00 × 10 ⁻⁴	9.65 × 10 ⁻³	5.79 × 10 ⁻³
1.00 × 10 ⁻⁴	1.16 × 10 ⁻²	6.83 × 10 ⁻³

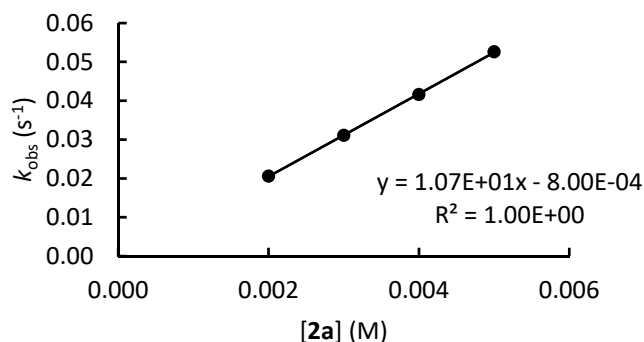
$$k_2 = (5.16 \pm 0.12) \times 10^{-1} \text{ M}^{-1} \text{ s}^{-1}$$



2a + 6c (from **6c**·HBr + 1 equiv KOTBu) in DMSO (sequential mixing stopped-flow – 1 measurement per concentration, detection at 425 nm) RM1002

[6c] ₀ , M	[2a] ₀ , M	<i>k</i> _{obs} , s ⁻¹
1.00 × 10 ⁻⁴	2.00 × 10 ⁻³	2.06 × 10 ⁻²
1.00 × 10 ⁻⁴	3.00 × 10 ⁻³	3.11 × 10 ⁻²
1.00 × 10 ⁻⁴	4.00 × 10 ⁻³	4.16 × 10 ⁻²
1.00 × 10 ⁻⁴	5.00 × 10 ⁻³	5.26 × 10 ⁻²

$$k_2 = (1.07 \pm 0.01) \times 10^1 \text{ M}^{-1} \text{ s}^{-1}$$

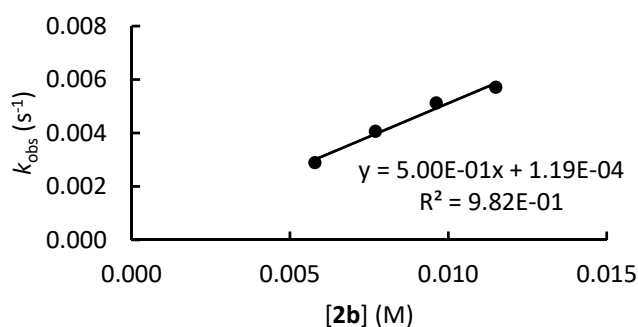


Reactions of 2-methylcyclohexenone (**2b**) with reference nucleophiles

2b + 6c (from **6c**·HBr + 1 equiv KOTBu) in DMSO (conventional UV/Vis, detection at 425 nm) RM1047

[6c] ₀ , M	[2b] ₀ , M	<i>k</i> _{obs} , s ⁻¹
1.00 × 10 ⁻⁴	5.79 × 10 ⁻³	2.89 × 10 ⁻³
1.00 × 10 ⁻⁴	7.70 × 10 ⁻³	4.06 × 10 ⁻³
1.00 × 10 ⁻⁴	9.62 × 10 ⁻³	5.12 × 10 ⁻³
1.00 × 10 ⁻⁴	1.15 × 10 ⁻²	5.71 × 10 ⁻³

$$k_2 = (5.00 \pm 0.49) \times 10^{-1} \text{ M}^{-1} \text{ s}^{-1}$$

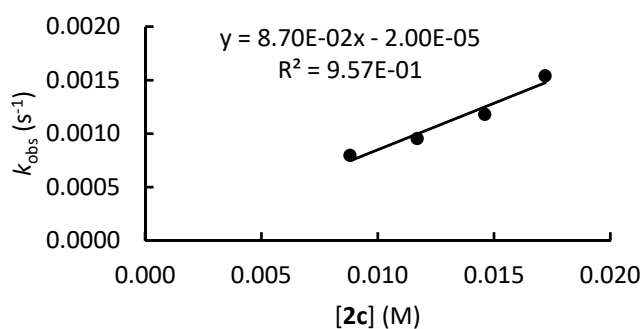


Reactions of 3-methylcyclohexenone (**2c**) with reference nucleophiles

2c + 6c (from **6c**·HBr + 1 equiv KOTBu) in DMSO (conventional UV/Vis, detection at 425 nm) RM901

[6c] ₀ , M	[2c] ₀ , M	<i>k</i> _{obs} , s ⁻¹
1.00 × 10 ⁻⁴	8.81 × 10 ⁻³	7.97 × 10 ⁻⁴
1.00 × 10 ⁻⁴	1.17 × 10 ⁻²	9.54 × 10 ⁻⁴
1.00 × 10 ⁻⁴	1.46 × 10 ⁻²	1.18 × 10 ⁻³
1.00 × 10 ⁻⁴	1.72 × 10 ⁻²	1.54 × 10 ⁻³

$$k_2 = (8.70 \pm 1.31) \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$$

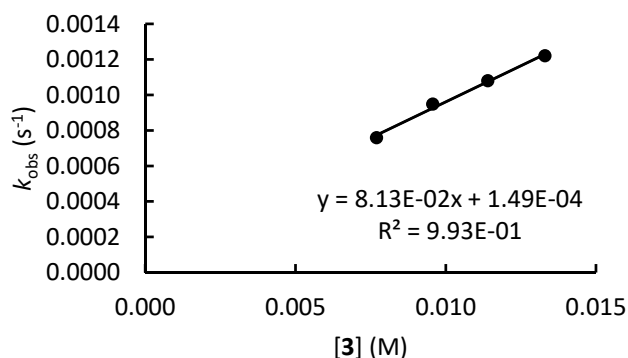


Reactions of cycloheptenone (**3**) with reference nucleophiles

3 + **6a** (from **6a**·HCl + 1 equiv K_{Ot}Bu) in DMSO (conventional UV/Vis, detection at 427 nm) RM559

[6a] ₀ , M	[3] ₀ , M	<i>k</i> _{obs} , s ⁻¹
1.00 × 10 ⁻⁴	7.70 × 10 ⁻³	7.59 × 10 ⁻⁴
1.00 × 10 ⁻⁴	9.57 × 10 ⁻³	9.48 × 10 ⁻⁴
1.00 × 10 ⁻⁴	1.14 × 10 ⁻²	1.08 × 10 ⁻³
1.00 × 10 ⁻⁴	1.33 × 10 ⁻²	1.22 × 10 ⁻³

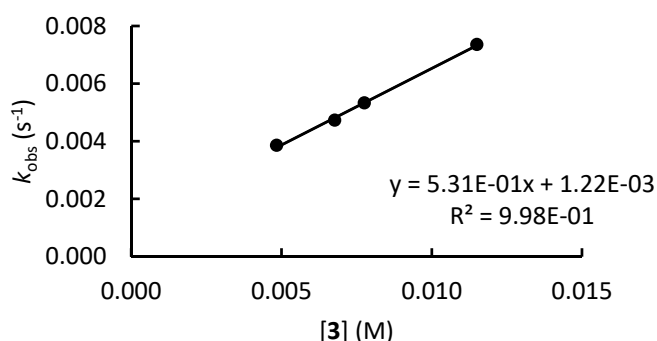
$$k_2 = (8.13 \pm 0.49) \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$$



3 + **7** (from **7**·HBF₄ + 1 equiv K_{Ot}Bu) in DMSO (conventional UV/Vis, detection at 378 nm) RM558

[7] ₀ , M	[3] ₀ , M	<i>k</i> _{obs} , s ⁻¹
1.00 × 10 ⁻⁴	4.84 × 10 ⁻³	3.86 × 10 ⁻³
1.00 × 10 ⁻⁴	6.77 × 10 ⁻³	4.73 × 10 ⁻³
1.00 × 10 ⁻⁴	7.76 × 10 ⁻³	5.33 × 10 ⁻³
1.00 × 10 ⁻⁴	1.15 × 10 ⁻²	7.36 × 10 ⁻³

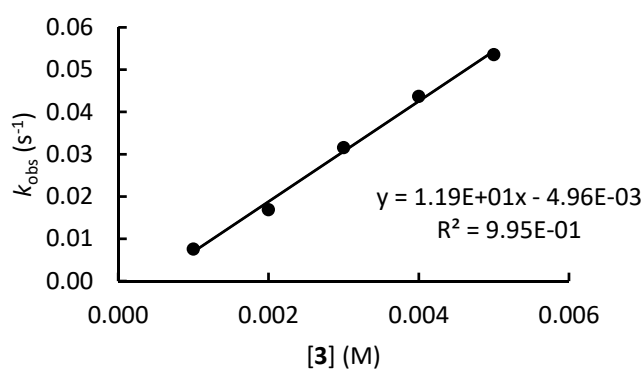
$$k_2 = (5.31 \pm 0.17) \times 10^{-1} \text{ M}^{-1} \text{ s}^{-1}$$



3 + **6c** (from **6c**·HBr + 1 equiv K_{Ot}Bu) in DMSO (sequential mixing stopped-flow, 1 repeat per concentration, detection at 425 nm) RM561

[6c] ₀ , M	[3] ₀ , M	<i>k</i> _{obs} , s ⁻¹
1.00 × 10 ⁻⁴	1.00 × 10 ⁻³	7.60 × 10 ⁻³
1.00 × 10 ⁻⁴	2.00 × 10 ⁻³	1.69 × 10 ⁻²
1.00 × 10 ⁻⁴	3.00 × 10 ⁻³	3.16 × 10 ⁻²
1.00 × 10 ⁻⁴	4.00 × 10 ⁻³	4.37 × 10 ⁻²
1.00 × 10 ⁻⁴	5.00 × 10 ⁻³	5.36 × 10 ⁻²

$$k_2 = (1.19 \pm 0.05) \times 10^1 \text{ M}^{-1} \text{ s}^{-1}$$

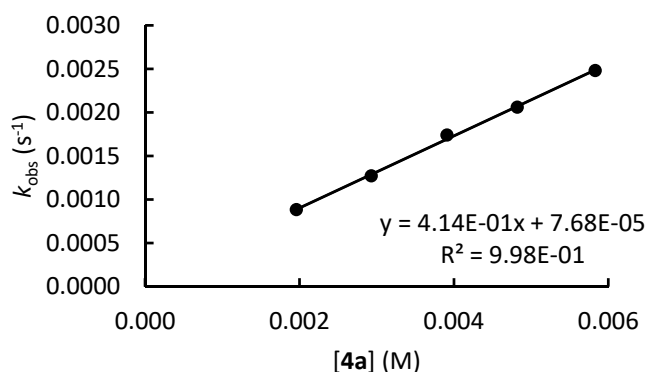


Reactions of furanone (4a) with reference nucleophiles

4a + 6a (from 6a·HCl + 1 equiv KOTBu) in DMSO (conventional UV/Vis, detection at 427 nm) RM493

[6a] ₀ , M	[4a] ₀ , M	k _{obs} , s ⁻¹
1.00 × 10 ⁻⁴	1.96 × 10 ⁻³	8.83 × 10 ⁻⁴
1.00 × 10 ⁻⁴	2.93 × 10 ⁻³	1.27 × 10 ⁻³
1.00 × 10 ⁻⁴	3.91 × 10 ⁻³	1.74 × 10 ⁻³
1.00 × 10 ⁻⁴	4.82 × 10 ⁻³	2.06 × 10 ⁻³
1.00 × 10 ⁻⁴	5.83 × 10 ⁻³	2.48 × 10 ⁻³

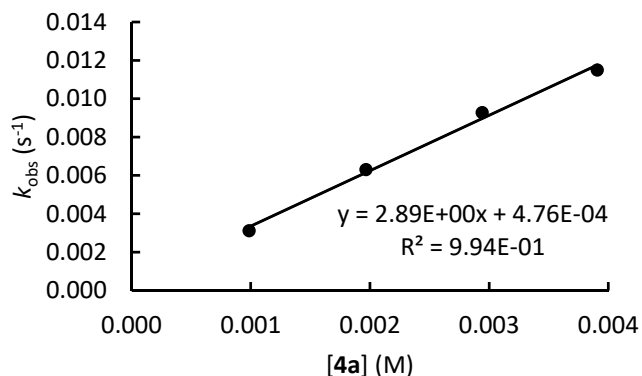
$$k_2 = (4.14 \pm 0.10) \times 10^{-1} \text{ M}^{-1} \text{ s}^{-1}$$



4a + 7 (from 7·HBF₄ + 1 equiv KOTBu) in DMSO (conventional UV/Vis, detection at 378 nm) RM442

[7] ₀ , M	[4a] ₀ , M	k _{obs} , s ⁻¹
1.00 × 10 ⁻⁴	9.87 × 10 ⁻⁴	3.12 × 10 ⁻³
1.00 × 10 ⁻⁴	1.97 × 10 ⁻³	6.31 × 10 ⁻³
1.00 × 10 ⁻⁴	2.94 × 10 ⁻³	9.28 × 10 ⁻³
1.00 × 10 ⁻⁴	3.91 × 10 ⁻³	1.15 × 10 ⁻²

$$k_2 = 2.89 \pm 0.16 \text{ M}^{-1} \text{ s}^{-1}$$

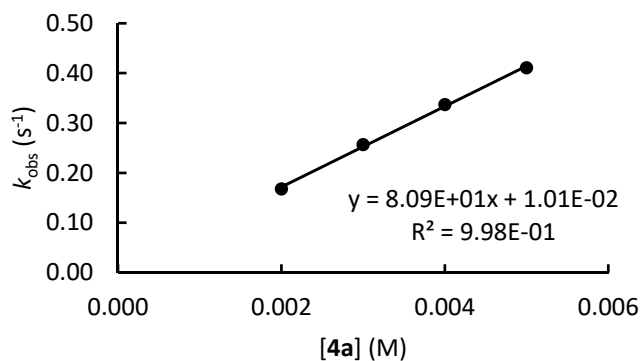


4a + 6c (from 6c·HBr + 1 equiv KOTBu) in DMSO (sequential mixing stopped-flow, detection at 425 nm)

RM500

[6c] ₀ , M	[4a] ₀ , M	k _{obs} , s ⁻¹
1.00 × 10 ⁻⁴	2.00 × 10 ⁻³	1.68 × 10 ⁻¹
1.00 × 10 ⁻⁴	3.00 × 10 ⁻³	2.57 × 10 ⁻¹
1.00 × 10 ⁻⁴	4.00 × 10 ⁻³	3.37 × 10 ⁻¹
1.00 × 10 ⁻⁴	5.00 × 10 ⁻³	4.11 × 10 ⁻¹

$$k_2 = (8.09 \pm 0.02) \times 10^1 \text{ M}^{-1} \text{ s}^{-1}$$

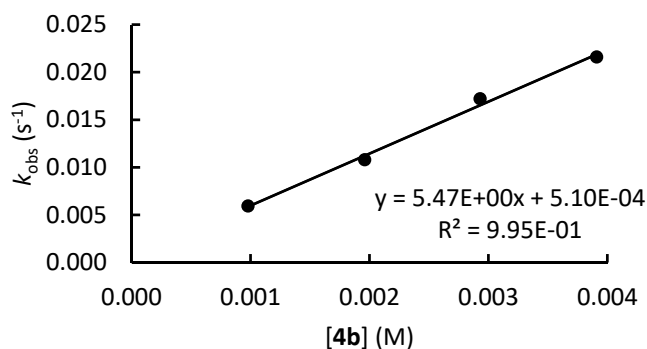


Reactions of methylene furanone (**4b**) with reference nucleophiles

4b + **6a** (from **6a**·HCl with 1 equiv KOtBu) in DMSO (conventional UV/Vis, detection at 427 nm) RM490

[6a] ₀ , M	[4b] ₀ , M	<i>k</i> _{obs} , s ⁻¹
1.00 × 10 ⁻⁴	9.79 × 10 ⁻⁴	5.93 × 10 ⁻³
1.00 × 10 ⁻⁴	1.96 × 10 ⁻³	1.08 × 10 ⁻²
1.00 × 10 ⁻⁴	2.93 × 10 ⁻³	1.72 × 10 ⁻²
1.00 × 10 ⁻⁴	3.91 × 10 ⁻³	2.16 × 10 ⁻²

$$k_2 = 5.47 \pm 0.27 \text{ M}^{-1} \text{ s}^{-1}$$

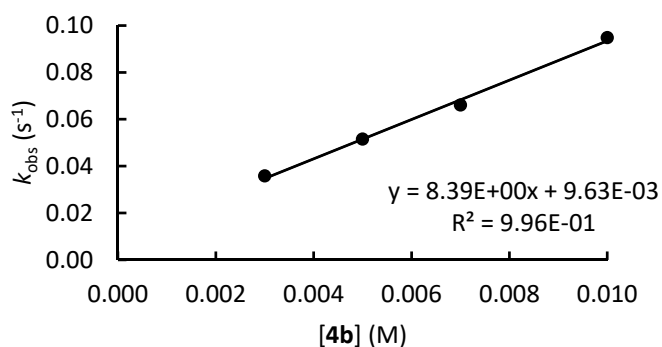


4b + **7** (from **7**-HBF₄ + 1 equiv KOtBu) in DMSO (sequential mixing stopped-flow, detection at 378 nm) RM487

RM487

[7] ₀ , M	[4b] ₀ , M	<i>k</i> _{obs} , s ⁻¹			
		1	2	3	average
1.00 × 10 ⁻⁴	3.00 × 10 ⁻³	3.24 × 10 ⁻²	3.50 × 10 ⁻²	4.00 × 10 ⁻²	3.58 × 10 ⁻²
1.00 × 10 ⁻⁴	5.00 × 10 ⁻³	4.65 × 10 ⁻²	5.02 × 10 ⁻²	5.78 × 10 ⁻²	5.15 × 10 ⁻²
1.00 × 10 ⁻⁴	7.00 × 10 ⁻³	6.15 × 10 ⁻²	6.42 × 10 ⁻²	7.25 × 10 ⁻²	6.61 × 10 ⁻²
1.00 × 10 ⁻⁴	1.00 × 10 ⁻²	9.82 × 10 ⁻²	9.15 × 10 ⁻²	9.46 × 10 ⁻²	9.48 × 10 ⁻²

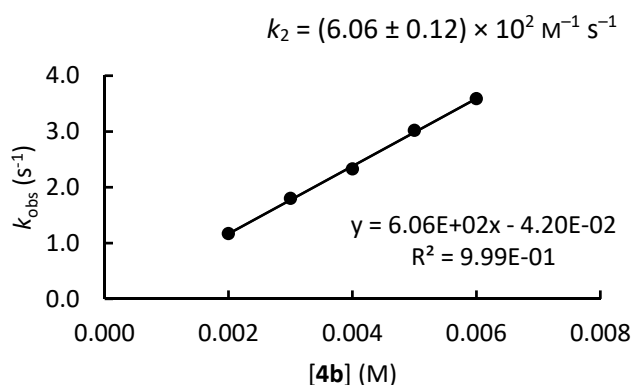
$$k_2 = 8.39 \pm 0.38 \text{ M}^{-1} \text{ s}^{-1}$$



4b + 6c (from **6c**·HBr + 1 equiv KOTBu) in DMSO (sequential mixing stopped-flow, detection at 425 nm)

RM501

[6c] ₀ , M	[4b] ₀ , M	<i>k</i> _{obs} , s ⁻¹				
		1	2	3	4	average
1.00 × 10 ⁻⁴	2.00 × 10 ⁻³	1.16	1.16	1.18	1.19	1.17
1.00 × 10 ⁻⁴	3.00 × 10 ⁻³	1.79	1.82	1.82	1.75	1.80
1.00 × 10 ⁻⁴	4.00 × 10 ⁻³	2.36	2.33	2.29	2.32	2.33
1.00 × 10 ⁻⁴	5.00 × 10 ⁻³	2.99	3.10	3.03	2.97	3.02
1.00 × 10 ⁻⁴	6.00 × 10 ⁻³	3.74	3.46	3.60	3.56	3.59

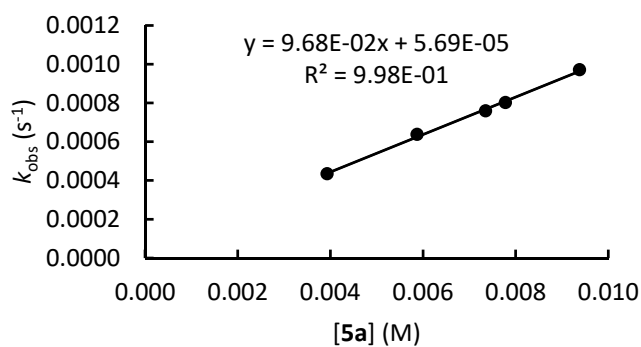


Reactions of pyranone (5a) with reference nucleophiles

5a + 6a (from **6a**·H + 1 equiv KOTBu) in DMSO (conventional UV/Vis, detection at 427 nm) RM492

[6a] ₀ , M	[5a] ₀ , M	<i>k</i> _{obs} , s ⁻¹
1.00 × 10 ⁻⁴	3.93 × 10 ⁻³	4.35 × 10 ⁻⁴
1.00 × 10 ⁻⁴	5.87 × 10 ⁻³	6.38 × 10 ⁻⁴
1.00 × 10 ⁻⁴	7.35 × 10 ⁻³	7.59 × 10 ⁻⁴
1.00 × 10 ⁻⁴	7.78 × 10 ⁻³	8.02 × 10 ⁻⁴
1.00 × 10 ⁻⁴	9.38 × 10 ⁻³	9.72 × 10 ⁻⁴

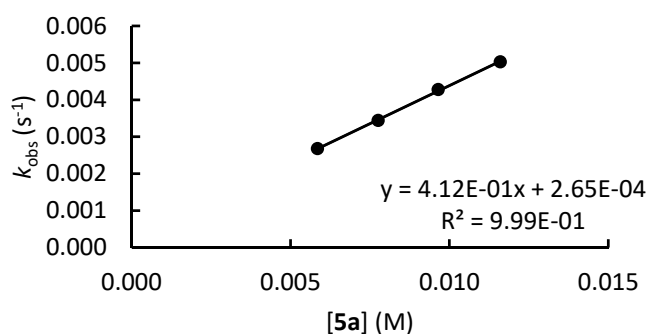
$$k_2 = (9.68 \pm 0.27) \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$$



5a + 7 (from **7**·HBF₄ + 1 equiv KOTBu) in DMSO (conventional UV/Vis, detection at 378 nm) RM498

[7] ₀ , M	[5a] ₀ , M	<i>k</i> _{obs} , s ⁻¹
1.00 × 10 ⁻⁴	5.85 × 10 ⁻³	2.68 × 10 ⁻³
1.00 × 10 ⁻⁴	7.76 × 10 ⁻³	3.44 × 10 ⁻³
1.00 × 10 ⁻⁴	9.65 × 10 ⁻³	4.28 × 10 ⁻³
1.00 × 10 ⁻⁴	1.16 × 10 ⁻²	5.03 × 10 ⁻³

$$k_2 = (4.12 \pm 0.08) \times 10^{-1} \text{ M}^{-1} \text{ s}^{-1}$$

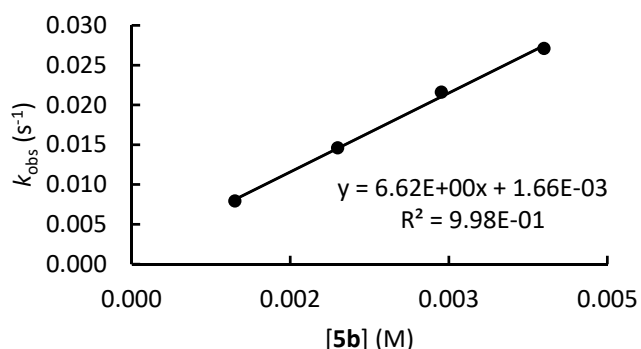


Reactions of methylene pyranone (5b) with reference nucleophiles

5b + 6a (from **6a**·HCl + 1 equiv KOTu) in DMSO (conventional UV/Vis, detection at 427 nm) RM890

[6a] ₀ , M	[5b] ₀ , M	k _{obs} , s ⁻¹
1.00 × 10 ⁻⁴	9.78 × 10 ⁻⁴	7.93 × 10 ⁻³
1.00 × 10 ⁻⁴	1.95 × 10 ⁻³	1.46 × 10 ⁻²
1.00 × 10 ⁻⁴	2.93 × 10 ⁻³	2.16 × 10 ⁻²
1.00 × 10 ⁻⁴	3.90 × 10 ⁻³	2.71 × 10 ⁻²

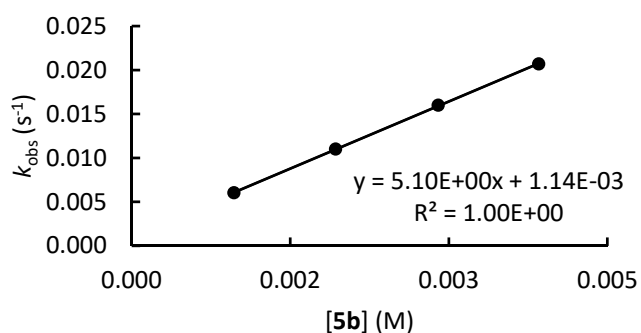
$$k_2 = 6.62 \pm 0.23 \text{ M}^{-1} \text{ s}^{-1}$$



5b + 7 (from **7**·HBF₄ + 1 equiv KOTu) in DMSO (conventional UV/Vis, detection at 378 nm) RM891

[7] ₀ , M	[5b] ₀ , M	k _{obs} , s ⁻¹
1.00 × 10 ⁻⁴	9.68 × 10 ⁻⁴	6.03 × 10 ⁻³
1.00 × 10 ⁻⁴	1.93 × 10 ⁻³	1.10 × 10 ⁻²
1.00 × 10 ⁻⁴	2.90 × 10 ⁻³	1.60 × 10 ⁻²
1.00 × 10 ⁻⁴	3.85 × 10 ⁻³	2.07 × 10 ⁻²

$$k_2 = 5.10 \pm 0.04 \text{ M}^{-1} \text{ s}^{-1}$$

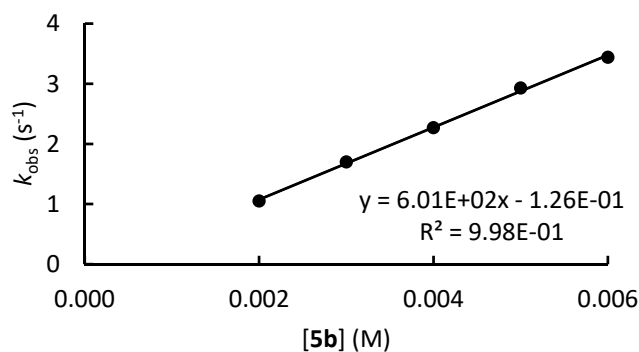


5b + 6c (from **6c**·HBr + 1 equiv KOTu) in DMSO (sequential mixing stopped-flow, detection at 425 nm)

RM896

[6c] ₀ , M	[5b] ₀ , M	k _{obs} , s ⁻¹			average
		1	2	3	
1.00 × 10 ⁻⁴	2.00 × 10 ⁻³	1.06	1.05	1.05	1.05
1.00 × 10 ⁻⁴	3.00 × 10 ⁻³	1.67	1.72	1.71	1.70
1.00 × 10 ⁻⁴	4.00 × 10 ⁻³	2.29	2.28	2.25	2.27
1.00 × 10 ⁻⁴	5.00 × 10 ⁻³	2.97	2.92	2.90	2.93
1.00 × 10 ⁻⁴	6.00 × 10 ⁻³	3.46	3.44	3.41	3.44

$$k_2 = (6.01 \pm 0.14) \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$$

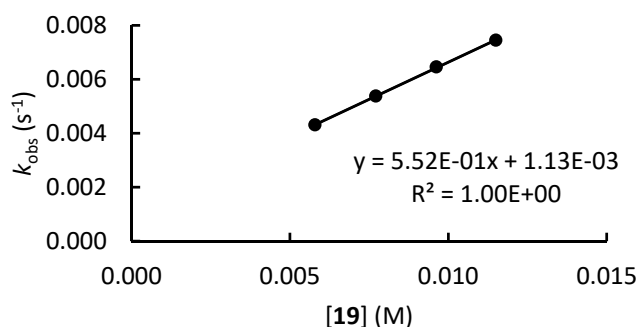


Reactions of carvone (19) with reference nucleophiles

19 + 6c (from 6c·HBr + 1 equiv KOTBu) in DMSO (conventional UV/Vis, detection at 425 nm) RM1055

[6c] ₀ , M	[19] ₀ , M	k _{obs} , s ⁻¹
1.00 × 10 ⁻⁴	5.79 × 10 ⁻³	4.31 × 10 ⁻³
1.00 × 10 ⁻⁴	7.71 × 10 ⁻³	5.38 × 10 ⁻³
1.00 × 10 ⁻⁴	9.62 × 10 ⁻³	6.46 × 10 ⁻³
1.00 × 10 ⁻⁴	1.15 × 10 ⁻²	7.45 × 10 ⁻³

$$k_2 = (5.52 \pm 0.06) \times 10^{-1} \text{ M}^{-1} \text{ s}^{-1}$$

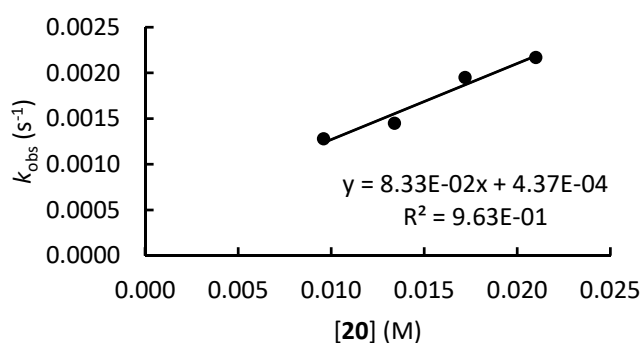


Reactions of verbenone (20) with reference nucleophiles

20 + 6c (from 6c·HBr + 1 equiv KOTBu) in DMSO (conventional UV/Vis, detection at 425 nm) RM1057

[6c] ₀ , M	[20] ₀ , M	k _{obs} , s ⁻¹
1.00 × 10 ⁻⁴	9.59 × 10 ⁻³	1.28 × 10 ⁻³
1.00 × 10 ⁻⁴	1.34 × 10 ⁻²	1.45 × 10 ⁻³
1.00 × 10 ⁻⁴	1.72 × 10 ⁻²	1.95 × 10 ⁻³
1.00 × 10 ⁻⁴	2.10 × 10 ⁻²	2.17 × 10 ⁻³

$$k_2 = (8.33 \pm 1.16) \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$$

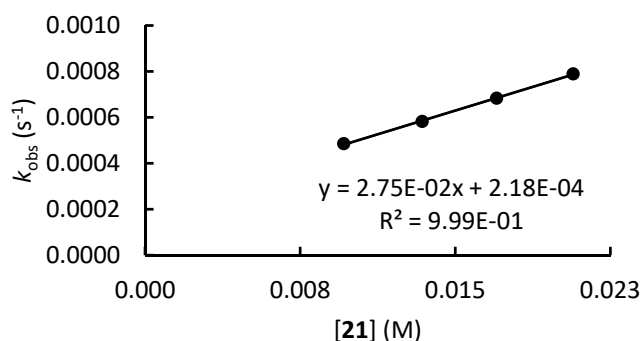


Reactions of nootkatone (21) with reference nucleophiles

21 + 6c (from 6c·HBr + 1 equiv KOTBu) in DMSO (conventional UV/Vis, detection at 425 nm) RM1061

[6c] ₀ , M	[21] ₀ , M	k _{obs} , s ⁻¹
1.00 × 10 ⁻⁴	9.61 × 10 ⁻³	4.85 × 10 ⁻⁴
1.00 × 10 ⁻⁴	1.34 × 10 ⁻²	5.82 × 10 ⁻⁴
1.00 × 10 ⁻⁴	1.70 × 10 ⁻²	6.83 × 10 ⁻⁴
1.00 × 10 ⁻⁴	2.07 × 10 ⁻²	7.89 × 10 ⁻⁴

$$k_2 = (2.75 \pm 0.05) \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$$



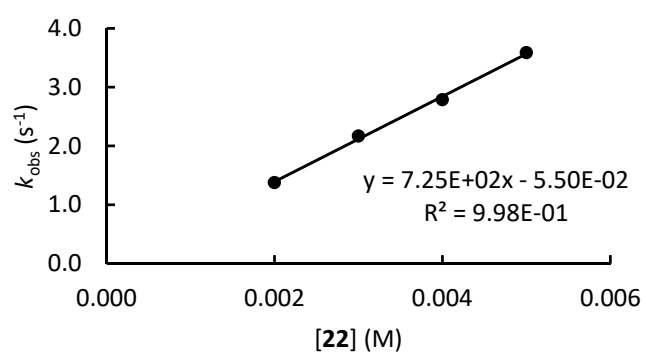
Reactions of parthenolide (**22**) with reference nucleophiles

22 + **6c** (from **6c**·HBr + 1 equiv KOtBu) in DMSO (sequential mixing stopped-flow, detection at 425 nm)

RM1052

[6c] ₀ , M	[22] ₀ , M	<i>k</i> _{obs} , s ⁻¹					<i>average</i>
		1	2	3	4	5	
1.00 × 10 ⁻⁴	2.00 × 10 ⁻³	1.40	1.38	1.39	1.37	1.38	1.38
1.00 × 10 ⁻⁴	3.00 × 10 ⁻³	2.20	2.18	2.16	2.18	2.14	2.17
1.00 × 10 ⁻⁴	4.00 × 10 ⁻³	2.82	2.80	2.75	2.77	2.81	2.79
1.00 × 10 ⁻⁴	5.00 × 10 ⁻³	3.58	3.59	3.62	3.55	3.62	3.59

$$k_2 = (7.25 \pm 0.25) \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$$



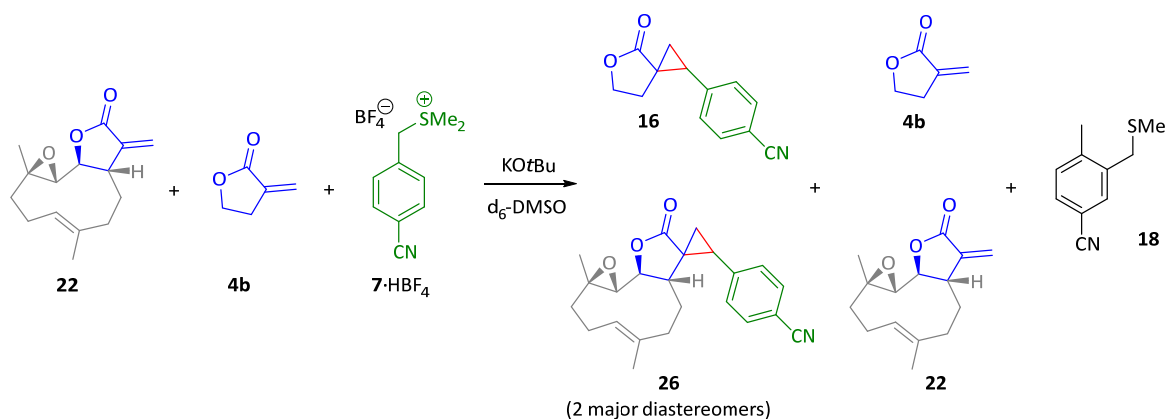
Competition Experiments

Competition experiments were performed as outlined in the main text. Reaction mixtures in d_6 -DMSO were analyzed without further workup. ^1H NMR spectra were recorded at 400 MHz with a pulse delay of 20 seconds and subsequently processed with phase and baseline correction (MestReNova version 12.0.4).

To identify the significant resonances in the reaction mixtures of the competition experiments, we also analyzed the solutions of the reactions of the sulfonium ylide **7** with the individual electrophiles in d_6 -DMSO. The comparison of the ^1H NMR spectra obtained for the different species under identical conditions facilitated the assignment of the resonances to be used for the determination of the competition constants.

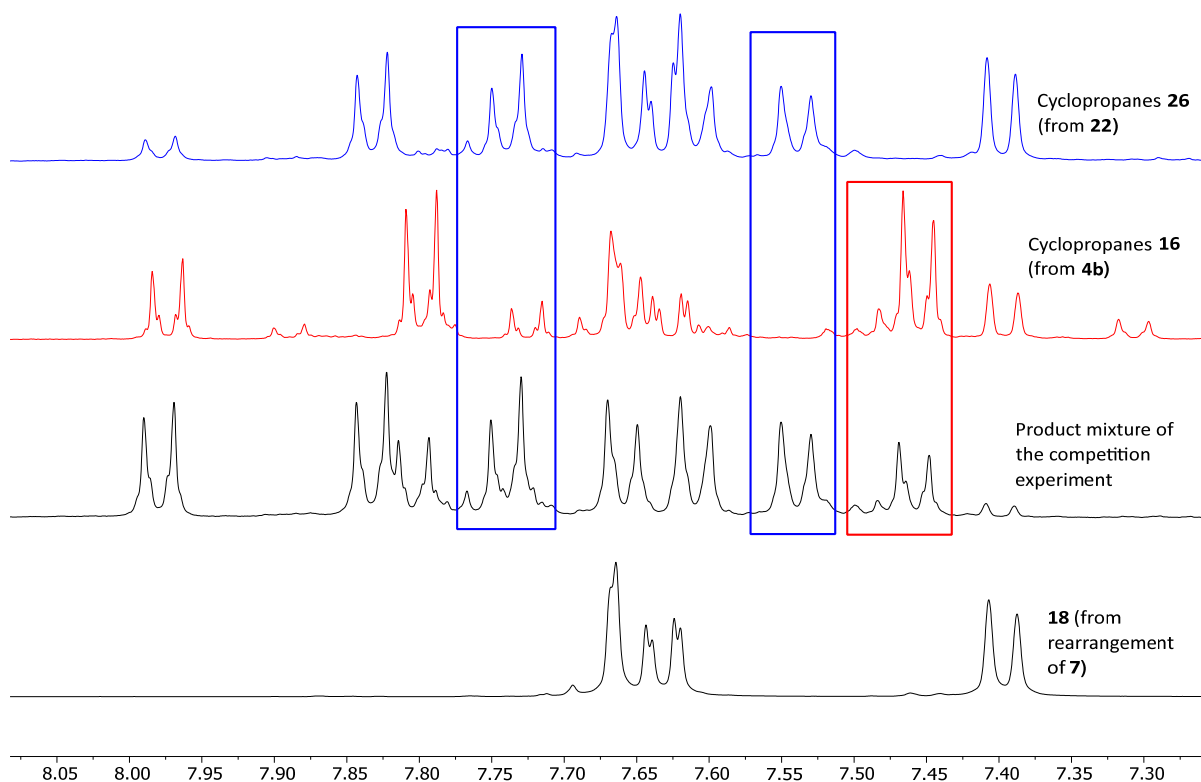
As a consequence, well-resolved resonances of the diastereomeric products were selected, integrated, and utilized for the determination of the competition constants κ . The spectral ranges and integrals used for the spectroscopic analysis are marked in each of the ^1H NMR spectra.

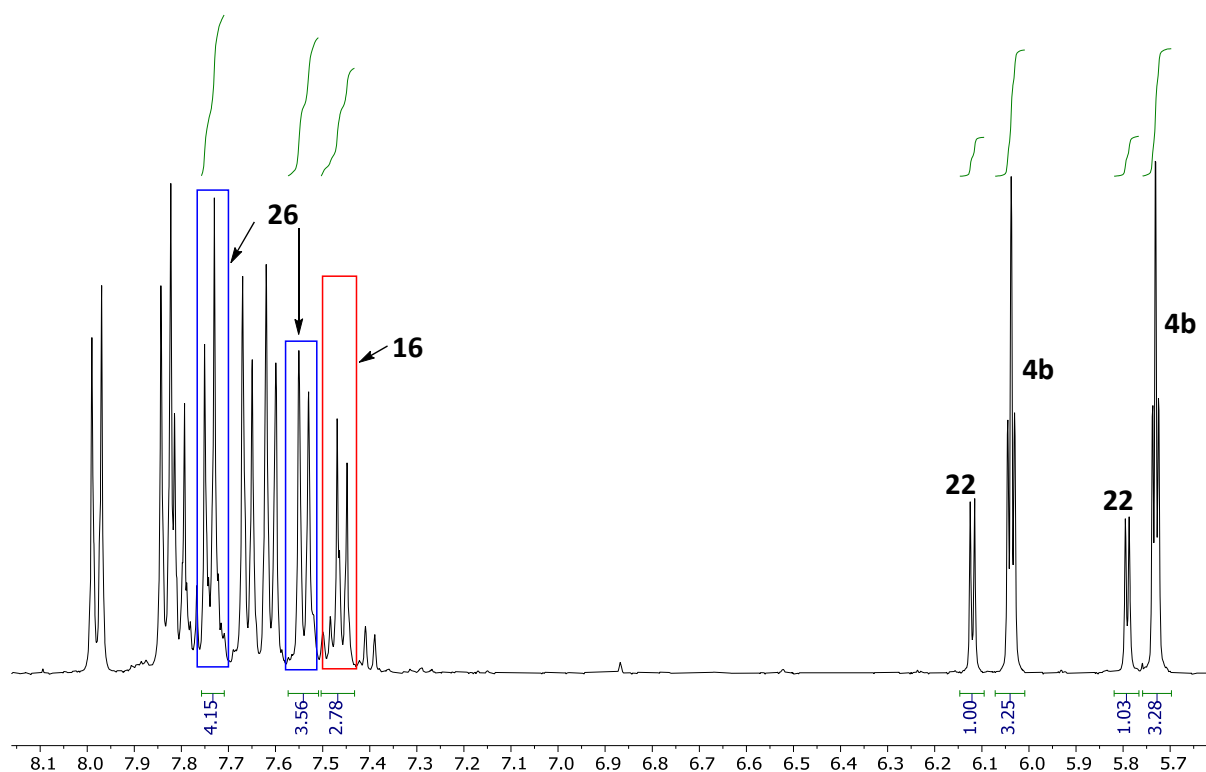
Competition experiment between **4b** and parthenolide (**22**)
(RNH513)



In a glovebox, parthenolide **22** (4.20 mg, 0.0169 mmol), α -methylenefuranone **4b** (1.66 mg, 0.0169 mmol) and the sulfonium tetrafluoroborate **7**-HBF₄ (3.73 mg, 0.0141 mmol) were dissolved in d₆-DMSO (0.4 mL) and then mixed with a solution of KOtBu (1.5 mg, 0.013 mmol) in d₆-DMSO (0.4 mL).

The resulting reaction mixture was transferred into an NMR tube and analyzed by ¹H NMR spectroscopy.



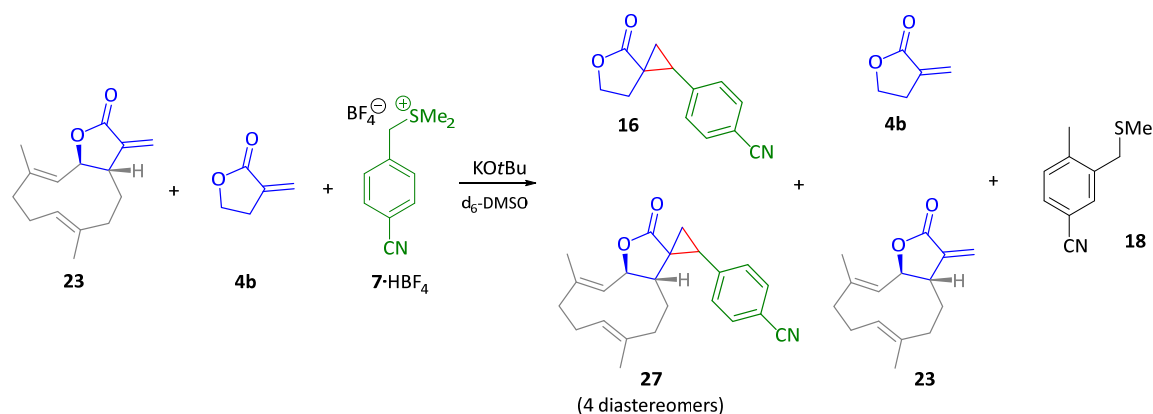


Well resolved resonances in the aromatic region of the ¹H NMR spectrum were selected for integration. Integrals over resonances assigned to both major diastereomers of **16** as well as those assigned to the two major diastereomers of **26** were used to determine the competition constant κ .

Species	Integrals / number of protons	Integral, normalized to 1 H
22	1.00 / 1 H	1.00 / 1 H
4b	3.25 / 1 H	3.25 / 1 H
26	two diastereomers: 7.71 / 2 H	3.86 / 1 H
16	two diastereomers: 2.78 / 2 H	1.39 / 1 H

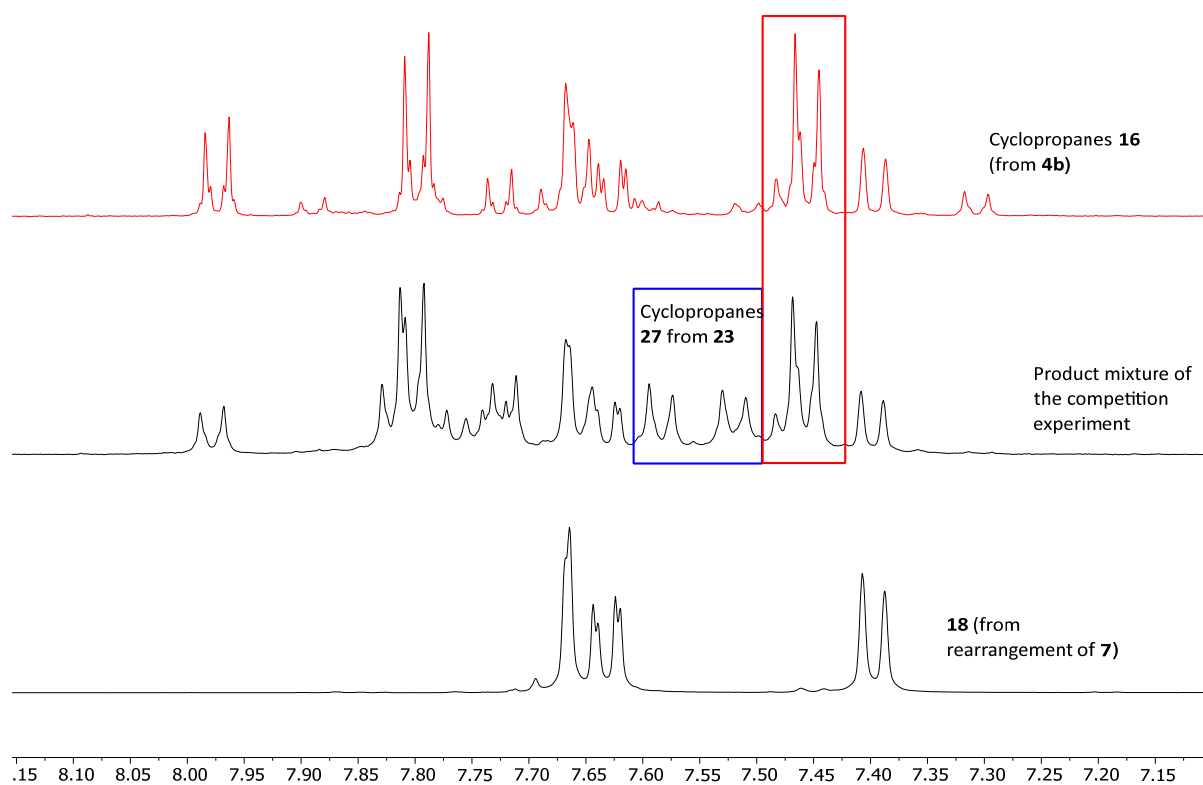
$$\kappa = \frac{\lg\left(1 + \frac{[\mathbf{26}]}{[\mathbf{22}]}\right)}{\lg\left(1 + \frac{[\mathbf{16}]}{[\mathbf{4b}]}\right)} = \frac{\lg\left(1 + \frac{3.86}{1.00}\right)}{\lg\left(1 + \frac{1.39}{3.25}\right)} = 4.4$$

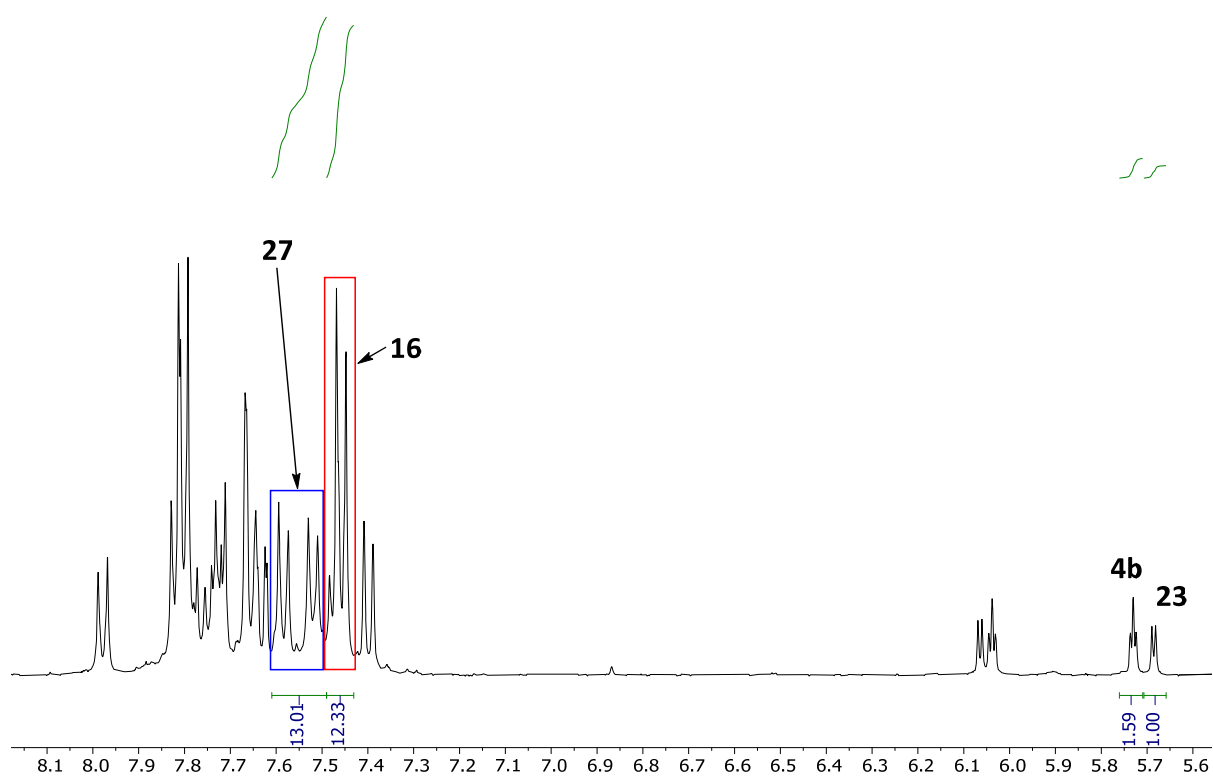
Competition experiment between **4b** and costunolid (**23**)
(RNH447)



In a glovebox, costunolid (**23**, 4.26 mg, 0.0183 mmol), α -methylenefuranone (**4b**, 1.80 mg, 0.0183 mmol) and the sulfonium tetrafluoroborate **7·HBF₄** (4.04 mg, 0.0152 mmol) were dissolved in **d₆-DMSO** (0.4 mL) and then mixed with a solution of **KOtBu** (1.6 mg, 0.014 mmol) in **d₆-DMSO** (0.4 mL).

The resulting reaction mixture was transferred into an NMR tube and analyzed by ¹H NMR spectroscopy.



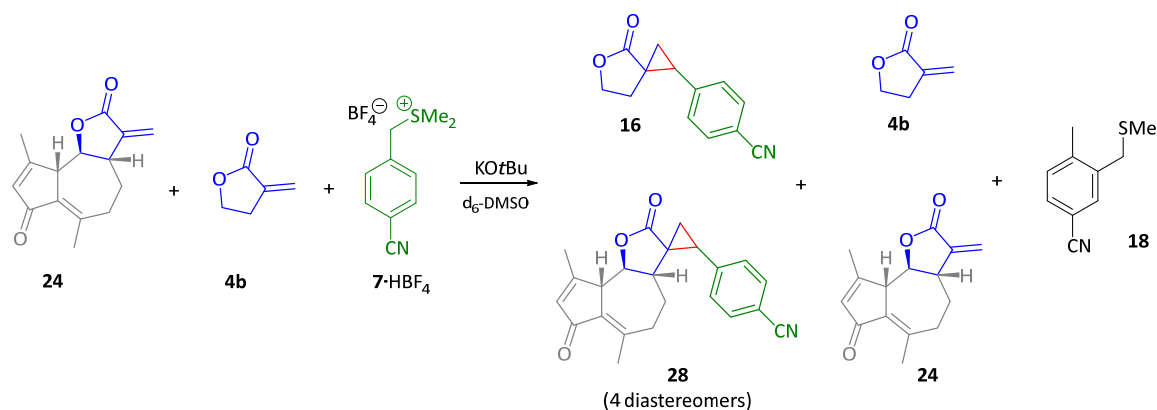


Well resolved resonances in the aromatic region of the ^1H NMR spectrum were selected for integration. Integrals over resonances assigned to both major diastereomers of **16** and **27**, respectively, were used to determine the competition constant κ .

Species	Integrals / number of protons	Integral, normalized to 1 H
23	1.00 / 1 H	1.00 / 1 H
4b	1.59 / 1 H	1.59 / 1 H
27	two diastereomers: 13.01 / 2 H	6.51 / 1 H
16	two diastereomers: 12.33 / 2 H	6.17 / 1 H

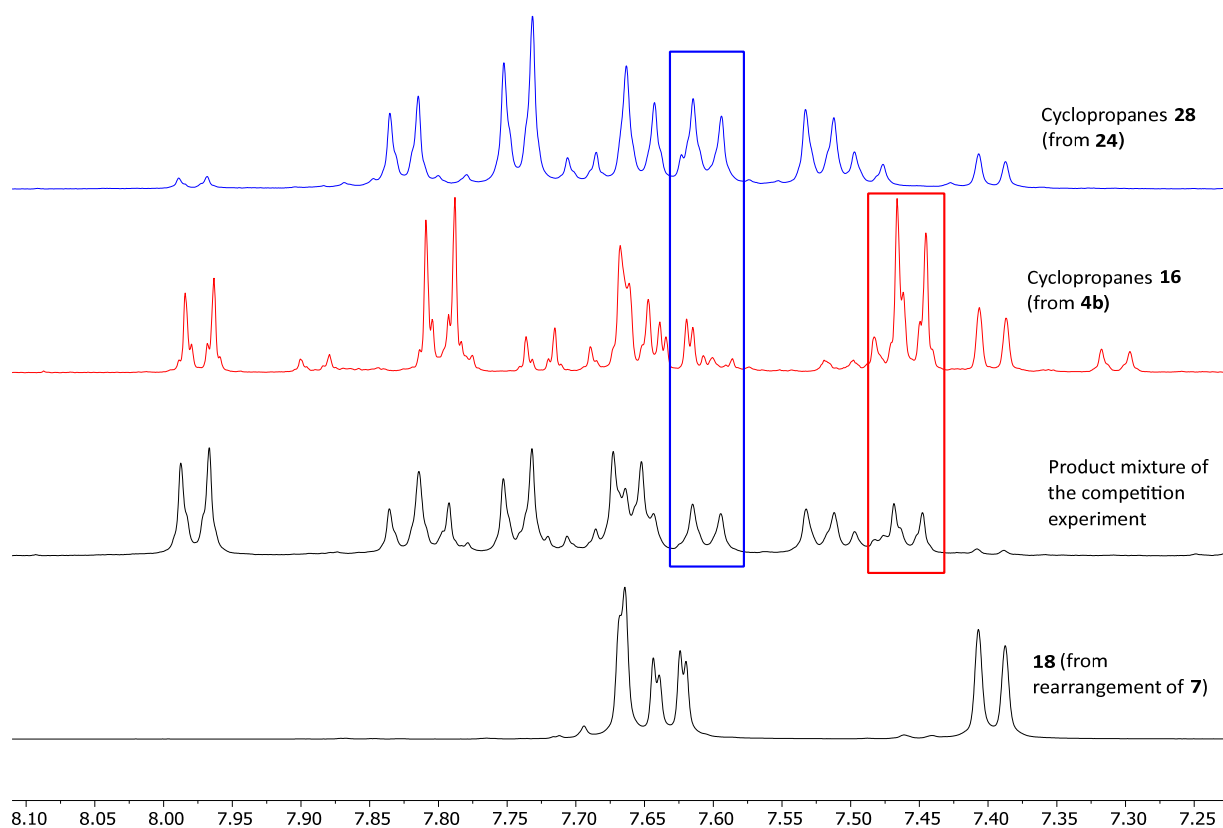
$$\kappa = \frac{\lg\left(1 + \frac{[\mathbf{27}]}{[\mathbf{23}]}\right)}{\lg\left(1 + \frac{[\mathbf{16}]}{[\mathbf{4b}]}\right)} = \frac{\lg\left(1 + \frac{6.51}{1.00}\right)}{\lg\left(1 + \frac{6.17}{1.59}\right)} = 1.3$$

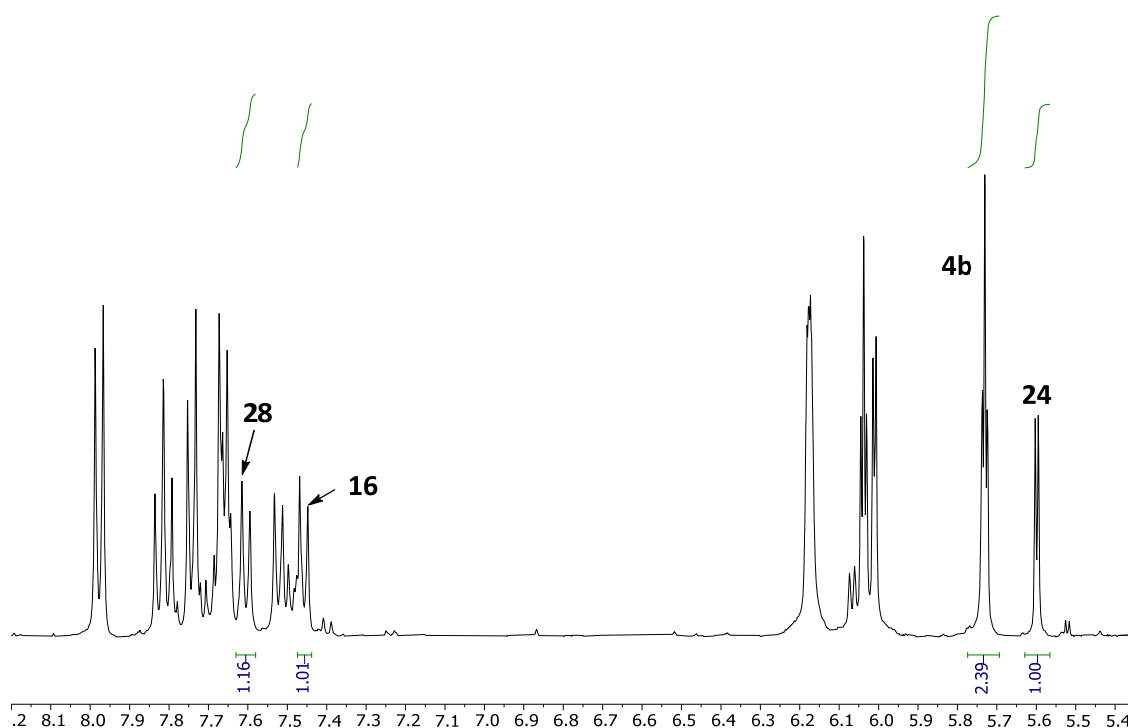
Competition experiment between **4b** and dehydroleucodine (**24**)
(RNH448)



In a glovebox, dehydroleucodine (**24**, 4.48 mg, 0.0183 mmol), α -methylene-furanone (**4b**, 1.85 mg, 0.0188 mmol) and the sulfonium tetrafluoroborate **7-HBF₄** (4.03 mg, 0.0152 mmol) were dissolved in $\text{d}_6\text{-DMSO}$ (0.4 mL) and then mixed with a solution of KOtBu (1.6 mg, 0.014 mmol) in $\text{d}_6\text{-DMSO}$ (0.4 mL).

The resulting reaction mixture was transferred into an NMR tube and analyzed by ^1H NMR spectroscopy.



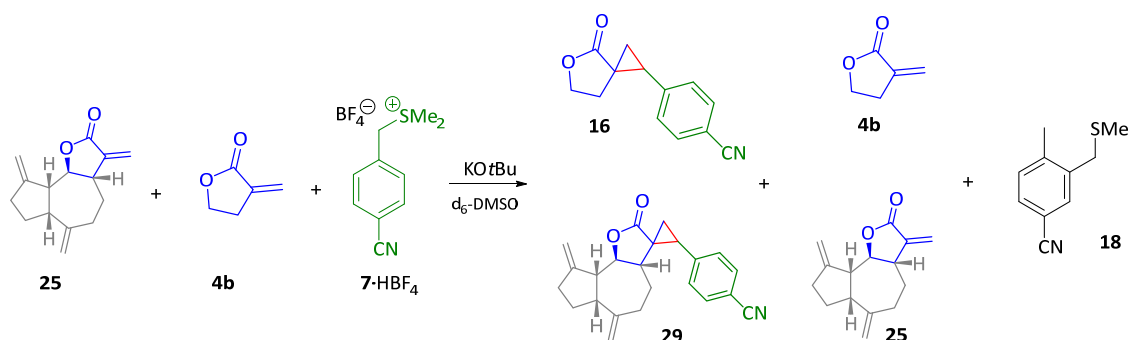


Well resolved resonances in the aromatic region of the ^1H NMR spectrum were selected for integration. Integrals over resonances assigned to one diastereomer of **16** and **28**, respectively, were used for the evaluation. Both integrals were corrected for the diastereomeric ratios for **16** and **28** (independently determined under identical conditions) to determine the competition constant κ .

Species	Integrals / number of protons	Integral, normalized to 1 H
24	1.00 / 1 H	1.00 / 1 H
4b	2.39 / 1 H	2.39 / 1 H
28	Single diastereomer: 1.16 / 2 H Corrected for a diastereomeric ratio of (dr: 0.294 : 1) to give 3.94 / 2 H	1.97 / 1 H
16	Single diastereomer: 1.01 / 2 H Corrected for a diastereomeric ratio of (dr: 0.810 : 1) to give 1.25 / 2 H	0.63 / 1 H

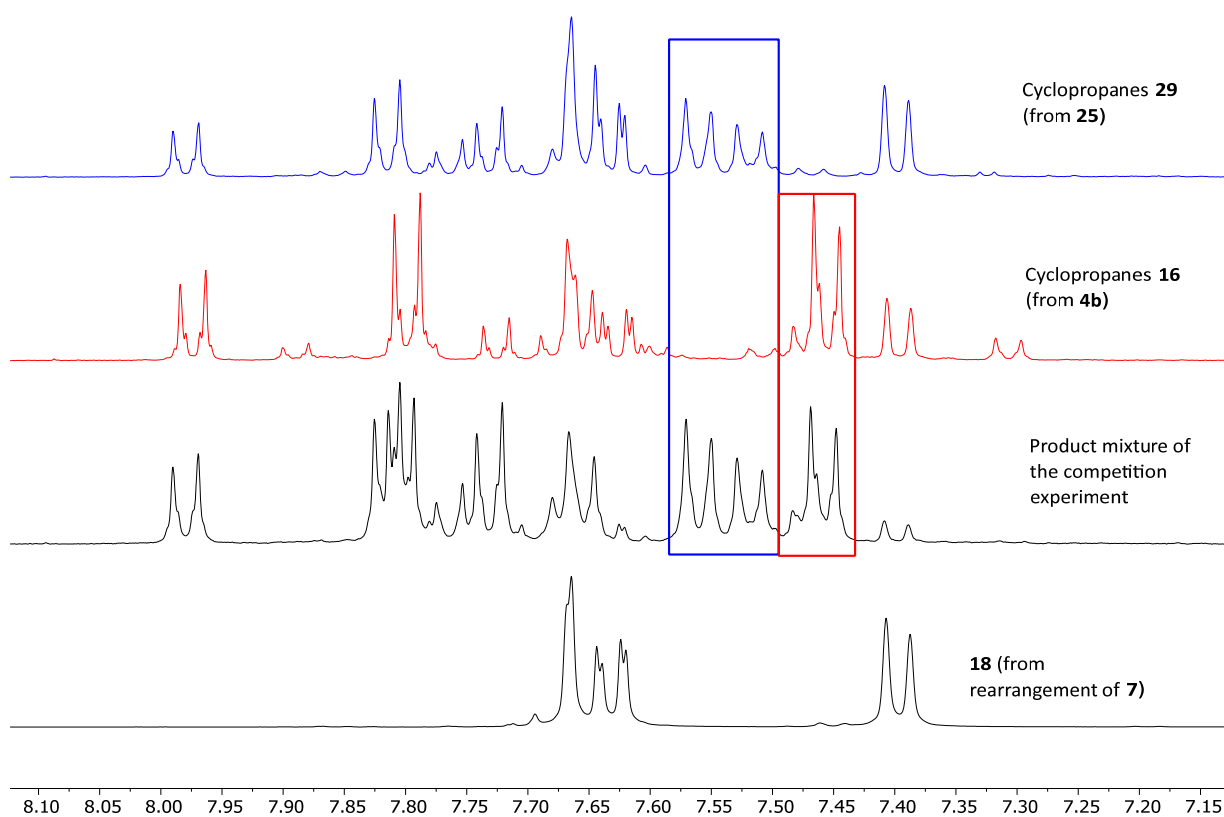
$$\kappa = \frac{\lg\left(1 + \frac{[\mathbf{28}]}{[\mathbf{24}]}\right)}{\lg\left(1 + \frac{[\mathbf{16}]}{[\mathbf{4b}]}\right)} = \frac{\lg\left(1 + \frac{1.97}{1.00}\right)}{\lg\left(1 + \frac{0.63}{2.39}\right)} = 4.6$$

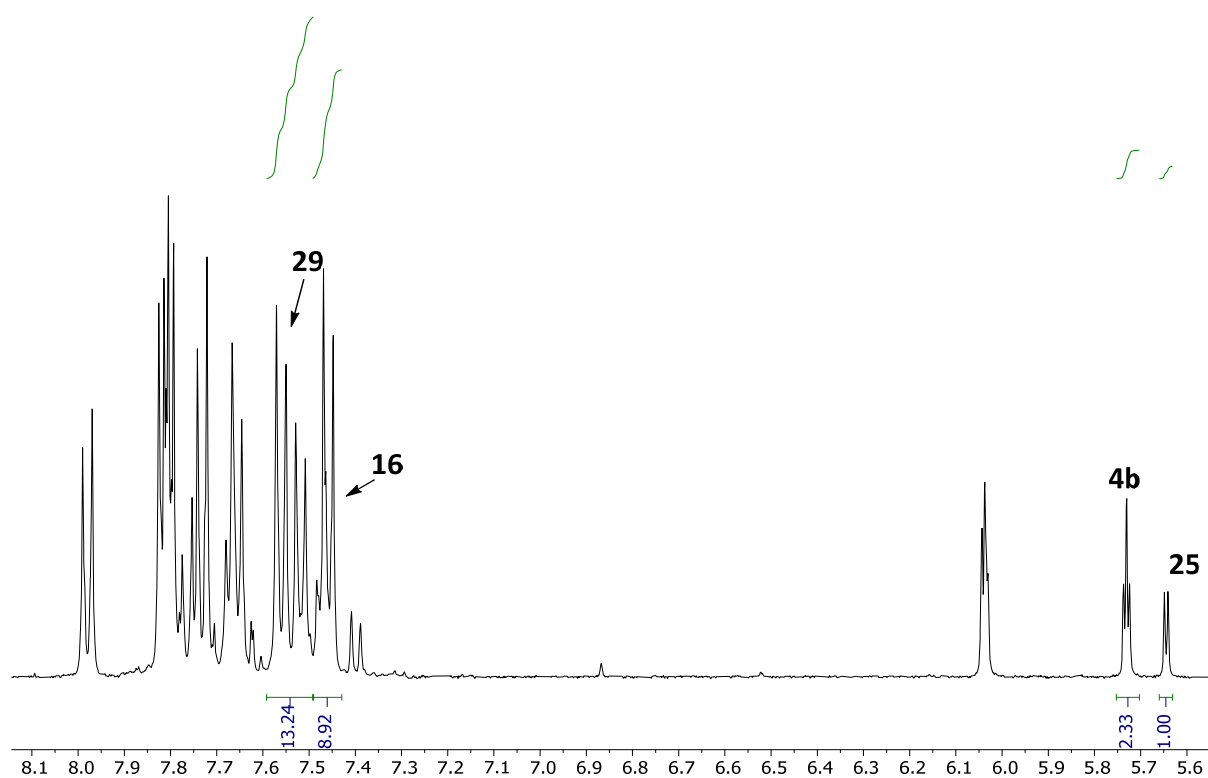
Competition experiment between **4b** and dehydrocostus lactone (**25**)
(RNH380)



In a glovebox, dehydrocostus lactone (**25**, 4.0 mg, 0.0174 mmol), α -methylene-furanone (**4b**, 1.7 mg, 0.0173 mmol) and the sulfonium tetrafluoroborate **7**·HBF₄ (3.8 mg, 0.0145 mmol) were dissolved in d₆-DMSO (0.4 mL) and then mixed with a solution of KOtBu (1.5 mg, 0.013 mmol) in d₆-DMSO (0.4 mL).

The resulting reaction mixture was transferred into an NMR tube and analyzed by ¹H NMR spectroscopy.





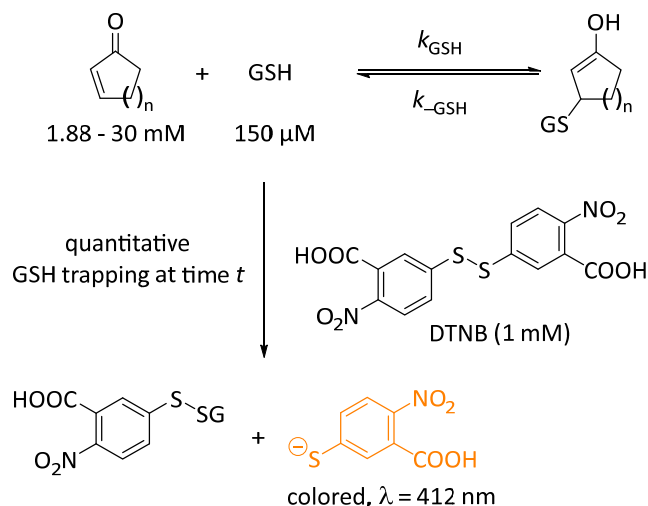
Well resolved resonances in the aromatic region of the ¹H NMR spectrum were selected for integration. Integrals over resonances assigned to both major diastereomers of **16** and **29**, respectively, were used to determine the competition constant κ .

Species	Integrals / number of protons	Integral, normalized to 1 H
25	1.00 / 1 H	1.00 / 1 H
4b	2.33 / 1 H	2.33 / 1 H
29	two diastereomers: 13.24 / 2 H	6.62 / 1 H
16	two diastereomers: 8.92 / 2 H	4.46 / 1 H

$$\kappa = \frac{\lg\left(1 + \frac{[\mathbf{29}]}{[\mathbf{25}]}\right)}{\lg\left(1 + \frac{[\mathbf{16}]}{[\mathbf{4b}]}\right)} = \frac{\lg\left(1 + \frac{6.62}{1.00}\right)}{\lg\left(1 + \frac{4.46}{2.33}\right)} = 1.9$$

Kinetic GSH Chemoassay

A kinetic glutathione (GSH) chemoassay was used to determine the reactivity of cyclic Michael acceptors in aqueous solution.⁵⁶



Second-order rate constants (k_2) for the reactions of GSH with cyclic enones and α,β -unsaturated lactones (electrophiles) were determined by a series of pseudo-first order kinetic measurements at variable electrophile concentrations. In aqueous solutions, the reactions of GSH with the electrophiles were monitored by following the consumption of GSH. For each kinetic run, 15-20 time-dependent GSH concentrations, $[\text{GSH}]_t$, were determined by quantitative trapping with DTNB (indicated by the formation of the colored thiophenolate, detected at $\lambda = 412$ nm). Assuming the validity of the Lambert-Beer law for the sub-millimolar solutions of the thiophenolate, the measured absorbance A (at 412 nm) is a measure of $[\text{GSH}]_t$.

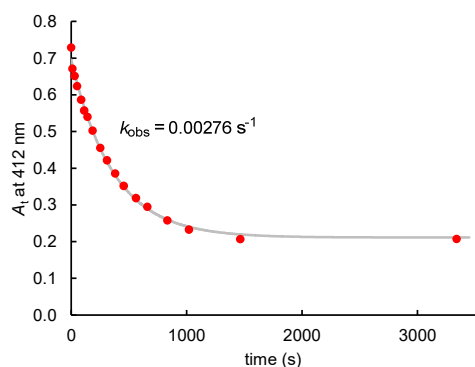
General Procedure.

180 μL of GSH solution (10 \times stock solution, pH 7.40; final concentration: 150 μM) in phosphate buffer (64.8 mM Na_2HPO_4 , 15.3 mM KH_2PO_4 , pH 7.40) were added to 1620 μL electrophile solution in phosphate buffer and incubated in a 2 mL Eppendorf tube at 20 $^\circ\text{C}$ with shaking at 300 rpm. After certain time intervals, 100 μL of the reaction mixture or control were added to 2 μL of DTNB solution in phosphate buffer (100 \times stock solution, pH 7.40; final concentration: 1 mM) in a transparent flat bottom 96-well plate (*Greiner*). The absorbance ($\lambda = 412$ nm) was measured at 20 $^\circ\text{C}$ using an Infinite M Nano Plus plate reader (*Tecan*). This procedure was repeated 15 to 20 times to determine a sufficient number of time-dependent GSH concentrations, $[\text{GSH}]_t$, during the course of a given reaction. Electrophile solutions were prepared in four different concentrations with equal concentration gaps (1x, 2x, 3x, 4x) and were in the range from 1.88 to 30 mM. As controls, solutions without electrophile were used containing either no GSH (blank; 0% relative absorbance) or 150 μM GSH (control; 100% relative absorbance). All solutions were pre-incubated at 20 $^\circ\text{C}$ prior to measurement.

Determination of the rate constants k_{GSH} and $k_{-\text{GSH}}$.

Contributions of the forward (expressed by k_{GSH}) and reverse reaction (expressed by $k_{-\text{GSH}}$) to k_{obs} in our experimental setup were considered by applying the equation $k_{\text{obs}} = k_{\text{GSH}}[\text{electrophile}] + k_{-\text{GSH}}$.^{S6b}

First-order rate constant k_{obs} (s^{-1}) for individual kinetic runs were determined by fitting the mono-exponential function $A_t = A_0 \cdot \exp^{-k_{\text{obs}}t} + C$ to the observed A_t (at 412 nm).



Decay of the thiophenolate absorbance (red dots) during the reaction of GSH (0.15 mM) with cyclopentenone **1a** (3.75 mM) in water (pH = 7.40, phosphate buffer) and fitted curve (grey, for k_{obs} determination).

At the end of our kinetic GSH chemoassays used to determine the rates of GSH adduct formation with excess Michael acceptors, the remaining (free) GSH is quantitatively trapped by the DTNB reagent. This GSH trapping eliminates the entire GSH from the equilibrium with the electrophile. Thus, it triggers the reverse reaction to re-establish the GSH/enone/Michael adduct equilibrium. In this way, the reverse reaction (that is, Michael adduct dissociation) can be monitored at 412 nm.^{S6c}

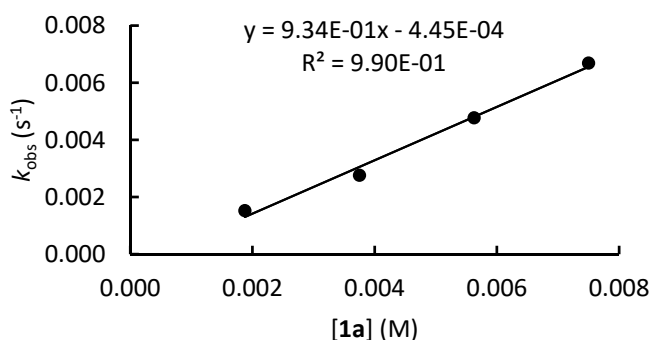
Photometric tracing the solutions of the chemoassays for the Michael acceptors **2a**, **4a**, **4b**, **5a**, and **5b** did not indicate GSH formation over a time of 10 hours (at r.t. under aerobic conditions). However, a significant increase of absorption due to further DTNB consumption by released GSH was observed for the GSH-cyclopentenone (**1a**) adduct and, in a much slower process, for the GSH-**1b** adduct. For the retro-Michael addition of the GSH-**1a** adduct a first-order rate constant of $k = 2.8 \times 10^{-4} \text{ s}^{-1}$ ($t_{1/2} = 40 \text{ min}$) was roughly determined. Esterbauer and colleagues reported $k(20 \text{ }^\circ\text{C}) = 5.16 \times 10^{-6} \text{ s}^{-1}$ ($t_{1/2} = 37 \text{ h}$) for the dissociation of the GSH-cyclohexenone (**2a**) adduct.^{S6c}

Linear correlations were obtained for all investigated GSH/electrophile couples by plotting k_{obs} vs [enone]. The slope of a k_{obs} vs [enone] plot corresponds to the second-order rate constant k_{GSH} ($\text{M}^{-1} \text{ s}^{-1}$) and intercept on the ordinate reflects (in theory) the contribution of the retro-Michael addition ($k_{-\text{GSH}}$). Our experiments do not allow to derive $k_{-\text{GSH}}$ reliably from the intercepts on the ordinate, however, because these intercepts are usually at least one order of magnitude smaller than the values of the slopes and, thus, in the range of the experimental error.

GSH + 1a in H₂O

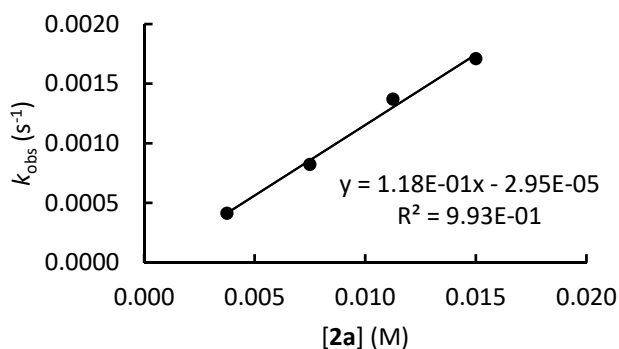
[GSH] ₀ , M	[1a] ₀ , M	k _{obs} , s ⁻¹
1.50 × 10 ⁻⁴	1.88 × 10 ⁻³	1.52 × 10 ⁻³
1.50 × 10 ⁻⁴	3.75 × 10 ⁻³	2.76 × 10 ⁻³
1.50 × 10 ⁻⁴	5.63 × 10 ⁻³	4.77 × 10 ⁻³
1.50 × 10 ⁻⁴	7.50 × 10 ⁻³	6.69 × 10 ⁻³

$$k_2 = (9.34 \pm 0.66) \times 10^{-1} \text{ M}^{-1} \text{ s}^{-1}$$

**GSH + 2a** in H₂O

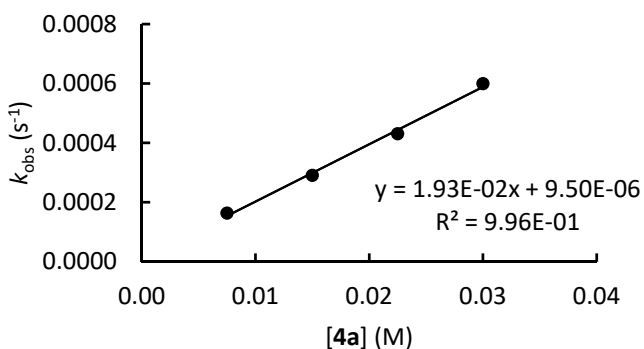
[GSH] ₀ , M	[2a] ₀ , M	k _{obs} , s ⁻¹
1.50 × 10 ⁻⁴	3.75 × 10 ⁻³	4.14 × 10 ⁻⁴
1.50 × 10 ⁻⁴	7.50 × 10 ⁻³	8.23 × 10 ⁻⁴
1.50 × 10 ⁻⁴	1.13 × 10 ⁻²	1.37 × 10 ⁻³
1.50 × 10 ⁻⁴	1.50 × 10 ⁻²	1.71 × 10 ⁻³

$$k_2 = (1.18 \pm 0.07) \times 10^{-1} \text{ M}^{-1} \text{ s}^{-1}$$

**GSH + 4a** in H₂O

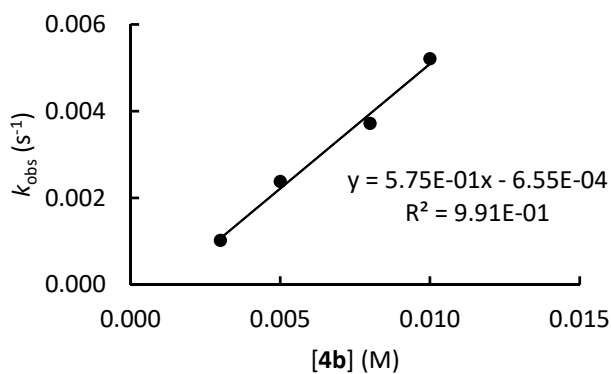
[GSH] ₀ , M	[4a] ₀ , M	k _{obs} , s ⁻¹
1.50 × 10 ⁻⁴	7.50 × 10 ⁻³	1.64 × 10 ⁻⁴
1.50 × 10 ⁻⁴	1.50 × 10 ⁻²	2.91 × 10 ⁻⁴
1.50 × 10 ⁻⁴	2.25 × 10 ⁻²	4.31 × 10 ⁻⁴
1.50 × 10 ⁻⁴	3.00 × 10 ⁻²	6.00 × 10 ⁻⁴

$$k_2 = (1.93 \pm 0.09) \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$$

**GSH + 4b** in H₂O

[GSH] ₀ , M	[4b] ₀ , M	k _{obs} , s ⁻¹
1.50 × 10 ⁻⁴	3.00 × 10 ⁻³	1.02 × 10 ⁻³
1.50 × 10 ⁻⁴	5.00 × 10 ⁻³	2.38 × 10 ⁻³
1.50 × 10 ⁻⁴	8.00 × 10 ⁻³	3.72 × 10 ⁻³
1.50 × 10 ⁻⁴	1.00 × 10 ⁻²	5.21 × 10 ⁻³

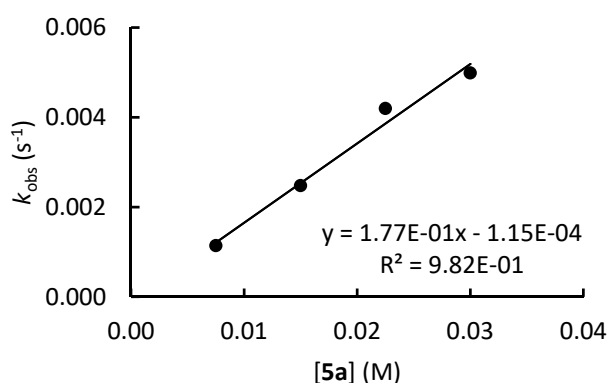
$$k_2 = (5.75 \pm 0.40) \times 10^{-1} \text{ M}^{-1} \text{ s}^{-1}$$



GSH + 5a in H₂O

[GSH] ₀ , M	[5a] ₀ , M	<i>k</i> _{obs} , s ⁻¹
1.50 × 10 ⁻⁴	7.50 × 10 ⁻³	1.14 × 10 ⁻³
1.50 × 10 ⁻⁴	1.50 × 10 ⁻²	2.48 × 10 ⁻³
1.50 × 10 ⁻⁴	2.25 × 10 ⁻²	4.20 × 10 ⁻³
1.50 × 10 ⁻⁴	3.00 × 10 ⁻²	4.99 × 10 ⁻³

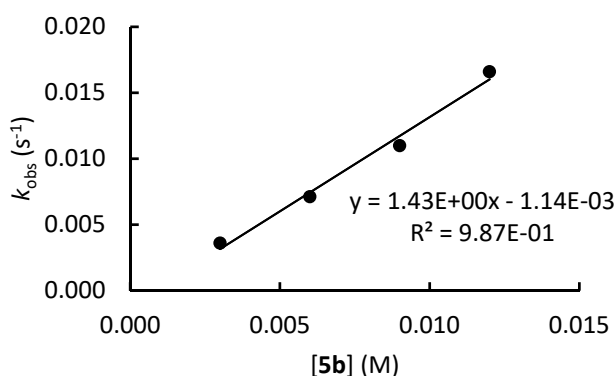
$$k_2 = (1.77 \pm 0.17) \times 10^{-1} \text{ M}^{-1} \text{ s}^{-1}$$



GSH + 5b in H₂O

[GSH] ₀ , M	[5b] ₀ , M	<i>k</i> _{obs} , s ⁻¹
1.50 × 10 ⁻⁴	3.00 × 10 ⁻³	3.60 × 10 ⁻³
1.50 × 10 ⁻⁴	6.00 × 10 ⁻³	7.13 × 10 ⁻³
1.50 × 10 ⁻⁴	9.00 × 10 ⁻³	1.10 × 10 ⁻²
1.50 × 10 ⁻⁴	1.20 × 10 ⁻²	1.66 × 10 ⁻²

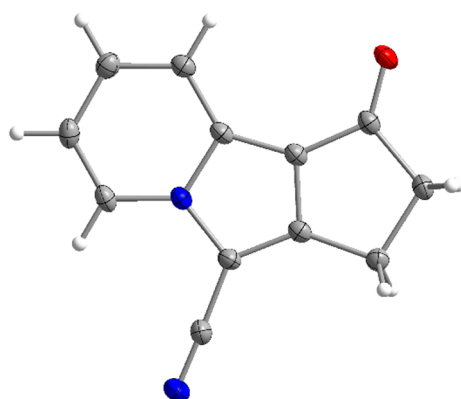
$$k_2 = 1.43 \pm 0.11 \text{ M}^{-1} \text{ s}^{-1}$$



Crystallographic Data

The X-ray intensity data of **8**, **12(D1)**, **15(D1)**, **16(D1)**, **17(D1)**, **18** and **26(D1)** were measured on a Bruker D8 Venture TXS system equipped with a multilayer mirror monochromator and a Mo K α rotating anode X-ray tube ($\lambda = 0.71073 \text{ \AA}$). The frames were integrated with the Bruker SAINT software package.⁵⁷ Data were corrected for absorption effects using the Multi-Scan method (SADABS).⁵⁸ The structures were solved and refined using the Bruker SHELXTL Software Package.⁵⁹ All hydrogen atoms have been calculated in ideal geometry riding on their parent atoms. In **12(D1)**, the O-atom is disordered; the site occupation factor ratio of the two parts refined to 0.966/0.034. The figures have been drawn at the 50% ellipsoid probability level. The less-occupied moieties of disordered parts have been omitted for the figures. Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre, CCDC, 12 Union Road, Cambridge CB21EZ, UK. Copies of the data can be obtained free of charge on quoting the depository numbers CCDC (<https://www.ccdc.cam.ac.uk/structures/>).

Crystallographic data for **8**.

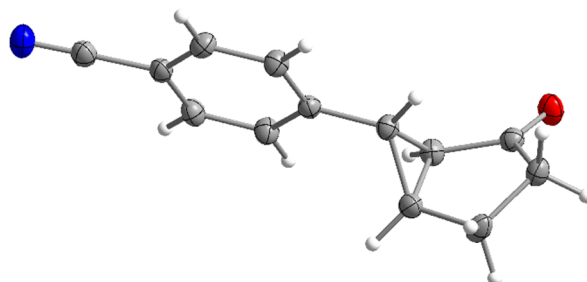


(wv580)

Molecular structure of **8** drawn at the 50% ellipsoid probability level at $T = 108$ K (CCDC 2044215).

net formula	$C_{12}H_8N_2O$
$M_r/g\ mol^{-1}$	196.20
crystal size/mm	$0.100 \times 0.030 \times 0.020$
T/K	108.(2)
radiation	MoK α
diffractometer	'Bruker D8 Venture TXS'
crystal system	monoclinic
space group	'P 1 21/c 1'
$a/\text{\AA}$	14.2681(7)
$b/\text{\AA}$	3.9182(2)
$c/\text{\AA}$	17.1782(10)
$\alpha/^\circ$	90
$\beta/^\circ$	109.954(2)
$\gamma/^\circ$	90
$V/\text{\AA}^3$	902.70(8)
Z	4
calc. density/ $g\ cm^{-3}$	1.444
μ/mm^{-1}	0.095
absorption correction	Multi-Scan
transmission factor range	0.86–1.00
refls. measured	8211
R_{int}	0.0394
mean $\sigma(I)/I$	0.0335
θ range	3.219–26.732
observed refls.	1521
x, y (weighting scheme)	0.0426, 0.5869
hydrogen refinement	constr
refls in refinement	1897
parameters	136
restraints	0
$R(F_{obs})$	0.0460
$R_w(F^2)$	0.1119
S	1.089
shift/error $_{max}$	0.001
max electron density/ $e\ \text{\AA}^{-3}$	0.243
min electron density/ $e\ \text{\AA}^{-3}$	-0.243

Crystallographic data for **12(D1)**

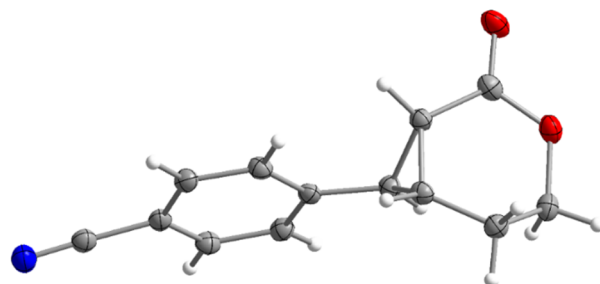


(yv471)

Molecular structure drawn at the 50% ellipsoid probability level at $T = 102$ K (CCDC 2044216).

net formula	$C_{13}H_{11}NO$
$M_r/g\ mol^{-1}$	197.23
crystal size/mm	$0.120 \times 0.100 \times 0.090$
T/K	102.(2)
radiation	MoK α
diffractometer	'Bruker D8 Venture TXS'
crystal system	monoclinic
space group	'P 1 21/c 1'
$a/\text{\AA}$	10.8844(9)
$b/\text{\AA}$	9.9707(7)
$c/\text{\AA}$	9.1680(7)
$\alpha/^\circ$	90
$\beta/^\circ$	91.835(3)
$\gamma/^\circ$	90
$V/\text{\AA}^3$	994.45(13)
Z	4
calc. density/ $g\ cm^{-3}$	1.317
μ/mm^{-1}	0.084
absorption correction	Multi-Scan
transmission factor range	0.93–0.99
refls. measured	17273
R_{int}	0.0482
mean $\sigma(I)/I$	0.0321
θ range	3.019–28.282
observed refls.	2059
x, y (weighting scheme)	0.0483, 0.4815
hydrogen refinement	constr
refls in refinement	2461
parameters	141
restraints	0
$R(F_{obs})$	0.0415
$R_w(F^2)$	0.1163
S	1.043
shift/error $_{max}$	0.001
max electron density/ $e\ \text{\AA}^{-3}$	0.241
min electron density/ $e\ \text{\AA}^{-3}$	-0.214

Crystallographic data for **15(D1)**

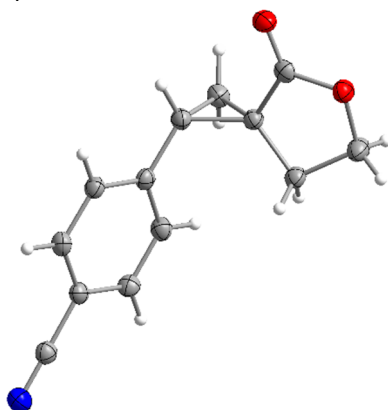


(wv581)

Molecular structure drawn at the 50% ellipsoid probability level at $T = 108$ K (CCDC 2044217).

net formula	$C_{13}H_{11}NO_2$
$M_r/g\ mol^{-1}$	213.23
crystal size/mm	$0.080 \times 0.060 \times 0.050$
T/K	108.(2)
radiation	MoK α
diffractometer	'Bruker D8 Venture TXS'
crystal system	monoclinic
space group	'P 1 21/c 1'
$a/\text{\AA}$	10.6358(4)
$b/\text{\AA}$	9.5636(4)
$c/\text{\AA}$	10.4269(4)
$\alpha/^\circ$	90
$\beta/^\circ$	100.187(2)
$\gamma/^\circ$	90
$V/\text{\AA}^3$	1043.87(7)
Z	4
calc. density/ $g\ cm^{-3}$	1.357
μ/mm^{-1}	0.092
absorption correction	Multi-Scan
transmission factor range	0.92–0.99
refls. measured	10661
R_{int}	0.0344
mean $\sigma(I)/I$	0.0279
θ range	2.885–27.081
observed refls.	1971
x, y (weighting scheme)	0.0433, 0.5066
hydrogen refinement	constr
Flack parameter	?
refls in refinement	2298
parameters	145
restraints	0
$R(F_{obs})$	0.0401
$R_w(F^2)$	0.1025
S	1.036
shift/error $_{max}$	0.001
max electron density/ $e\ \text{\AA}^{-3}$	0.243
min electron density/ $e\ \text{\AA}^{-3}$	-0.205

Crystallographic data for **16(D1)**

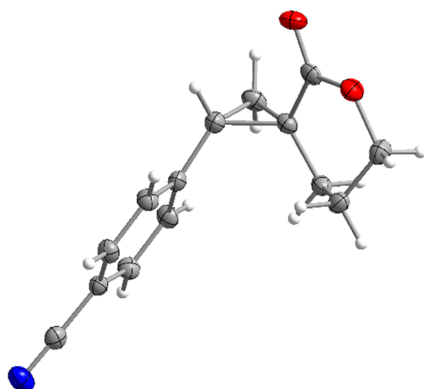


(vv629)

Molecular structure drawn at the 50% ellipsoid probability level at $T = 103$ K (CCDC 2044218).

net formula	$C_{13}H_{11}NO_2$
$M_r/g\ mol^{-1}$	213.23
crystal size/mm	$0.100 \times 0.080 \times 0.050$
T/K	103.(2)
radiation	MoK α
diffractometer	'Bruker D8 Venture TXS'
crystal system	monoclinic
space group	'P 1 21/n 1'
$a/\text{\AA}$	12.1957(10)
$b/\text{\AA}$	7.1469(5)
$c/\text{\AA}$	12.4085(11)
$\alpha/^\circ$	90
$\beta/^\circ$	105.197(3)
$\gamma/^\circ$	90
$V/\text{\AA}^3$	1043.72(15)
Z	4
calc. density/ $g\ cm^{-3}$	1.357
μ/mm^{-1}	0.092
absorption correction	Multi-Scan
transmission factor range	0.94–0.99
refls. measured	14056
R_{int}	0.0402
mean $\sigma(I)/I$	0.0254
θ range	3.320–26.371
observed refls.	1670
x, y (weighting scheme)	0.0342, 0.9886
hydrogen refinement	constr
refls in refinement	2124
parameters	145
restraints	0
$R(F_{obs})$	0.0431
$R_w(F^2)$	0.1092
S	1.054
shift/error $_{max}$	0.001
max electron density/ $e\ \text{\AA}^{-3}$	0.181
min electron density/ $e\ \text{\AA}^{-3}$	-0.261

Crystallographic data for **17(D1)**

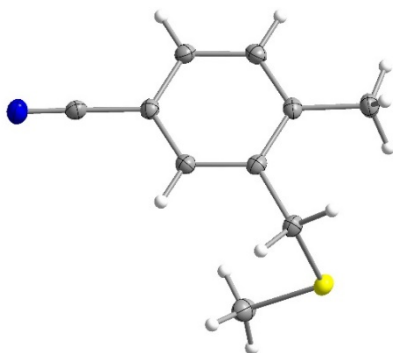


(wv638)

Molecular structure drawn at the 50% ellipsoid probability level at $T = 112$ K (CCDC 2044219).

net formula	$C_{14}H_{13}NO_2$
$M_r/g\ mol^{-1}$	227.25
crystal size/mm	$0.080 \times 0.030 \times 0.030$
T/K	112.(2)
radiation	MoK α
diffractometer	'Bruker D8 Venture TXS'
crystal system	monoclinic
space group	'P 1 21/c 1'
$a/\text{\AA}$	11.6656(4)
$b/\text{\AA}$	9.4061(4)
$c/\text{\AA}$	10.7626(5)
$\alpha/^\circ$	90
$\beta/^\circ$	97.797(2)
$\gamma/^\circ$	90
$V/\text{\AA}^3$	1170.04(8)
Z	4
calc. density/ $g\ cm^{-3}$	1.290
μ/mm^{-1}	0.087
absorption correction	Multi-Scan
transmission factor range	0.92–1.00
refls. measured	11194
R_{int}	0.0421
mean $\sigma(I)/I$	0.0367
θ range	3.246–26.363
observed refls.	1856
x, y (weighting scheme)	0.0360, 0.5952
hydrogen refinement	constr
refls in refinement	2388
parameters	154
restraints	0
$R(F_{obs})$	0.0434
$R_w(F^2)$	0.1005
S	1.032
shift/error $_{max}$	0.001
max electron density/ $e\ \text{\AA}^{-3}$	0.226
min electron density/ $e\ \text{\AA}^{-3}$	-0.199

Crystallographic data for **18**

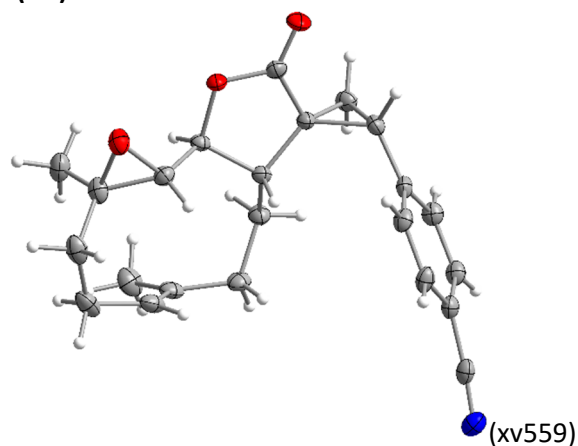


(vv592)

Molecular structure drawn at the 50% ellipsoid probability level at $T = 103$ K (CCDC 2044220).

net formula	$C_{10}H_{11}NS$
$M_r/g\ mol^{-1}$	177.26
crystal size/mm	$0.080 \times 0.060 \times 0.030$
T/K	103.(2)
radiation	MoK α
diffractometer	'Bruker D8 Venture TXS'
crystal system	triclinic
space group	'P -1'
$a/\text{\AA}$	7.3211(2)
$b/\text{\AA}$	7.9973(2)
$c/\text{\AA}$	8.7918(3)
$\alpha/^\circ$	69.1780(10)
$\beta/^\circ$	74.1170(10)
$\gamma/^\circ$	83.7140(10)
$V/\text{\AA}^3$	462.72(2)
Z	2
calc. density/ $g\ cm^{-3}$	1.272
μ/mm^{-1}	0.291
absorption correction	Multi-Scan
transmission factor range	0.9226–0.9705
refls. measured	8722
R_{int}	0.0244
mean $\sigma(I)/I$	0.0205
θ range	3.345–27.099
observed refls.	1867
x, y (weighting scheme)	0.0274, 0.2230
hydrogen refinement	constr
refls in refinement	2031
parameters	111
restraints	0
$R(F_{obs})$	0.0266
$R_w(F^2)$	0.0704
S	1.065
shift/error $_{max}$	0.001
max electron density/ $e\ \text{\AA}^{-3}$	0.295
min electron density/ $e\ \text{\AA}^{-3}$	-0.192

Crystallographic data for **26(D1)**



Molecular structure drawn at the 50% ellipsoid probability level at $T = 103$ K (CCDC 2044221).

net formula	$C_{23}H_{25}NO_3$
$M_r/g\ mol^{-1}$	363.44
crystal size/mm	$0.100 \times 0.040 \times 0.020$
T/K	103.(2)
radiation	MoK α
diffractometer	'Bruker D8 Venture TXS'
crystal system	monoclinic
space group	'C 1 2 1'
$a/\text{\AA}$	21.9099(11)
$b/\text{\AA}$	6.5137(4)
$c/\text{\AA}$	14.4743(8)
$\alpha/^\circ$	90
$\beta/^\circ$	115.663(2)
$\gamma/^\circ$	90
$V/\text{\AA}^3$	1861.93(18)
Z	4
calc. density/ $g\ cm^{-3}$	1.297
μ/mm^{-1}	0.085
absorption correction	Multi-Scan
transmission factor range	0.94–1.00
refls. measured	10760
R_{int}	0.0360
mean $\sigma(I)/I$	0.0431
θ range	3.080–26.370
observed refls.	3410
x, y (weighting scheme)	0.0438, 1.4361
hydrogen refinement	constr
Flack parameter	-0.2(6)
refls in refinement	3790
parameters	246
restraints	1
$R(F_{obs})$	0.0423
$R_w(F^2)$	0.1041
S	1.070
shift/error $_{max}$	0.001
max electron density/ $e\ \text{\AA}^{-3}$	0.177
min electron density/ $e\ \text{\AA}^{-3}$	-0.185

Computational Details

Initially, all structures were subjected to a conformational search with the OPLS3^{S10} force field as implemented in MacroModel^{S11} with the MCMC method in gas phase. All subsequent quantum-chemical calculations were performed with the Gaussian 16 A.03 set of codes.^{S12} All structures were optimized at the M06-2X/6-31+G(d,p)^{S13} level of theory considering solvation by the SMD model for DMSO.^{S14} Thermal corrections at 298 K were obtained at the same level of theory from vibrational frequencies and are unscaled. Transition states were validated by the presence of one imaginary frequency and IRC calculations. All conformers were Boltzmann weighted. Finally, a free energy correction +7.91 kJ mol⁻¹ was applied to all free energies to consider the conversion from gas phase (1 atm) to liquid phase (1 M).

The distortion-interaction analysis was performed either on the whole reaction pathway obtained from IRC calculations (the Hessian was recalculated every 3 steps) or alternatively, when two transition states with highly similar C-C bond lengths were compared, directly at the TS geometries. Input files for the DIA calculations were prepared using the autoDIAS python script.^{S15} For a recent protocols article on the method, see ref. S16.

SAPT^{S17} calculations were performed with the PSI4 (v1.3.2) package^{S18} on the same points used for the distortion-interaction analysis. For the computations, the SAPT0 method was used together with the jun-cc-pvdz basis set applying “df” as option for scf_type. Such a computation produces both the SAPT0/jun-cc-pvdz as well as the scaled sSAPT0/jun-cc-pvdz energies as output of which we used the latter for our analysis as recommended recently.^{S17b}

Table S2. Electronic and Gibbs energies for all species at the SMD(DMSO)/M06-2X/6-31+G(d,p) level.

Compound	Filename (.log)	E_{tot} (hartree)	G_{298} (hartree)	Weighting
7	sy_1	-840.355846	-840.212336	0.8595
	sy_2	-840.354449	-840.210628	0.1405
	weighted:		-840.212096	
	dimethylsulfide	-477.935305	-477.885651	
1a + 7				
1a	1a	-269.254647	-269.184823	
<i>trans</i> -TS1 (1a+7)	1a_sy_tr_1_ts1	-1109.598903	-1109.362268	0.0063
	1a_sy_tr_3_ts1	-1109.604033	-1109.366342	0.4716
	1a_sy_tr_3_ts1_rot1	-1109.598903	-1109.362272	0.0063
	1a_sy_tr_5_ts1	-1109.598272	-1109.361096	0.0018
	1a_sy_tr_7_ts1	-1109.600123	-1109.364118	0.0446
	1a_sy_tr_8_ts1	-1109.604033	-1109.366334	0.4676
	1a_sy_tr_9_ts1	-1109.600799	-1109.361046	0.0017
	weighted:		-1109.366169	
<i>trans</i> -IM (1a+7)	1a_sy_tr_1	-1109.625308	-1109.385434	0.0112
	1a_sy_tr_2	-1109.625716	-1109.384735	0.0053

	1a_sy_tr_3	-1109.629946	-1109.389085	0.5385
	1a_sy_tr_4	-1109.626523	-1109.387140	0.0685
	1a_sy_tr_5	-1109.628148	-1109.388018	0.1738
	1a_sy_tr_6	-1109.628036	-1109.387753	0.1312
	1a_sy_tr_7	-1109.626480	-1109.386745	0.0451
	1a_sy_tr_8	-1109.622710	-1109.380750	0.0001
	1a_sy_tr_9	-1109.625757	-1109.385433	0.0112
	1a_sy_tr_10	-1109.620392	-1109.379087	0.0000
	1a_sy_tr_11	-1109.623366	-1109.382999	0.0008
	1a_sy_tr_12	-1109.623916	-1109.384662	0.0050
	1a_sy_tr_13	-1109.625495	-1109.383970	0.0024
	1a_sy_tr_14	-1109.619529	-1109.378647	0.0000
	1a_sy_tr_15	-1109.623600	-1109.382813	0.0007
	1a_sy_tr_16	-1109.616295	-1109.375284	0.0000
	1a_sy_tr_17	-1109.624947	-1109.384889	0.0063
	1a_sy_tr_18	-1109.617760	-1109.375792	0.0000
	weighted:		-1109.388310	
<i>trans</i> -TS2 (1a+7)	1a_sy_tr_5_ts2	-1109.619245	-1109.380612	0.3755
	1a_sy_tr_7_ts2	-1109.618109	-1109.379913	0.1789
	1a_sy_tr_15_ts2	-1109.615788	-1109.376805	0.0066
	1a_sy_tr_17_ts2	-1109.618447	-1109.380759	0.4390
	weighted:		-1109.380526	
<i>trans</i> -product (1a+7)	1a_sy_tr_prod_1	-631.741910	-631.572455	1.0000
	weighted:		-631.572455	
		$G_{\text{trans}}^{\ddagger}$	73.5	kJ mol^{-1}
		$G_{\text{IM, trans}}^0$	15.3	kJ mol^{-1}
		$G_{\text{cp, trans}}^{\ddagger}$	35.8	kJ mol^{-1}
		G_{trans}^0	-160.0	kJ mol^{-1}
<i>cis</i> -TS1 (1a+7)	1a_sy_c_1_ts1	-1109.594532	-1109.357683	0.0023
	1a_sy_c_2_ts1	-1109.596717	-1109.358648	0.0063
	1a_sy_c_3_ts1	-1109.599461	-1109.363347	0.9131
	1a_sy_c_4_ts1	-1109.596602	-1109.360183	0.0319
	1a_sy_c_7_ts1	-1109.597215	-1109.360538	0.0465
	weighted:		-1109.363073	
<i>cis</i> -IM (1a+7)	1a_sy_c_1	-1109.619867	-1109.379193	0.0000
	1a_sy_c_1_r	-1109.619199	-1109.377574	0.0000
	1a_sy_c_2	-1109.628122	-1109.387720	0.1514
	1a_sy_c_2_r	-1109.626722	-1109.386229	0.0311
	1a_sy_c_3	-1109.627767	-1109.388073	0.2202
	1a_sy_c_4	-1109.626849	-1109.386179	0.0295
	1a_sy_c_5	-1109.623616	-1109.382361	0.0005
	1a_sy_c_6	-1109.627832	-1109.386436	0.0388

	1a_sy_c_7	-1109.628358	-1109.388215	0.2558
	1a_sy_c_8	-1109.629117	-1109.388271	0.2715
	1a_sy_c_8_r	-1109.622692	-1109.380877	0.0001
	1a_sy_c_9	-1109.623551	-1109.383077	0.0011
	weighted:		-1109.387923	
<i>cis</i> -TS2 (1a+7)	1a_sy_tr_1_ts2	-1109.609851	-1109.370427	0.0024
	1a_sy_tr_2_ts2	-1109.613865	-1109.376055	0.9392
	1a_sy_tr_8_ts2	-1109.611967	-1109.373435	0.0584
	weighted:		-1109.375888	
<i>cis</i> -product (1a+7)	1a_sy_c_prod_1	-631.738876	-631.569661	1.0000
	weighted:		-631.569661	

G_{cis}^{\ddagger}	81.6	kJ mol^{-1}
$G_{IM, cis}^0$	16.3	kJ mol^{-1}
$G_{cp, cis}^{\ddagger}$	47.9	kJ mol^{-1}
G_{cis}^0	-152.7	kJ mol^{-1}

1b + 7				
1b	1b	-308.557006	-308.461468	
<i>trans</i> -TS1 (1b+7)	1b_sy_tr_1_ts1	-1148.899282	-1148.637808	0.1926
	1b_sy_tr_2_ts1	-1148.903732	-1148.639159	0.8071
	1b_sy_tr_4_ts1	-1148.894302	-1148.631711	0.0003
	weighted:		-1148.638897	
<i>trans</i> -IM (1b+7)	1b_sy_tr_1	-1148.924233	-1148.656123	0.0148
	1b_sy_tr_1_r	-1148.921115	-1148.653803	0.0013
	1b_sy_tr_2	-1148.926530	-1148.660045	0.9451
	1b_sy_tr_3	-1148.915723	-1148.648427	0.0000
	1b_sy_tr_3_r	-1148.919162	-1148.652944	0.0005
	1b_sy_tr_4	-1148.914301	-1148.646533	0.0000
	1b_sy_tr_4_r	-1148.918291	-1148.650342	0.0000
	1b_sy_tr_5_r	-1148.923961	-1148.656632	0.0253
	1b_sy_tr_6	-1148.922404	-1148.655817	0.0107
	1b_sy_tr_	-1148.921184	-1148.654353	0.0023
	weighted:		-1148.659831	
<i>trans</i> -TS2 (1b+7)	1b_sy_tr_1_ts2	-1148.915553	-1148.651428	0.5113
	1b_sy_tr_3_ts2	-1148.912492	-1148.648567	0.0246
	1b_sy_tr_5_ts2	-1148.916502	-1148.651336	0.4641
	weighted:		-1148.651315	
<i>trans</i> -product (1b+7)	1b_sy_tr_prod_1	-671.039596	-670.845628	1.0000
	weighted:		-670.845628	

		$G_{\text{trans}}^{\ddagger}$	83.7	kJ mol^{-1}
		$G_{\text{IM, trans}}^0$	28.8	kJ mol^{-1}
		$G_{\text{cp, trans}}^{\ddagger}$	51.1	kJ mol^{-1}
		G_{trans}^0	-150.9	kJ mol^{-1}
<i>cis</i> -TS1 (1b+7)	1b_sy_c_1_ts1	-1148.898970	-1148.636706	0.0374
	1b_sy_c_2_ts1	-1148.895924	-1148.631604	0.0002
	1b_sy_c_5_ts1	-1148.903091	-1148.639735	0.9272
	1b_sy_c_7_ts1	-1148.895968	-1148.631432	0.0001
	1b_sy_c_9_ts1	-1148.900072	-1148.636649	0.0352
	weighted:		-1148.639511	
<i>cis</i> -IM (1b+7)	1b_sy_c_1	-1148.923877	-1148.656831	0.0988
	1b_sy_c_2	-1148.924549	-1148.657560	0.2139
	1b_sy_c_2_r	-1148.920525	-1148.653822	0.0041
	1b_sy_c_3	-1148.921817	-1148.654560	0.0089
	1b_sy_c_3_r	-1148.923673	-1148.657351	0.1714
	1b_sy_c_4	-1148.922023	-1148.655541	0.0252
	1b_sy_c_5	-1148.924316	-1148.658191	0.4179
	1b_sy_c_6	-1148.922539	-1148.655652	0.0283
	1b_sy_c_7	-1148.921669	-1148.654367	0.0072
	1b_sy_c_8	-1148.920771	-1148.655049	0.0149
	1b_sy_c_9	-1148.922391	-1148.654605	0.0093
	weighted:		-1148.657481	
<i>cis</i> -TS2 (1b+7)	1b_sy_c_2_ts2	-1148.909187	-1148.644906	0.0522
	1b_sy_c_3_ts2	-1148.911075	-1148.647641	0.9478
	weighted:		-1148.647499	
<i>cis</i> -product (1b+7)	1b_sy_c_prod_1	-671.038631	-670.843098	1.0000
	weighted:		-670.843098	
		$G_{\text{cis}}^{\ddagger}$	82.1	kJ mol^{-1}
		$G_{\text{IM, cis}}^0$	34.9	kJ mol^{-1}
		$G_{\text{cp, cis}}^{\ddagger}$	61.2	kJ mol^{-1}
		G_{cis}^0	-144.3	kJ mol^{-1}

1c + 7

1c	1c	-308.559579	-308.464111	
<i>trans</i> -TS1 (1c+7)	1c_sy_tr_1_ts1	-1148.897964	-1148.633780	0.1002
	1c_sy_tr_3_ts1	-1148.900288	-1148.634393	0.1921
	1c_sy_tr_4_ts1	-1148.890393	-1148.625291	0.0000
	1c_sy_tr_5_ts1	-1148.897964	-1148.633779	0.1001
	1c_sy_tr_6_ts1	-1148.893354	-1148.629890	0.0016
	1c_sy_tr_7_ts1	-1148.900280	-1148.635477	0.6060
	1c_sy_tr_8_ts1	-1148.883946	-1148.619500	0.0000

	weighted:		-1148.634920	
<i>trans</i> -IM (1c+7)	1c_sy_tr_1	-1148.923895	-1148.656063	0.3364
	1c_sy_tr_1_r	-1148.921621	-1148.654207	0.0470
	1c_sy_tr_2	-1148.923706	-1148.655727	0.2356
	1c_sy_tr_2_r	-1148.921327	-1148.653884	0.0334
	1c_sy_tr_3	-1148.922801	-1148.655927	0.2912
	1c_sy_tr_3_r	-1148.921652	-1148.653689	0.0272
	1c_sy_tr_4	-1148.915933	-1148.648386	0.0001
	1c_sy_tr_4_r	-1148.914135	-1148.645211	0.0000
	1c_sy_tr_6	-1148.922026	-1148.653756	0.0292
	1c_sy_tr_8	-1148.912723	-1148.644372	0.0000
	weighted:		-1148.655651	
<i>trans</i> -TS2 (1c+7)	1c_sy_tr_1_ts2	-1148.913277	-1148.648062	0.5173
	1c_sy_tr_3_ts2	-1148.913536	-1148.647973	0.4708
	1c_sy_tr_4_ts2	-1148.909209	-1148.644509	0.0120
	weighted:		-1148.647978	
<i>trans</i> -product (1c+7)	1c_sy_tr_prod_1	-671.038783	-670.844292	1.0000
	weighted:		-670.844292	
		G_{trans}^{\ddagger}	101.1	kJ mol^{-1}
		$G_{IM, trans}^0$	46.7	kJ mol^{-1}
		$G_{cp, trans}^{\ddagger}$	66.8	kJ mol^{-1}
		G_{trans}^0	-140.5	kJ mol^{-1}
<i>cis</i> -TS1 (1c+7)	1c_sy_c_1_ts1	-1148.896350	-1148.631598	0.0143
	1c_sy_c_2_ts1	-1148.898837	-1148.635293	0.7188
	1c_sy_c_2_ts1_rot2	-1148.899003	-1148.633883	0.1613
	1c_sy_c_3_ts1	-1148.889646	-1148.623554	0.0000
	1c_sy_c_4_ts1	-1148.894568	-1148.631059	0.0081
	1c_sy_c_5_ts1	-1148.894166	-1148.629198	0.0011
	1c_sy_c_6_ts1	-1148.897410	-1148.633399	0.0965
	weighted:		-1148.634789	
<i>cis</i> -IM (1c+7)	1c_sy_c_1	-1148.925402	-1148.657742	0.8734
	1c_sy_c_1_r	-1148.919706	-1148.651395	0.0010
	1c_sy_c_2	-1148.922955	-1148.655814	0.1131
	1c_sy_c_2_r	-1148.920616	-1148.652602	0.0038
	1c_sy_c_3	-1148.915104	-1148.646643	0.0000
	1c_sy_c_3_r	-1148.910035	-1148.641648	0.0000
	1c_sy_c_5	-1148.916494	-1148.647842	0.0000
	1c_sy_c_5_r	-1148.915963	-1148.647959	0.0000
	1c_sy_c_6	-1148.921622	-1148.653379	0.0086
	weighted:		-1148.657460	

<i>cis</i> -TS2 (1c+7)	1c_sy_c_1_ts2	-1148.912371	-1148.645824	0.2601
	1c_sy_c_2_ts2	-1148.913310	-1148.646798	0.7309
	1c_sy_c_4_ts2	-1148.909111	-1148.642647	0.0090
	weighted:		-1148.646507	
<i>cis</i> -product (1c+7)	1c_sy_c_prod_1	-671.038738	-670.843261	1.0000
	weighted:		-670.843261	
	G_{cis}^{\ddagger}		101.5	kJ mol ⁻¹
	$G_{IM, cis}^0$		41.9	kJ mol ⁻¹
	$G_{cp, cis}^{\ddagger}$		70.7	kJ mol ⁻¹
	G_{cis}^0		-137.7	kJ mol ⁻¹

2a + 7				
2a	2a	-308.554827	-308.456692	
<i>trans</i> -TS1 (2a+7)	2a_sy_tr_1_ts1	-1148.894884	-1148.629917	0.0034
	2a_sy_tr_2_ts1	-1148.897692	-1148.631838	0.0260
	2a_sy_tr_3_ts1	-1148.899940	-1148.633875	0.2251
	2a_sy_tr_4_ts1	-1148.900930	-1148.634997	0.7397
	2a_sy_tr_5_ts1	-1148.890743	-1148.625570	0.0000
	2a_sy_tr_6_ts1	-1148.897008	-1148.629291	0.0017
	2a_sy_tr_9_ts1	-1148.895747	-1148.630080	0.0040
	2a_sy_tr_10_ts1	-1148.891534	-1148.624931	0.0000
	weighted:		-1148.634615	
<i>trans</i> -IM (2a+7)	2a_sy_tr_1	-1148.924672	-1148.656669	0.0399
	2a_sy_tr_1_r	-1148.925066	-1148.657470	0.0932
	2a_sy_tr_2	-1148.921535	-1148.652694	0.0006
	2a_sy_tr_2_r	-1148.925047	-1148.656087	0.0215
	2a_sy_tr_3	-1148.926550	-1148.659311	0.6566
	2a_sy_tr_4	-1148.926753	-1148.658092	0.1803
	2a_sy_tr_5	-1148.918379	-1148.648867	0.0000
	2a_sy_tr_5_r	-1148.920812	-1148.651445	0.0002
	2a_sy_tr_6	-1148.923445	-1148.654919	0.0062
	2a_sy_tr_7	-1148.919293	-1148.649629	0.0000
	2a_sy_tr_8	-1148.922771	-1148.653554	0.0015
	2a_sy_tr_9	-1148.919112	-1148.648765	0.0000
	2a_sy_tr_10	-1148.913664	-1148.645527	0.0000
	weighted:		-1148.658703	
<i>trans</i> -TS2 (2a+7)	2a_sy_tr_1_ts2	-1148.913683	-1148.647659	0.0668
	2a_sy_tr_2_ts2	-1148.917918	-1148.650050	0.8422
	2a_sy_tr_5_ts2	-1148.911014	-1148.644646	0.0027
	2a_sy_tr_6_ts2	-1148.914344	-1148.647922	0.0883
	weighted:		-1148.649687	

<i>trans</i> -product (2a+7)	2a_sy_tr_prod_1	-671.042180	-670.845110	0.7933
	2a_sy_tr_prod_3	-671.041286	-670.843842	0.2067
	weighted:		-670.844848	

G_{trans}^{\ddagger}	82.4	kJ mol^{-1}
$G_{IM, trans}^0$	19.2	kJ mol^{-1}
$G_{cp, trans}^{\ddagger}$	42.9	kJ mol^{-1}
G_{trans}^0	-161.4	kJ mol^{-1}

<i>cis</i> -TS1 (2a+7)	2a_sy_c_1_ts1	-1148.899474	-1148.634535	0.5156
	2a_sy_c_1_ts1_rot1	-1148.899949	-1148.634444	0.4681
	2a_sy_c_2_ts1	-1148.893432	-1148.627928	0.0005
	2a_sy_c_3_ts1	-1148.896106	-1148.630073	0.0046
	2a_sy_c_5_ts1	-1148.894081	-1148.629270	0.0019
	2a_sy_c_6_ts1	-1148.885578	-1148.619405	0.0000
	2a_sy_c_9_ts1	-1148.894657	-1148.630732	0.0091
	2a_sy_c_10_ts1	-1148.892092	-1148.626848	0.0001
	weighted:		-1148.634423	

<i>cis</i> -IM (2a+7)	2a_sy_c_1	-1148.926606	-1148.658355	0.1470
	2a_sy_c_1_r	-1148.923134	-1148.655454	0.0068
	2a_sy_c_2	-1148.921443	-1148.653821	0.0012
	2a_sy_c_2_r	-1148.920176	-1148.650347	0.0000
	2a_sy_c_3	-1148.925093	-1148.656159	0.0143
	2a_sy_c_3_r	-1148.917886	-1148.647668	0.0000
	2a_sy_c_4	-1148.927681	-1148.658100	0.1121
	2a_sy_c_5	-1148.925303	-1148.656483	0.0202
	2a_sy_c_5_r	-1148.924186	-1148.656302	0.0167
	2a_sy_c_6	-1148.917717	-1148.648975	0.0000
	2a_sy_c_9	-1148.924544	-1148.656358	0.0177
	2a_sy_c_10	-1148.926757	-1148.658008	0.1018
	2a_sy_c_11	-1148.926589	-1148.659620	0.5622
weighted:		-1148.658838		

<i>cis</i> -TS2 (2a+7)	2a_sy_c_1_ts2	-1148.908680	-1148.642389	0.4933
	2a_sy_c_2_ts2	-1148.905568	-1148.638389	0.0071
	2a_sy_c_3_ts2	-1148.905715	-1148.638639	0.0093
	2a_sy_c_5_ts2	-1148.908244	-1148.642383	0.4904
	weighted:		-1148.642323	

<i>cis</i> -product (2a+7)	2a_sy_c_prod_1	-671.036095	-670.838777	0.6317
	2a_sy_c_prod_2	-671.035810	-670.838268	0.3683
	weighted:		-670.838590	

G_{cis}^{\ddagger}	82.9	kJ mol^{-1}
$G_{IM, cis}^0$	18.8	kJ mol^{-1}
$G_{cp, cis}^{\ddagger}$	62.2	kJ mol^{-1}

G_{cis}^0 -145.0 kJ mol⁻¹

2b + 7				
2b	2b	-347.855437	-347.731078	
<i>trans</i> -TS1 (2b+7)	2b_sy_tr_1_ts1	-1188.194723	-1187.903549	0.1179
	2b_sy_tr_2_ts1	-1188.196708	-1187.905447	0.8820
	2b_sy_tr_4_ts1	-1188.190142	-1187.897392	0.0002
	weighted:		-1187.905222	
<i>trans</i> -IM (2b+7)	2b_sy_tr_1	-1188.219901	-1187.924348	0.4926
	2b_sy_tr_1_r	-1188.215150	-1187.919531	0.0030
	2b_sy_tr_2	-1188.217872	-1187.923122	0.1343
	2b_sy_tr_2_r	-1188.219526	-1187.924078	0.3700
	2b_sy_tr_3	-1188.213041	-1187.916449	0.0001
	2b_sy_tr_3_r	-1188.210536	-1187.913962	0.0000
	2b_sy_tr_4	-1188.209724	-1187.913235	0.0000
	weighted:		-1187.924068	
<i>trans</i> -TS2 (2b+7)	2b_sy_tr_2_ts2	-1188.213398	-1187.919527	1.0000
	weighted:		-1187.919527	
<i>trans</i> -product (2b+7)	2b_sy_tr_prod_1	-710.338002	-710.114710	0.2676
	2b_sy_tr_prod_2	-710.338504	-710.115660	0.7324
	weighted:		-710.115406	
		G_{trans}^\ddagger	92.4	kJ mol ⁻¹
		$G_{IM, trans}^0$	42.9	kJ mol ⁻¹
		$G_{cp, trans}^\ddagger$	54.8	kJ mol ⁻¹
		G_{trans}^0	-151.3	kJ mol ⁻¹
<i>cis</i> -TS1 (2b+7)	2b_sy_c_1_ts1	-1188.197351	-1187.906244	0.2079
	2b_sy_c_3_ts1	-1188.192173	-1187.900576	0.0005
	2b_sy_c_4_ts1	-1188.199021	-1187.906695	0.3352
	2b_sy_c_5_ts1	-1188.191938	-1187.900444	0.0004
	2b_sy_c_6_ts1	-1188.199549	-1187.906976	0.4516
	2b_sy_c_8_ts1	-1188.191256	-1187.898463	0.0001
	2b_sy_c_9_ts1	-1188.188341	-1187.897608	0.0000
	2b_sy_c_10_ts1	-1188.195169	-1187.902587	0.0043
	weighted:		-1187.906704	
<i>cis</i> -IM (2b+7)	2b_sy_c_1	-1188.221650	-1187.925979	0.3991
	2b_sy_c_2	-1188.221040	-1187.925393	0.2144
	2b_sy_c_3	-1188.216998	-1187.921815	0.0048
	2b_sy_c_4	-1188.219190	-1187.924424	0.0767
	2b_sy_c_5	-1188.221138	-1187.925413	0.2192
	2b_sy_c_5_r	-1188.213091	-1187.917522	0.0001

	2b_sy_c_6	-1188.218403	-1187.924305	0.0677
	2b_sy_c_8	-1188.218087	-1187.921415	0.0032
	2b_sy_c_9	-1188.216787	-1187.921593	0.0038
	2b_sy_c_10	-1188.216412	-1187.921139	0.0024
	2b_sy_c_11	-1188.216023	-1187.921224	0.0026
	2b_sy_c_12	-1188.216527	-1187.922003	0.0059
	2b_sy_c_13	-1188.214075	-1187.918434	0.0001
	weighted:		-1187.925397	
<i>cis</i> -TS2 (2b+7)	2b_sy_c_3_ts2	-1188.204776	-1187.912026	0.9947
	2b_sy_c_5_ts2	-1188.200729	-1187.907087	0.0053
	weighted:		-1187.912000	
<i>cis</i> -product (2b+7)	2b_sy_c_prod_1	-710.334261	-710.111105	0.5710
	2b_sy_c_prod_2	-710.334347	-710.110835	0.4290
	weighted:		-710.110989	

G_{cis}^{\ddagger}	88.5	kJ mol^{-1}
$G_{IM, cis}^0$	39.4	kJ mol^{-1}
$G_{cp, cis}^{\ddagger}$	74.6	kJ mol^{-1}
G_{cis}^0	-139.7	kJ mol^{-1}

2c + 7				
2c	2c	-347.858736	-347.734627	
<i>trans</i> -TS1 (2c+7)	2c_sy_tr_1_ts1	-1188.193159	-1187.900369	0.0053
	2c_sy_tr_2_ts1	-1188.196459	-1187.904146	0.2916
	2c_sy_tr_2_ts1_rot1	-1188.197381	-1187.904938	0.6750
	2c_sy_tr_3_ts1	-1188.194255	-1187.901401	0.0159
	2c_sy_tr_4_ts1	-1188.186984	-1187.894064	0.0000
	2c_sy_tr_5_ts1	-1188.194165	-1187.901153	0.0122
	weighted:			-1187.904581
<i>trans</i> -IM (2c+7)	2c_sy_tr_1	-1188.223312	-1187.926841	0.7749
	2c_sy_tr_1_r	-1188.218497	-1187.921981	0.0045
	2c_sy_tr_2	-1188.222035	-1187.925091	0.1212
	2c_sy_tr_2_r	-1188.219126	-1187.922576	0.0084
	2c_sy_tr_3	-1188.219683	-1187.924555	0.0686
	2c_sy_tr_3_r	-1188.217718	-1187.921957	0.0044
	2c_sy_tr_4	-1188.215194	-1187.917228	0.0000
	2c_sy_tr_4_r	-1188.211473	-1187.913923	0.0000
	2c_sy_tr_5	-1188.218650	-1187.922762	0.0103
	2c_sy_tr_5_r	-1188.218692	-1187.922493	0.0077
	weighted:			-1187.926317
<i>trans</i> -TS2 (2c+7)	2c_sy_tr_1_ts2	-1188.209239	-1187.915302	0.0641
	2c_sy_tr_2_ts2	-1188.212485	-1187.917664	0.7841

	2c_sy_tr_3_ts2	-1188.209102	-1187.916115	0.1518
	weighted:		-1187.917277	
<i>trans</i> -product (2c+7)	2c_sy_tr_prod_1	-710.339129	-710.116305	0.9043
	2c_sy_tr_prod_2	-710.337435	-710.114186	0.0957
	weighted:		-710.116102	
	$G_{\text{trans}}^{\ddagger}$		103.4	kJ mol^{-1}
	$G_{\text{IM, trans}}^0$		46.3	kJ mol^{-1}
	$G_{\text{cp, trans}}^{\ddagger}$		70.0	kJ mol^{-1}
	G_{trans}^0		-143.9	kJ mol^{-1}
<i>cis</i> -TS1 (2c+7)	2c_sy_c_1_ts1	-1188.197325	-1187.905200	0.9687
	2c_sy_c_2_ts1	-1188.190157	-1187.898392	0.0007
	2c_sy_c_3_ts1	-1188.194357	-1187.901557	0.0204
	2c_sy_c_4_ts1	-1188.191200	-1187.898661	0.0009
	2c_sy_c_5_ts1	-1188.192721	-1187.900656	0.0078
	2c_sy_c_6_ts1	-1188.181433	-1187.887990	0.0000
	2c_sy_c_7_ts1	-1188.190960	-1187.897350	0.0002
	2c_sy_c_8_ts1	-1188.191867	-1187.898887	0.0012
	weighted:		-1187.905070	
<i>cis</i> -IM (2c+7)	2c_sy_c_1	-1188.221464	-1187.925398	0.3036
	2c_sy_c_1_r	-1188.215464	-1187.919253	0.0004
	2c_sy_c_2	-1188.222327	-1187.925863	0.4970
	2c_sy_c_2_r	-1188.216957	-1187.920097	0.0011
	2c_sy_c_3	-1188.219690	-1187.923455	0.0387
	2c_sy_c_3_r	-1188.213699	-1187.917754	0.0001
	2c_sy_c_4	-1188.221039	-1187.924680	0.1418
	2c_sy_c_4_r	-1188.215831	-1187.919912	0.0009
	2c_sy_c_5	-1188.218014	-1187.921647	0.0057
	2c_sy_c_6	-1188.211850	-1187.914347	0.0000
	2c_sy_c_7	-1188.213307	-1187.917057	0.0000
	2c_sy_c_8	-1188.219059	-1187.922248	0.0108
	weighted:		-1187.925383	
<i>cis</i> -TS2 (2c+7)	2c_sy_c_1_ts2	-1188.206877	-1187.912240	0.3551
	2c_sy_c_2_ts2	-1188.206186	-1187.912588	0.5136
	2c_sy_c_3_ts2	-1188.204986	-1187.911301	0.1313
	weighted:		-1187.912295	
<i>cis</i> -product (2c+7)	2c_sy_c_prod_1	-710.335667	-710.112280	0.7692
	2c_sy_c_prod_2	-710.334844	-710.111144	0.2308
	weighted:		-710.112018	
	$G_{\text{cis}}^{\ddagger}$		102.1	kJ mol^{-1}
	$G_{\text{IM, cis}}^0$		48.7	kJ mol^{-1}

$G_{cp, cis}^{\ddagger}$	83.1	kJ mol^{-1}
G_{cis}^0	-133.1	kJ mol^{-1}

3 + 7				
3	3_1	-347.841829	-347.717170	0.5769
	3_2	-347.842288	-347.716448	0.2683
	3_3	-347.841624	-347.715929	0.1548
	weighted:		-347.716784	
<i>trans</i> -TS1 (3+7)	3_sy_tr_1_ts1	-1188.184029	-1187.889922	0.0027
	3_sy_tr_2_ts1	-1188.183718	-1187.891680	0.0176
	3_sy_tr_2_ts1_rot1	-1188.189309	-1187.895467	0.9766
	3_sy_tr_3_ts1	-1188.149303	-1187.859282	0.0000
	3_sy_tr_4_ts1	-1188.147624	-1187.857305	0.0000
	3_sy_tr_28_ts1	-1188.184841	-1187.890034	0.0031
	weighted:		-1187.895369	
<i>trans</i> -IM (3+7)	3_sy_tr_1	-1188.207326	-1187.911047	0.0001
	3_sy_tr_1_r	-1188.209881	-1187.913528	0.0009
	3_sy_tr_2	-1188.208322	-1187.913153	0.0006
	3_sy_tr_3	-1188.216597	-1187.919563	0.5474
	3_sy_tr_3_r	-1188.211486	-1187.915408	0.0067
	3_sy_tr_4	-1188.210041	-1187.914807	0.0035
	3_sy_tr_5	-1188.210590	-1187.913495	0.0009
	3_sy_tr_5_r	-1188.209506	-1187.913446	0.0008
	3_sy_tr_6	-1188.212937	-1187.917412	0.0559
	3_sy_tr_7	-1188.212463	-1187.915778	0.0099
	3_sy_tr_8	-1188.212677	-1187.916733	0.0272
	3_sy_tr_9	-1188.210529	-1187.912761	0.0004
	3_sy_tr_10	-1188.209132	-1187.912577	0.0003
	3_sy_tr_11	-1188.209338	-1187.913773	0.0012
	3_sy_tr_12	-1188.205200	-1187.906442	0.0000
	3_sy_tr_13	-1188.209593	-1187.911592	0.0001
	3_sy_tr_14	-1188.210222	-1187.912824	0.0004
	3_sy_tr_15	-1188.205831	-1187.908595	0.0000
	3_sy_tr_16	-1188.203612	-1187.906745	0.0000
	3_sy_tr_17	-1188.213285	-1187.916867	0.0314
	3_sy_tr_18	-1188.209489	-1187.913496	0.0009
	3_sy_tr_19	-1188.206143	-1187.909305	0.0000
	3_sy_tr_20	-1188.204846	-1187.908400	0.0000
	3_sy_tr_21	-1188.202158	-1187.904658	0.0000
	3_sy_tr_22	-1188.204891	-1187.908924	0.0000
	3_sy_tr_23	-1188.211905	-1187.916194	0.0154
	3_sy_tr_24	-1188.207351	-1187.909305	0.0000
	3_sy_tr_25	-1188.209144	-1187.912435	0.0003
3_sy_tr_26	-1188.205010	-1187.908473	0.0000	
3_sy_tr_28	-1188.215766	-1187.918948	0.2851	

	3_sy_tr_30	-1188.203749	-1187.908468	0.0000
	3_sy_tr_31	-1188.201950	-1187.904686	0.0000
	3_sy_tr_32	-1188.204204	-1187.906718	0.0000
	3_sy_tr_33	-1188.213534	-1187.915842	0.0106
	weighted:		-1187.918889	
<i>trans</i> -TS2 (3+7)	3_sy_tr_1_ts2	-1188.201534	-1187.907174	0.1258
	3_sy_tr_3_ts2	-1188.189189	-1187.896800	0.0000
	3_sy_tr_4_ts2	-1188.174825	-1187.884660	0.0000
	3_sy_tr_5_ts2	-1188.204024	-1187.909002	0.8742
	weighted:		-1187.908772	
<i>trans</i> -product (3+7)	3_sy_tr_prod_1	-710.333932	-710.108814	0.2154
	3_sy_tr_prod_3	-710.328888	-710.104027	0.0013
	3_sy_tr_prod_4	-710.335303	-710.109820	0.6258
	3_sy_tr_prod_5	-710.331802	-710.107889	0.0808
	3_sy_tr_prod_6	-710.325079	-710.102268	0.0002
	3_sy_tr_prod_7	-710.333263	-710.107837	0.0765
	weighted:		-710.109286	

G_{trans}^{\ddagger}	80.7	kJ mol^{-1}
$G_{IM, trans}^0$	19.0	kJ mol^{-1}
$G_{cp, trans}^{\ddagger}$	45.5	kJ mol^{-1}
G_{trans}^0	-172.8	kJ mol^{-1}

<i>cis</i> -TS1 (3+7)	3_sy_c_1_ts1	-1188.185890	-1187.893970	0.6639
	3_sy_c_2_ts1	-1188.186643	-1187.892858	0.2043
	3_sy_c_3_ts1	-1188.180471	-1187.887218	0.0005
	3_sy_c_4_ts1	-1188.177862	-1187.885701	0.0001
	3_sy_c_5_ts1	-1188.183749	-1187.891186	0.0347
	3_sy_c_6_ts1	-1188.149506	-1187.859207	0.0000
	3_sy_c_7_ts1	-1188.182986	-1187.889490	0.0057
	3_sy_c_9_ts1	-1188.182786	-1187.890041	0.0103
	3_sy_c_10_ts1	-1188.184416	-1187.891969	0.0796
	3_sy_c_11_ts1	-1188.174490	-1187.881602	0.0000
	3_sy_c_14_ts1	-1188.180926	-1187.887748	0.0009
	3_sy_c_15_ts1	-1188.144571	-1187.853562	0.0000
	3_sy_c_16_ts1	-1188.145192	-1187.855855	0.0000
	3_sy_c_18_ts1	-1188.144341	-1187.853174	0.0000
	weighted:		-1187.893411	
<i>cis</i> -IM (3+7)	3_sy_c_1	-1188.219004	-1187.921972	0.6639
	3_sy_c_1_r	-1188.209494	-1187.912810	0.0000
	3_sy_c_2	-1188.214634	-1187.917953	0.0094
	3_sy_c_2_r	-1188.206945	-1187.909878	0.0000
	3_sy_c_3	-1188.213514	-1187.915601	0.0008
	3_sy_c_3_r	-1188.203491	-1187.905974	0.0000

	3_sy_c_4	-1188.209052	-1187.912496	0.0000
	3_sy_c_4_r	-1188.199929	-1187.902293	0.0000
	3_sy_c_5	-1188.212430	-1187.914097	0.0002
	3_sy_c_5_r	-1188.202315	-1187.906217	0.0000
	3_sy_c_6	-1188.212155	-1187.916524	0.0021
	3_sy_c_7	-1188.209216	-1187.912247	0.0000
	3_sy_c_8	-1188.218091	-1187.920458	0.1334
	3_sy_c_9	-1188.210105	-1187.913571	0.0001
	3_sy_c_10	-1188.213830	-1187.917055	0.0036
	3_sy_c_11	-1188.203218	-1187.906152	0.0000
	3_sy_c_12	-1188.215197	-1187.917715	0.0073
	3_sy_c_13	-1188.214574	-1187.918247	0.0128
	3_sy_c_14	-1188.211194	-1187.915060	0.0004
	3_sy_c_15	-1188.211851	-1187.916059	0.0013
	3_sy_c_16	-1188.211006	-1187.914012	0.0001
	3_sy_c_17	-1188.204376	-1187.908324	0.0000
	3_sy_c_18	-1188.218447	-1187.920655	0.1644
	3_sy_c_19	-1188.210132	-1187.914059	0.0002
	3_sy_c_20	-1188.208113	-1187.912387	0.0000
	weighted:		-1187.921387	
<i>cis</i> -TS2 (3+7)	3_sy_c_1_ts2	-1188.198829	-1187.904510	0.9969
	3_sy_c_2_ts2	-1188.191007	-1187.896588	0.0002
	3_sy_c_3_ts2	-1188.194080	-1187.898992	0.0029
	3_sy_c_4_ts2	-1188.187454	-1187.891773	0.0000
	weighted:		-1187.904493	
<i>cis</i> -product (3+7)	3_sy_c_prod_1	-710.326302	-710.101515	0.3846
	3_sy_c_prod_2	-710.325325	-710.101286	0.3019
	3_sy_c_prod_3	-710.321169	-710.095727	0.0008
	3_sy_c_prod_4	-710.327045	-710.101123	0.2538
	3_sy_c_prod_5	-710.325137	-710.099745	0.0589
	weighted:		-710.101237	
	G_{cis}^{\ddagger}	85.8		kJ mol^{-1}
	$G_{IM, cis}^0$	12.4		kJ mol^{-1}
	$G_{cp, cis}^{\ddagger}$	56.7		kJ mol^{-1}
	G_{cis}^0	-151.7		kJ mol^{-1}
4a + 7				
4a	4a	-305.169162	-305.121481	
<i>trans</i> -TS1 (4a+7)	4a_tr_sy_1_ts1	-1145.513164	-1145.299771	0.0260
	4a_tr_sy_1_ts1_rot1	-1145.517009	-1145.303189	0.9733
	4a_tr_sy_2_ts1	-1145.509975	-1145.295422	0.0003
	4a_tr_sy_3_ts1	-1145.510896	-1145.296046	0.0005
	weighted:		-1145.303094	

<i>trans</i> -IM (4a+7)	4a_tr_sy_1	-1145.539079	-1145.321585	0.0761
	4a_tr_sy_1_r	-1145.538032	-1145.322058	0.1257
	4a_tr_sy_2	-1145.532897	-1145.315260	0.0001
	4a_tr_sy_2_r	-1145.534954	-1145.317944	0.0016
	4a_tr_sy_3	-1145.538633	-1145.322024	0.1213
	4a_tr_sy_3_r	-1145.540568	-1145.323644	0.6752
	weighted:		-1145.323081	
<i>trans</i> -TS2 (4a+7)	4a_tr_sy_1_ts2	-1145.528959	-1145.314181	0.1338
	4a_tr_sy_2_ts2	-1145.526993	-1145.313160	0.0453
	4a_tr_sy_3_ts2	-1145.530449	-1145.315892	0.8208
	weighted:		-1145.315539	
<i>trans</i> -product (4a+7)	4a_sy_tr_prod_1	-667.656198	-667.508900	1.0000
	weighted:		-667.508900	
		G_{trans}^{\ddagger}	72.8	kJ mol^{-1}
		$G_{IM, trans}^0$	20.3	kJ mol^{-1}
		$G_{cp, trans}^{\ddagger}$	40.1	kJ mol^{-1}
		G_{trans}^0	-159.5	kJ mol^{-1}
<i>cis</i> -TS1 (4a+7)	4a_c_sy_1_ts1	-1145.510167	-1145.295519	0.0030
	4a_c_sy_2_ts1	-1145.510667	-1145.295834	0.0042
	4a_c_sy_3_ts1	-1145.513676	-1145.300727	0.7511
	4a_c_sy_4_ts1	-1145.513067	-1145.299588	0.2244
	4a_c_sy_5_ts1	-1145.509046	-1145.294380	0.0009
	4a_c_sy_6_ts1	-1145.511051	-1145.297118	0.0164
	weighted:		-1145.300371	
<i>cis</i> -IM (4a+7)	4a_c_sy_1	-1145.534119	-1145.316808	0.0001
	4a_c_sy_1_r	-1145.533225	-1145.315769	0.0000
	4a_c_sy_2	-1145.541329	-1145.323806	0.2088
	4a_c_sy_2_r	-1145.536344	-1145.318996	0.0013
	4a_c_sy_3	-1145.541560	-1145.323898	0.2301
	4a_c_sy_4	-1145.540016	-1145.323299	0.1220
	4a_c_sy_5	-1145.536186	-1145.319337	0.0018
	4a_c_sy_6	-1145.541383	-1145.324500	0.4358
weighted:		-1145.324052		
<i>cis</i> -TS2 (4a+7)	4a_c_sy_1_ts2	-1145.523943	-1145.307249	0.0963
	4a_c_sy_2_ts2	-1145.525706	-1145.309361	0.9037
	weighted:		-1145.309158	
<i>cis</i> -product (4a+7)	4a_sy_c_prod_1	-667.654360	-667.507922	1.0000
	weighted:		-667.507922	

G_{cis}^{\ddagger}	79.9	kJ mol^{-1}
$G_{IM, cis}^0$	17.7	kJ mol^{-1}
$G_{cp, cis}^{\ddagger}$	56.8	kJ mol^{-1}
G_{cis}^0	-156.9	kJ mol^{-1}

4b + 7				
4b	4b	-344.460189	-344.386215	
TS1 (4b+7)	4b_sy_1_ts1	-1184.805843	-1184.565470	0.0318
	4b_sy_2_ts1	-1184.804409	-1184.564051	0.0071
	4b_sy_3_ts1	-1184.804612	-1184.565061	0.0206
	4b_sy_4_ts1	-1184.802892	-1184.561105	0.0003
	4b_sy_5_ts1	-1184.809791	-1184.567745	0.3546
	4b_sy_5_ts1_rot1	-1184.809658	-1184.567323	0.2267
	4b_sy_7_ts1	-1184.806622	-1184.567714	0.3432
	4b_sy_8_ts1	-1184.806199	-1184.564178	0.0081
	4b_sy_9_ts1	-1184.807422	-1184.564135	0.0077
		weighted:		-1184.567427
IM (4b+7)	4b_sy_1	-1184.836314	-1184.591825	0.0050
	4b_sy_1_r	-1184.835794	-1184.593051	0.0185
	4b_sy_2	-1184.837004	-1184.591934	0.0057
	4b_sy_2_r	-1184.833907	-1184.589561	0.0005
	4b_sy_3	-1184.841202	-1184.596529	0.7380
	4b_sy_3_r	-1184.835577	-1184.593157	0.0207
	4b_sy_5	-1184.838755	-1184.595005	0.1467
	4b_sy_5_r	-1184.834609	-1184.593099	0.0194
	4b_sy_6	-1184.833774	-1184.588194	0.0001
	4b_sy_7	-1184.837589	-1184.593869	0.0440
	4b_sy_8	-1184.833581	-1184.587721	0.0001
	4b_sy_9	-1184.835301	-1184.590555	0.0013
		weighted:		-1184.595925
<i>cis</i> -TS2 (4b+7)	4b_sy_c_1_ts2	-1184.826011	-1184.585731	1.0000
	weighted:		-1184.585731	
<i>cis</i> -product (4b+7)	4b_sy_c_prod_1	-706.954852	-706.781326	0.5723
	4b_sy_c_prod_2	-706.954584	-706.781051	0.4277
	weighted:		-706.781209	
<i>trans</i> -TS2 (4b+7)	4b_sy_tr_2_ts2	-1184.826876	-1184.585464	0.2818
	4b_sy_tr_3_ts2	-1184.828172	-1184.586346	0.7182
	weighted:		-1184.586098	
<i>trans</i> -product (4b+7)	4b_sy_tr_prod_1	-706.952817	-706.780289	0.7928
	4b_sy_tr_prod_2	-706.951166	-706.779023	0.2072
	weighted:		-706.780026	

		G^\ddagger	73.8	kJ mol^{-1}	
		G_{IM}^0	-1.0	kJ mol^{-1}	
		$G_{\text{cp, cis}}^\ddagger$	25.8	kJ mol^{-1}	
		G_{cis}^0	-179.3	kJ mol^{-1}	
		$G_{\text{cp, trans}}^\ddagger$	24.8	kJ mol^{-1}	
		G_{trans}^0	-179.7	kJ mol^{-1}	
5a + 7					
5a	5a		-344.464791	-344.389281	
<i>trans</i> -TS1 (5a+7)	5a_sy_tr_1_ts1		-1184.806162	-1184.564227	0.0045
	5a_sy_tr_2_ts1		-1184.807952	-1184.566052	0.0313
	5a_sy_tr_3_ts1		-1184.802698	-1184.560344	0.0001
	5a_sy_tr_4_ts1		-1184.811847	-1184.569146	0.8317
	5a_sy_tr_5_ts1		-1184.809270	-1184.567367	0.1262
	5a_sy_tr_6_ts1		-1184.807480	-1184.564358	0.0052
	5a_sy_tr_9_ts1		-1184.803884	-1184.561259	0.0002
	5a_sy_tr_10_ts1		-1184.806991	-1184.562699	0.0009
		weighted:			-1184.568770
<i>trans</i> -IM (5a+7)	5a_sy_tr_1		-1184.835642	-1184.590990	0.0504
	5a_sy_tr_1_r		-1184.835938	-1184.590648	0.0350
	5a_sy_tr_2		-1184.831928	-1184.587004	0.0007
	5a_sy_tr_2_r		-1184.835128	-1184.590051	0.0186
	5a_sy_tr_3		-1184.829438	-1184.582809	0.0000
	5a_sy_tr_3_r		-1184.832276	-1184.586730	0.0005
	5a_sy_tr_4		-1184.837388	-1184.593467	0.6958
	5a_sy_tr_5		-1184.836886	-1184.592249	0.1912
	5a_sy_tr_6		-1184.829806	-1184.583446	0.0000
	5a_sy_tr_7		-1184.833221	-1184.587679	0.0015
	5a_sy_tr_8		-1184.833795	-1184.589014	0.0062
	5a_sy_tr_9		-1184.825549	-1184.578730	0.0000
	5a_sy_tr_10		-1184.829851	-1184.584542	0.0001
	weighted:			-1184.592902	
<i>trans</i> -TS2 (5a+7)	5a_sy_tr_1_ts2		-1184.824604	-1184.581885	0.9320
	5a_sy_tr_3_ts2		-1184.822244	-1184.579416	0.0680
		weighted:			-1184.581718
<i>trans</i> -product (5a+7)	5a_sy_tr_prod_1		-706.950864	-706.776810	0.0728
	5a_sy_tr_prod_2		-706.954244	-706.779210	0.9272
		weighted:			-706.779035
		$G_{\text{trans}}^\ddagger$	78.3	kJ mol^{-1}	
		$G_{\text{IM, trans}}^0$	15.0	kJ mol^{-1}	
		$G_{\text{cp, trans}}^\ddagger$	44.3	kJ mol^{-1}	
		G_{trans}^0	-165.6	kJ mol^{-1}	

<i>cis</i> -TS1 (5a+7)	5a_sy_c_1_ts1	-1184.797740	-1184.554515	0.0000
	5a_sy_c_2_ts1	-1184.806708	-1184.564583	0.0146
	5a_sy_c_3_ts1	-1184.805021	-1184.561146	0.0004
	5a_sy_c_4_ts1	-1184.810520	-1184.568525	0.9502
	5a_sy_c_5_ts1	-1184.807181	-1184.564958	0.0216
	5a_sy_c_6_ts1	-1184.806080	-1184.564399	0.0120
	5a_sy_c_7_ts1	-1184.804524	-1184.562001	0.0009
	5a_sy_c_9_ts1	-1184.803155	-1184.560819	0.0003
	weighted:		-1184.568330	
<i>cis</i> -IM (5a+7)	5a_sy_c_1	-1184.828479	-1184.583478	0.0000
	5a_sy_c_1_r	-1184.827150	-1184.581328	0.0000
	5a_sy_c_2	-1184.836086	-1184.590896	0.0749
	5a_sy_c_2_r	-1184.834393	-1184.590451	0.0467
	5a_sy_c_3	-1184.836586	-1184.590964	0.0805
	5a_sy_c_3_r	-1184.831011	-1184.585385	0.0002
	5a_sy_c_4	-1184.837415	-1184.592573	0.4432
	5a_sy_c_4_r	-1184.834335	-1184.588763	0.0078
	5a_sy_c_5	-1184.835094	-1184.589432	0.0159
	5a_sy_c_5_r	-1184.829238	-1184.582795	0.0000
	5a_sy_c_6	-1184.835378	-1184.590568	0.0529
	5a_sy_c_7	-1184.832311	-1184.587040	0.0013
5a_sy_c_9	-1184.837641	-1184.592129	0.2766	
	weighted:		-1184.591901	
<i>cis</i> -TS2 (5a+7)	5a_sy_c_1_ts2	-1184.817478	-1184.573220	0.0082
	5a_sy_c_2_ts2	-1184.819665	-1184.577333	0.6432
	5a_sy_c_3_ts2	-1184.818810	-1184.575771	0.1228
	5a_sy_c_4_ts2	-1184.819507	-1184.576287	0.2121
	5a_sy_c_5_ts2	-1184.816684	-1184.573704	0.0137
	weighted:		-1184.576836	
<i>cis</i> -product (5a+7)	5a_sy_c_prod_1	-706.946613	-706.772324	0.0863
	5a_sy_c_prod_2	-706.949332	-706.774549	0.9137
	weighted:		-706.774357	

G_{cis}^{\ddagger}	79.5	kJ mol^{-1}
$G_{IM, cis}^0$	17.6	kJ mol^{-1}
$G_{cp, cis}^{\ddagger}$	57.2	kJ mol^{-1}
G_{cis}^0	-153.3	kJ mol^{-1}

5b + 7				
5b	5b	-383.756315	-383.654836	
TS1 (5b+7)	5b_sy_1_ts1	-1224.100343	-1223.831375	0.0002
	5b_sy_2_ts1	-1224.101024	-1223.833043	0.0014

	5b_sy_5_ts1	-1224.109021	-1223.838310	0.3825
	5b_sy_5_ts1_rot1	-1224.105940	-1223.836293	0.0451
	5b_sy_5_ts1_rot2	-1224.102673	-1223.835417	0.0178
	5b_sy_6_ts1	-1224.101417	-1223.832618	0.0009
	5b_sy_7_ts1	-1224.103166	-1223.835392	0.0173
	5b_sy_8_ts1	-1224.103061	-1223.835508	0.0196
	5b_sy_9_ts1	-1224.103900	-1223.836508	0.0566
	5b_sy_10_ts1	-1224.108368	-1223.838480	0.4584
	weighted:		-1223.838023	
IM (5b+7)	5b_sy_1	-1224.135225	-1223.861724	0.0016
	5b_sy_1_r	-1224.132898	-1223.862576	0.0040
	5b_sy_2	-1224.134619	-1223.860940	0.0007
	5b_sy_2_r2	-1224.132990	-1223.861002	0.0008
	5b_sy_2_r3	-1224.133619	-1223.861551	0.0014
	5b_sy_2_r4	-1224.134822	-1223.862744	0.0048
	5b_sy_2_r	-1224.132985	-1223.862451	0.0035
	5b_sy_3	-1224.139800	-1223.866229	0.1940
	5b_sy_3_r	-1224.134609	-1223.863511	0.0109
	5b_sy_4	-1224.136769	-1223.864097	0.0202
	5b_sy_5	-1224.139418	-1223.866172	0.1825
	5b_sy_5_r	-1224.133617	-1223.861611	0.0014
	5b_sy_6	-1224.139000	-1223.865617	0.1014
	5b_sy_6_r	-1224.134754	-1223.863392	0.0096
	5b_sy_8	-1224.135715	-1223.863432	0.0100
	5b_sy_9	-1224.135248	-1223.863493	0.0107
	5b_sy_10	-1224.138546	-1223.866859	0.3784
	5b_sy_11	-1224.135620	-1223.861248	0.0010
	5b_sy_12	-1224.131082	-1223.859022	0.0001
	5b_sy_13	-1224.131722	-1223.857915	0.0000
	5b_sy_14	-1224.135394	-1223.864316	0.0255
	5b_sy_15	-1224.135189	-1223.864677	0.0374
	5b_sy_16	-1224.131624	-1223.859344	0.0001
	weighted:		-1223.866052	
trans-TS2 (5b+7)	5b_tr_1_ts2	-1224.125656	-1223.856115	0.0366
	5b_tr_2_ts2	-1224.125901	-1223.856194	0.0398
	5b_tr_3_ts2	-1224.127012	-1223.856848	0.0797
	5b_tr_4_ts2	-1224.127615	-1223.858876	0.6839
	5b_tr_6_ts2	-1224.127318	-1223.857505	0.1599
	weighted:		-1223.858287	
trans-product (5b+7)	5b_sy_tr_prod_1	-746.248951	-746.048930	0.8079
	5b_sy_tr_prod_2	-746.246987	-746.046869	0.0908
	5b_sy_tr_prod_3	-746.248289	-746.046959	0.0999
	5b_sy_tr_prod_5	-746.243114	-746.042902	0.0014
	weighted:		-746.048538	

<i>cis</i> -TS2 (5b+7)	5b_c_2_r2_ts2	-1224.122817	-1223.853019	0.0554
	5b_c_2_r3_ts2	-1224.124495	-1223.855387	0.6815
	5b_c_2_r4_ts2	-1224.124738	-1223.854489	0.2632
	weighted:		-1223.855019	
<i>cis</i> -product (5b+7)	5b_sy_c_prod_1	-746.250103	-746.049796	0.1640
	5b_sy_c_prod_2	-746.250315	-746.051214	0.7373
	5b_sy_c_prod_4	-746.250173	-746.049317	0.0987
	weighted:		-746.050794	

G^\ddagger	68.6	kJ mol^{-1}
G_{IM}^0	-5.0	kJ mol^{-1}
$G_{\text{cp, cis}}^\ddagger$	24.0	kJ mol^{-1}
G_{cis}^0	-181.9	kJ mol^{-1}
$G_{\text{cp, trans}}^\ddagger$	15.4	kJ mol^{-1}
G_{trans}^0	-176.0	kJ mol^{-1}

(*E*)/(*Z*)-Pentenone + 7

	e_pentenone_1	-270.451269	-270.363875	0.5909
	e_pentenone_2	-270.450203	-270.363528	0.4091
	weighted:		-270.363733	
	z_pentenone_1	-270.444870	-270.357441	0.0683
	z_pentenone_2	-270.446077	-270.359906	0.9317
	weighted:		-270.359738	
TS1 ((<i>E</i>) + 7)	e_pent_sr_oe_1_ts1	-1110.795242	-1110.539755	0.0004
	e_pent_sr_oe_2_ts1	-1110.790301	-1110.534896	0.0000
	e_pent_sr_oe_3_ts1	-1110.788381	-1110.532292	0.0000
	e_pent_sr_oe_4_ts1	-1110.790716	-1110.535082	0.0000
	e_pent_sr_oe_5_ts1	-1110.796443	-1110.540731	0.0012
	e_pent_sr_oz_1_ts1	-1110.801484	-1110.546202	0.4026
	e_pent_sr_oz_2_ts1	-1110.796298	-1110.542684	0.0097
	e_pent_sr_oz_3_ts1	-1110.788832	-1110.532474	0.0000
	e_pent_sr_oz_4_ts1	-1110.792300	-1110.536466	0.0000
	e_pent_sr_oz_5_ts1	-1110.792847	-1110.538800	0.0002
	e_pent_ss_oe_1_ts1	-1110.786641	-1110.531790	0.0000
	e_pent_ss_oe_2_ts1	-1110.795386	-1110.541174	0.0020
	e_pent_ss_oe_3_ts1	-1110.795054	-1110.538157	0.0001
	e_pent_ss_oe_4_ts1	-1110.789144	-1110.532308	0.0000
	e_pent_ss_oe_6_ts1	-1110.786268	-1110.531902	0.0000
	e_pent_ss_oe_8_ts1	-1110.795454	-1110.539326	0.0003
	e_pent_ss_oe_9_ts1	-1110.797873	-1110.543229	0.0172/OE
	e_pent_ss_oz_1_ts1	-1110.792437	-1110.538884	0.0002
	e_pent_ss_oz_2_ts1	-1110.799715	-1110.546510	0.5582/OZ

e_pent_ss_oz_3_ts1	-1110.795402	-1110.542361	0.0069
e_pent_ss_oz_4_ts1	-1110.792524	-1110.538930	0.0002
e_pent_ss_oz_7_ts1	-1110.792911	-1110.538552	0.0001
e_pent_ss_oz_9_ts1	-1110.793003	-1110.537945	0.0001
e_pent_ss_oz_10_ts1	-1110.794199	-1110.540323	0.0008

OE/OZ indicates the conformers used for calculating the individual barriers.

weighted: -1110.546230

TS1 ((Z) + 7)

z_pent_sr_oe_1_ts1	-1110.786849	-1110.531722	0.0001
z_pent_sr_oe_2_ts1	-1110.791650	-1110.533101	0.0003
z_pent_sr_oe_3_ts1	-1110.789976	-1110.532492	0.0001
z_pent_sr_oe_4_ts1	-1110.782538	-1110.525927	0.0000
z_pent_sr_oe_5_ts1	-1110.794017	-1110.537695	0.0358
z_pent_sr_oz_1_ts1	-1110.793767	-1110.539544	0.2540
z_pent_sr_oz_2_ts1	-1110.792782	-1110.538747	0.1091
z_pent_sr_oz_3_ts1	-1110.789926	-1110.535578	0.0038
z_pent_sr_oz_4_ts1	-1110.791960	-1110.534964	0.0020
z_pent_sr_oz_5_ts1	-1110.789497	-1110.535227	0.0026
z_pent_ss_oe_1_ts1	-1110.783853	-1110.529108	0.0000
z_pent_ss_oe_2_ts1	-1110.788299	-1110.534079	0.0008
z_pent_ss_oe_3_ts1	-1110.785720	-1110.528311	0.0000
z_pent_ss_oe_4_ts1	-1110.786007	-1110.530420	0.0000
z_pent_ss_oe_7_ts1	-1110.786640	-1110.531784	0.0001
z_pent_ss_oe_8_fr_ts1	-1110.795242	-1110.537716	0.0366/OE
z_pent_ss_oz_1_ts1	-1110.787994	-1110.534438	0.0011
z_pent_ss_oz_2_ts1	-1110.785855	-1110.532474	0.0001
z_pent_ss_oz_3_ts1 ^[a]	-1110.793031	-1110.539616	0.2741/OZ
z_pent_ss_oz_6_ts1 ^[a]	-1110.795465	-1110.539590	0.2666/OZ
z_pent_ss_oz_9_ts1	-1110.791775	-1110.536726	0.0128

OE/OZ indicates the conformers used for calculating the individual barriers.

weighted: -1110.539269

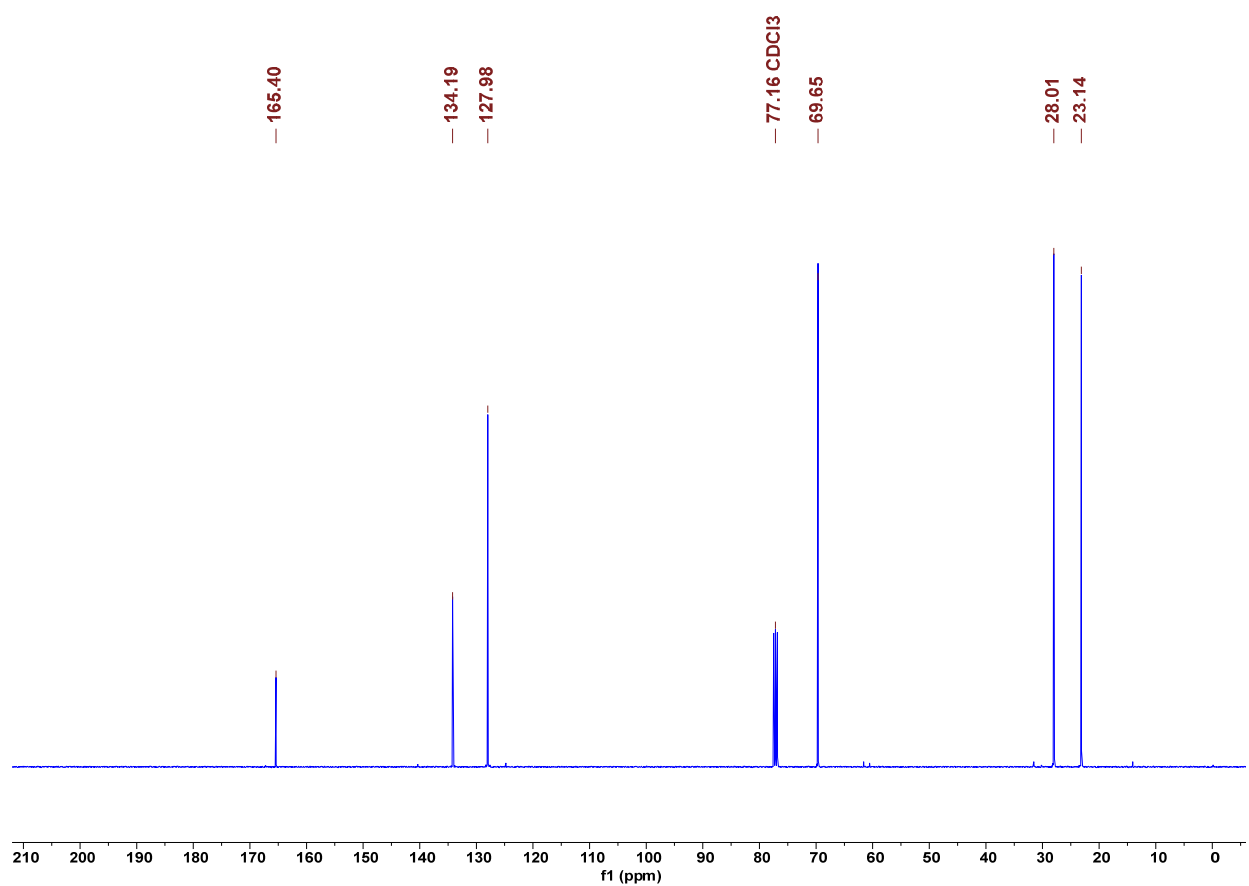
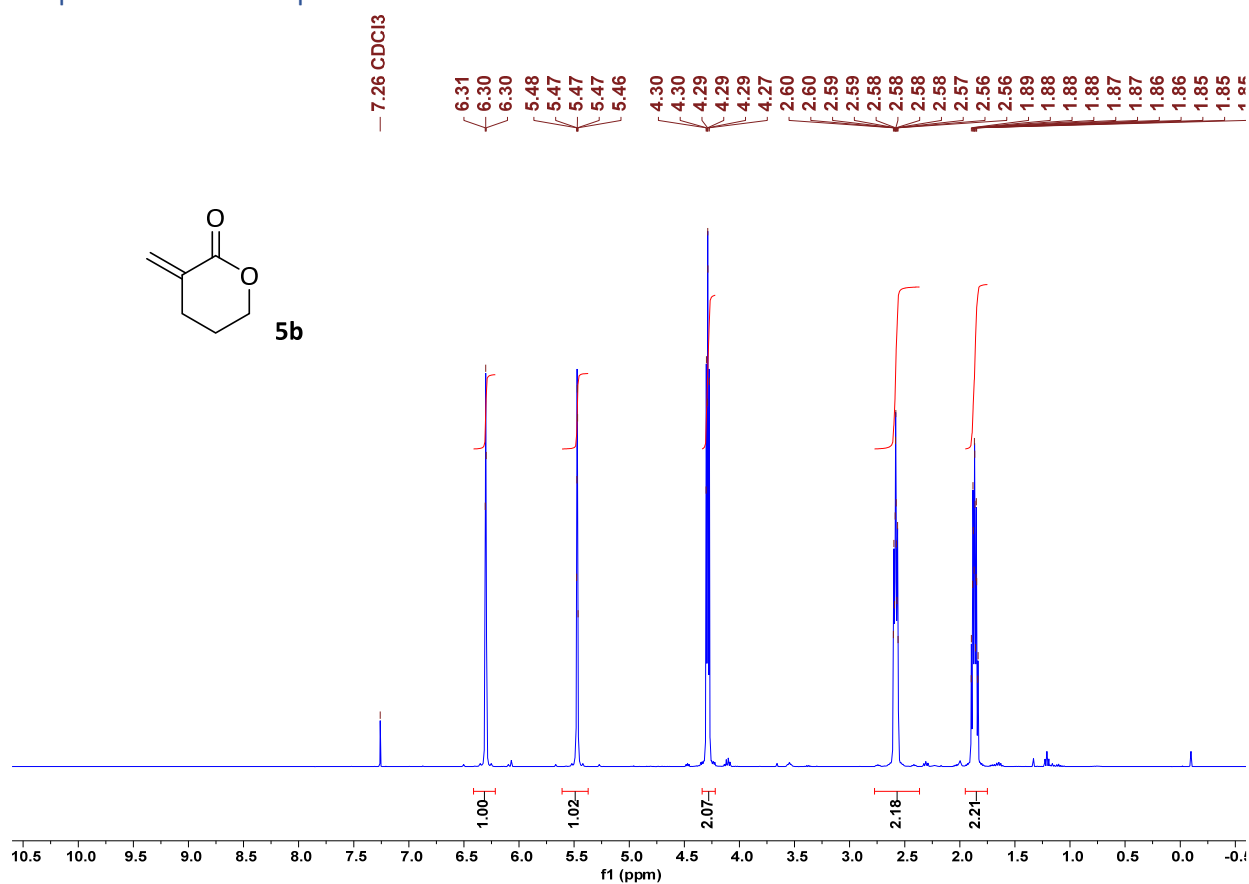
$G_{(E),\text{weighted}}^\ddagger$	70.4	kJ mol^{-1}
$G_{(Z),\text{weighted}}^\ddagger$	78.2	kJ mol^{-1}

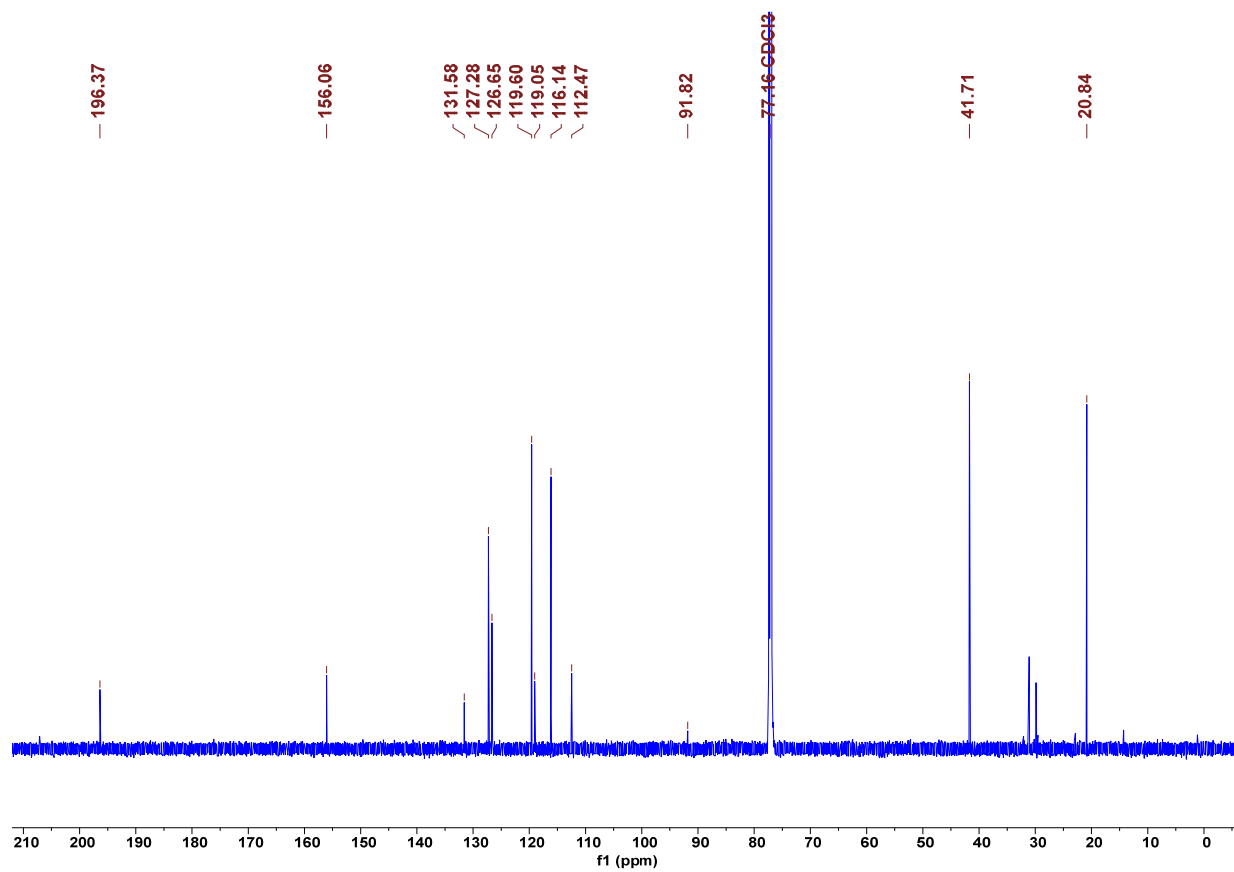
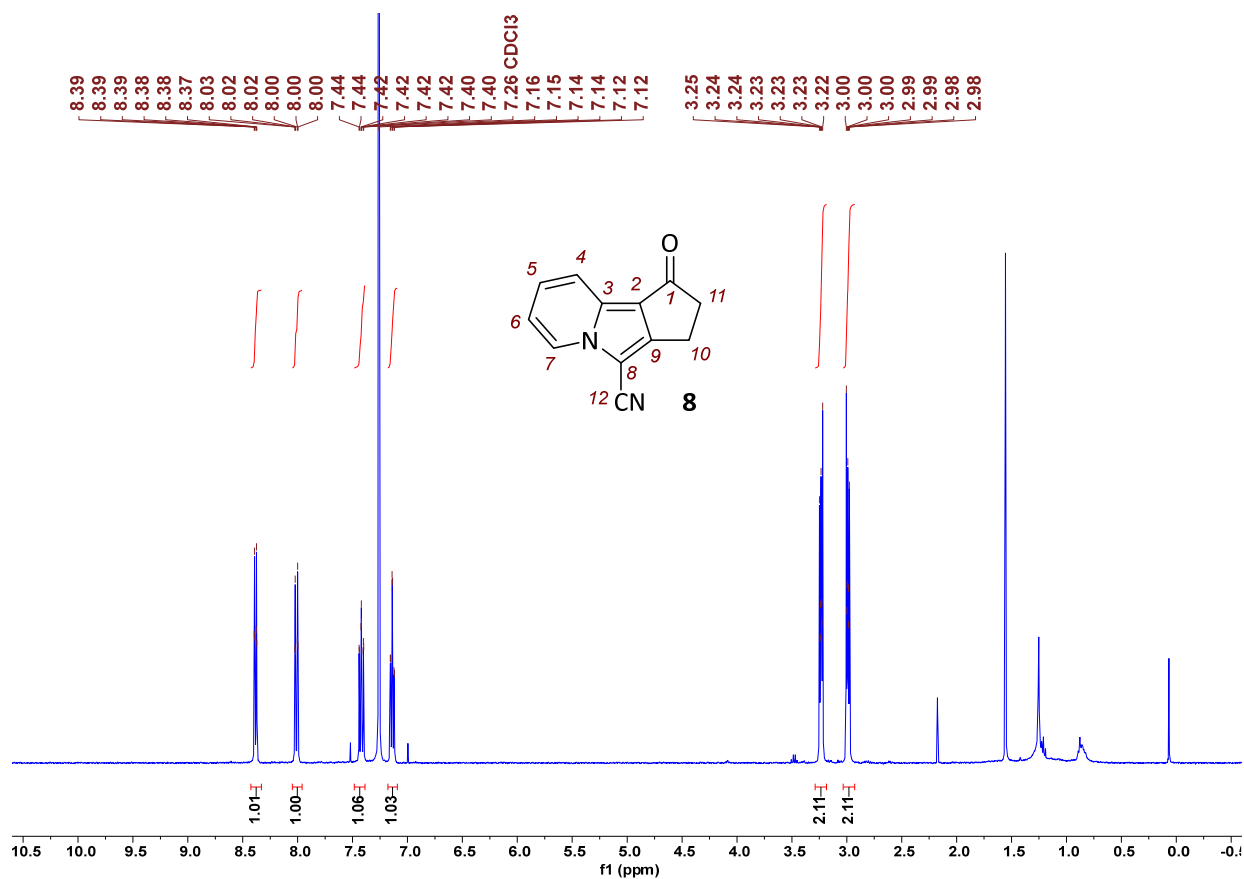
G^\ddagger of most favorable conformer for each transition state (highlighted in green):

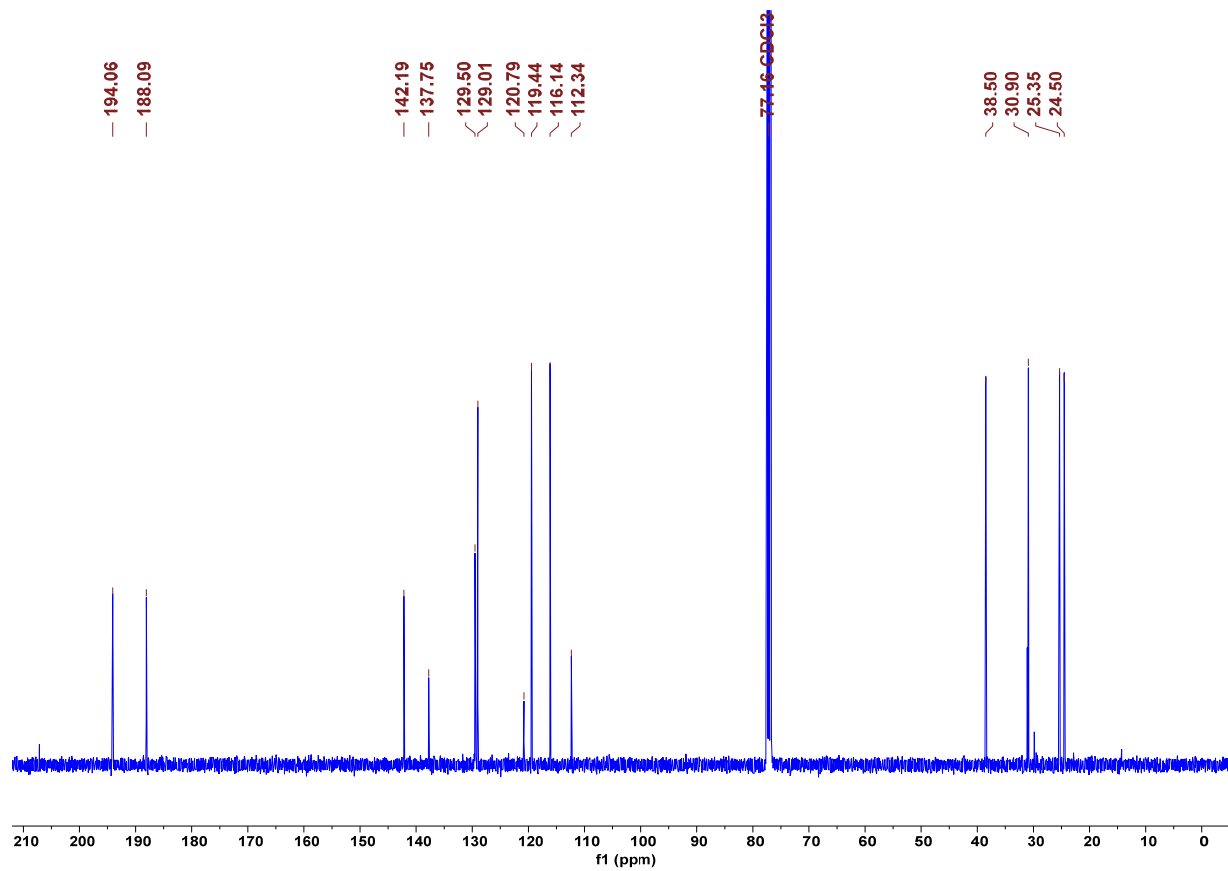
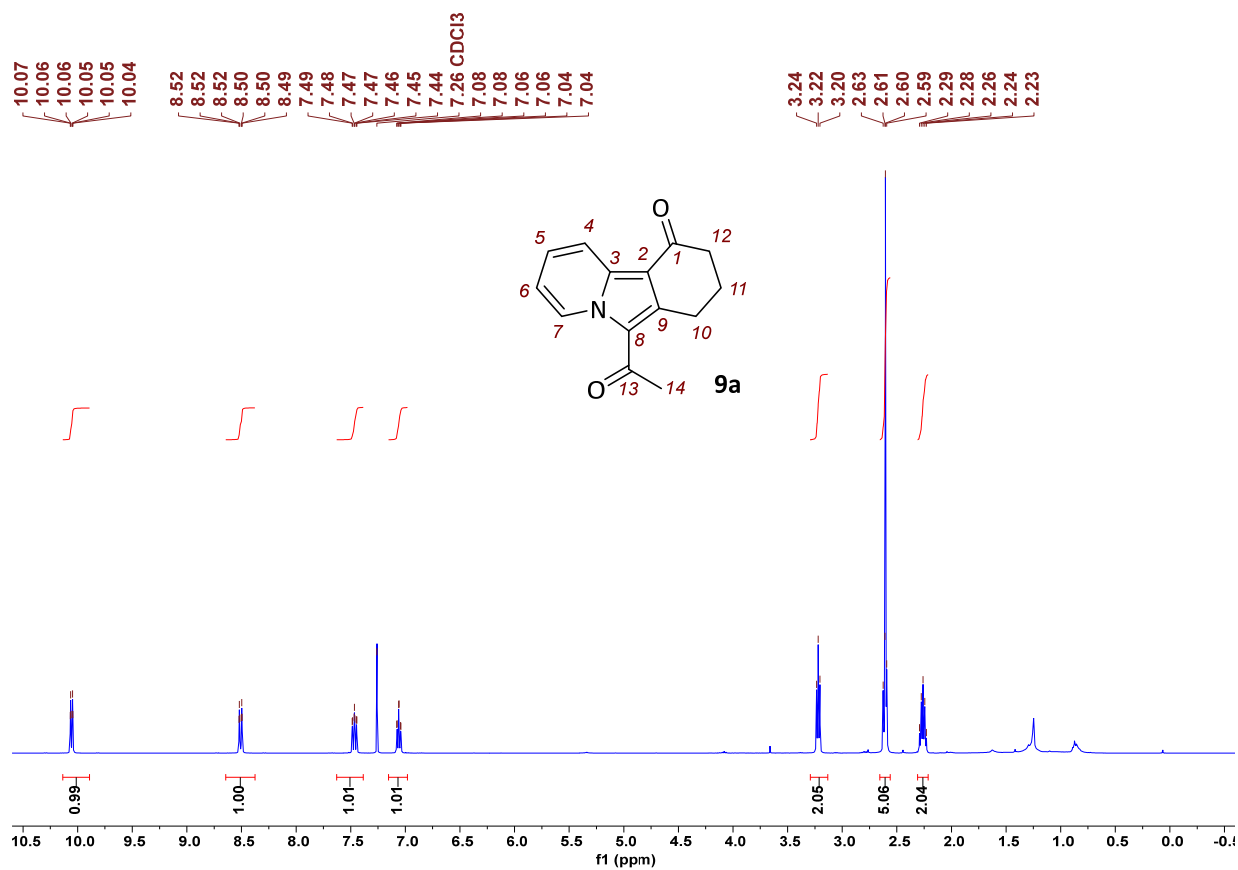
$G_{(E),\text{s-trans}}^\ddagger$	78.3	kJ mol^{-1}
$G_{(Z),\text{s-trans}}^\ddagger$	82.3	kJ mol^{-1}
$G_{(E),\text{s-cis}}^\ddagger$	69.7	kJ mol^{-1}
$G_{(Z),\text{s-cis}}^\ddagger$	77.3	kJ mol^{-1}

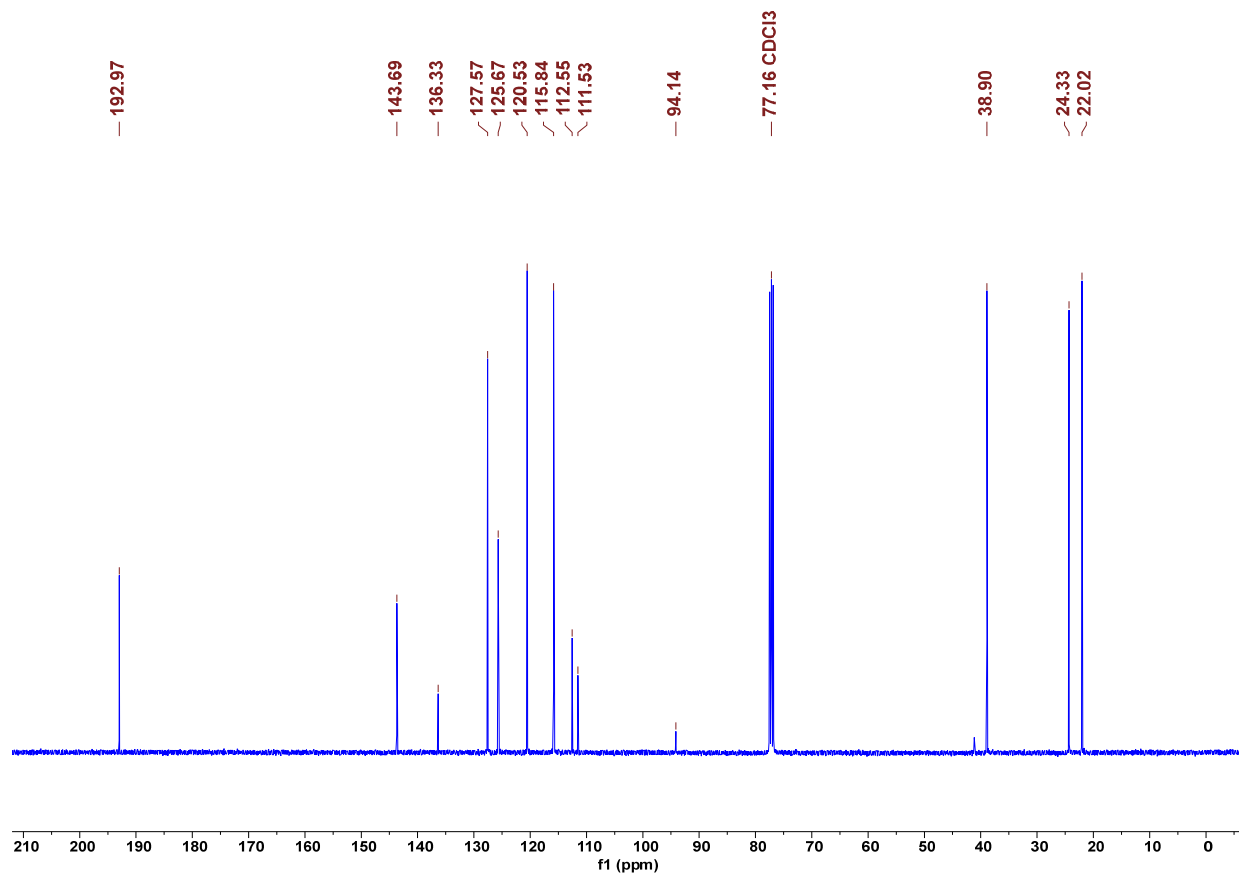
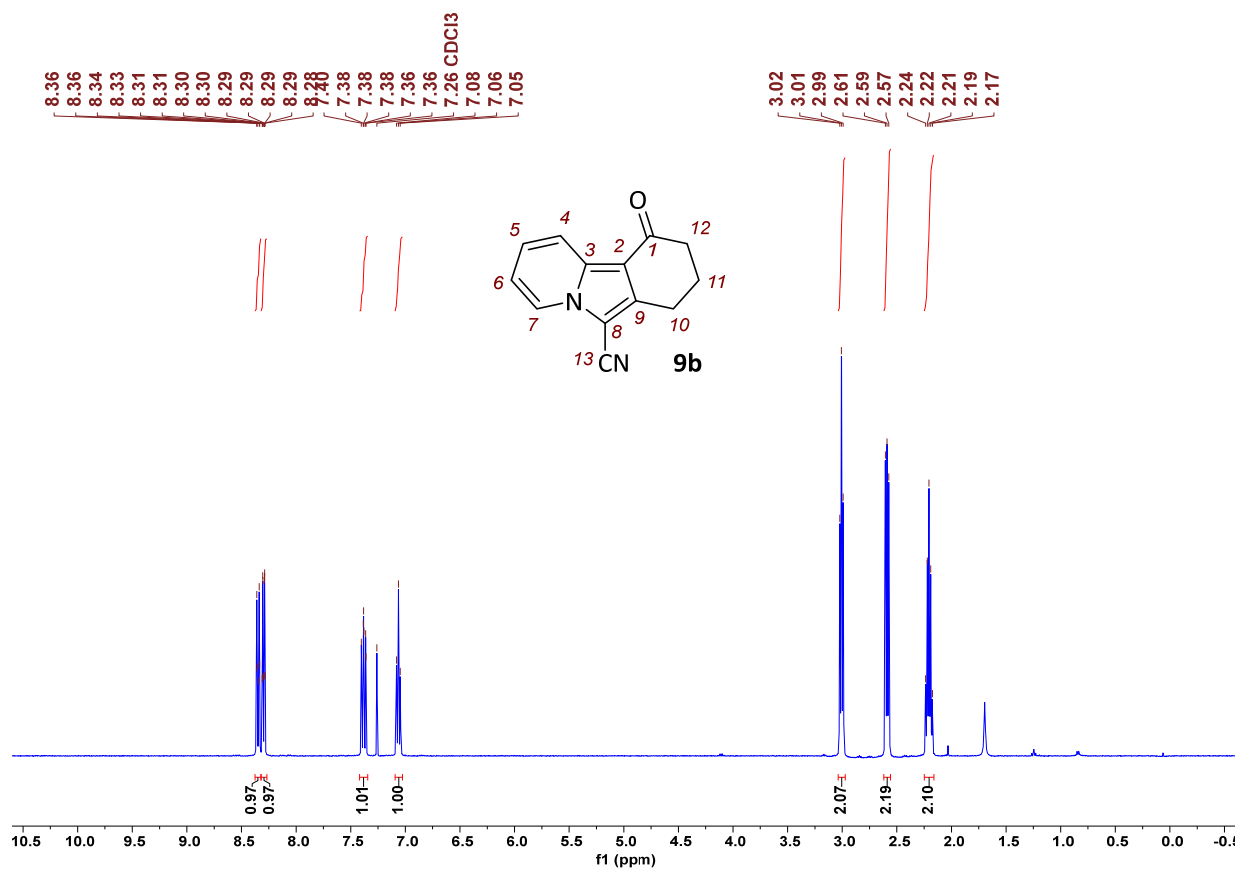
[a] For the picture shown in Figure 6 in the main text, the structure for “z_pent_ss_oz_6_ts1” was used as it has a similar conformation as the other systems. This conformer is slightly disfavored by 0.04 kJ/mol relative to the most favorable conformer, “z_pent_ss_oz_3_ts1”.

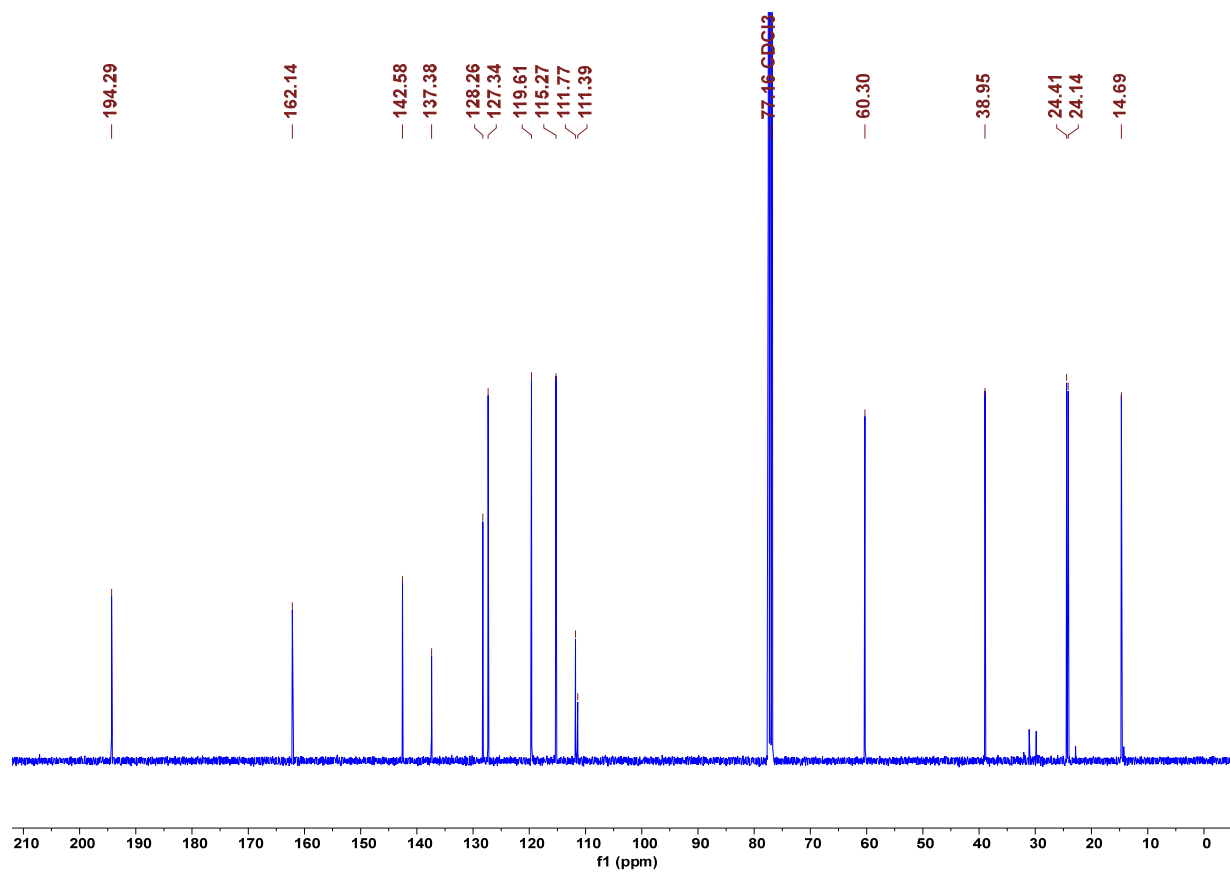
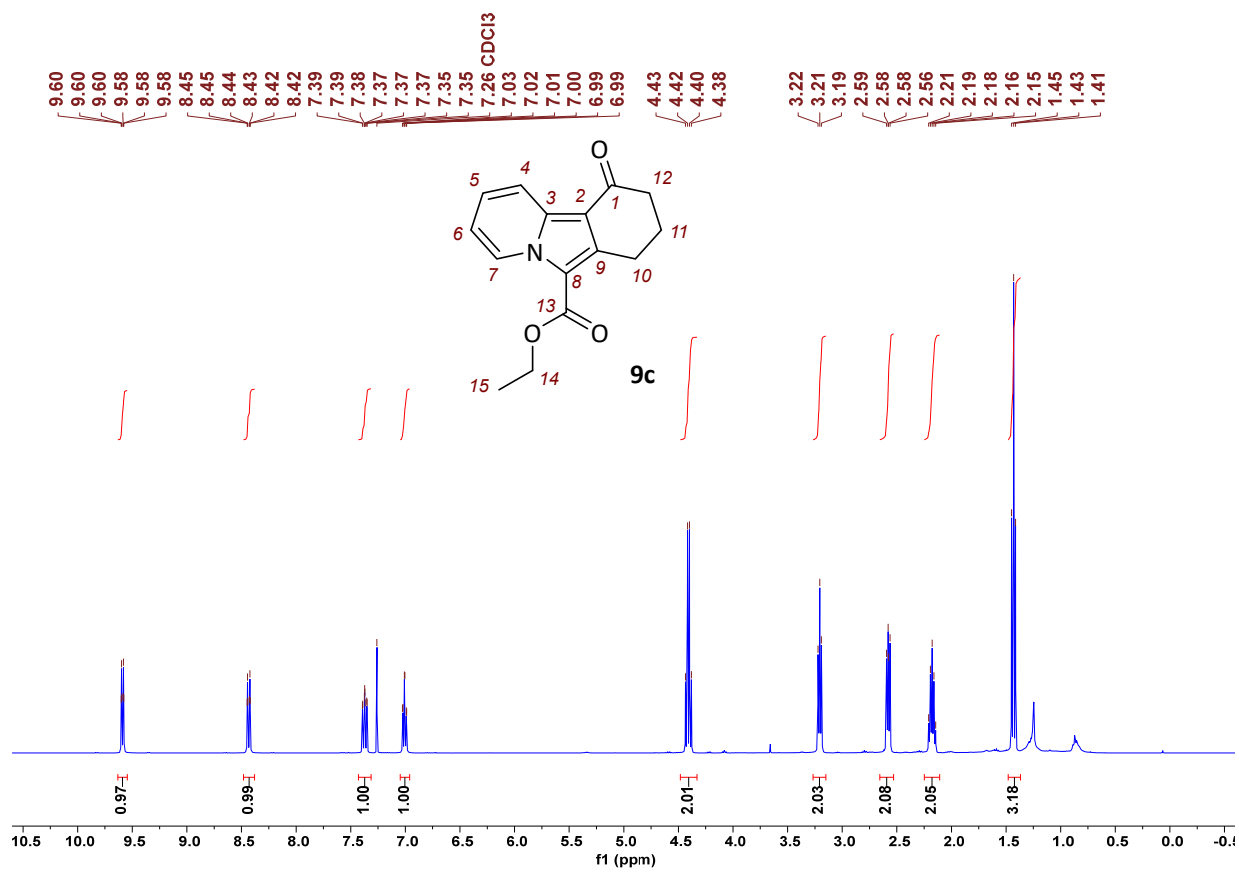
Copies of NMR Spectra of Isolated Products

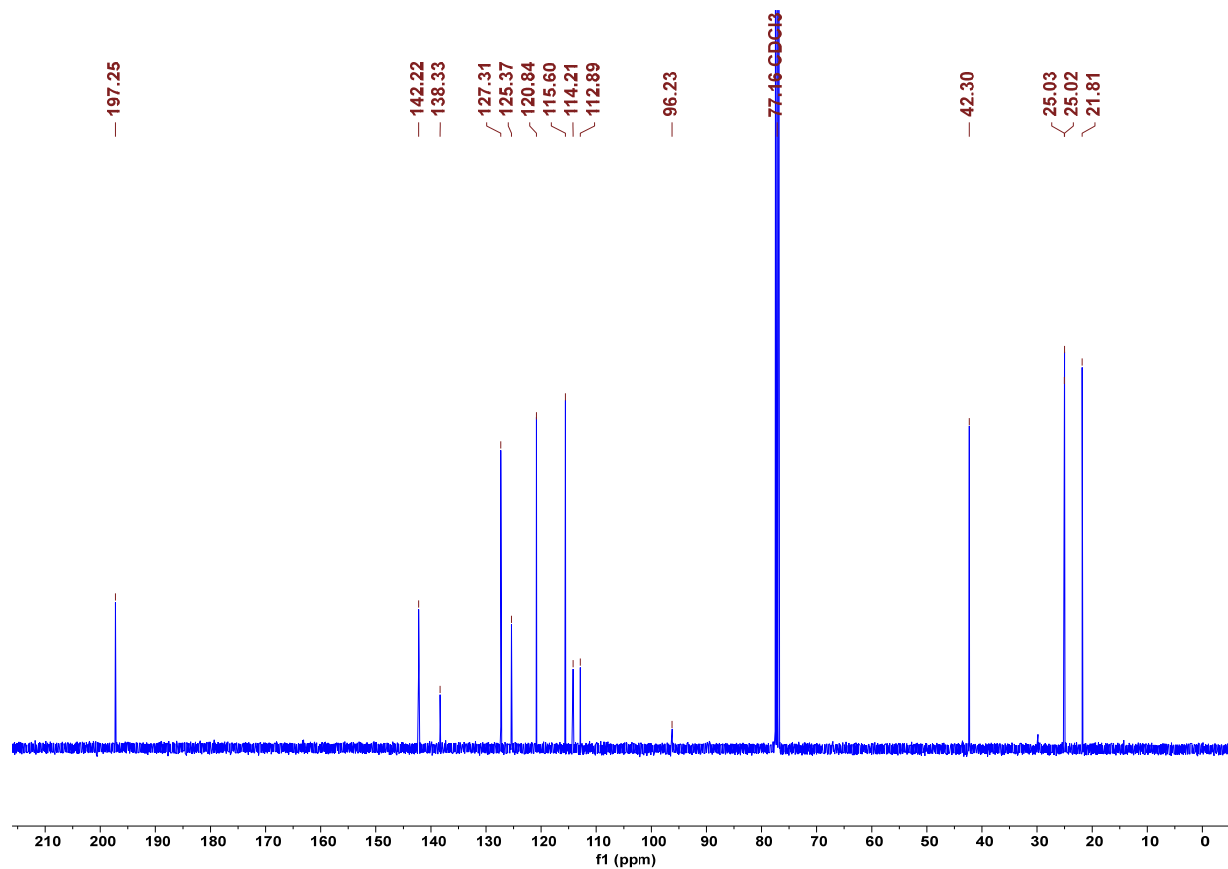
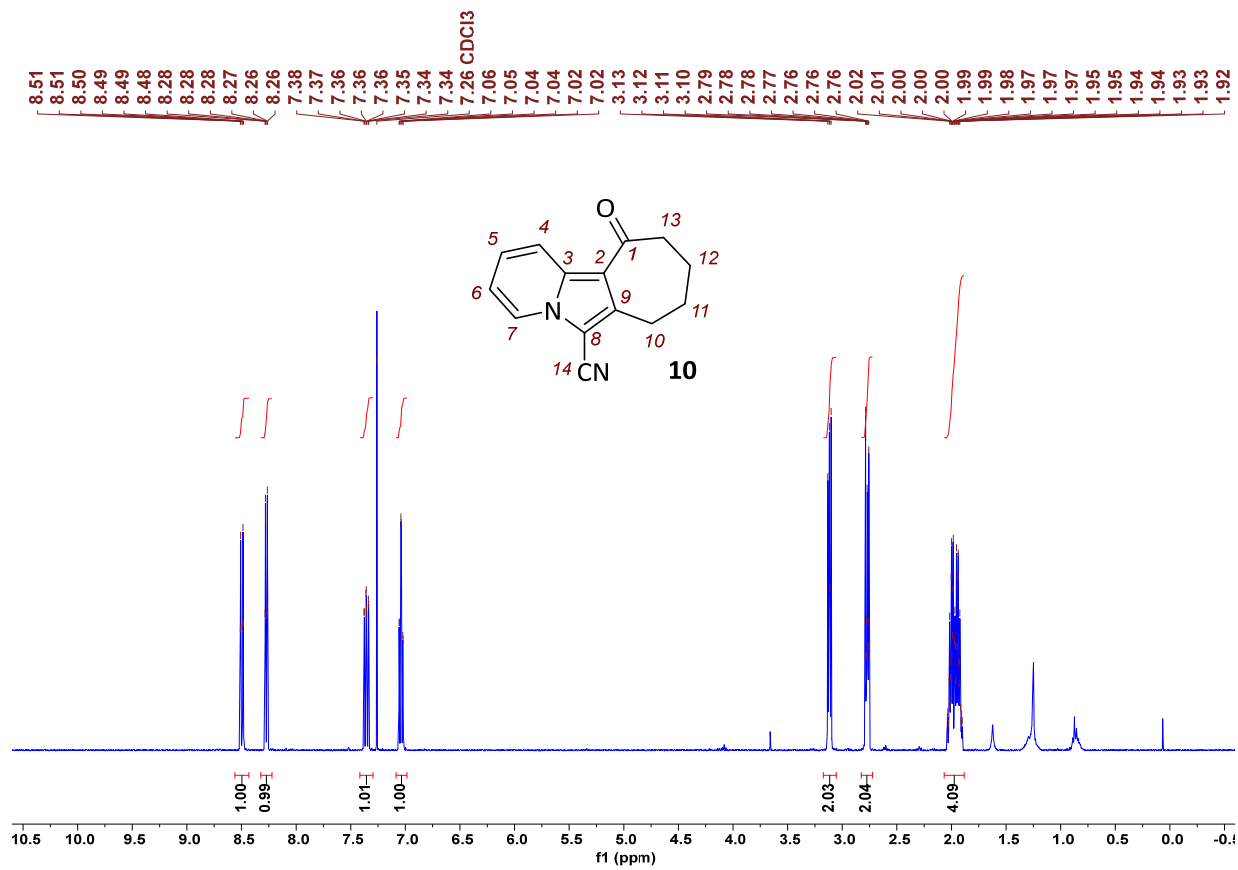


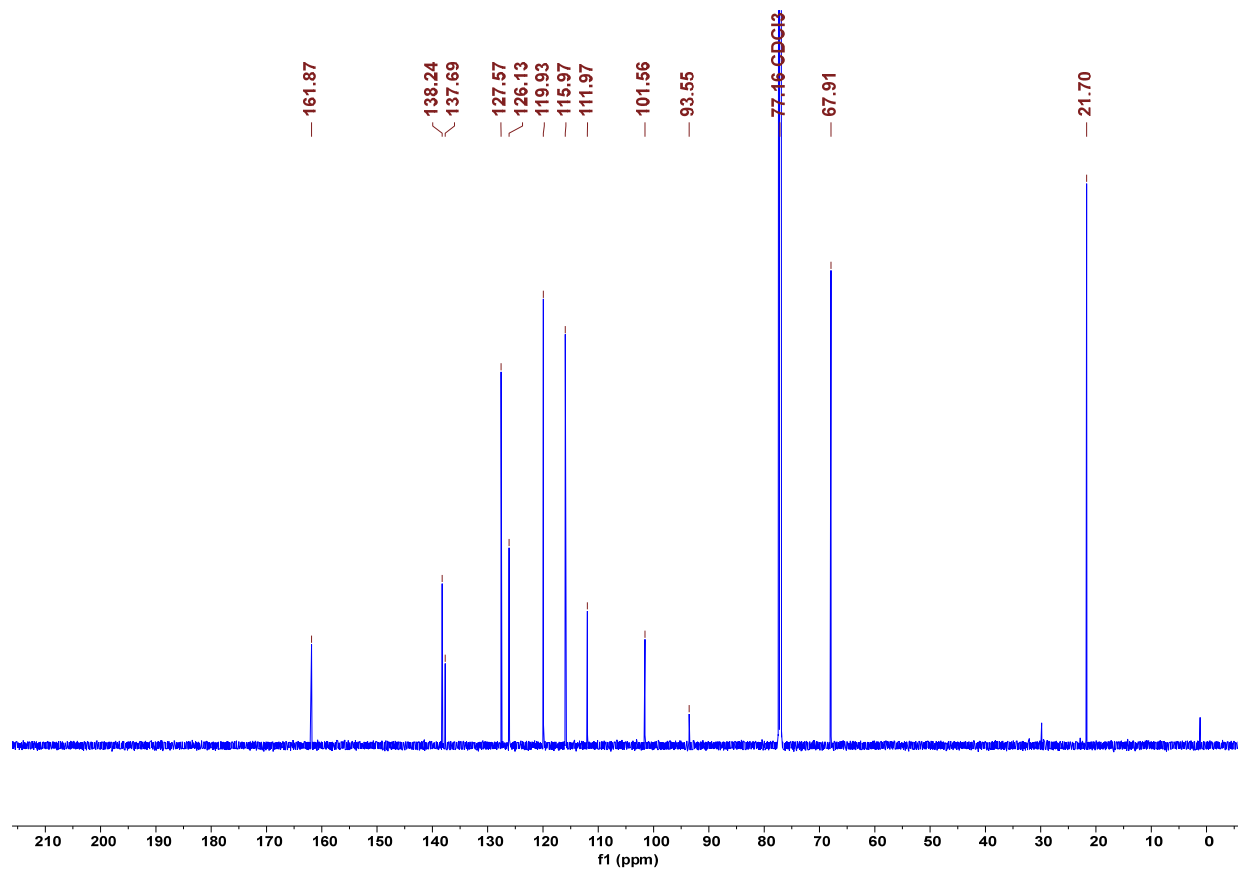
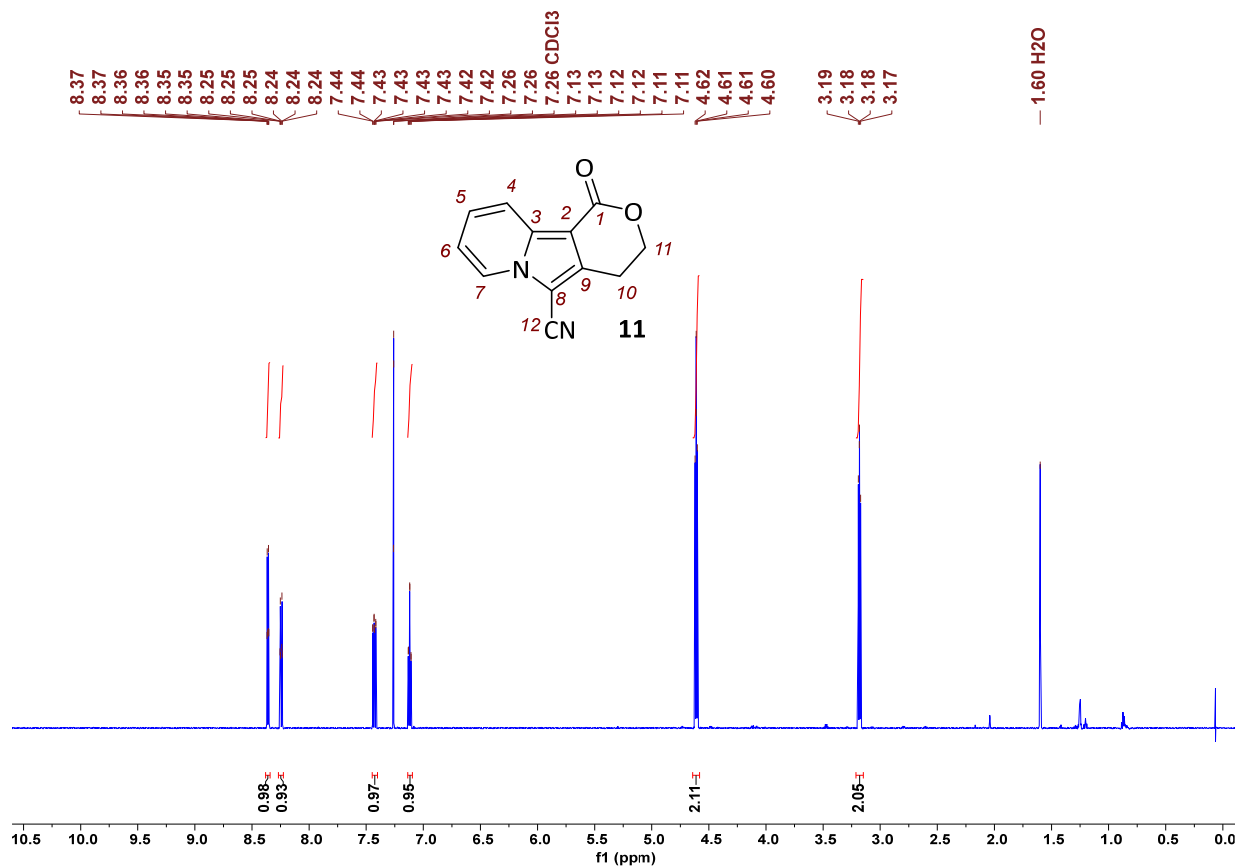


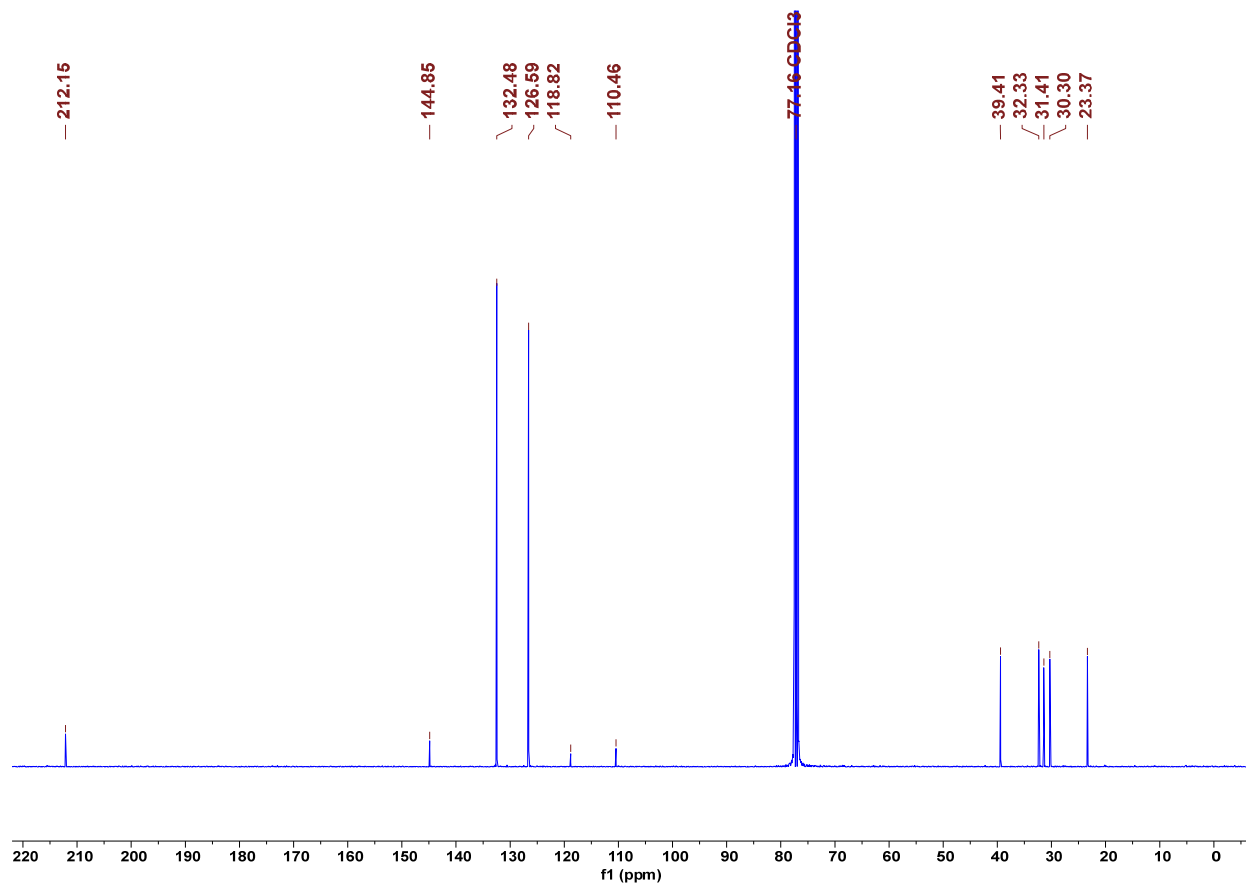
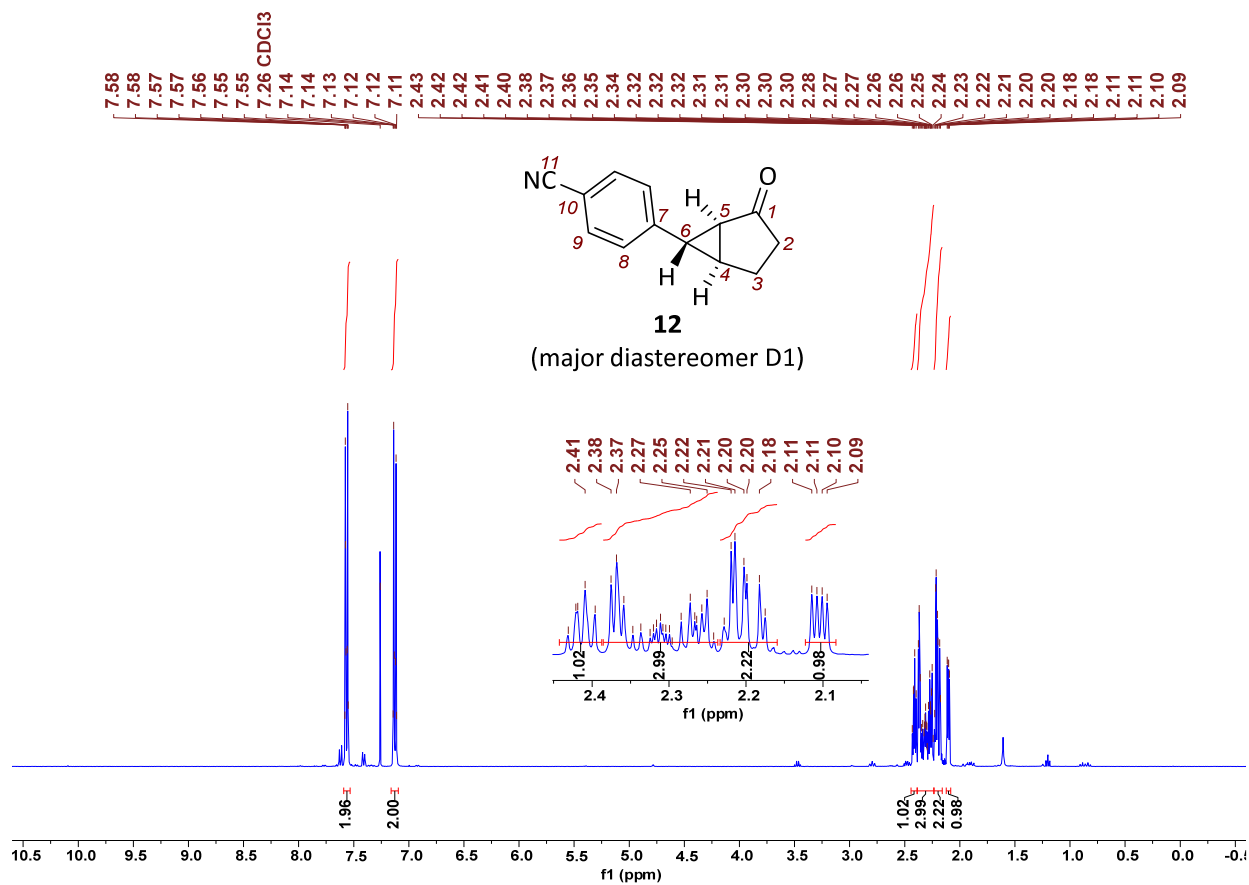


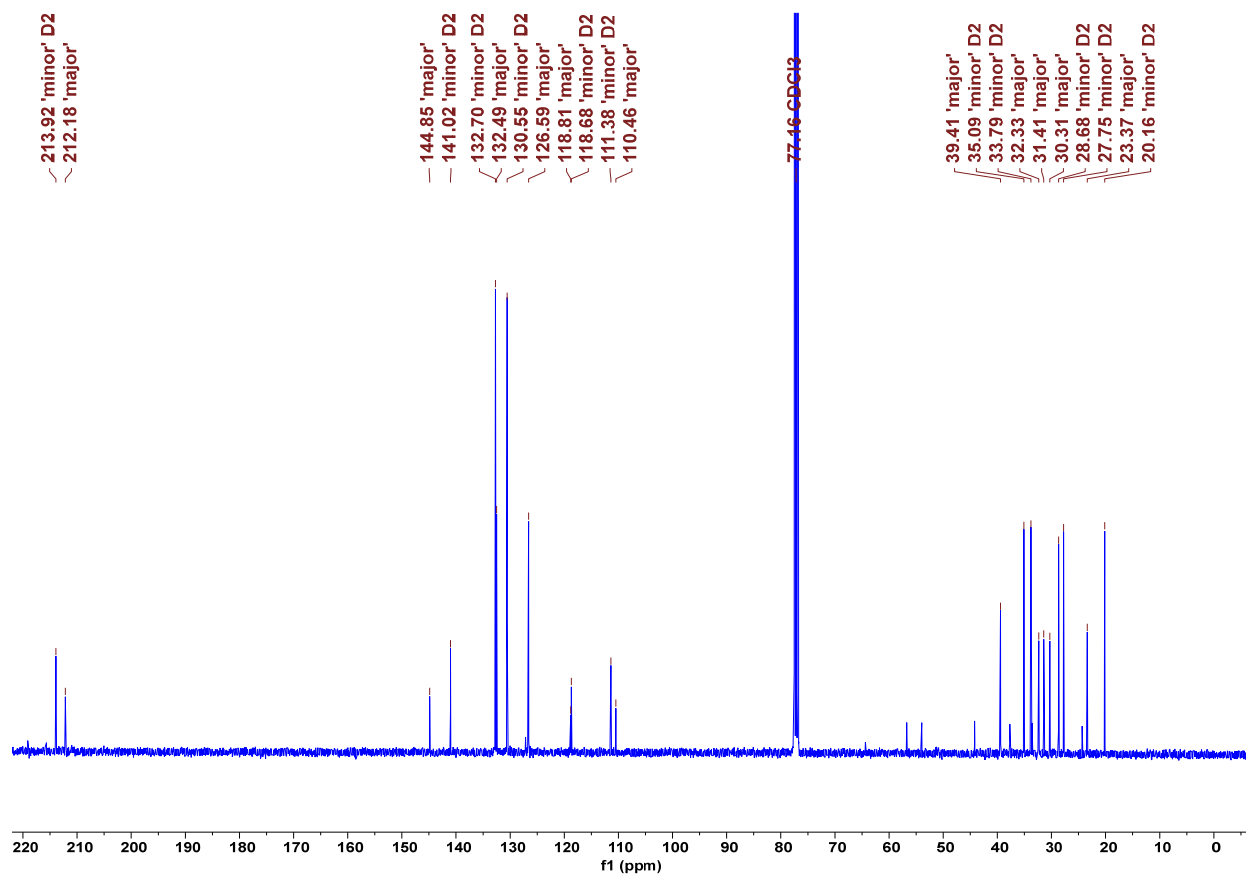
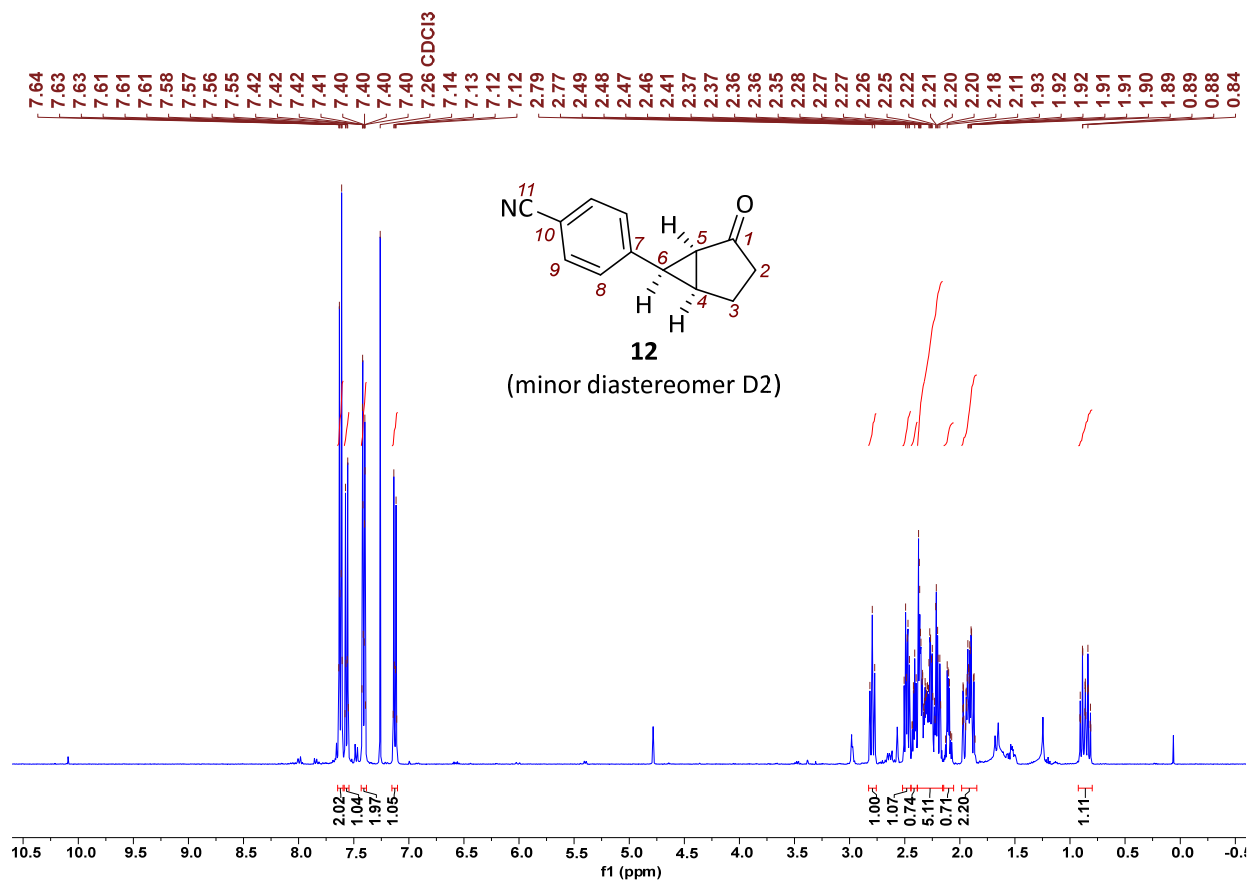


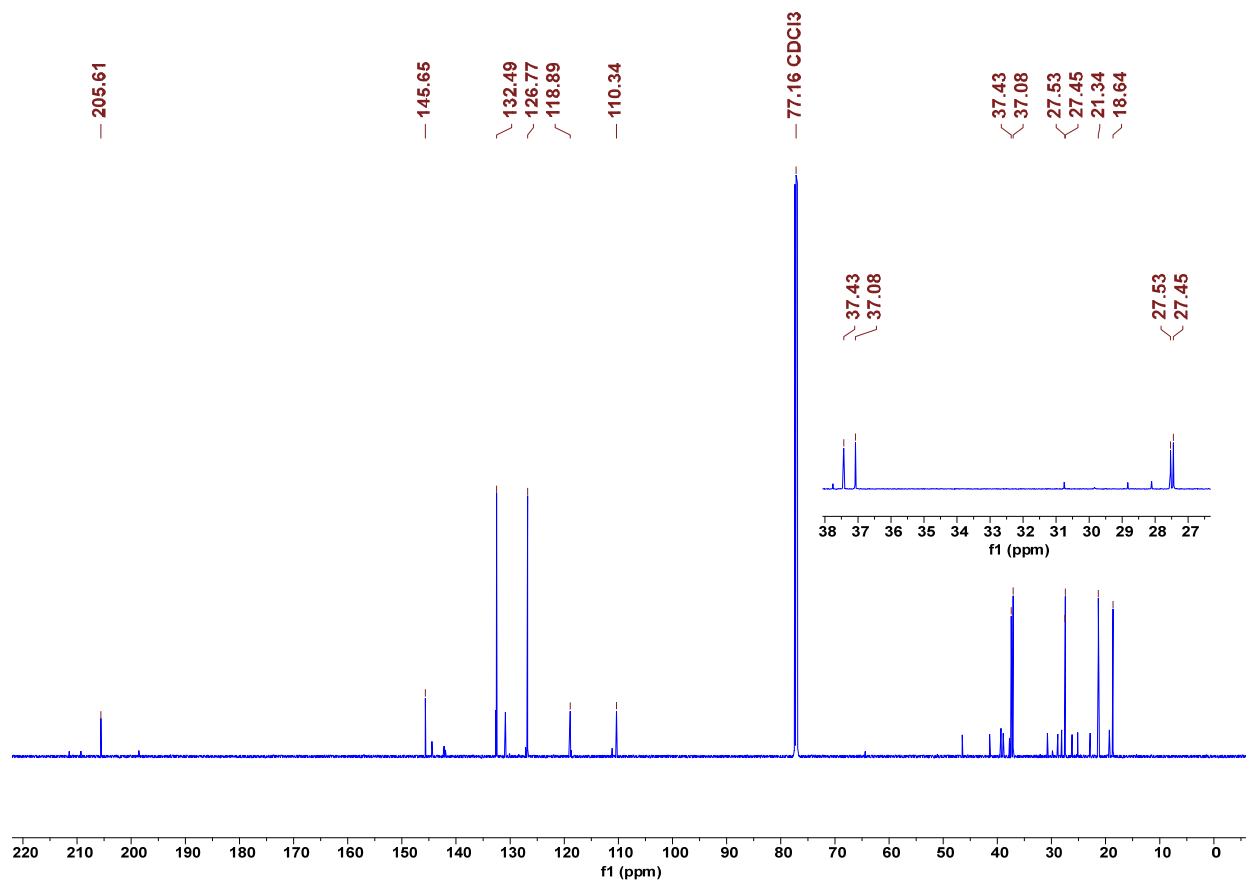
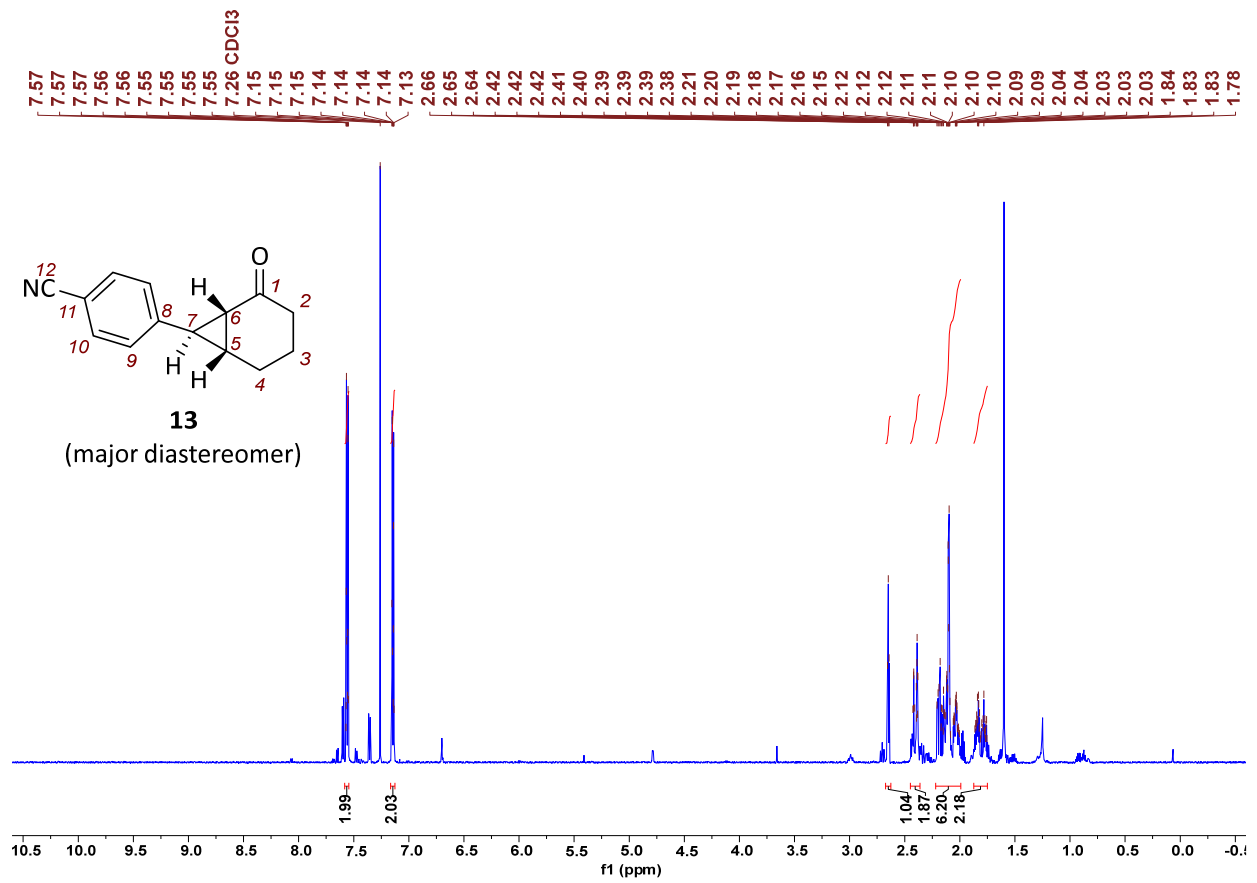


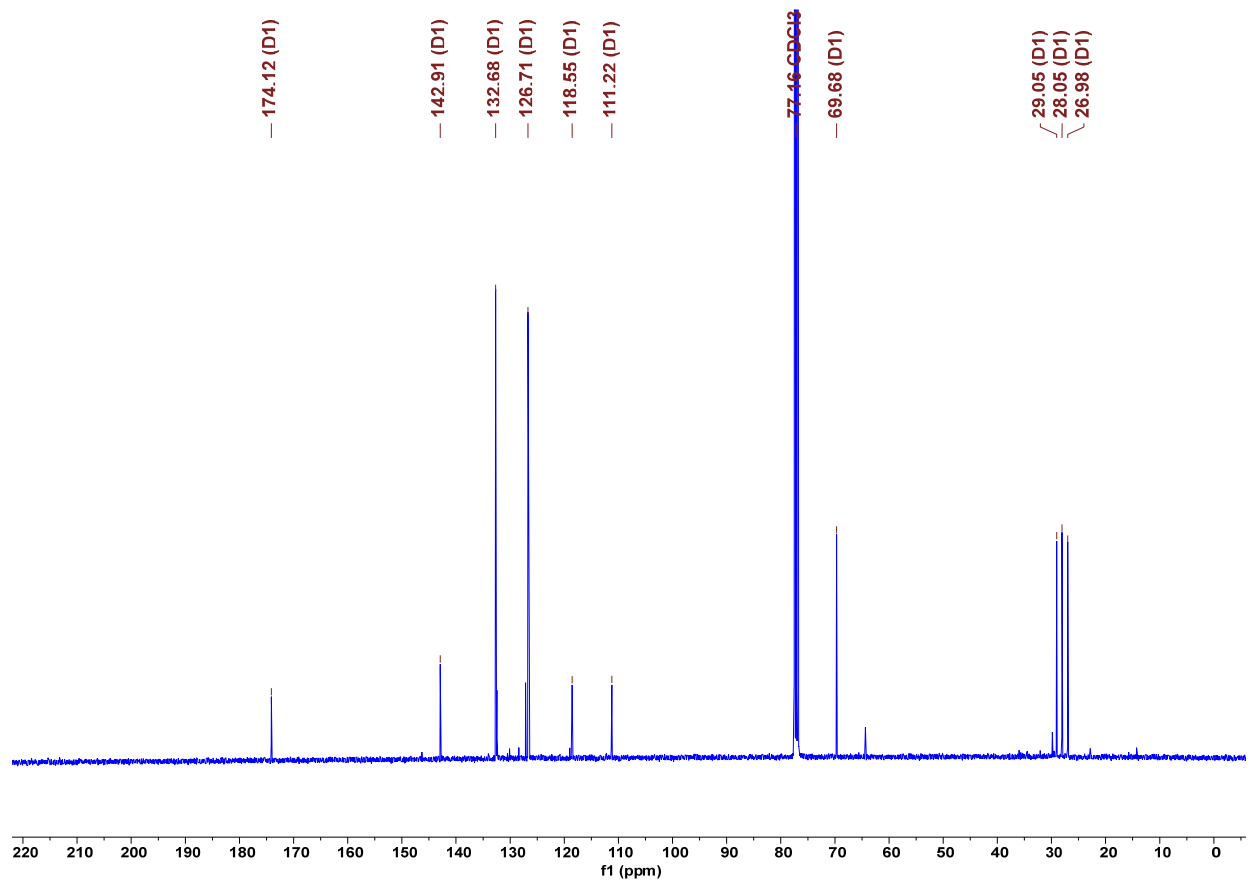
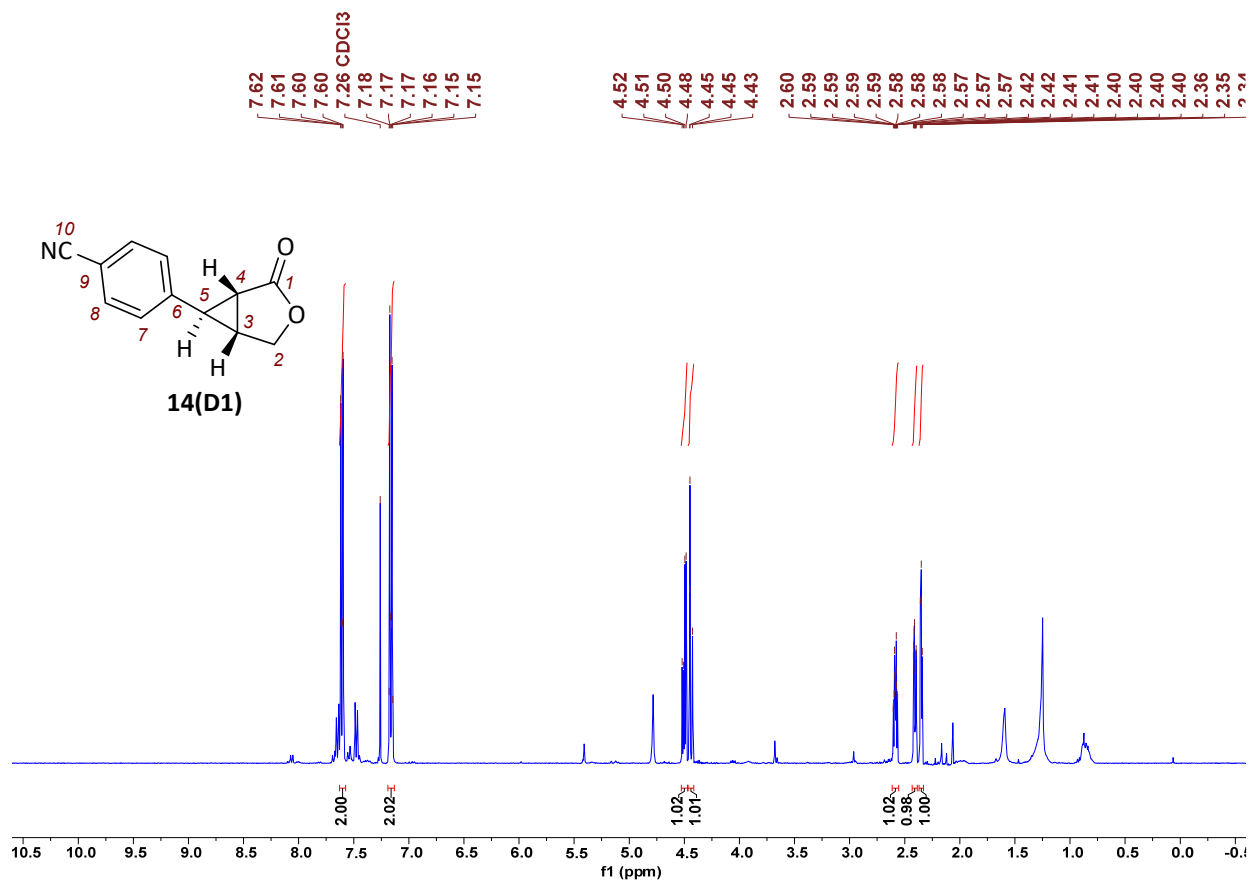


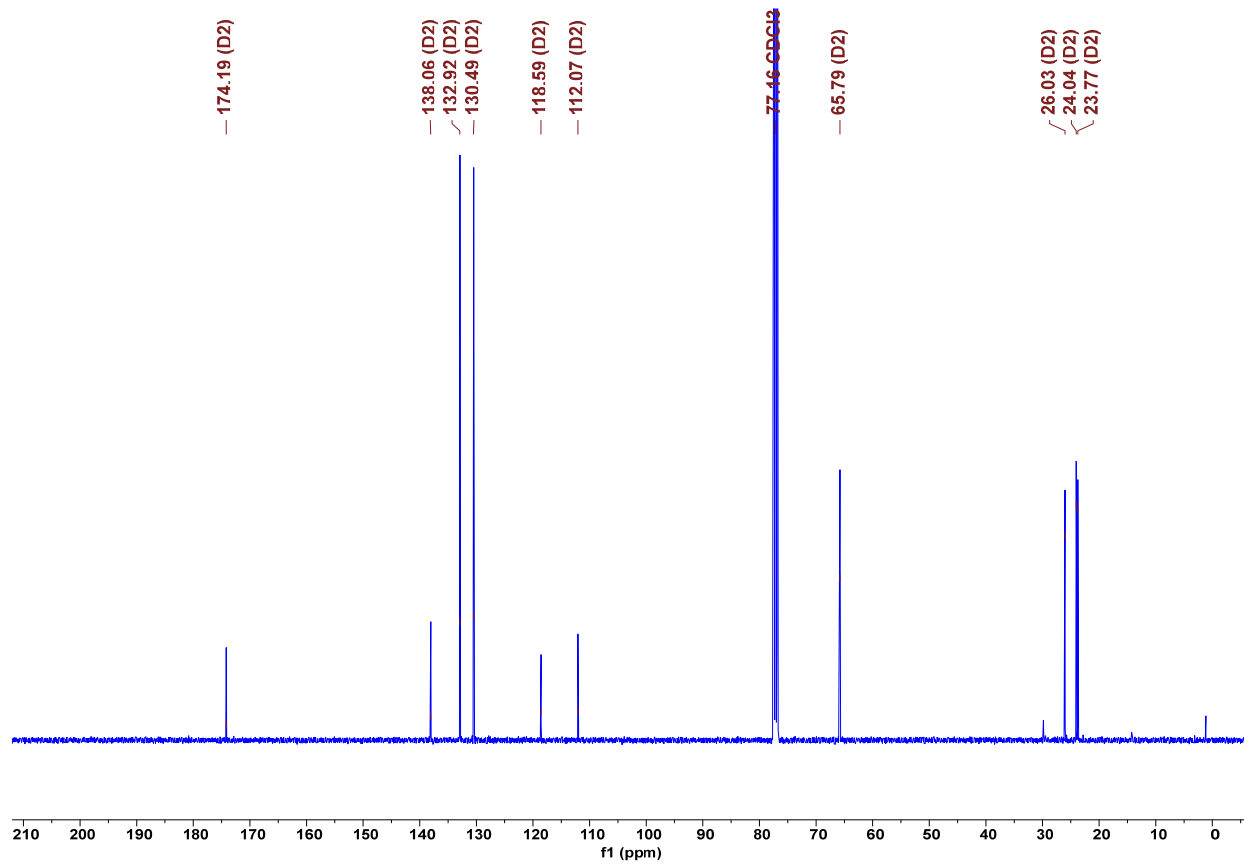
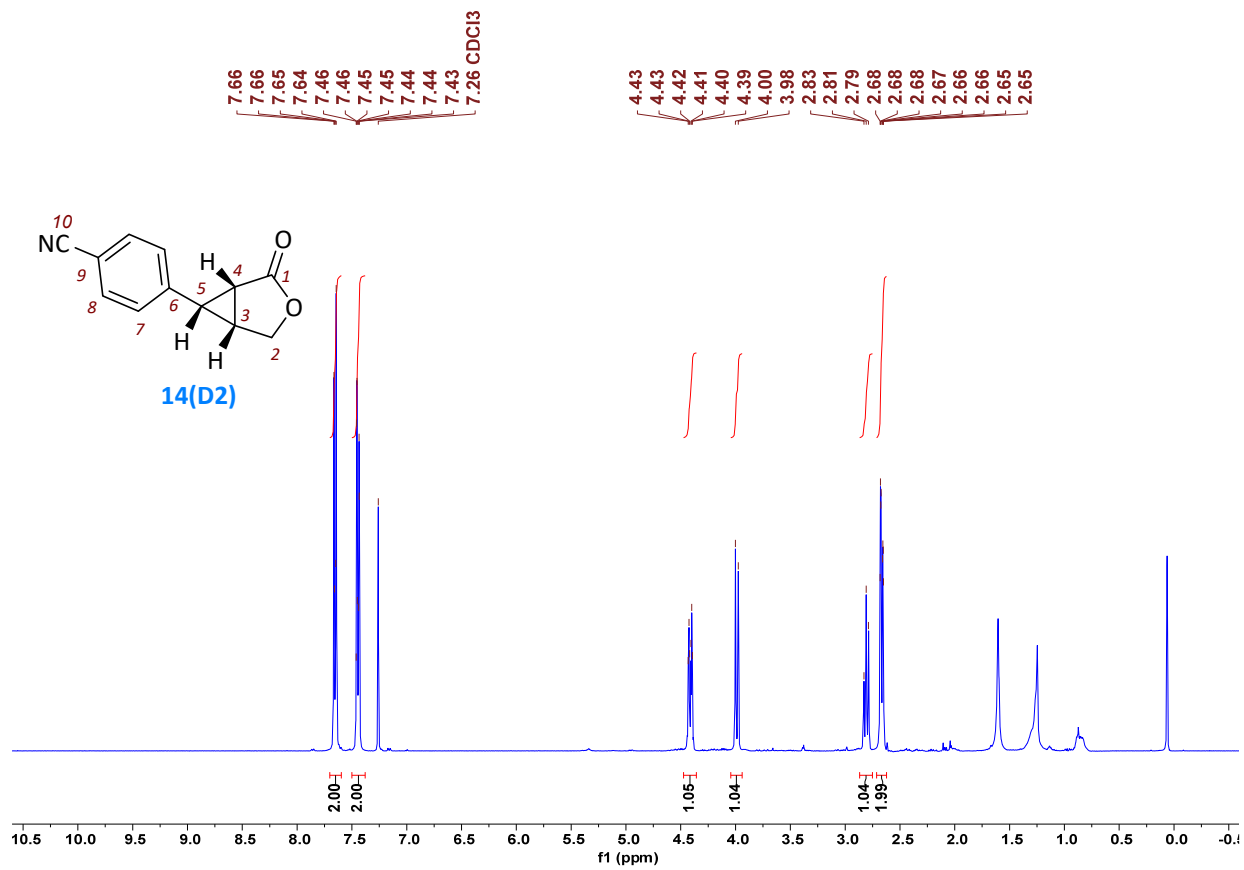


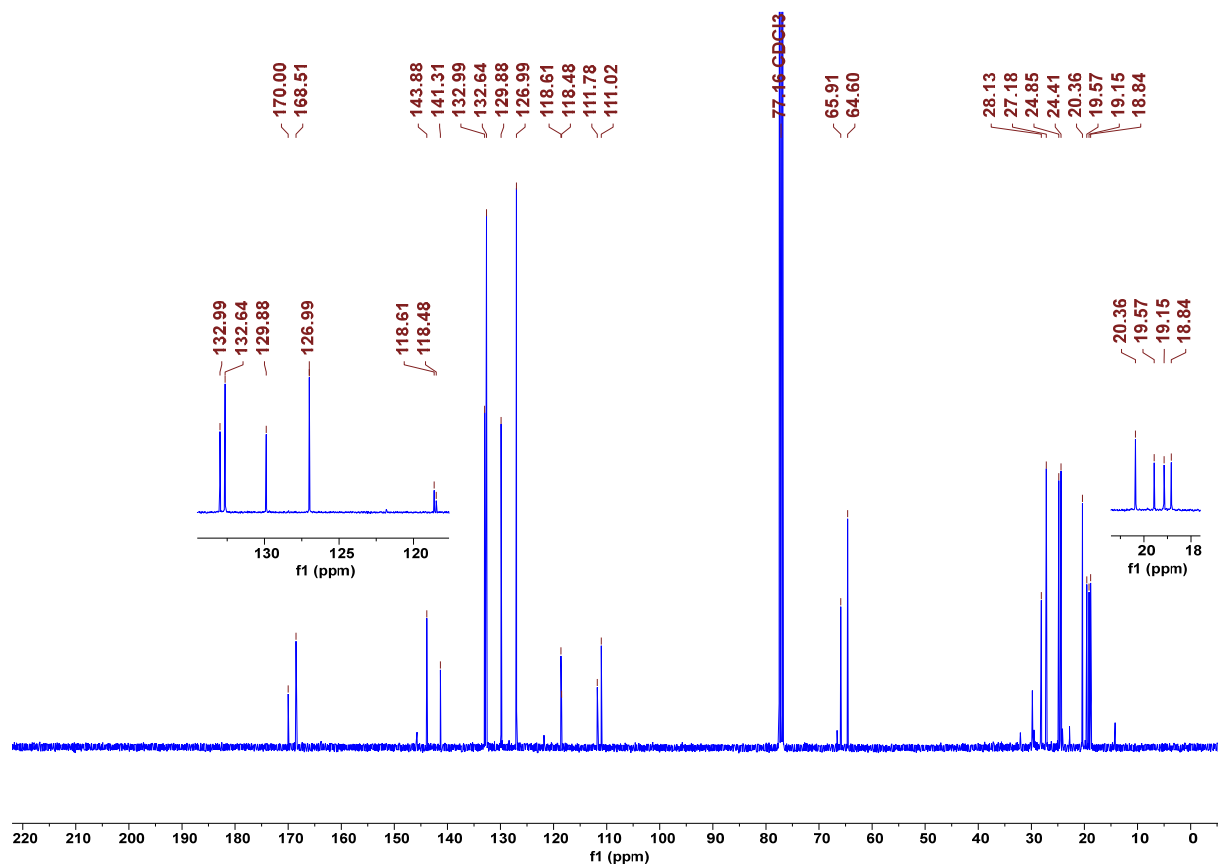
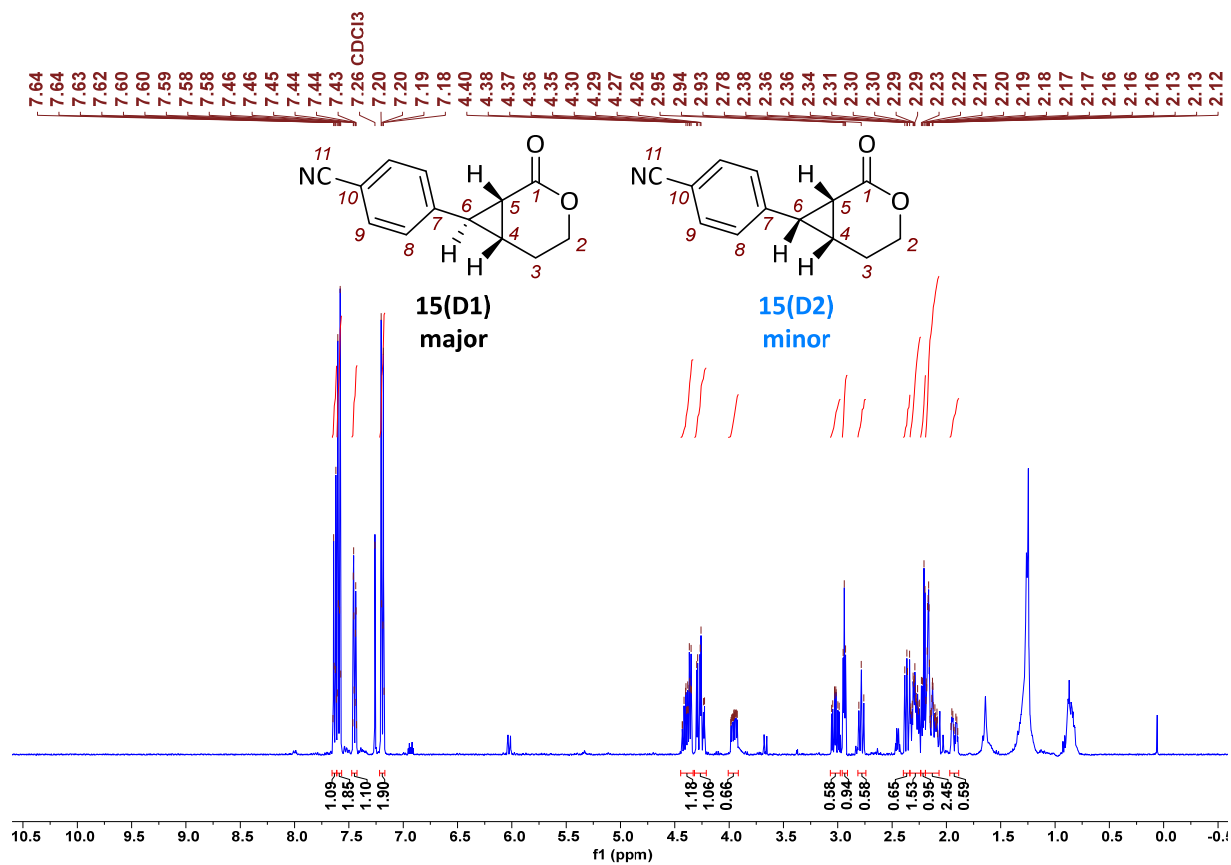


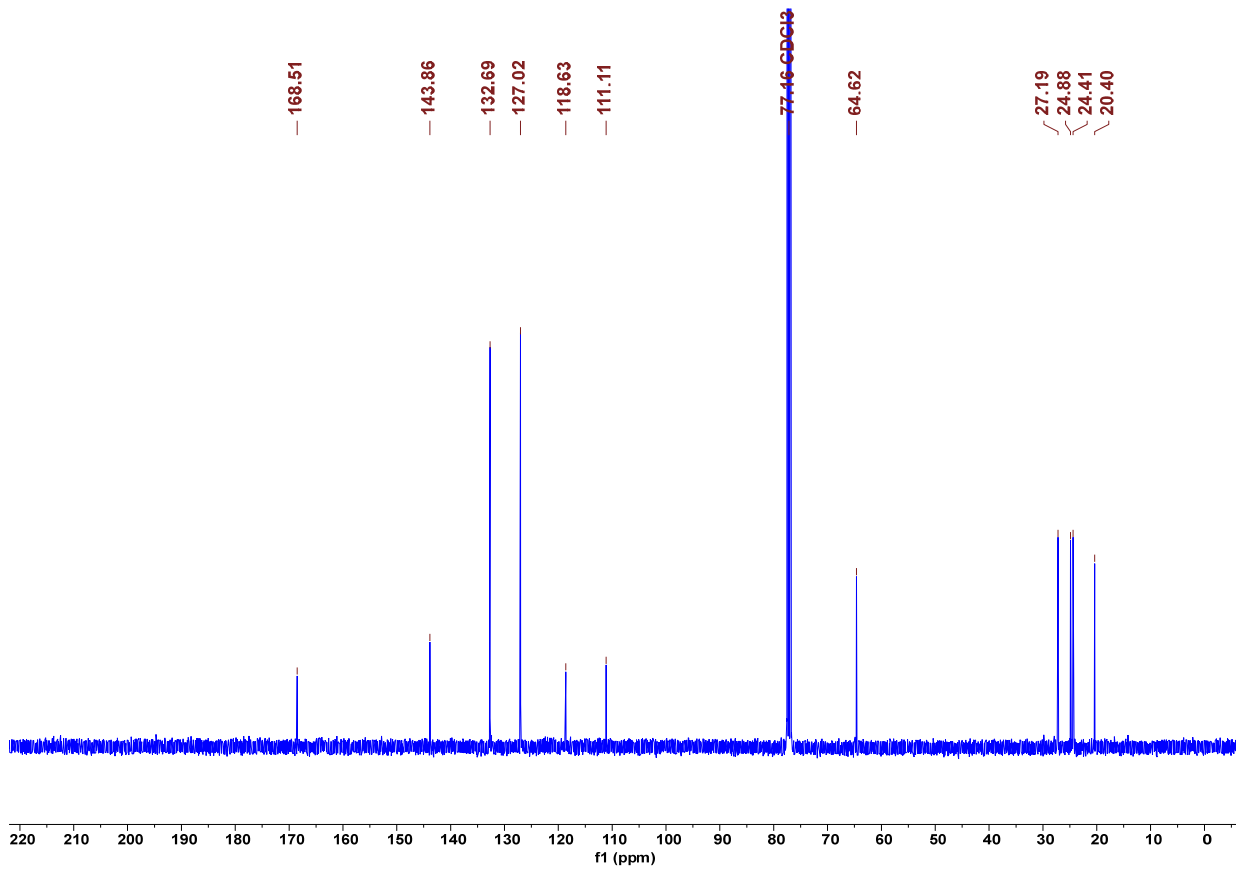
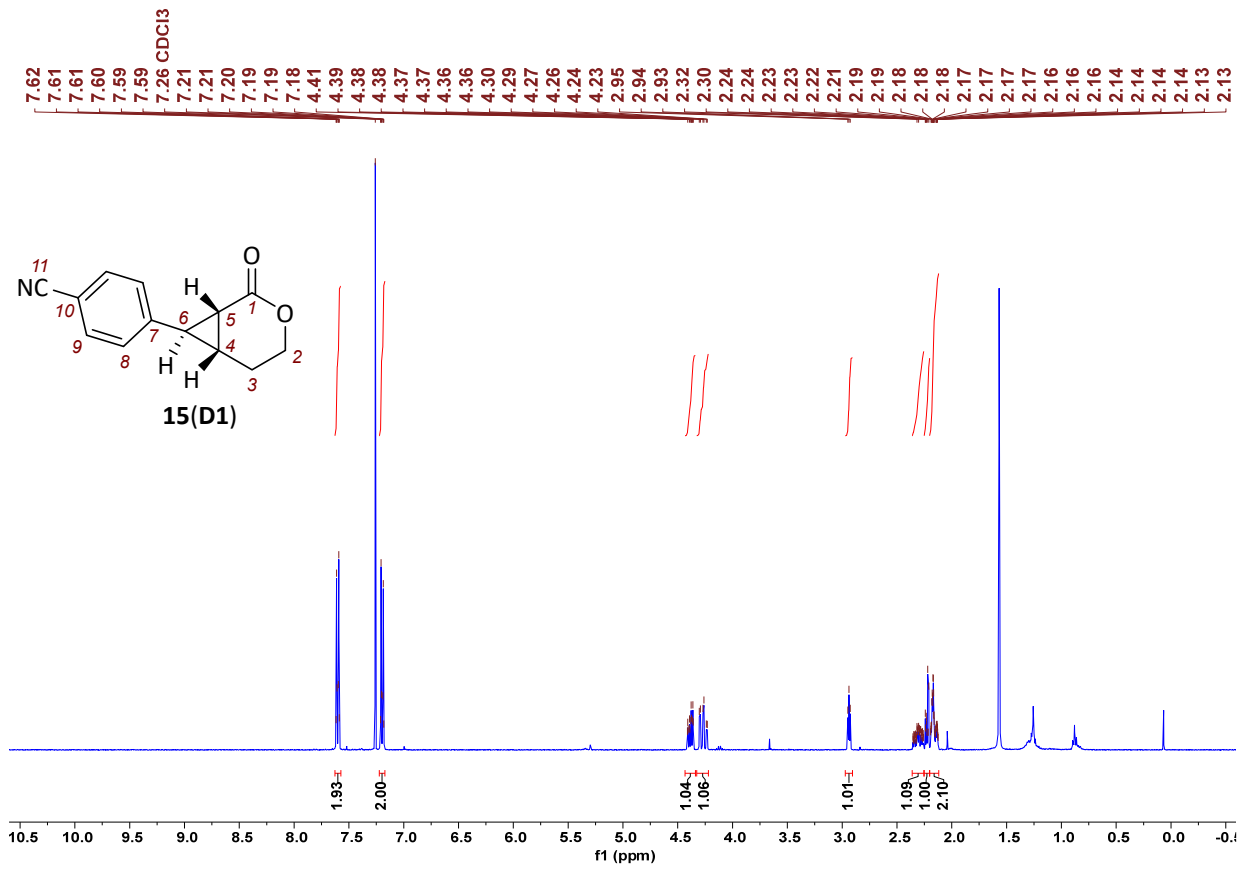


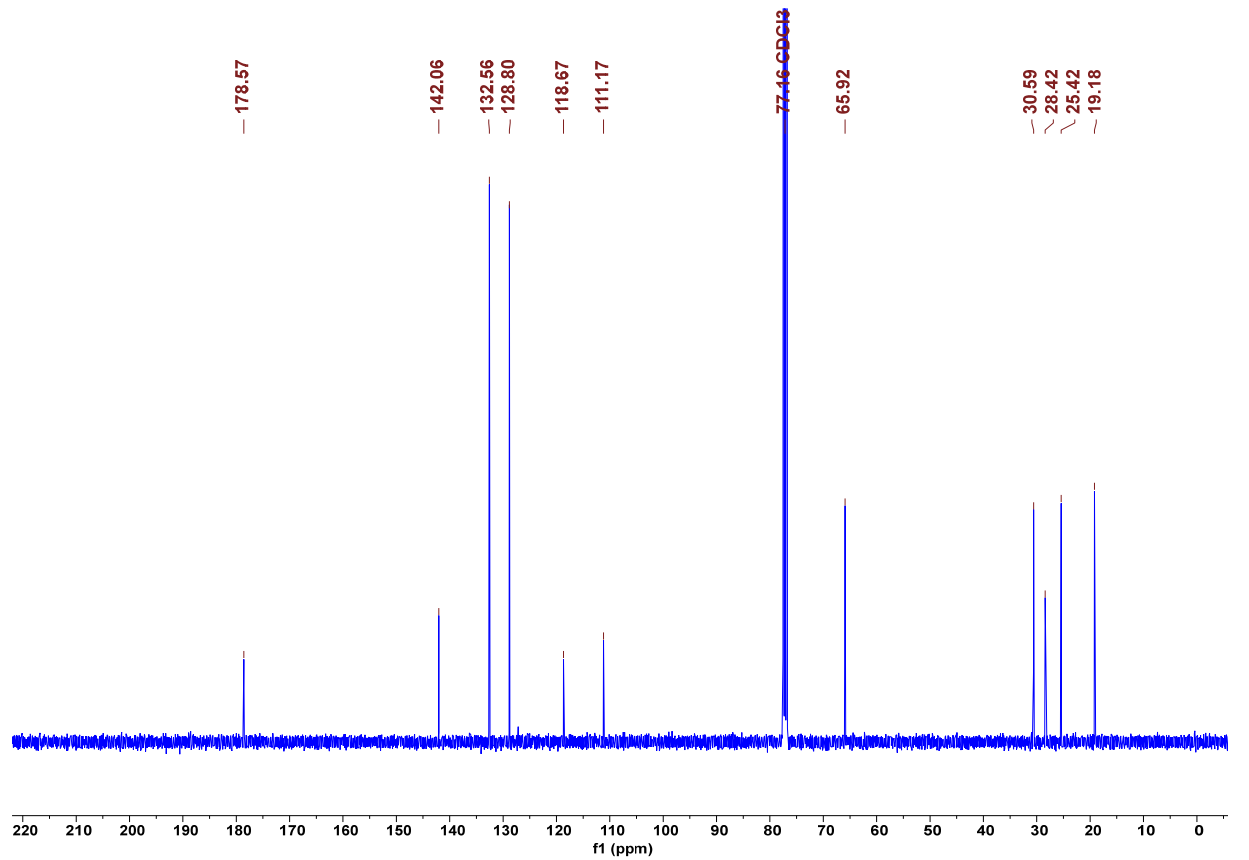
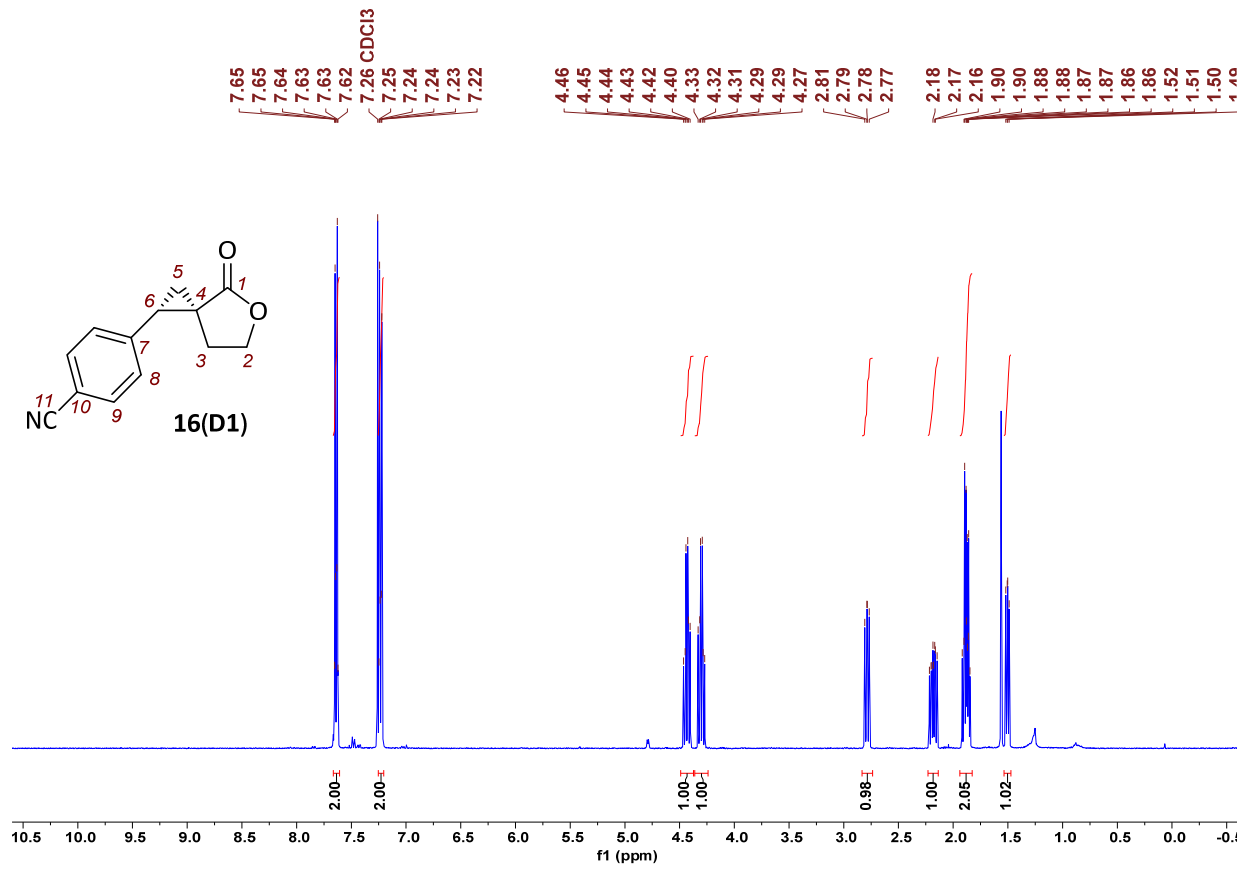


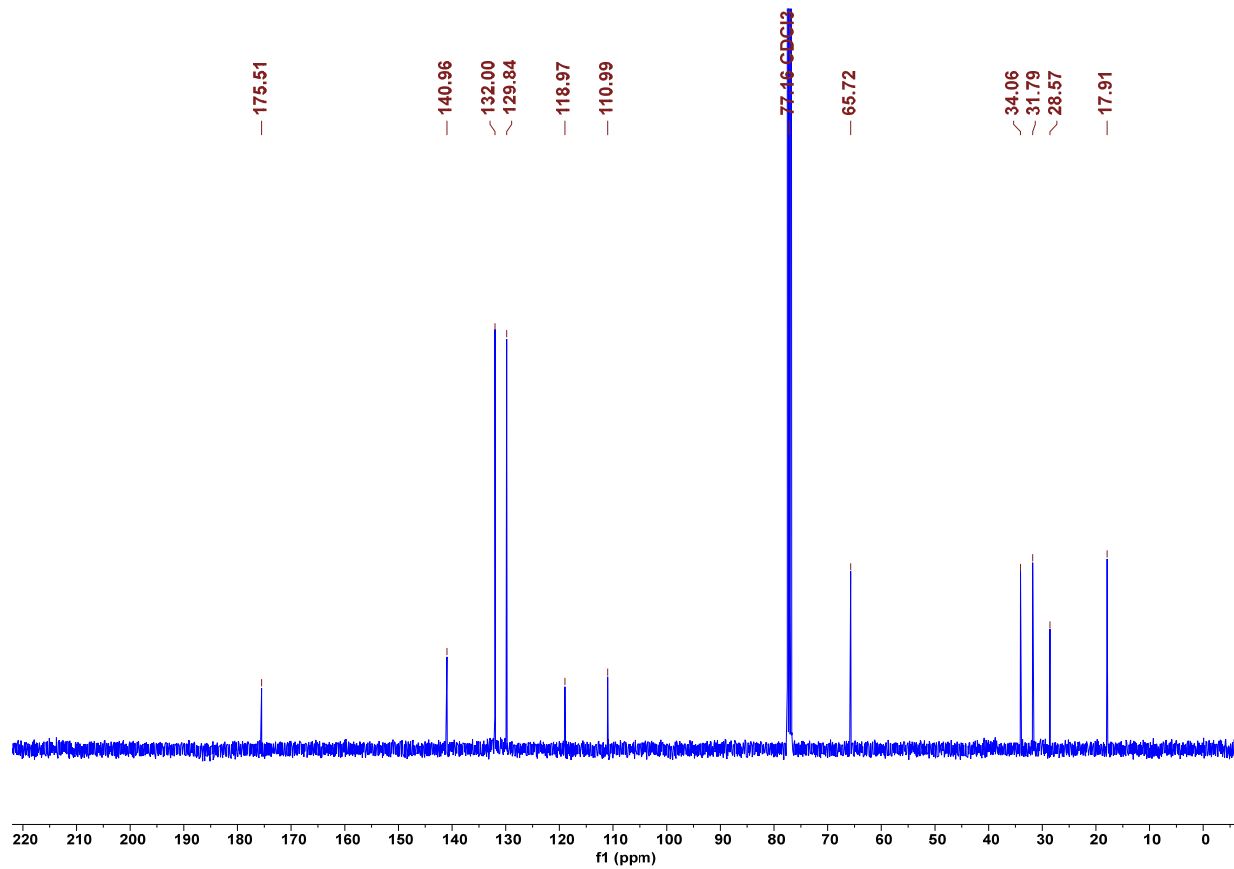
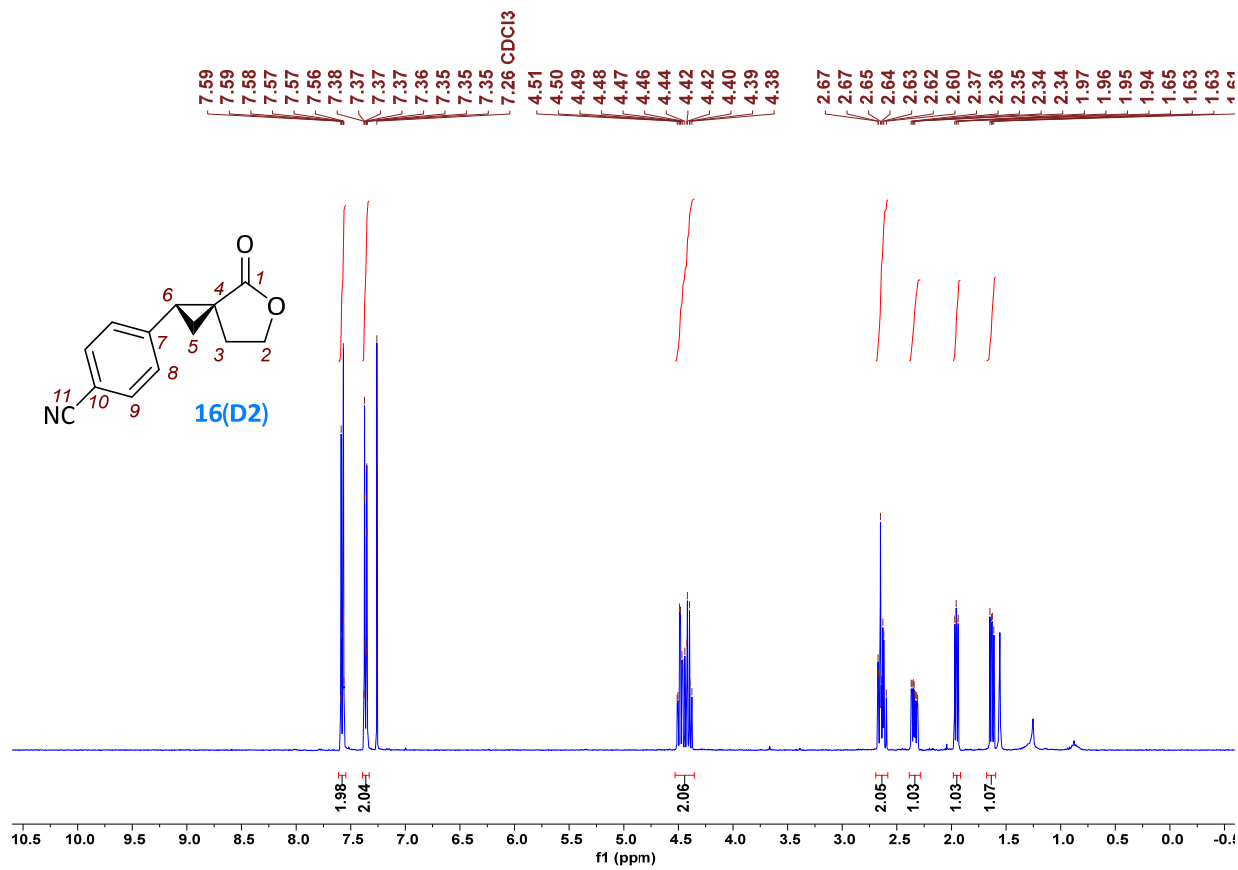


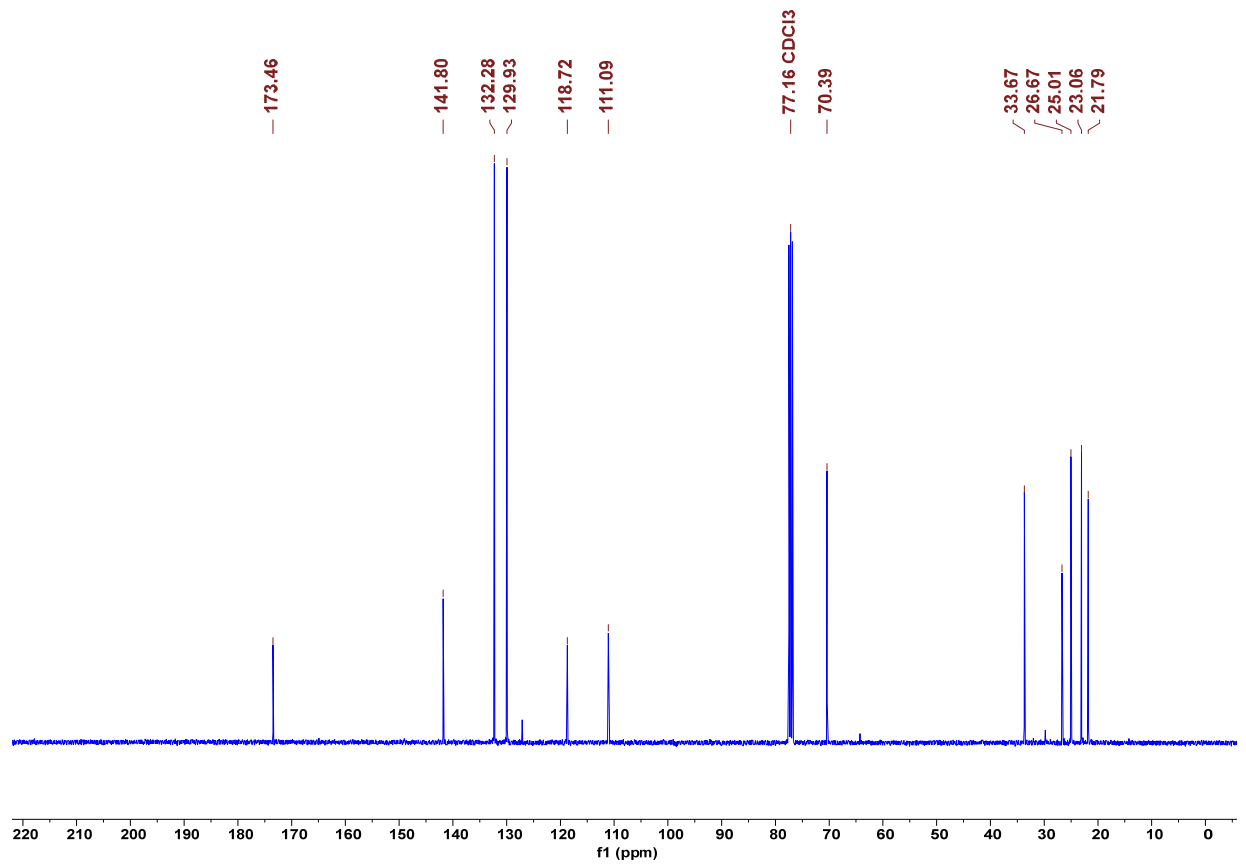
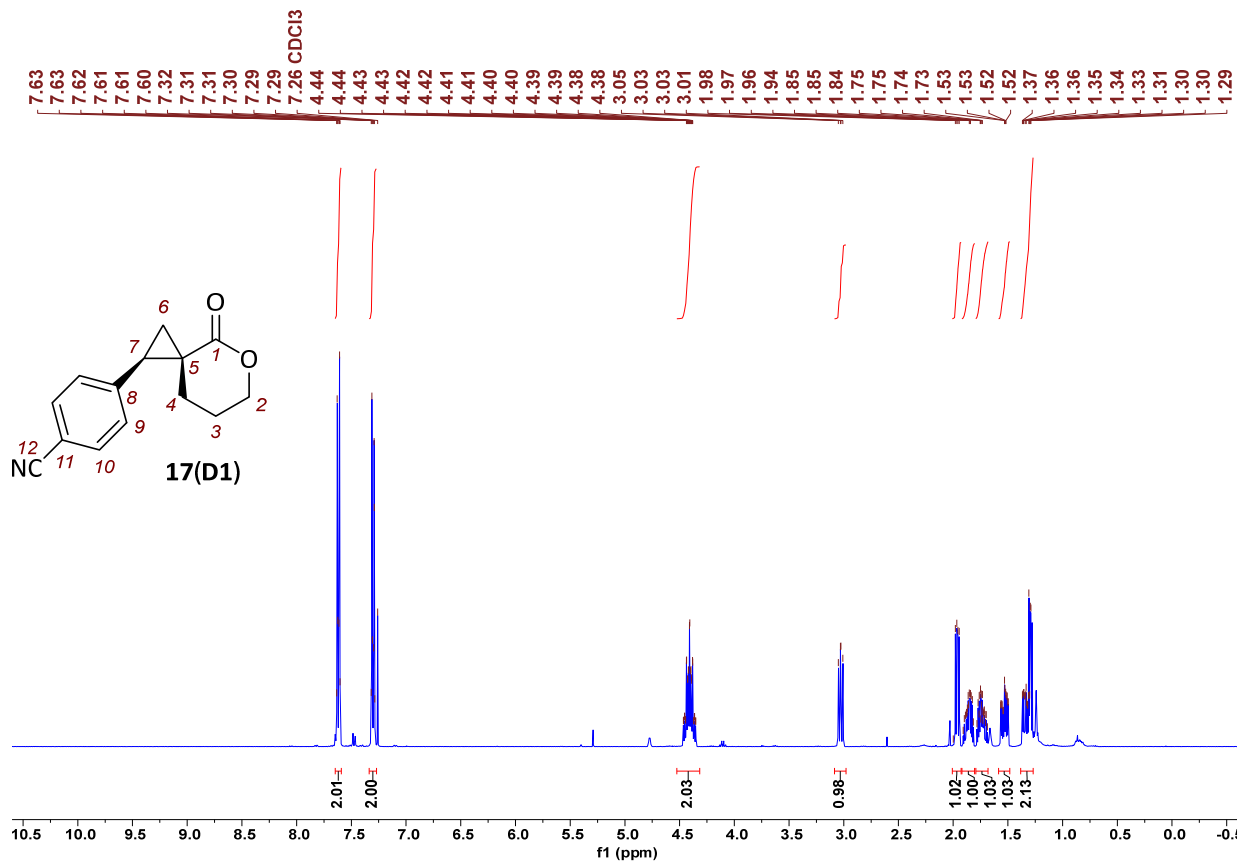


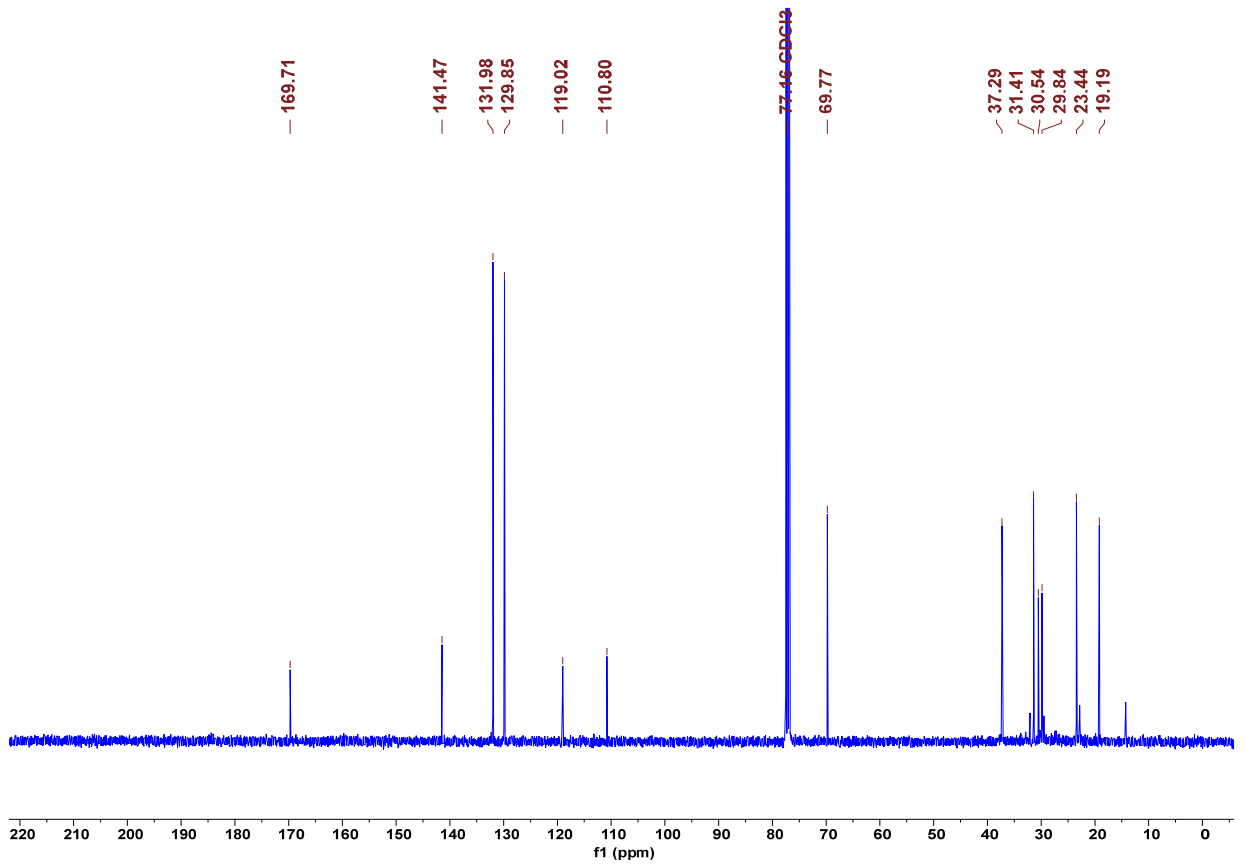
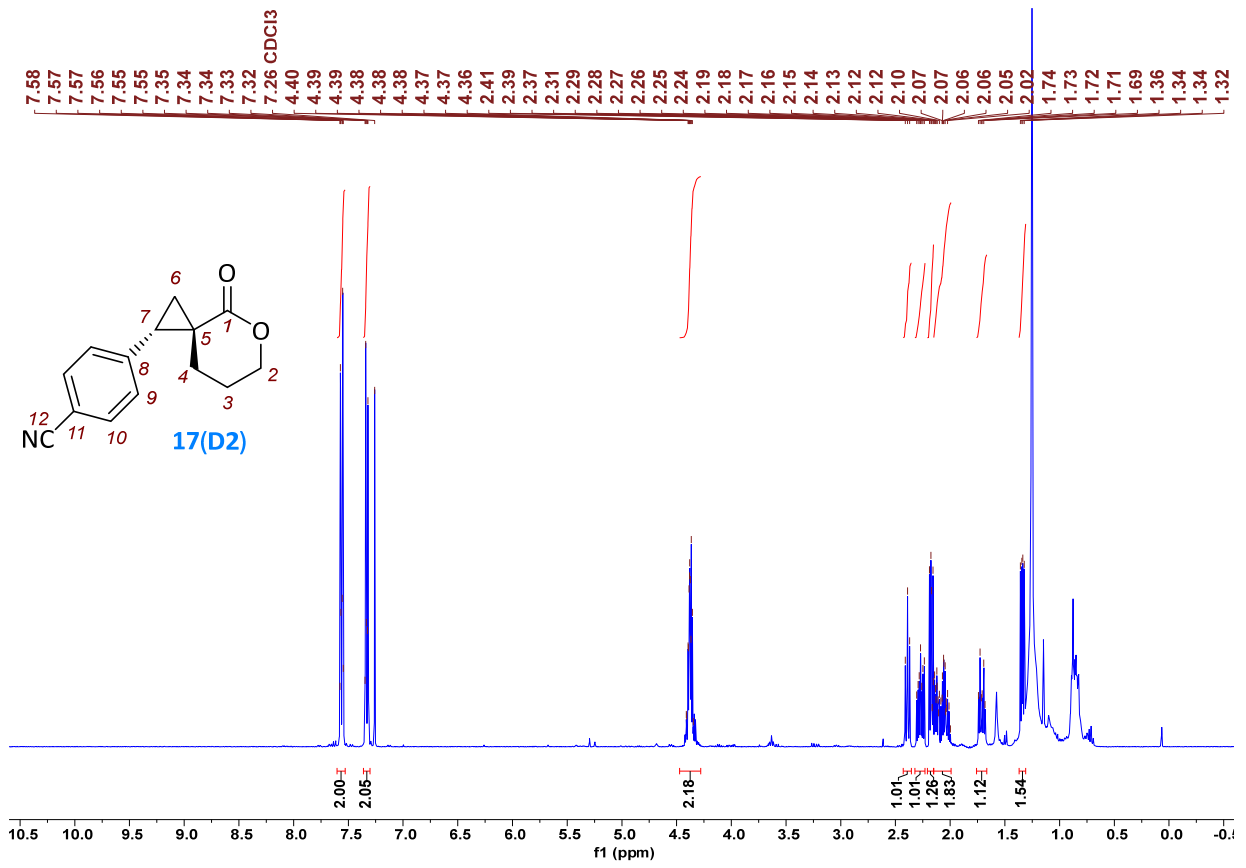


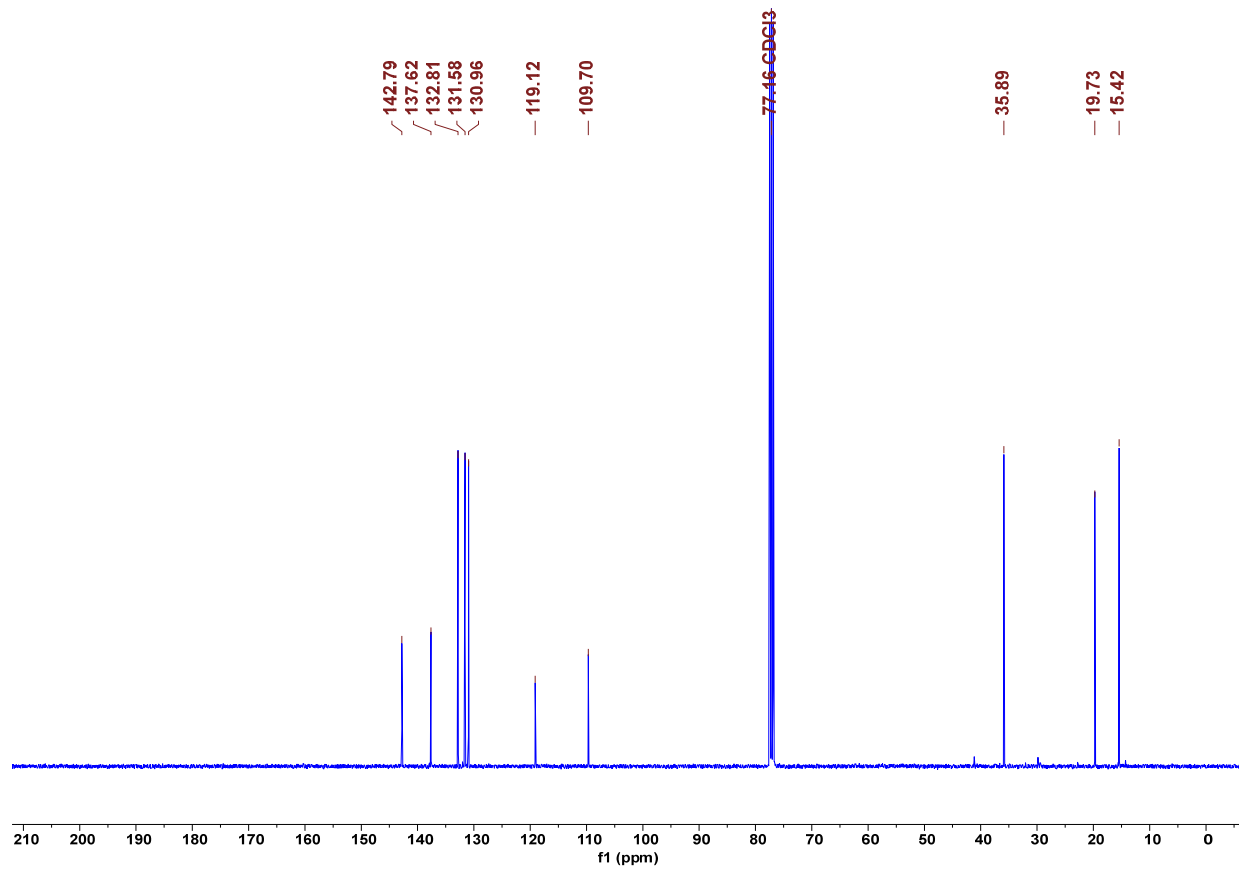
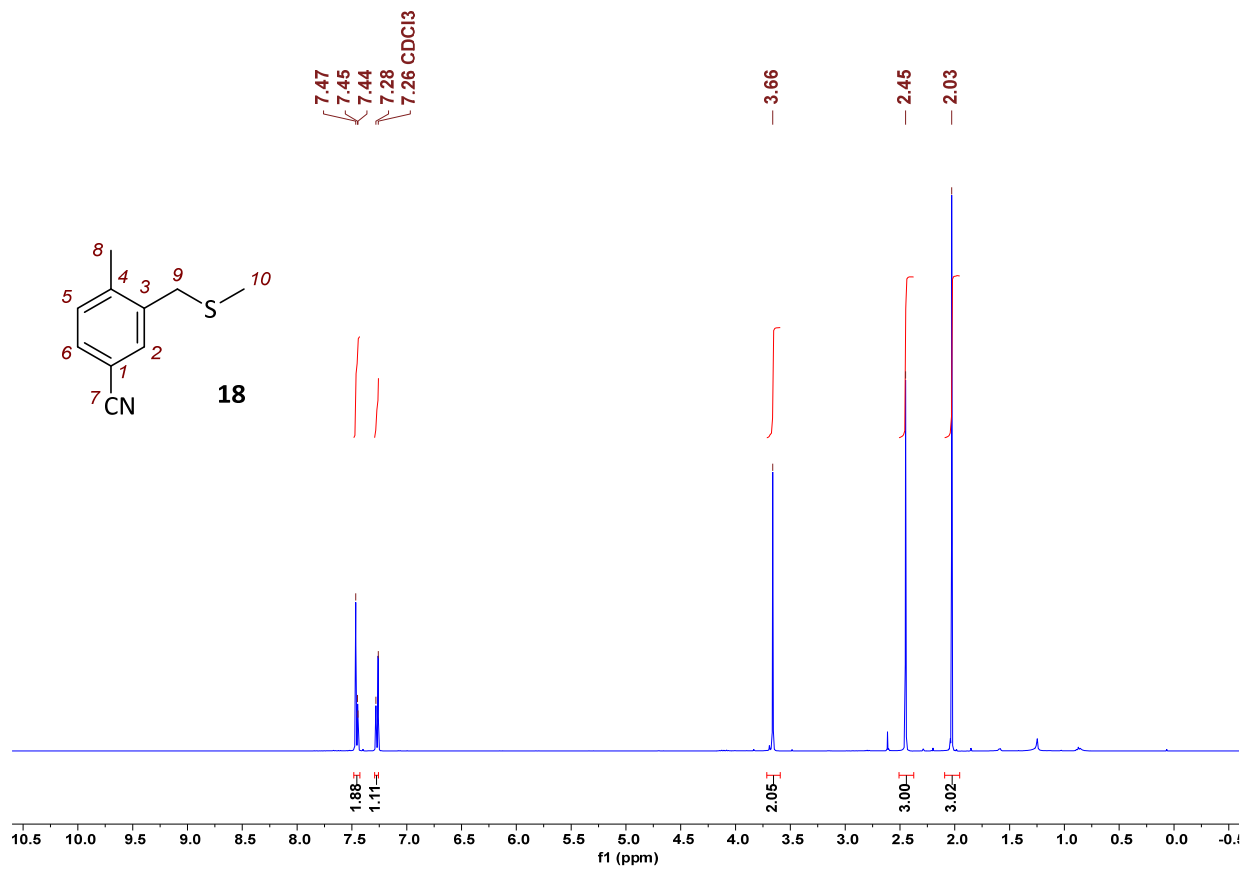


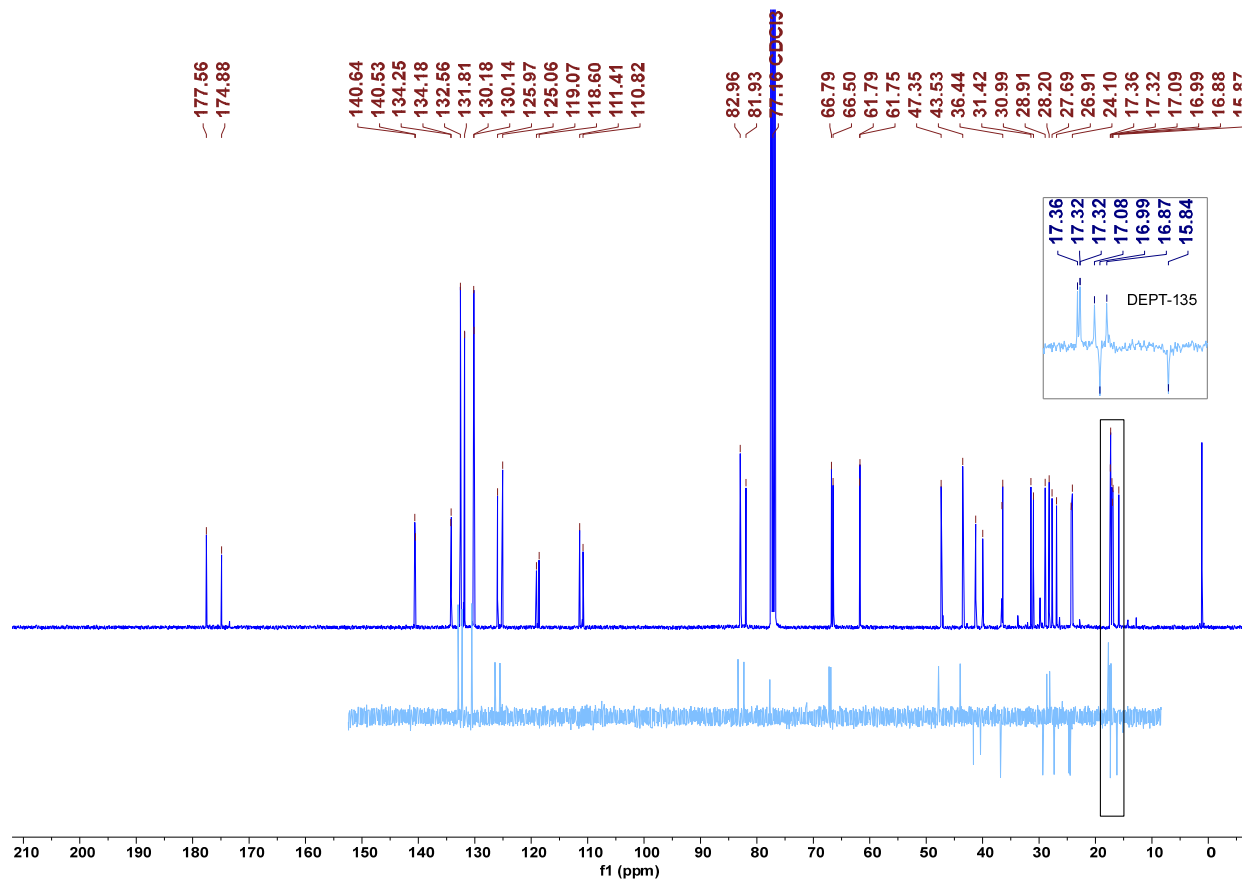
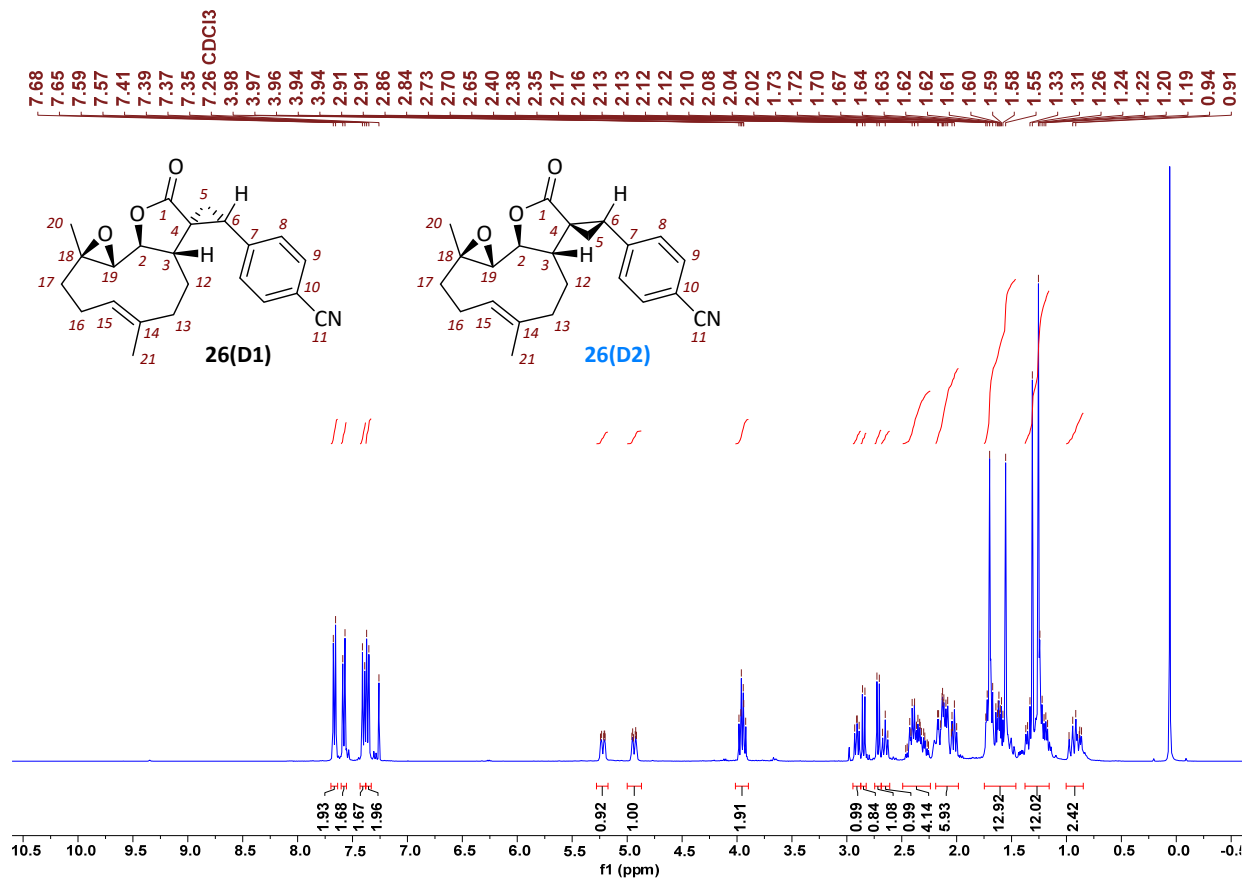












Geometries of Optimized Structures

Filename (cf. Table S2), cartesian coordinates (in Å), electronic energies (in Hartree), enthalpies (in Hartree), Gibbs free energies (in Hartree), and the number of the imaginary vibrational frequencies (NImag) for all stationary points at the SMD(DMSO)/M06-2X/6-31+G(d,p) level of theory.

1a.log

E = -269.254647

H = -269.150003

G = -269.184822

NImag=0

C	-1.0203441	0.1290731	-0.5485736
C	-0.2196870	1.3540136	-0.1936494
C	1.2056527	0.8232277	0.0132978
C	1.1148917	-0.6763319	-0.2400737
C	-0.2884637	-0.9943957	-0.5756443
O	2.0440005	-1.4638806	-0.1744684
H	-2.0852381	0.1826537	-0.7569641
H	-0.6289976	1.8279859	0.7047834
H	-0.2824361	2.0947835	-0.9978192
H	1.9293794	1.2577125	-0.6825554
H	1.5814155	0.9898885	1.0270998
H	-0.6318732	-1.9973302	-0.8027328

1a_sy_c_1.log

E = -1109.619867

H = -1109.314207

G = -1109.379194

NImag=0

C	2.6910487	3.5066805	0.7322146
C	1.6315231	2.5668680	0.2254245
C	2.6695367	3.6834528	2.1040234
O	3.4041492	4.4002643	2.8557700
C	0.6476738	3.0562902	-0.8680736
C	1.1383422	2.9715953	-2.3013709
C	2.5011281	3.0171943	-2.6142673
C	2.9232420	2.9419197	-3.9369740
C	1.9730184	2.8230059	-4.9569119
C	0.6061138	2.7722681	-4.6598248
C	0.1998407	2.8451277	-3.3336710
C	1.5248217	2.8504856	2.7012745
C	0.8957416	2.0944597	1.5218005
S	-0.0474248	4.7805634	-0.7202788
C	-0.3177889	5.1183874	1.0304997
C	1.3020390	5.9149490	-1.0971997
C	2.4069418	2.7450085	-6.3269274
N	2.7558406	2.6828730	-7.4293936
H	3.4293757	3.9816131	0.0923301
H	2.0545319	1.6762322	-0.2690471
H	-0.2756709	2.4674024	-0.8019991
H	3.2435746	3.1058843	-1.8287320
H	3.9802295	2.9742896	-4.1795003
H	-0.1224534	2.6701974	-5.4570915
H	-0.8601179	2.7931016	-3.0982569
H	1.9269576	2.1748537	3.4647354
H	0.8155961	3.5149532	3.2132604
H	-0.1840221	2.2612681	1.4507208
H	1.0301507	1.0148060	1.6319300
H	-0.7366123	6.1264812	1.0731503

H	-1.0501169	4.4028102	1.4062342
H	0.6284164	5.0616270	1.5662723
H	0.8814863	6.9182220	-0.9970380
H	1.6029496	5.7479083	-2.1326146
H	2.1277374	5.7553562	-0.4053684

1a_sy_c_1_r.log

E = -1109.619199

H = -1109.313354

G = -1109.377575

NImag=0

C	-0.6483422	-1.9312622	-0.4576022
C	-1.3709077	-0.7347737	-1.0161392
C	-1.2651490	-2.4713529	0.6597322
O	-0.9210691	-3.4377244	1.4095567
C	-0.4687702	0.5170325	-0.8491401
C	0.0451344	0.8711706	0.5290163
C	-0.8034924	1.0723800	1.6256483
C	-0.2822123	1.3728340	2.8777088
C	1.1039486	1.4833732	3.0389262
C	1.9660310	1.2965603	1.9538050
C	1.4283700	0.9934132	0.7085668
C	-2.5608878	-1.6890288	0.9331718
C	-2.7406232	-0.7682356	-0.2835228
S	-1.0774095	2.1055878	-1.6592038
C	-2.2295485	1.5535495	-2.9334855
C	-2.2025204	2.9449982	-0.5261290
C	1.6462665	1.7984056	4.3340780
N	2.0829627	2.0536542	5.3758193
H	0.3062821	-2.2710052	-0.8524519
H	-1.5337850	-0.8111307	-2.0980754
H	0.4062130	0.3385674	-1.4842197
H	-1.8794719	1.0025391	1.5160789
H	-0.9422046	1.5241191	3.7253956
H	3.0390943	1.3841452	2.0868688
H	2.0942020	0.8383293	-0.1355958
H	-3.4006617	-2.3812595	1.0596733
H	-2.4572354	-1.1412199	1.8787200
H	-3.1238534	0.2232783	-0.0259096
H	-3.4683877	-1.2084793	-0.9728269
H	-2.6046336	2.4581579	-3.4164627
H	-1.6732969	0.9544977	-3.6559493
H	-3.0467530	0.9849107	-2.4874272
H	-2.6297937	3.7696856	-1.1016955
H	-1.6151898	3.3465367	0.2998217
H	-2.9886880	2.2772994	-0.1749635

1a_sy_c_1_ts1.log

E = -1109.594532

H = -1109.292116

G = -1109.357683

NImag=1

C	-2.9258991	-0.5828908	0.8577836
C	-1.5541670	-0.6376377	1.0908991
C	-3.3493363	-1.7150809	0.0844580
O	-4.4852695	-1.9832566	-0.3308433
C	-0.4556054	0.4901510	-0.4608850
C	0.9665075	0.2783080	-0.3489145
C	1.7825541	1.0311335	0.5318668
C	3.1333956	0.7608785	0.6727937

C	3.7202488	-0.2884107	-0.0517284
C	2.9288021	-1.0608750	-0.9222442
C	1.5838465	-0.7793846	-1.0650753
C	-2.1204269	-2.5861453	-0.1807990
C	-1.0533823	-2.0327687	0.7690100
S	-0.9400191	2.1923214	-0.3922609
C	-2.4458628	2.1937150	-1.3825133
C	-1.6307766	2.5731045	1.2435888
C	5.1141872	-0.5726665	0.0968851
N	6.2456186	-0.8033840	0.2165953
H	-3.6014053	0.2169819	1.1389212
H	-1.0499656	-0.0521283	1.8552121
H	-0.9571549	0.0095069	-1.2982468
H	1.3534157	1.8354536	1.1248774
H	3.7401768	1.3539288	1.3501805
H	3.3816357	-1.8695835	-1.4876516
H	0.9829111	-1.3718001	-1.7502122
H	-2.3491310	-3.6452865	-0.0361409
H	-1.8266577	-2.4483170	-1.2300917
H	-0.0406819	-2.0533032	0.3628096
H	-1.0373479	-2.6056444	1.7047022
H	-2.9186589	3.1702161	-1.2632504
H	-2.1551452	2.0393923	-2.4224615
H	-3.1017471	1.3936829	-1.0344836
H	-1.8806219	3.6362290	1.2200052
H	-0.8493491	2.3982234	1.9851050
H	-2.5150912	1.9742148	1.4534581

1a_sy_c_2.log

E = -1109.628122

H = -1109.322708

G = -1109.387720

NImag=0

C	2.8497975	3.2555513	0.8135849
C	1.7272651	2.3756227	0.3239393
C	2.6772417	3.6922958	2.1197700
O	3.3855048	4.4756288	2.8242885
C	0.7898470	3.0123258	-0.7363766
C	1.2332366	2.9687292	-2.1750784
C	2.5845025	3.0418273	-2.5378504
C	2.9610521	2.9947532	-3.8742707
C	1.9773398	2.8716749	-4.8628688
C	0.6241897	2.7861247	-4.5188917
C	0.2637835	2.8318165	-3.1773012
C	1.3797033	3.0856743	2.6758354
C	0.9515376	2.0436135	1.6337254
S	0.4592055	4.7546762	-0.1600265
C	1.6214238	5.8183776	-1.0368969
C	-1.0514098	5.1695586	-1.0586220
C	2.3640182	2.8225111	-6.2482563
N	2.6747455	2.7840606	-7.3631842
H	3.6954208	3.5589129	0.2031884
H	2.0613020	1.4429213	-0.1535105
H	-0.2101173	2.5663922	-0.6753474
H	3.3523276	3.1323245	-1.7782208
H	4.0079953	3.0502929	-4.1534662
H	-0.1299527	2.6780306	-5.2912299
H	-0.7845899	2.7486350	-2.9034149
H	1.5573365	2.6479755	3.6640373
H	0.6374573	3.8844052	2.8082099
H	-0.1320252	2.0133121	1.4719924

H	1.2535573	1.0447468	1.9630199
H	1.3614961	6.8425158	-0.7593910
H	2.6244193	5.5744147	-0.6883444
H	1.5201783	5.6750937	-2.1141809
H	-1.3071117	6.1966431	-0.7908049
H	-1.8391353	4.4928775	-0.7233754
H	-0.8918426	5.0874840	-2.1353812

la_sy_c_2_r.log

E = -1109.626722
H = -1109.321416
G = -1109.386229

NImag=0

C	0.2315518	-1.7888184	-1.3663476
C	-0.7653785	-0.7323031	-1.7530262
C	-0.3510424	-2.8556619	-0.6986784
O	0.1690997	-3.8823067	-0.1613767
C	-0.6197135	0.5135244	-0.8239616
C	-0.9899408	0.2855224	0.6226165
C	-2.3067243	0.3639921	1.0934308
C	-2.6029299	0.0803265	2.4213228
C	-1.5715499	-0.2954326	3.2889979
C	-0.2487562	-0.3688568	2.8376463
C	0.0333941	-0.0669123	1.5110019
C	-1.8729943	-2.6257333	-0.6529577
C	-2.1241472	-1.4651483	-1.6254206
S	-1.6122836	1.9384538	-1.4773261
C	-1.0105013	3.2956376	-0.4509999
C	-0.7627140	2.3057008	-3.0260737
C	-1.8720601	-0.5953732	4.6636889
N	-2.1136361	-0.8358531	5.7705457
H	1.3040997	-1.6485758	-1.4776328
H	-0.6216430	-0.3622766	-2.7765742
H	0.4149704	0.8705554	-0.8839981
H	-3.1233336	0.6435848	0.4334650
H	-3.6237127	0.1436589	2.7828173
H	0.5455376	-0.6513184	3.5205092
H	1.0584369	-0.1108040	1.1563297
H	-2.4123876	-3.5373686	-0.9321157
H	-2.1614862	-2.3811405	0.3787809
H	-2.9468785	-0.8077039	-1.3219869
H	-2.3828975	-1.8620941	-2.6121381
H	-1.3975966	4.2216777	-0.8798218
H	-1.4062660	3.1586715	0.5561398
H	0.0814801	3.2897116	-0.4507595
H	-1.0472584	3.3226737	-3.3035257
H	-1.1107912	1.6076749	-3.7867171
H	0.3164985	2.2307653	-2.8761283

la_sy_c_2_ts1.log

E = -1109.596717
H = -1109.293713
G = -1109.358648

NImag=1

C	-1.4693990	-1.8705846	0.1249581
C	-1.3770451	-1.1889140	-1.0888573
C	-2.8007528	-1.7963997	0.6461940
O	-3.2464713	-2.2602552	1.7063823
C	-0.4359173	0.7509447	-0.9743689
C	0.9182441	0.4458459	-0.5660606

C	1.3487088	0.3794501	0.7784506
C	2.6322563	-0.0344919	1.1025732
C	3.5270411	-0.4105549	0.0913381
C	3.1182523	-0.3679468	-1.2528586
C	1.8399569	0.0541107	-1.5681779
C	-3.6543213	-0.9991149	-0.3455479
C	-2.7756661	-0.8707621	-1.5955184
S	-1.4372416	1.9025269	-0.1196177
C	-1.7840383	1.2845853	1.5564969
C	-0.4340009	3.3594090	0.2866632
C	4.8521914	-0.8377500	0.4269766
N	5.9259683	-1.1841160	0.6975999
H	-0.6503635	-2.3637497	0.6379598
H	-0.5894118	-1.3997493	-1.8076710
H	-0.5697455	0.9580460	-2.0344387
H	0.6827821	0.6533319	1.5886792
H	2.9446749	-0.0726007	2.1415011
H	3.8094004	-0.6583567	-2.0379771
H	1.5331288	0.0938783	-2.6099052
H	-4.6091074	-1.5013932	-0.5234327
H	-3.8831976	-0.0213580	0.1000223
H	-2.8470040	0.1011931	-2.0914602
H	-3.0472503	-1.6321867	-2.3365438
H	-2.8204893	1.5362322	1.7857929
H	-1.6428259	0.2036804	1.5675723
H	-1.1129212	1.7661451	2.2691183
H	-1.0550583	4.0234802	0.8925088
H	-0.1714727	3.8421640	-0.6557751
H	0.4600098	3.0576275	0.8349675

1a_sy_c_3.log

E = -1109.627767

H = -1109.322417

G = -1109.388074

NImag=0

C	2.5893875	3.9935605	1.4774016
C	2.5444006	3.3145599	0.1370121
C	1.9750525	3.2372563	2.4651411
O	1.7043861	3.5156845	3.6732645
C	1.3393486	3.7372283	-0.7576901
C	1.4850697	3.3633299	-2.2091676
C	0.5169972	2.5554111	-2.8136827
C	0.6423360	2.1743774	-4.1449903
C	1.7469850	2.6179172	-4.8801933
C	2.7224927	3.4322056	-4.2905653
C	2.5888701	3.7960187	-2.9570640
C	1.5800642	1.8802252	1.8502903
C	2.3376254	1.8268940	0.5172962
S	1.0889966	5.5750702	-0.6033565
C	-0.0070034	5.9510710	-1.9890816
C	-0.1111089	5.6906966	0.7432900
C	1.8826384	2.2330112	-6.2602064
N	1.9910973	1.9233022	-7.3708319
H	2.9305839	5.0168132	1.6185561
H	3.4514670	3.4496040	-0.4647395
H	0.4077452	3.3214804	-0.3563591
H	-0.3404026	2.2211492	-2.2364927
H	-0.1063120	1.5440173	-4.6132517
H	3.5724204	3.7708601	-4.8734802
H	3.3485828	4.4279457	-2.5039176
H	1.8319781	1.0541564	2.5235361

H	0.4900898	1.8590320	1.7065810
H	1.8198594	1.2573987	-0.2637915
H	3.3214374	1.3700518	0.6653906
H	-0.3812668	6.9634435	-1.8231695
H	0.5737530	5.9183349	-2.9112741
H	-0.8296850	5.2333441	-2.0142737
H	-0.4165732	6.7373134	0.8064939
H	0.3886761	5.3754092	1.6589030
H	-0.9633891	5.0481262	0.5127230

1a_sy_c_3_ts1.log

E = -1109.599461
H = -1109.297106
G = -1109.363346

NImag=1

C	2.5412308	-0.8786370	-1.2452133
C	1.2722264	-1.1446965	-0.7352918
C	3.5482298	-1.3975635	-0.3657298
O	4.7808818	-1.3227225	-0.4698012
C	0.4205283	0.4720623	0.4957670
C	-0.9907755	0.2605567	0.3131790
C	-1.7041968	-0.4962051	1.2774959
C	-3.0342899	-0.8262632	1.0975437
C	-3.7128454	-0.4065766	-0.0608125
C	-3.0293359	0.3428683	-1.0315032
C	-1.6955500	0.6651377	-0.8490124
C	2.8356022	-2.0628494	0.8142915
C	1.3807425	-2.1972594	0.3519529
S	1.1247296	1.8843578	-0.2808535
C	0.3456694	3.3377322	0.4713226
C	2.7328788	1.9630977	0.5273303
C	-5.0911292	-0.7395928	-0.2493694
N	-6.2094722	-1.0105526	-0.4025443
H	2.7613221	-0.2973741	-2.1347402
H	0.3765649	-1.0829551	-1.3497427
H	0.8089706	0.3456673	1.5059070
H	-1.1922915	-0.8129896	2.1820031
H	-3.5612921	-1.4019291	1.8523654
H	-3.5497641	0.6663205	-1.9278662
H	-1.1924127	1.2378672	-1.6244508
H	3.3158132	-3.0043573	1.0927180
H	2.9102443	-1.3794459	1.6721339
H	0.6441229	-2.0769648	1.1502270
H	1.2134707	-3.1802754	-0.1059209
H	0.8539033	4.2262052	0.0893378
H	-0.7013079	3.3473187	0.1626829
H	0.4307632	3.2683393	1.5572802
H	3.2094141	2.8921591	0.2101781
H	3.3210700	1.1088597	0.1944754
H	2.5849004	1.9489892	1.6091634

1a_sy_c_4.log

E = -1109.626849
H = -1109.321183
G = -1109.386179

NImag=0

C	2.7615693	3.3574711	0.7698546
C	1.5978874	2.5999384	0.1862207
C	2.7535058	3.4088868	2.1549203
O	3.5752004	3.9396830	2.9645113

C	0.7578016	3.3643849	-0.8786098
C	1.1960046	3.1613638	-2.3104810
C	2.5253905	3.3698325	-2.7007579
C	2.9127111	3.1669004	-4.0190799
C	1.9614010	2.7467400	-4.9571702
C	0.6309834	2.5325763	-4.5821279
C	0.2567869	2.7467439	-3.2602461
C	1.5141671	2.6653654	2.6767394
C	0.7415546	2.2027140	1.4319598
S	0.8556222	5.1836511	-0.5489827
C	-0.3910331	5.7985666	-1.7049005
C	-0.0454952	5.3955614	0.9991023
C	2.3584656	2.5324958	-6.3237600
N	2.6778192	2.3608816	-7.4236093
H	3.5796772	3.7496804	0.1717443
H	1.9012953	1.6866816	-0.3485897
H	-0.3066962	3.1174898	-0.7934031
H	3.2676571	3.6914432	-1.9766175
H	3.9413423	3.3289889	-4.3235216
H	-0.0972750	2.2064968	-5.3171755
H	-0.7754355	2.5868317	-2.9621299
H	1.8421702	1.8257642	3.3010698
H	0.9258772	3.3277776	3.3251517
H	-0.2465631	2.6703414	1.3825178
H	0.5715640	1.1226137	1.4347409
H	-0.5615820	6.8479920	-1.4566980
H	0.0150947	5.7227097	-2.7144592
H	-1.3137358	5.2232322	-1.6064206
H	-0.2244208	6.4675375	1.1066895
H	0.5918155	5.0405542	1.8088431
H	-0.9892277	4.8492083	0.9544750

la_sy_c_4_ts1.log

E = -1109.596603

H = -1109.294017

G = -1109.360184

NImag=1

C	1.7588144	-1.4811927	-0.8166067
C	1.2197508	-1.3122527	0.4596718
C	3.1871041	-1.5583148	-0.7738860
O	3.9850166	-1.6785885	-1.7160008
C	0.3110758	0.6654573	0.7286593
C	-1.0701924	0.3913740	0.4189934
C	-1.6063847	0.4148931	-0.8922067
C	-2.9110647	0.0231497	-1.1423133
C	-3.7303047	-0.4162184	-0.0906855
C	-3.2169431	-0.4611897	1.2174969
C	-1.9148981	-0.0663619	1.4615571
C	3.6262615	-1.5496209	0.6948238
C	2.3270995	-1.4098230	1.5041813
S	1.1595668	1.6908176	-0.4118164
C	0.5096013	3.3652084	-0.1740299
C	2.7696912	1.8720632	0.3670728
C	-5.0794373	-0.8166872	-0.3487231
N	-6.1738979	-1.1424147	-0.5567786
H	1.1863810	-1.5641277	-1.7350128
H	0.2286022	-1.6704217	0.7223972
H	0.5392476	0.9298157	1.7608696
H	-0.9996152	0.7440741	-1.7316800
H	-3.3030702	0.0540729	-2.1542603
H	-3.8466826	-0.8030694	2.0332018

H	-1.5267188	-0.1016165	2.4758946
H	4.1422179	-2.4927747	0.9033559
H	4.3504938	-0.7481266	0.8752244
H	2.3377738	-0.5432668	2.1716277
H	2.1445706	-2.2895742	2.1303376
H	1.0871937	4.0450837	-0.8044991
H	-0.5338167	3.3564133	-0.4942030
H	0.5899096	3.6374387	0.8798574
H	3.2824664	2.6920649	-0.1385232
H	3.3247921	0.9482352	0.2157175
H	2.6373236	2.0909176	1.4285393

1a_sy_c_5.log

E = -1109.623616
H = -1109.317751
G = -1109.382360

NImag=0

C	2.1012286	4.0976199	1.5565838
C	2.3429015	3.7353566	0.1149485
C	1.9322358	2.9836437	2.3659557
O	1.6553257	2.8920171	3.6019896
C	1.0933640	3.7907624	-0.8086552
C	1.3357934	3.3322566	-2.2303212
C	2.3941655	3.8504810	-2.9876450
C	2.6180467	3.4032009	-4.2843293
C	1.7775654	2.4248793	-4.8281879
C	0.7167579	1.8968688	-4.0829189
C	0.5027235	2.3569266	-2.7894164
C	2.1161547	1.7273944	1.4955938
C	2.7858148	2.2473073	0.2201418
S	0.2915578	5.4639342	-0.9505943
C	-0.7117767	5.6289513	0.5386295
C	1.6032557	6.6688203	-0.6724877
C	2.0092830	1.9548503	-6.1682282
N	2.1956603	1.5762557	-7.2467555
H	2.0030472	5.1157695	1.9216425
H	3.1271800	4.3297867	-0.3716038
H	0.2847586	3.1963053	-0.3652361
H	3.0580507	4.6020611	-2.5703950
H	3.4375423	3.8033226	-4.8721276
H	0.0731066	1.1373026	-4.5141341
H	-0.3163611	1.9495985	-2.2034003
H	2.7137451	0.9725597	2.0173411
H	1.1326652	1.2798245	1.2930932
H	2.5475970	1.6606289	-0.6731870
H	3.8738151	2.2331386	0.3429920
H	-1.1665890	6.6209216	0.4957994
H	-1.4876402	4.8627345	0.4878521
H	-0.0948883	5.5069867	1.4269255
H	1.1236125	7.6495427	-0.7006807
H	2.3138714	6.5870855	-1.4966570
H	2.0862291	6.4999044	0.2892727

1a_sy_c_6.log

E = -1109.627832
H = -1109.322223
G = -1109.386436

NImag=0

C	2.7090650	3.5619201	0.8762186
C	1.6435279	2.6260849	0.3581492

C	2.8719421	3.4577003	2.2529149
O	3.7201387	3.9972046	3.0253170
C	0.7056882	3.1605515	-0.7448607
C	1.1821121	3.0444202	-2.1685182
C	2.5398326	3.1540590	-2.4957972
C	2.9588930	3.0434121	-3.8153429
C	2.0112685	2.8168943	-4.8209770
C	0.6530398	2.6911106	-4.5103458
C	0.2493236	2.8028252	-3.1848277
C	1.8254978	2.4684972	2.7940125
C	0.8410583	2.2826472	1.6379402
S	0.2859989	4.9221423	-0.2952500
C	1.4388126	5.9705879	-1.2026539
C	-1.2039127	5.2120668	-1.2742303
C	2.4420463	2.7022255	-6.1893880
N	2.7883592	2.6112983	-7.2906956
H	3.4318490	4.0707931	0.2444253
H	2.0505133	1.6953859	-0.0757328
H	-0.2760122	2.6760784	-0.6655838
H	3.2781592	3.3224150	-1.7188521
H	4.0104181	3.1279256	-4.0686852
H	-0.0708743	2.5014303	-5.2957738
H	-0.8020066	2.6893660	-2.9343966
H	2.3361243	1.5294227	3.0481353
H	1.3583816	2.8432055	3.7110394
H	0.0168250	2.9997534	1.7470636
H	0.3964239	1.2840171	1.5805261
H	1.1306025	6.9988878	-1.0004398
H	2.4392101	5.7951128	-0.8095284
H	1.3806983	5.7547790	-2.2708357
H	-1.5128689	6.2411924	-1.0809050
H	-1.9749177	4.5227012	-0.9262920
H	-0.9989174	5.0712858	-2.3369295

1a_sy_c_7.log

E = -1109.628358

H = -1109.322813

G = -1109.388215

NImag=0

C	1.7270994	3.8818607	1.7375521
C	2.0743893	3.5764877	0.3034944
C	2.3081238	2.9804709	2.6193534
O	2.3284981	2.9581172	3.8879278
C	0.9088061	3.6882215	-0.6944982
C	1.2203878	3.3244884	-2.1221858
C	2.4166895	3.7129787	-2.7407853
C	2.6817700	3.3466715	-4.0552441
C	1.7441540	2.5817839	-4.7585162
C	0.5482796	2.1789658	-4.1531793
C	0.2963609	2.5538674	-2.8394675
C	3.0562082	1.9148374	1.7980957
C	2.5513236	2.1013526	0.3643871
S	0.1772151	5.3906604	-0.5413386
C	1.4755879	6.5116820	-1.0886906
C	-0.9700401	5.4956891	-1.9256788
C	2.0169146	2.1988328	-6.1186065
N	2.2359961	1.8910548	-7.2132760
H	1.2637798	4.8115070	2.0605374
H	2.8951578	4.2041534	-0.0825464
H	0.0763250	3.0736376	-0.3297917
H	3.1558162	4.2947699	-2.1989079

H	3.6083201	3.6453888	-4.5340265
H	-0.1685268	1.5808920	-4.7058195
H	-0.6281749	2.2427984	-2.3609159
H	4.1348094	2.1090988	1.8774827
H	2.8775945	0.9089658	2.1927746
H	1.6877104	1.4465708	0.1904755
H	3.2969418	1.8762363	-0.4045081
H	1.0397681	7.5130161	-1.0722894
H	2.2969232	6.4572048	-0.3723776
H	1.8017802	6.2542031	-2.0976167
H	-1.4284469	6.4855866	-1.8781582
H	-1.7331587	4.7275756	-1.7853460
H	-0.4382830	5.3592722	-2.8688100

1a_sy_c_7_ts1.log

E = -1109.597215

H = -1109.294348

G = -1109.360538

NImag=1

C	-2.9563358	-0.4458108	0.9853411
C	-1.6155514	-0.8166252	0.9218933
C	-3.7474811	-1.2839621	0.1312394
O	-4.9668691	-1.2384140	-0.0821232
C	-0.5014649	0.3513205	-0.5713157
C	0.9084873	0.1293155	-0.3647464
C	1.6678378	0.7568541	0.6528314
C	2.9976962	0.4315630	0.8653126
C	3.6194810	-0.5476863	0.0761537
C	2.8847271	-1.1974223	-0.9313820
C	1.5612544	-0.8601047	-1.1442913
C	-2.8101532	-2.2996784	-0.5274972
C	-1.5010079	-2.1768171	0.2597089
S	-1.2554987	1.9215690	-0.4447421
C	-1.1957165	2.5145209	1.2715531
C	-0.1700782	3.1446454	-1.2198241
C	4.9924729	-0.8849147	0.2986042
N	6.1058745	-1.1586372	0.4787861
H	-3.3621924	0.3985573	1.5334185
H	-0.8765105	-0.5187420	1.6625585
H	-0.9309345	-0.1241792	-1.4513672
H	1.2151931	1.5002143	1.2993199
H	3.5598076	0.9283774	1.6501159
H	3.3625962	-1.9537770	-1.5464330
H	1.0063293	-1.3555744	-1.9363999
H	-3.2479176	-3.3013711	-0.5195633
H	-2.6726954	-2.0037271	-1.5757842
H	-0.6003829	-2.2881578	-0.3490791
H	-1.4547352	-2.9345620	1.0516899
H	-2.0140791	3.2288962	1.3782774
H	-1.3489158	1.6735627	1.9469871
H	-0.2434463	3.0072908	1.4686300
H	-0.6024889	4.1316525	-1.0394559
H	-0.1518429	2.9298177	-2.2892495
H	0.8320891	3.0776668	-0.7921568

1a_sy_c_8.log

E = -1109.629117

H = -1109.323353

G = -1109.388271

NImag=0

C	2.1969190	4.1198793	1.6431375
C	2.4347350	3.6665600	0.2277301
C	2.0542954	3.0562731	2.5237124
O	1.7884381	3.0357246	3.7644641
C	1.1604172	3.6724975	-0.6618723
C	1.3524845	3.3126855	-2.1115219
C	2.4309585	3.8061440	-2.8583573
C	2.5899252	3.4455571	-4.1916119
C	1.6645319	2.5799431	-4.7853213
C	0.5855550	2.0724219	-4.0518506
C	0.4384705	2.4433404	-2.7215112
C	2.2589297	1.7490955	1.7340504
C	2.8889084	2.1932428	0.4092492
S	0.3118634	5.3087463	-0.4449271
C	1.5054586	6.5278346	-1.0208937
C	-0.8936354	5.3578183	-1.7831280
C	1.8269409	2.2029127	-6.1645388
N	1.9566508	1.8997364	-7.2746689
H	2.0715650	5.1622935	1.9275078
H	3.2052498	4.2428496	-0.2991347
H	0.4193517	2.9999833	-0.2113544
H	3.1607090	4.4700331	-2.4061992
H	3.4253435	3.8270554	-4.7690521
H	-0.1228309	1.3972566	-4.5202519
H	-0.3954428	2.0519032	-2.1453128
H	2.8886235	1.0497990	2.2941271
H	1.2851725	1.2612260	1.5881700
H	2.6195485	1.5585683	-0.4425616
H	3.9802507	2.1834011	0.4953621
H	1.0111688	7.4986425	-0.9465396
H	2.3674046	6.5021223	-0.3523282
H	1.7909002	6.3239695	-2.0540235
H	-1.4148959	6.3133544	-1.6962843
H	-1.5979580	4.5380475	-1.6278552
H	-0.3954064	5.2742812	-2.7505103

1a_sy_c_8_r.log

E = -1109.622692

H = -1109.316830

G = -1109.380877

NImag=0

C	-1.1520157	-0.0348257	2.1228427
C	-1.7022955	-0.4365054	0.7834591
C	-2.0534054	0.6851253	2.8913175
O	-1.9198202	1.2319910	4.0302733
C	-0.9338776	0.3048953	-0.3446920
C	-0.8630760	1.8106196	-0.3315437
C	-2.0026788	2.6252851	-0.2841019
C	-1.8832463	4.0087918	-0.2477686
C	-0.6104552	4.5915995	-0.2657827
C	0.5383313	3.7963599	-0.3241236
C	0.4012368	2.4137124	-0.3584579
C	-3.3880044	0.7734710	2.1305739
C	-3.2266935	-0.1686378	0.9282075
S	-1.4350517	-0.3776376	-2.0183303
C	-2.6530582	0.7396232	-2.7396786
C	-0.0011870	0.0312717	-3.0326760
C	-0.4839951	6.0246142	-0.2299588
N	-0.3819343	7.1778537	-0.2029857
H	-0.1153359	-0.2085066	2.4022608
H	-1.5449717	-1.4999641	0.5489531

H	0.0930015	-0.0786593	-0.3046487
H	-2.9955604	2.1905300	-0.2819063
H	-2.7678860	4.6355353	-0.2073618
H	1.5209088	4.2558736	-0.3390290
H	1.2908255	1.7911559	-0.3973675
H	-4.2170934	0.4785535	2.7833361
H	-3.5673033	1.8175174	1.8429500
H	-3.6974844	0.2045065	0.0124557
H	-3.7058230	-1.1271502	1.1497346
H	-2.8581396	0.3472286	-3.7381112
H	-3.5632711	0.7057919	-2.1405020
H	-2.2488162	1.7510070	-2.8006001
H	-0.2354936	-0.2643710	-4.0572283
H	0.8446426	-0.5491407	-2.6609776
H	0.1978416	1.1034779	-2.9759196

la_sy_c_9.log

E = -1109.623551
H = -1109.317825
G = -1109.383077

NImag=0

C	1.6625500	3.8930771	1.6009635
C	1.9927905	3.6398378	0.1528754
C	2.2065724	2.9290502	2.4402876
O	2.2293802	2.8558499	3.7066848
C	0.8581681	3.8253240	-0.8721770
C	1.2129579	3.3558549	-2.2652624
C	0.4117494	2.3936307	-2.8873789
C	0.7276421	1.9200130	-4.1556646
C	1.8582204	2.4218709	-4.8091908
C	2.6705589	3.3856897	-4.1991506
C	2.3456526	3.8457106	-2.9292225
C	2.9032279	1.8686274	1.5717741
C	2.3946257	2.1373526	0.1543886
S	0.2386433	5.5752275	-1.0542339
C	-0.9702139	5.7633716	0.2702859
C	1.5846924	6.6375221	-0.4972346
C	2.1903121	1.9417890	-6.1242522
N	2.4568781	1.5555513	-7.1830156
H	1.2672782	4.8290278	1.9839671
H	2.8479021	4.2370106	-0.2092252
H	-0.0398567	3.3012751	-0.5233825
H	-0.4642394	2.0090768	-2.3729939
H	0.1073178	1.1711308	-4.6368648
H	3.5460585	3.7644909	-4.7158443
H	2.9889451	4.5851969	-2.4598035
H	3.9892665	2.0171605	1.6483056
H	2.6873276	0.8544151	1.9238371
H	1.4962767	1.5346111	-0.0318637
H	3.1177495	1.9039434	-0.6331151
H	-1.3209907	6.7963787	0.2250614
H	-1.7947183	5.0828686	0.0513857
H	-0.5223853	5.5413163	1.2370802
H	1.1950346	7.6573697	-0.5244175
H	2.4052416	6.5413376	-1.2097033
H	1.8972841	6.3648398	0.5109997

la_sy_c_prod_1.log

E = -631.738876
H = -631.517360

G = -631.569661
 NImag=0

C	1.3273116	0.0752224	-3.1443791
C	-0.1143880	0.4543975	-3.1417364
C	-0.8774831	-0.7322537	-3.7125871
C	0.1175723	-1.8489560	-4.0267529
C	1.5173824	-1.2205411	-3.9212160
O	2.2111675	0.6797459	-2.5670201
C	-0.7901536	0.5300440	-4.5024121
C	-0.0325720	0.6555678	-5.7869229
C	0.9642138	1.6271803	-5.9398895
C	1.6502960	1.7585900	-7.1408453
C	1.3344381	0.9053194	-8.2059281
C	0.3343915	-0.0659113	-8.0729376
C	-0.3430086	-0.1822913	-6.8645449
H	-1.6910622	1.1398757	-4.4743912
H	-0.4815493	1.0858035	-2.3413634
H	-1.8402646	-1.0003830	-3.2921564
C	2.0428082	1.0306838	-9.4514049
N	2.6132338	1.1319339	-10.4546066
H	0.0045398	-2.6347284	-3.2748254
H	-0.0665097	-2.2989035	-5.0067418
H	1.9500632	-0.9750441	-4.8986034
H	2.2363343	-1.8540586	-3.3961935
H	1.2067346	2.2836693	-5.1085548
H	2.4241821	2.5102720	-7.2579930
H	0.0968829	-0.7185167	-8.9067299
H	-1.1209611	-0.9324177	-6.7542638

1a_sy_tr_1.log
 E = -1109.625308
 H = -1109.319791
 G = -1109.385435
 NImag=0

C	5.1854047	1.2381520	1.8128887
C	3.7037935	1.4464244	1.9712516
C	3.3322244	2.2564809	0.7062173
C	4.3756719	1.8347882	-0.3334817
C	5.5956771	1.3967417	0.4955180
O	6.7230801	1.2014708	-0.0525826
C	3.2868064	2.0792639	3.3139874
C	1.8020449	2.3187999	3.4565970
C	1.1254744	3.3151646	2.7397108
C	-0.2490622	3.4663928	2.8664972
C	-0.9600907	2.6059397	3.7122595
C	-0.3003607	1.6060354	4.4336771
C	1.0778709	1.4745237	4.3045428
S	4.2461361	3.6550586	3.5835261
C	5.7299271	3.1076743	4.4603575
C	3.3661748	4.3809039	4.9884816
C	-2.3847165	2.7580453	3.8463519
N	-3.5311121	2.8812081	3.9546009
H	5.7979121	0.7745427	2.5830024
H	3.1287548	0.5007849	1.9715841
H	3.4530811	3.3282400	0.9070610
H	2.2977147	2.0932315	0.3891241
H	4.6320688	2.6313005	-1.0401402
H	4.0318526	0.9731160	-0.9229493
H	3.6234328	1.4346418	4.1335069
H	1.6641363	3.9925171	2.0834960
H	-0.7706714	4.2422364	2.3161600

H	-0.8597229	0.9475659	5.0898215
H	1.5972941	0.7049873	4.8680278
H	6.4216594	2.7013553	3.7260635
H	6.1512052	3.9953894	4.9373468
H	5.4538916	2.3612219	5.2078337
H	2.4267062	4.8045265	4.6345317
H	4.0054864	5.1756403	5.3771798
H	3.1929543	3.6168343	5.7494488

la_sy_tr_10.log

E = -1109.620392
H = -1109.314675
G = -1109.379087

NImag=0

C	4.5251204	2.6000321	1.5391890
C	4.3071186	1.5485144	2.5954493
C	3.6759482	0.3772223	1.7952436
C	4.2133841	0.5558277	0.3729008
C	4.5283326	2.0583773	0.2624582
O	4.7818885	2.5903653	-0.8631154
C	3.4354819	1.8411589	3.8365834
C	1.9711462	2.1631569	3.6442595
C	1.5247499	3.0924688	2.6939944
C	0.1657264	3.3349088	2.5324666
C	-0.7574373	2.6491610	3.3303775
C	-0.3281399	1.7219983	4.2862272
C	1.0333115	1.4861660	4.4338841
S	4.1393092	3.1301719	4.9914758
C	3.7486401	4.7469991	4.2956903
C	5.9214223	3.0532914	4.7278941
C	-2.1647819	2.9003475	3.1650099
N	-3.2974223	3.1020989	3.0324376
H	4.8654505	3.6112324	1.7446069
H	5.2564779	1.1814328	3.0225382
H	2.5860020	0.4914452	1.7844108
H	3.9061448	-0.5940624	2.2448986
H	3.5066585	0.2363976	-0.4004539
H	5.1450737	-0.0060577	0.2169871
H	3.4972411	0.9613788	4.4887596
H	2.2408912	3.6173178	2.0724925
H	-0.1809258	4.0503781	1.7940827
H	-1.0514220	1.1944814	4.8988851
H	1.3731771	0.7612971	5.1685555
H	2.6890126	4.9402910	4.4643288
H	4.3455255	5.4617146	4.8671505
H	4.0030542	4.7904017	3.2375487
H	6.2607802	2.0589766	5.0217430
H	6.3595879	3.8025046	5.3899648
H	6.1593719	3.2656037	3.6844751

la_sy_tr_11.log

E = -1109.623366
H = -1109.317970
G = -1109.382998

NImag=0

C	4.6602085	2.4149752	1.4336181
C	4.3911805	1.4414442	2.5498569
C	3.7108372	0.2522367	1.8257518
C	4.2338150	0.3281383	0.3876846
C	4.6237050	1.8046998	0.1894962

O	4.8910460	2.2583070	-0.9671481
C	3.5447513	1.9047314	3.7598957
C	2.0894035	2.2368535	3.5661612
C	1.6302655	3.0312680	2.5049225
C	0.2734859	3.2906876	2.3555407
C	-0.6372860	2.7567128	3.2753632
C	-0.1969830	1.9628601	4.3395343
C	1.1628264	1.7086903	4.4747746
S	4.4759187	3.2872944	4.5930576
C	3.7678998	3.2840784	6.2505285
C	3.7917041	4.8339832	3.9681754
C	-2.0426225	3.0266496	3.1233922
N	-3.1736638	3.2440377	3.0021830
H	5.0543887	3.4173136	1.5889250
H	5.3238817	1.0766391	3.0181597
H	2.6255900	0.4036787	1.8223610
H	3.9121771	-0.7001259	2.3266802
H	3.4993483	0.0048280	-0.3579081
H	5.1329406	-0.2883294	0.2480972
H	3.6192096	1.1296793	4.5330491
H	2.3382595	3.4393976	1.7923467
H	-0.0816791	3.9030676	1.5333606
H	-0.9101721	1.5510208	5.0456842
H	1.5096382	1.0851513	5.2943172
H	4.0468904	2.3450511	6.7309603
H	4.2097173	4.1253746	6.7879718
H	2.6830617	3.3935705	6.1896487
H	3.9790722	4.8923649	2.8959237
H	4.3348475	5.6292066	4.4835426
H	2.7252361	4.8871632	4.1918913

la_sy_tr_12.log

E = -1109.623916

H = -1109.318575

G = -1109.384663

NImag=0

C	5.0178458	0.8142725	1.9231682
C	3.6353226	1.3977247	1.8205342
C	3.7664288	2.4319547	0.6671180
C	5.0113514	2.0072501	-0.1247148
C	5.8149353	1.1084476	0.8295257
O	6.9910207	0.7325576	0.5299174
C	3.1300438	1.9276419	3.1812706
C	1.6668909	2.2473899	3.3371995
C	0.9465902	2.9347662	2.3510723
C	-0.4034081	3.2105267	2.5262667
C	-1.0437500	2.7959788	3.7007187
C	-0.3410801	2.1072353	4.6945915
C	1.0091911	1.8374146	4.5034489
S	4.2217364	3.3479841	3.7202643
C	4.2448133	3.1265488	5.5091702
C	3.2055129	4.8363913	3.6081558
C	-2.4428724	3.0785993	3.8852423
N	-3.5683552	3.3064612	4.0347492
H	5.2901037	0.1050960	2.7024656
H	2.8667235	0.6501166	1.5549376
H	3.9229715	3.4401837	1.0731070
H	2.8675315	2.4777259	0.0466413
H	5.6135413	2.8569478	-0.4653940
H	4.7464316	1.4228275	-1.0160479
H	3.3956192	1.1764940	3.9335672

H	1.4369375	3.2696224	1.4435600
H	-0.9607535	3.7430995	1.7629902
H	-0.8476236	1.7850453	5.5982189
H	1.5585070	1.2921821	5.2660620
H	4.8071837	2.2159772	5.7213343
H	4.7579421	3.9912821	5.9342503
H	3.2236679	3.0578534	5.8898247
H	2.9805778	5.0253532	2.5571930
H	3.8227267	5.6466530	4.0028577
H	2.2928948	4.7244952	4.1958334

1a_sy_tr_13.log

E = -1109.625495

H = -1109.319769

G = -1109.383970

NImag=0

C	4.8612448	0.6405883	1.7534507
C	3.5339527	1.3358576	1.6549513
C	3.7799327	2.4364509	0.5753401
C	5.3026679	2.5314518	0.3876646
C	5.8827425	1.2838725	1.0729421
O	7.1170627	1.0024227	0.9681284
C	3.0601293	1.8535118	3.0362389
C	1.6060500	2.2083974	3.2146017
C	0.8323139	2.7098958	2.1603328
C	-0.5063657	3.0279723	2.3558415
C	-1.0806370	2.8410205	3.6185520
C	-0.3267923	2.3261111	4.6790497
C	1.0086539	2.0075552	4.4659603
S	4.2007726	3.2607445	3.5115732
C	4.4503116	2.9893240	5.2759948
C	3.1621885	4.7366273	3.5523913
C	-2.4656242	3.1723705	3.8256169
N	-3.5797154	3.4404200	3.9930109
H	4.9982041	-0.2612242	2.3463923
H	2.7123643	0.6767454	1.3366723
H	3.3345075	3.4023757	0.8413503
H	3.2989952	2.1251356	-0.3567612
H	5.7307801	3.4286507	0.8548987
H	5.5941641	2.5532384	-0.6682126
H	3.3265035	1.1018535	3.7870663
H	1.2659253	2.8523530	1.1762704
H	-1.1055541	3.4152818	1.5385070
H	-0.7853851	2.1719821	5.6500910
H	1.5952327	1.5907021	5.2802761
H	5.0146905	2.0614051	5.3843134
H	5.0359967	3.8301642	5.6525030
H	3.4879596	2.9291657	5.7875081
H	2.8209020	4.9406999	2.5361578
H	3.8067293	5.5495222	3.8939302
H	2.3196958	4.5983545	4.2321956

1a_sy_tr_14.log

E = -1109.619529

H = -1109.313997

G = -1109.378647

NImag=0

C	5.0280423	1.0588229	2.0674048
C	3.5670868	1.3548614	2.2064423
C	3.1878138	2.1049671	0.8929182

C	4.4765639	2.2048769	0.0580252
C	5.5752842	1.5102878	0.8803513
O	6.7626150	1.4323475	0.4307852
C	3.1423041	2.0618150	3.5304891
C	1.6516516	2.3068692	3.6064085
C	1.0457458	3.4904651	3.1705728
C	-0.3367758	3.6319456	3.2016364
C	-1.1247156	2.5738020	3.6669245
C	-0.5346977	1.3815175	4.1030359
C	0.8482087	1.2590246	4.0728494
S	4.0331747	3.6041321	4.0376214
C	4.6614604	4.4630595	2.5781047
C	5.5744369	2.9919806	4.7476100
C	-2.5558585	2.7145312	3.7002648
N	-3.7082188	2.8275127	3.7270909
H	5.5828087	0.5011701	2.8184604
H	2.9539032	0.4409235	2.2825040
H	2.7589992	3.0911349	1.0940972
H	2.4119107	1.5440168	0.3647082
H	4.7712342	3.2418739	-0.1527330
H	4.3828895	1.7039125	-0.9124564
H	3.4268797	1.3979576	4.3555187
H	1.6387462	4.3227270	2.7998199
H	-0.8029770	4.5522983	2.8664162
H	-1.1535275	0.5681677	4.4670867
H	1.3130920	0.3399977	4.4186523
H	3.8207536	4.8587450	2.0079554
H	5.2551974	5.2911858	2.9725006
H	5.2782198	3.7859814	1.9893951
H	5.3174961	2.3289393	5.5753176
H	6.1070284	3.8674229	5.1256089
H	6.1480240	2.4717268	3.9812128

la_sy_tr_15.log

E = -1109.623600

H = -1109.317826

G = -1109.382813

NImag=0

C	3.4698261	1.5069331	1.0888579
C	3.9670263	2.5964576	2.0133878
C	5.5044338	2.4144561	1.9581959
C	5.7765365	1.7606253	0.5995378
C	4.4665553	1.0374432	0.2458822
O	4.4181388	0.2050366	-0.7116332
C	3.3723932	2.4136086	3.4144855
C	1.8577663	2.4009251	3.4603628
C	1.1029045	3.2995891	2.6971750
C	-0.2853583	3.2827100	2.7600998
C	-0.9233493	2.3549796	3.5917689
C	-0.1813840	1.4489049	4.3583877
C	1.2059593	1.4812302	4.2887431
S	3.8617310	3.6914517	4.6971756
C	4.0300098	5.2402949	3.7907556
C	5.5756475	3.3329639	5.1328567
C	-2.3607473	2.3300978	3.6565357
N	-3.5174463	2.3111061	3.7095043
H	2.4164197	1.2689088	0.9696284
H	3.7006316	3.6069148	1.6612380
H	5.8093695	1.7276955	2.7577779
H	6.0468208	3.3554828	2.0978207
H	6.6256708	1.0690881	0.6160993

H	5.9822667	2.5093964	-0.1779328
H	3.7567527	1.4901204	3.8644458
H	1.5934101	4.0129059	2.0414697
H	-0.8732271	3.9764716	2.1683052
H	-0.6876215	0.7311637	4.9952415
H	1.7909609	0.7810775	4.8789535
H	3.0549498	5.4942940	3.3710471
H	4.3212472	5.9935230	4.5257925
H	4.7874750	5.1447383	3.0125033
H	5.6194965	2.2958945	5.4701578
H	5.8230020	4.0008383	5.9606421
H	6.2380322	3.5054726	4.2866311

1a_sy_tr_15_ts2.log
E = -1109.615788
H = -1109.311787
G = -1109.376805

NImag=1

C	1.6262229	1.8075266	0.6162962
C	1.9069105	0.3228913	0.6615783
C	3.3676654	0.2267981	0.1671896
C	3.5962600	1.4822175	-0.6850305
C	2.5570589	2.4914185	-0.1805629
O	2.6055128	3.7097095	-0.4848327
C	0.9116255	-0.0706784	-0.3815512
C	-0.5481986	0.1408316	-0.1745148
C	-1.1022638	0.2611693	1.1086719
C	-2.4740710	0.3857543	1.2729058
C	-3.3065393	0.3803366	0.1450349
C	-2.7694880	0.2564230	-1.1416156
C	-1.3936895	0.1390972	-1.2919516
S	0.8339468	-2.2881397	-0.6775993
C	-0.2902519	-2.8067472	0.6383191
C	2.3714796	-2.9604212	-0.0041499
C	-4.7296054	0.5051187	0.3116543
N	-5.8758429	0.6045141	0.4455776
H	0.7553743	2.2704895	1.0646545
H	1.7407548	-0.1792327	1.6204327
H	3.5741974	-0.6950142	-0.3803910
H	4.0204902	0.2455068	1.0455689
H	3.4228603	1.2955356	-1.7531235
H	4.6079274	1.8876905	-0.5884186
H	1.2386582	0.1361533	-1.4012436
H	-0.4609569	0.2610688	1.9846623
H	-2.9046397	0.4833540	2.2639498
H	-3.4235116	0.2562680	-2.0071599
H	-0.9667915	0.0453248	-2.2870154
H	-1.3043253	-2.5149417	0.3618614
H	-0.2335113	-3.8948407	0.7145953
H	-0.0035529	-2.3459135	1.5866837
H	3.1621394	-2.8225350	-0.7418412
H	2.2166970	-4.0291220	0.1609942
H	2.6272069	-2.4678904	0.9363912

1a_sy_tr_16.log
E = -1109.616295
H = -1109.310697
G = -1109.375284

NImag=0

C	4.8502958	0.7150452	1.6979242
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C	3.5514827	1.4648898	1.7550154
C	3.7707126	2.6887537	0.8096827
C	5.1803363	2.5344110	0.2108208
C	5.7944827	1.2907707	0.8718961
O	6.9929166	0.9509741	0.6114717
C	3.0747602	1.7307196	3.2030889
C	1.6197529	2.0959005	3.4025600
C	0.9207892	2.8582232	2.4593242
C	-0.4114845	3.1918717	2.6719088
C	-1.0494368	2.7633188	3.8417910
C	-0.3653377	1.9978427	4.7926683
C	0.9645016	1.6667709	4.5631495
S	4.0431871	2.9485029	4.2632401
C	3.2702356	4.5638817	4.0322663
C	5.6781095	3.2507450	3.5534569
C	-2.4278985	3.1104441	4.0668359
N	-3.5367598	3.3906699	4.2481104
H	5.0171096	-0.1910025	2.2769036
H	2.7017915	0.8693698	1.3768690
H	3.6704225	3.6369654	1.3453555
H	3.0041355	2.7013869	0.0300667
H	5.8222958	3.4071299	0.3893329
H	5.1528521	2.3873047	-0.8754962
H	3.2683416	0.8136285	3.7694542
H	1.4105372	3.1988674	1.5536745
H	-0.9557426	3.7804633	1.9408723
H	-0.8719323	1.6644845	5.6921610
H	1.4985058	1.0631250	5.2926848
H	2.2899548	4.5423425	4.5094850
H	3.9162755	5.2735312	4.5537125
H	3.1915651	4.8214341	2.9762464
H	6.2421557	2.3204014	3.5849714
H	6.1308332	3.9943693	4.2143261
H	5.5998538	3.6356630	2.5382693

la_sy_tr_17.log

E = -1109.624947

H = -1109.319485

G = -1109.384888

NImag=0

C	3.3667570	1.8337283	0.8288459
C	4.0628032	2.8315892	1.7194473
C	5.5510800	2.3969728	1.6086859
C	5.5171480	0.9158292	1.2155141
C	4.1463132	0.7210656	0.5493164
O	3.8791165	-0.3336794	-0.1055522
C	3.5261044	2.7279165	3.1748868
C	2.0224882	2.6182334	3.2800163
C	1.4525302	1.5675759	4.0029607
C	0.0706022	1.4478990	4.1047120
C	-0.7441117	2.3991996	3.4818032
C	-0.1855746	3.4629285	2.7606521
C	1.1954808	3.5661338	2.6639554
S	3.9341219	4.2632625	4.1623321
C	5.7200981	4.2376449	4.4091856
C	3.3817366	3.8043593	5.8176932
C	-2.1748783	2.2838722	3.5831106
N	-3.3263398	2.1912293	3.6654468
H	2.3252356	1.9306448	0.5357618
H	3.9368419	3.8757314	1.3942472
H	6.1251663	2.5724860	2.5207427

H	6.0173937	2.9835337	0.8104025
H	5.5883472	0.2531192	2.0890994
H	6.3281817	0.6376549	0.5340143
H	4.0046514	1.8993692	3.7110797
H	2.0944128	0.8345037	4.4829673
H	-0.3750276	0.6286384	4.6590941
H	-0.8299908	4.1924245	2.2816872
H	1.6290467	4.3843725	2.0945224
H	6.2009001	4.5465131	3.4811159
H	5.9268326	4.9739715	5.1890988
H	6.0410004	3.2423715	4.7220563
H	2.2913049	3.8028161	5.8233814
H	3.7542913	4.5705462	6.5003800
H	3.7818358	2.8222429	6.0779366

la_sy_tr_17_ts2.log

E = -1109.618448

H = -1109.314824

G = -1109.380760

NImag=1

C	1.8765822	-1.6479354	-0.6383780
C	1.9007946	-0.1675490	-0.9352113
C	3.3513205	0.2451467	-0.6205621
C	3.8496565	-0.7896704	0.3976962
C	2.9683995	-2.0265650	0.1625001
O	3.2472463	-3.1475429	0.6532522
C	0.9420985	0.1964365	0.1445031
C	-0.4874998	-0.1914748	0.0726638
C	-1.2218607	-0.3154386	1.2609655
C	-2.5710538	-0.6432090	1.2319804
C	-3.1962233	-0.8495955	-0.0035357
C	-2.4773171	-0.7314050	-1.2009020
C	-1.1300766	-0.4018680	-1.1577431
S	0.8092613	2.4537461	0.1255905
C	-0.2750758	2.8531135	1.5113578
C	-0.3029496	2.7951134	-1.2528512
C	-4.5929861	-1.1905976	-0.0444978
N	-5.7181389	-1.4637604	-0.0771135
H	1.0683417	-2.3087695	-0.9294622
H	1.5703786	0.1441678	-1.9305840
H	3.4288596	1.2781254	-0.2670168
H	3.9300956	0.1648449	-1.5459026
H	3.7159627	-0.4519307	1.4340909
H	4.9073790	-1.0398045	0.2737986
H	1.3622938	0.1676776	1.1505776
H	-0.7249803	-0.1599929	2.2149031
H	-3.1366892	-0.7432382	2.1522977
H	-2.9747679	-0.8967509	-2.1508082
H	-0.5765475	-0.3129233	-2.0874661
H	0.2296505	2.5516198	2.4313423
H	-0.4441111	3.9321798	1.5242492
H	-1.2269322	2.3265345	1.4097145
H	0.1814571	2.4567694	-2.1709674
H	-0.4713134	3.8731292	-1.3058532
H	-1.2520171	2.2733738	-1.1091832

la_sy_tr_18.log

E = -1109.617759

H = -1109.312020

G = -1109.375792

NImag=0

C	4.8056861	0.7852582	1.5901890
C	3.4835798	1.4905430	1.6773559
C	3.6549517	2.6966389	0.7053910
C	5.1645684	2.8439082	0.4672995
C	5.7874030	1.5290193	0.9643602
O	7.0289676	1.3023398	0.8039173
C	3.0356314	1.7734184	3.1331454
C	1.5706892	2.1151957	3.3536777
C	0.7821161	2.6737315	2.3421245
C	-0.5608996	2.9575278	2.5692629
C	-1.1210108	2.6807241	3.8200220
C	-0.3477950	2.1147422	4.8411597
C	0.9895769	1.8340055	4.5981090
S	3.9584271	3.0090466	4.1789068
C	3.8038497	4.6313756	3.4083764
C	5.7337425	2.7031338	4.0542603
C	-2.5098520	2.9733515	4.0580417
N	-3.6271442	3.2095247	4.2501315
H	4.9896169	-0.1617523	2.0933885
H	2.6436122	0.8678987	1.3278605
H	3.1860672	3.6163556	1.0639852
H	3.1553119	2.4406158	-0.2342128
H	5.6103806	3.6836444	1.0210806
H	5.4085866	3.0093638	-0.5878691
H	3.2512621	0.8673863	3.7142626
H	1.2008631	2.8828911	1.3645550
H	-1.1719862	3.3875124	1.7826751
H	-0.7942854	1.8927398	5.8046152
H	1.5885546	1.3807892	5.3841153
H	2.7489932	4.8017929	3.1829964
H	4.1380500	5.3499369	4.1594842
H	4.4236919	4.6966579	2.5153566
H	5.9164831	1.6715687	4.3578590
H	6.1895326	3.3906643	4.7712686
H	6.0995776	2.8871498	3.0459483

la_sy_tr_1_ts1.log

E = -1109.598903
H = -1109.296457
G = -1109.362268

NImag=1

C	2.5670005	-1.4077189	1.0989586
C	1.2418092	-1.3537804	0.6708458
C	1.1676750	-1.7546672	-0.7928676
C	2.6077117	-1.5833559	-1.2909187
C	3.4544996	-1.5295115	-0.0155889
O	4.6947788	-1.5638567	-0.0209458
C	0.3733495	0.6420800	0.6930609
C	-1.0183133	0.3807506	0.4064611
C	-1.6108835	0.4970080	-0.8753628
C	-2.9256829	0.1246092	-1.0970656
C	-3.7024133	-0.3848434	-0.0440748
C	-3.1373749	-0.5142617	1.2358189
C	-1.8246544	-0.1368007	1.4518750
S	1.1949653	1.7217506	-0.4217691
C	2.8562401	1.8455776	0.2690537
C	0.5999752	3.3932324	-0.0349734
C	-5.0629215	-0.7651076	-0.2721780
N	-6.1662370	-1.0745048	-0.4568194
H	2.9052710	-1.2962331	2.1236636

H	0.4089917	-1.5897829	1.3292877
H	0.4307123	-1.1800623	-1.3616046
H	0.8622622	-2.8065299	-0.8451077
H	2.7435560	-0.6379608	-1.8345287
H	2.9495356	-2.3859126	-1.9502601
H	0.6110928	0.8947655	1.7263177
H	-1.0406887	0.8872392	-1.7143354
H	-3.3598795	0.2278442	-2.0867073
H	-3.7356047	-0.9047076	2.0534213
H	-1.3998172	-0.2298035	2.4477684
H	3.4377054	0.9755740	-0.0301141
H	3.3006854	2.7484657	-0.1535983
H	2.7895139	1.9184611	1.3566132
H	-0.4620255	3.4243291	-0.2847528
H	1.1520468	4.1037478	-0.6545346
H	0.7562492	3.5876829	1.0281989

la_sy_tr_1_ts2.log

E = -1109.609852

H = -1109.305550

G = -1109.370427

NImag=1

C	-1.5632511	2.0112265	0.9927931
C	-2.1134055	0.8144946	0.2594842
C	-0.8863468	2.8870867	0.1272315
O	-0.2570783	3.9392993	0.3949894
C	-1.0983760	-0.1260630	0.8274866
C	0.3558764	-0.1624594	0.4916443
C	0.8507578	-0.1784193	-0.8211246
C	2.2168258	-0.2573026	-1.0624243
C	3.1060019	-0.3393915	0.0147809
C	2.6306651	-0.3511947	1.3321510
C	1.2643042	-0.2691634	1.5574731
C	-1.0397403	2.3780210	-1.3125514
C	-2.0437737	1.2153124	-1.2280784
S	-1.6669180	-2.2828929	0.4379482
C	-3.4411827	-2.1244961	0.1355928
C	-1.1168607	-2.6908701	-1.2337642
C	4.5198811	-0.4250210	-0.2344405
N	5.6586105	-0.4945779	-0.4347357
H	-1.6529374	2.1500098	2.0645798
H	-3.1168606	0.5043050	0.5604823
H	-1.2620235	-0.2702212	1.8953152
H	0.1757585	-0.1481010	-1.6673880
H	2.5933431	-0.2654931	-2.0798775
H	3.3252514	-0.4224281	2.1624943
H	0.8907690	-0.2742660	2.5775381
H	-1.3947277	3.1906711	-1.9544050
H	-0.0560488	2.0787872	-1.6940379
H	-1.8120364	0.3747378	-1.8889733
H	-3.0399349	1.5719728	-1.5068508
H	-3.8385299	-3.1094984	-0.1191777
H	-3.9113895	-1.7694895	1.0543284
H	-3.6233260	-1.4222265	-0.6809580
H	-1.5913977	-3.6312449	-1.5246827
H	-0.0343469	-2.8238886	-1.2145668
H	-1.3942483	-1.8993650	-1.9326445

la_sy_tr_2.log

E = -1109.625716

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H =      -1109.320001
G =      -1109.384735
NImag=0
C      4.9556630      0.8211800      1.9090951
C      3.5063472      1.1982286      1.9796295
C      3.2722385      1.9474153      0.6406581
C      4.6584416      2.4313018      0.1876000
C      5.6572079      1.5761716      0.9855154
O      6.9096217      1.6785008      0.7893015
C      3.1688329      2.0169934      3.2641302
C      1.6967460      2.3139669      3.4286002
C      1.0471048      3.3864612      2.8038913
C      -0.3255805      3.5563457      2.9374259
C      -1.0618076      2.6395751      3.6964757
C      -0.4283563      1.5627000      4.3266325
C      0.9461863      1.4123629      4.1928061
S      4.1525946      3.5893596      3.3203038
C      5.7984281      3.1003903      3.8972958
C      3.5349608      4.3312496      4.8490014
C      -2.4835039      2.8099045      3.8354523
N      -3.6281360      2.9462852      3.9473739
H      5.4344547      0.2119964      2.6728286
H      2.8164361      0.3451307      2.0621951
H      2.5356209      2.7527432      0.7158659
H      2.8767455      1.2261879      -0.0807683
H      4.8353012      3.4919709      0.4158468
H      4.8177106      2.3113148      -0.8896865
H      3.5215726      1.4552659      4.1367582
H      1.6000378      4.1125489      2.2135476
H      -0.8245585      4.3918640      2.4580868
H      -1.0057496      0.8602429      4.9184641
H      1.4452269      0.5829775      4.6859009
H      6.3822946      2.7622220      3.0408046
H      6.2371887      4.0008691      4.3339517
H      5.6955227      2.3152823      4.6489132
H      2.5279504      4.7094670      4.6752864
H      4.2046618      5.1594912      5.0869889
H      3.5446947      3.5823329      5.6440274

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1a_sy_tr_2_ts2.log
E =      -1109.613865
H =      -1109.310184
G =      -1109.376054
NImag=1
C      1.6916791      1.9525600      -0.9442660
C      2.1501405      0.9683281      0.1021292
C      0.7968116      2.8959581      -0.4062904
O      0.1540484      3.8014139      -0.9885686
C      1.2522319      -0.1029802      -0.4144344
C      -0.2304188      -0.1496537      -0.2249119
C      -0.8250270      -0.2194307      1.0425723
C      -2.2043494      -0.3312551      1.1724536
C      -3.0019590      -0.3840487      0.0241595
C      -2.4238443      -0.3375133      -1.2509907
C      -1.0446238      -0.2311314      -1.3643523
C      0.6941743      2.6690170      1.1092384
C      1.7950502      1.6476665      1.4373427
S      1.8331079      -2.0534685      0.5292753
C      0.8436672      -3.1350816      -0.5260440
C      3.4441263      -2.2293138      -0.2678199
C      -4.4298313      -0.4978917      0.1546160

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N	-5.5796982	-0.5898715	0.2592751
H	1.9748863	1.8952343	-1.9894090
H	3.1984481	0.6577508	0.0489302
H	1.5501090	-0.4482203	-1.4065016
H	-0.2145464	-0.2031117	1.9390836
H	-2.6614084	-0.3833882	2.1550060
H	-3.0499878	-0.3871004	-2.1355533
H	-0.5873093	-0.1978833	-2.3492671
H	0.8294488	3.6176257	1.6381802
H	-0.3140189	2.3086476	1.3485833
H	1.5291921	0.9370687	2.2254810
H	2.6930452	2.1757439	1.7723346
H	1.2299061	-4.1537284	-0.4539763
H	-0.1854263	-3.1087338	-0.1624206
H	0.8863415	-2.7860158	-1.5617301
H	3.7347106	-3.2816532	-0.2507786
H	4.1677748	-1.6445092	0.3018578
H	3.3952532	-1.8685059	-1.2990712

la_sy_tr_3.log

E = -1109.629946

H = -1109.324552

G = -1109.389085

NImag=0

C	4.5856214	2.3975522	1.4594287
C	4.5232885	1.5967453	2.7266279
C	3.8642288	0.2669776	2.2715795
C	3.0768909	0.6182280	1.0032556
C	3.7344315	1.9084985	0.4773793
O	3.4509121	2.3609451	-0.6740201
C	3.6807801	2.2365391	3.8796758
C	2.2100351	2.3866653	3.5870123
C	1.3157249	1.5034976	4.2028390
C	-0.0390079	1.5343474	3.8957878
C	-0.5064738	2.4737136	2.9690535
C	0.3706213	3.3820527	2.3648216
C	1.7239395	3.3369350	2.6782231
S	4.3585506	3.9074864	4.2504966
C	6.0573983	3.5413304	4.7259533
C	3.6179506	4.2387449	5.8605304
C	-1.9074763	2.5149574	2.6437447
N	-3.0352883	2.5476668	2.3821846
H	5.1304761	3.3357508	1.3706747
H	5.5008703	1.3847956	3.1794738
H	3.2558775	-0.1942702	3.0576724
H	4.6672651	-0.4353379	2.0266713
H	2.0157987	0.8184176	1.2097790
H	3.1156461	-0.1725510	0.2461267
H	3.8185743	1.6642593	4.8051427
H	1.6869450	0.7778683	4.9209596
H	-0.7291590	0.8432453	4.3679372
H	-0.0063391	4.1119752	1.6560611
H	2.4000568	4.0366592	2.1984898
H	6.6307598	3.3494869	3.8186767
H	6.4423592	4.4329149	5.2247020
H	6.0735737	2.6812348	5.3982975
H	2.5439621	4.3651814	5.7112492
H	4.0519457	5.1689727	6.2315625
H	3.8275604	3.4089140	6.5382502

la_sy_tr_3_ts1.log
E = -1109.604033
H = -1109.301434
G = -1109.366342

NImag=1

C	-1.1598034	2.1085941	-0.5378447
C	-1.4548702	1.5817338	0.7166977
C	-0.3331885	1.9119265	1.6865087
C	0.8299730	2.3549742	0.7876665
C	0.1950300	2.5768811	-0.5895233
O	0.7917169	3.1149679	-1.5340570
C	-1.3530961	-0.6146096	0.6784298
C	0.0324454	-0.8557550	0.3745592
C	0.9281691	-1.1740418	1.4285435
C	2.2917545	-1.2337817	1.2235982
C	2.8187202	-0.9867390	-0.0594657
C	1.9523588	-0.7062741	-1.1258888
C	0.5842683	-0.6435111	-0.9141263
S	-2.4818680	-1.0154174	-0.6027150
C	-4.0467256	-0.3055033	-0.0582010
C	-2.8580560	-2.7740337	-0.3893915
C	4.2320399	-1.0452271	-0.2782377
N	5.3785584	-1.0920236	-0.4531611
H	-1.8347537	2.1449496	-1.3877170
H	-2.4636335	1.4997523	1.1083184
H	-0.0835269	1.0784243	2.3488819
H	-0.6719541	2.7380563	2.3231554
H	1.6076461	1.5865063	0.6982301
H	1.3139263	3.2756843	1.1274439
H	-1.7164856	-0.9385354	1.6543834
H	0.5267024	-1.3642389	2.4202036
H	2.9603917	-1.4728093	2.0448614
H	2.3584101	-0.5274171	-2.1170002
H	-0.0613158	-0.4167880	-1.7564937
H	-4.0439171	0.7598855	-0.2882007
H	-4.8349318	-0.8003272	-0.6284612
H	-4.1757515	-0.4827946	1.0116818
H	-1.9365799	-3.3254959	-0.5843764
H	-3.6234073	-3.0518264	-1.1174366
H	-3.2047814	-2.9442253	0.6317825

la_sy_tr_3_ts1_rot1.log

E = -1109.598903
H = -1109.296458
G = -1109.362272

NImag=1

C	-2.5486144	1.4362597	1.1271682
C	-1.2205710	1.3634999	0.7108713
C	-1.1219897	1.8018932	-0.7405896
C	-2.5602077	1.6770294	-1.2573421
C	-3.4213605	1.6083747	0.0076077
O	-4.6604133	1.6713132	-0.0090846
C	-0.3979011	-0.6517375	0.6873724
C	1.0022609	-0.4147840	0.4217567
C	1.8091070	0.0557966	1.4887589
C	3.1322393	0.4087373	1.2960175
C	3.7076069	0.3009269	0.0187259
C	2.9306252	-0.1620254	-1.0553407
C	1.6054759	-0.5100181	-0.8568378
S	-1.2319866	-1.6818350	-0.4644747
C	-2.9028908	-1.7860960	0.2060129

C	-0.6792832	-3.3763710	-0.1172513
C	5.0786952	0.6559076	-0.1855177
N	6.1906106	0.9447907	-0.3507930
H	-2.9000734	1.3050149	2.1450716
H	-0.3895663	1.5624445	1.3836848
H	-0.3922481	1.2261361	-1.3174151
H	-0.7923762	2.8475290	-0.7611706
H	-2.7116484	0.7498689	-1.8275917
H	-2.8768463	2.5045621	-1.8981210
H	-0.6522023	-0.9265883	1.7109819
H	1.3760583	0.1316576	2.4825665
H	3.7305454	0.7631973	2.1297972
H	3.3727280	-0.2484783	-2.0430889
H	1.0354248	-0.8643051	-1.7117046
H	-3.4611135	-0.8949646	-0.0746650
H	-3.3633363	-2.6664691	-0.2460009
H	-2.8494385	-1.8904494	1.2917372
H	0.3843438	-3.4251728	-0.3570844
H	-1.2407178	-4.0570676	-0.7613904
H	-0.8513000	-3.5956964	0.9386252

la_sy_tr_4.log

E = -1109.626523

H = -1109.321249

G = -1109.387140

NImag=0

C	4.4137503	2.5147135	1.3645747
C	4.3353540	1.6646127	2.6032693
C	3.7314689	0.3382556	2.0793902
C	4.1820666	0.2758121	0.6163691
C	4.3780484	1.7483159	0.2085036
O	4.5199910	2.0744351	-1.0103086
C	3.5235023	2.2195350	3.7999749
C	2.0401613	2.3927625	3.5944210
C	1.5173923	3.3260711	2.6893032
C	0.1435016	3.4284053	2.5006595
C	-0.7146318	2.5921904	3.2236394
C	-0.2066590	1.6612187	4.1374727
C	1.1678992	1.5732397	4.3197022
S	4.2076346	3.8715975	4.2647343
C	5.9240595	3.4939243	4.6612362
C	3.5131157	4.0886588	5.9140167
C	-2.1370416	2.6966630	3.0315590
N	-3.2818352	2.7804831	2.8776953
H	4.6620978	3.5746384	1.3723142
H	5.3269512	1.4370137	3.0325858
H	2.6379261	0.3991043	2.1134490
H	4.0389578	-0.5221029	2.6826409
H	3.4628772	-0.2283636	-0.0378219
H	5.1437272	-0.2457570	0.5094217
H	3.6975297	1.5913355	4.6816972
H	2.1791976	3.9761957	2.1268583
H	-0.2633728	4.1497964	1.7999181
H	-0.8814430	1.0224019	4.6974762
H	1.5714492	0.8543500	5.0270884
H	6.4654774	3.3612860	3.7239468
H	6.3193405	4.3591443	5.1975245
H	5.9704629	2.5966256	5.2816624
H	2.4361733	4.2270476	5.8047773
H	3.9602704	4.9889594	6.3393373
H	3.7381991	3.2114306	6.5237114

la_sy_tr_5.log

E = -1109.628148
H = -1109.322722
G = -1109.388018

NImag=0

C	3.5954943	1.3111382	1.0367959
C	4.0741530	2.4580674	1.8928965
C	5.6134350	2.2803799	1.8886993
C	5.9174972	1.5226809	0.5922039
C	4.6142386	0.7724772	0.2638834
O	4.5925967	-0.1392286	-0.6196141
C	3.4808926	2.3845750	3.3069424
C	1.9791068	2.4491292	3.3965497
C	1.2312092	3.2923839	2.5641204
C	-0.1545670	3.3286911	2.6599053
C	-0.8002948	2.5091735	3.5933364
C	-0.0689061	1.6536940	4.4244037
C	1.3165548	1.6307761	4.3191797
S	4.2951236	3.6985165	4.3614663
C	3.4669571	3.5504814	5.9537946
C	3.6242928	5.2625655	3.7727862
C	-2.2354917	2.5421178	3.6944637
N	-3.3902156	2.5696634	3.7772960
H	2.5443857	1.0622690	0.9163707
H	3.8187089	3.4447888	1.4697330
H	5.9000665	1.6603296	2.7482838
H	6.1479965	3.2326587	1.9745824
H	6.7638588	0.8335793	0.6823193
H	6.1433067	2.2091195	-0.2355209
H	3.8401805	1.4708651	3.7964071
H	1.7253483	3.9210912	1.8296345
H	-0.7348372	3.9804586	2.0154360
H	-0.5808003	1.0167744	5.1379784
H	1.8916950	0.9655916	4.9573304
H	3.6669067	2.5498274	6.3416780
H	3.9141565	4.2994035	6.6105775
H	2.3961168	3.7268787	5.8396833
H	3.9676860	5.4186654	2.7489299
H	4.0386540	6.0369533	4.4218517
H	2.5349943	5.2542637	3.8352155

la_sy_tr_5_ts1.log

E = -1109.598272
H = -1109.295366
G = -1109.361096

NImag=1

C	-1.1415892	-1.9130105	0.8447741
C	-1.6904734	-0.6359526	0.9530891
C	-3.1410234	-0.6801517	0.4946661
C	-3.1868977	-1.9230736	-0.4021576
C	-1.9720248	-2.7491076	0.0308899
O	-1.7983456	-3.9311404	-0.3006940
C	-0.8139915	0.6312581	-0.5476645
C	0.6046920	0.4064829	-0.3753545
C	1.4240643	1.0932101	0.5496306
C	2.7474398	0.7329993	0.7440571
C	3.2957408	-0.3445096	0.0299975
C	2.4968856	-1.0580091	-0.8762888
C	1.1780975	-0.6836168	-1.0720477

S	-1.5372233	2.2255253	-0.4776410
C	-0.3402627	3.4933077	-0.9761218
C	-1.7977323	2.6891616	1.2524777
C	4.6639217	-0.7174954	0.2318124
N	5.7723024	-1.0189339	0.3955091
H	-0.1881200	-2.2298552	1.2530488
H	-1.3835332	0.0538954	1.7353401
H	-3.4793091	0.2314368	-0.0069744
H	-3.7752691	-0.8194804	1.3788355
H	-3.0582321	-1.6541945	-1.4587291
H	-4.1083292	-2.5051294	-0.3167328
H	-1.2504051	0.1390018	-1.4149555
H	1.0287939	1.9113265	1.1416839
H	3.3608098	1.2763546	1.4561072
H	2.9165395	-1.8952321	-1.4253988
H	0.5687455	-1.2314830	-1.7854214
H	-0.0092828	3.2393328	-1.9844532
H	-0.8746312	4.4456720	-0.9859096
H	0.5033834	3.5350359	-0.2876343
H	-2.5952847	2.0603652	1.6506601
H	-2.1295241	3.7296994	1.2395305
H	-0.8879188	2.5865126	1.8427665

la_sy_tr_5_ts2.log

E = -1109.619245

H = -1109.315585

G = -1109.380612

NImag=1

C	-1.9449361	-1.5720455	0.5435110
C	-1.8657444	-0.0871637	0.8056539
C	-3.2841250	0.4198232	0.4849013
C	-3.8501119	-0.5970499	-0.5163419
C	-3.0587792	-1.8894574	-0.2514648
O	-3.4209667	-2.9983630	-0.7165280
C	-0.8843780	0.2039194	-0.2793141
C	0.5269701	-0.2405466	-0.1776203
C	1.1564603	-0.4144101	1.0640414
C	2.4962230	-0.7746283	1.1285540
C	3.2162343	-0.9647120	-0.0577808
C	2.6014123	-0.7975314	-1.3051816
C	1.2628279	-0.4352509	-1.3554209
S	-0.6535777	2.4445759	-0.3532353
C	1.0571218	2.7758016	-0.8273606
C	-0.5463269	2.7861114	1.4151436
C	4.6039523	-1.3378280	0.0054956
N	5.7217187	-1.6371345	0.0557041
H	-1.1821938	-2.2781745	0.8511963
H	-1.5153780	0.2138878	1.7958813
H	-3.2952729	1.4507412	0.1129058
H	-3.8667970	0.3954918	1.4110210
H	-3.6873077	-0.2895802	-1.5580022
H	-4.9234636	-0.7689598	-0.3941006
H	-1.2979864	0.1419742	-1.2847999
H	0.6011943	-0.2788926	1.9867621
H	2.9847874	-0.9109840	2.0875261
H	3.1686729	-0.9520787	-2.2169691
H	0.7765637	-0.2996573	-2.3177652
H	1.1762767	2.5073746	-1.8783879
H	1.2466575	3.8441233	-0.6991456
H	1.7420712	2.1935188	-0.2057767
H	-1.5389498	2.6501047	1.8480082

H	-0.2307611	3.8231979	1.5477940
H	0.1725356	2.1113957	1.8879959

1a_sy_tr_6.log

E = -1109.628036
H = -1109.322477
G = -1109.387752

NImag=0

C	3.5217944	1.7624959	0.7525315
C	4.1203536	2.7643195	1.7086368
C	5.6356080	2.4427420	1.6346999
C	5.7133441	0.9730262	1.2060383
C	4.3839699	0.7108842	0.4763513
O	4.2134459	-0.3405316	-0.2148865
C	3.5594488	2.5317878	3.1321116
C	2.0593667	2.5286125	3.2607109
C	1.2680654	3.4237194	2.5283066
C	-0.1148013	3.4081966	2.6540732
C	-0.7148377	2.4852477	3.5203199
C	0.0602870	1.5815187	4.2546208
C	1.4436438	1.6111018	4.1193106
S	4.3243940	3.7838258	4.3023741
C	3.6676399	3.3322056	5.9176719
C	3.4453725	5.3252924	3.9928277
C	-2.1477553	2.4610591	3.6509552
N	-3.3008001	2.4417874	3.7572441
H	2.4871840	1.8034187	0.4240386
H	3.9321207	3.8108937	1.4304210
H	6.1692707	2.6493618	2.5689782
H	6.0800919	3.0778452	0.8618473
H	5.7885686	0.2928215	2.0657512
H	6.5679216	0.7631745	0.5541698
H	3.9675459	1.5946948	3.5316344
H	1.7306475	4.1318596	1.8471055
H	-0.7291387	4.0983309	2.0854011
H	-0.4163229	0.8656878	4.9159513
H	2.0533547	0.9073500	4.6797123
H	4.0221671	2.3267740	6.1517411
H	4.0765237	4.0459884	6.6357267
H	2.5772717	3.3774736	5.9074082
H	3.6217684	5.6154280	2.9556825
H	3.8841060	6.0687267	4.6616430
H	2.3810793	5.2030800	4.1991896

1a_sy_tr_7.log

E = -1109.626480
H = -1109.320959
G = -1109.386745

NImag=0

C	3.4988199	1.2682825	1.1462591
C	3.9400757	2.5649451	1.7801930
C	5.4809758	2.5059380	1.6410704
C	5.7276246	1.6201833	0.4156946
C	4.4802213	0.7243639	0.3292713
O	4.4549777	-0.2898176	-0.4329876
C	3.4504041	2.6558818	3.2337331
C	1.9478373	2.5707563	3.3632734
C	1.1132926	3.4402564	2.6493281
C	-0.2668329	3.3523665	2.7769881
C	-0.8170436	2.3802694	3.6221831

C	0.0050040	1.5018229	4.3359500
C	1.3854058	1.6074882	4.2052024
S	3.9544255	4.2855270	4.0038231
C	5.6529069	4.0086899	4.5556795
C	3.1206159	4.2206268	5.6045520
C	-2.2465109	2.2847904	3.7584126
N	-3.3967544	2.2090398	3.8690951
H	2.4689311	0.9215606	1.1663851
H	3.5573057	3.4579543	1.2539422
H	5.8985707	2.0161709	2.5297695
H	5.9357730	3.4986204	1.5553892
H	6.6453700	1.0270231	0.4881149
H	5.7946208	2.2140947	-0.5064733
H	3.9307930	1.8902811	3.8547749
H	1.5345572	4.1914188	1.9866094
H	-0.9164345	4.0257099	2.2277082
H	-0.4332744	0.7510275	4.9849564
H	2.0322183	0.9329918	4.7587302
H	6.3225059	4.1112762	3.7039095
H	5.8658652	4.7920460	5.2861744
H	5.7317923	3.0206449	5.0129213
H	2.0537862	4.3774006	5.4439567
H	3.5296927	5.0365818	6.2034077
H	3.3141815	3.2552869	6.0774025

la_sy_tr_7_ts1.log

E = -1109.600123

H = -1109.297596

G = -1109.364118

NImag=1

C	0.3595394	-1.9528871	-1.0677460
C	1.4999932	-1.1536868	-0.9448707
C	2.5187744	-1.8876707	-0.0806881
C	1.6546211	-2.8641337	0.7249615
C	0.3677676	-3.0003461	-0.0942998
O	-0.4716062	-3.8938618	0.1015517
C	1.0852763	0.5571861	0.3020559
C	-0.3525216	0.6908455	0.2372779
C	-1.0416635	1.4997827	-0.6960451
C	-2.4219331	1.4629817	-0.7975603
C	-3.1665557	0.6056570	0.0296519
C	-2.5048510	-0.2174443	0.9530153
C	-1.1236129	-0.1753661	1.0466764
S	1.9965099	1.9286329	-0.3134706
C	3.7043645	1.3606880	-0.2530553
C	2.0390387	3.1659738	1.0100146
C	-4.5943010	0.5702085	-0.0731573
N	-5.7513415	0.5422359	-0.1568891
H	-0.4649681	-1.7788792	-1.7514414
H	1.8415320	-0.5289640	-1.7676934
H	3.1271960	-1.2299953	0.5432670
H	3.2006180	-2.4347439	-0.7437803
H	1.3921406	-2.4438094	1.7053086
H	2.1184426	-3.8395691	0.8950852
H	1.4876910	0.2148206	1.2564593
H	-0.4968392	2.1676398	-1.3575072
H	-2.9320353	2.0960018	-1.5170157
H	-3.0768264	-0.8860869	1.5891237
H	-0.6182327	-0.8158486	1.7644155
H	3.8402307	0.5939197	-1.0165581
H	4.3332755	2.2233509	-0.4809047

H	3.9255518	0.9740612	0.7437382
H	1.0190556	3.5315882	1.1411657
H	2.6927526	3.9824446	0.6947067
H	2.4053989	2.6965532	1.9251532

la_sy_tr_7_ts2.log
E = -1109.618109
H = -1109.314514
G = -1109.379913
NImag=1

C	1.7863197	-1.7652787	-0.4561499
C	1.7627954	-0.3786249	-1.0510209
C	3.2169206	0.1039408	-0.9078333
C	3.7704576	-0.6695338	0.2958164
C	2.9161327	-1.9474068	0.3609906
O	3.2449018	-2.9335865	1.0644481
C	0.8512151	0.1992072	-0.0252707
C	-0.5836680	-0.1824346	0.0204697
C	-1.2888057	-0.5136878	-1.1457840
C	-2.6429906	-0.8124170	-1.0862886
C	-3.3020232	-0.7789393	0.1501661
C	-2.6122640	-0.4476314	1.3226047
C	-1.2580538	-0.1494298	1.2483084
S	0.7189702	2.3946222	-0.4602420
C	1.6120788	2.9914281	0.9921801
C	-0.9567280	2.9096088	-0.0248330
C	-4.7051374	-1.0894652	0.2149437
N	-5.8350463	-1.3387057	0.2670824
H	0.9815853	-2.4831674	-0.5670760
H	1.3761593	-0.2796561	-2.0691337
H	3.3000466	1.1922710	-0.8093532
H	3.7562961	-0.1853173	-1.8152197
H	3.6477604	-0.1147638	1.2365928
H	4.8320398	-0.9153027	0.2009484
H	1.3037324	0.3378019	0.9577987
H	-0.7825302	-0.5378076	-2.1057035
H	-3.1916261	-1.0701164	-1.9861569
H	-3.1336386	-0.4264484	2.2737039
H	-0.7115519	0.1106430	2.1511160
H	2.6549371	2.6821325	0.8972017
H	1.5566344	4.0812953	1.0230911
H	1.1738488	2.5630681	1.8970489
H	-1.6454279	2.4643750	-0.7458005
H	-1.0109561	3.9985900	-0.0912776
H	-1.2029734	2.5795731	0.9866172

la_sy_tr_8.log
E = -1109.622710
H = -1109.316948
G = -1109.380750
NImag=0

C	4.6411446	2.4500279	1.5940829
C	4.4669669	1.4796860	2.7246084
C	3.7895241	0.2571415	2.0365093
C	3.1290462	0.8119209	0.7690750
C	3.8698468	2.1317880	0.4861619
O	3.7016680	2.7509804	-0.6099854
C	3.5796080	1.9063596	3.9331781
C	2.1276044	2.2051223	3.6421827
C	1.7253167	3.1905306	2.7278123

C	0.3780062	3.3760173	2.4406160
C	-0.5797962	2.5735729	3.0708818
C	-0.1967381	1.5907896	3.9903366
C	1.1531328	1.4173105	4.2692858
S	4.2778371	3.2693339	4.9873842
C	4.0862075	4.8391615	4.1199339
C	6.0622170	3.0352224	4.8730826
C	-1.9745878	2.7634437	2.7715414
N	-3.0971464	2.9160212	2.5310804
H	5.2426214	3.3528291	1.6638915
H	5.4100706	1.1528699	3.1805538
H	3.0938338	-0.2677919	2.7013235
H	4.5778262	-0.4520386	1.7649731
H	2.0596631	1.0223103	0.9100353
H	3.2142940	0.1322438	-0.0858672
H	3.6112688	1.0904324	4.6658291
H	2.4621081	3.7982411	2.2173286
H	0.0679181	4.1337072	1.7286376
H	-0.9462778	0.9745514	4.4754107
H	1.4569189	0.6516173	4.9774492
H	3.0399740	5.1380714	4.1833985
H	4.7009172	5.5508373	4.6765501
H	4.4255671	4.7561706	3.0882422
H	6.2945417	2.0346005	5.2411213
H	6.5111689	3.7836123	5.5287528
H	6.3960282	3.1694056	3.8433020

la_sy_tr_8_ts1.log

E = -1109.604033

H = -1109.301433

G = -1109.366335

NImag=1

C	-0.8912074	2.2070739	-0.8252749
C	-1.3311076	1.8369706	0.4428137
C	-0.2506851	2.1391600	1.4670681
C	1.0152199	2.3693099	0.6294125
C	0.5077896	2.5233999	-0.8085789
O	1.2260631	2.9026925	-1.7455632
C	-1.4734562	-0.3513763	0.6057484
C	-0.1056650	-0.7647181	0.4368642
C	0.5559878	-0.7363168	-0.8168003
C	1.9199574	-0.9623933	-0.9112962
C	2.6720600	-1.2285320	0.2419666
C	2.0315472	-1.2945247	1.4951070
C	0.6721828	-1.0725749	1.5834607
S	-2.5468143	-0.7526828	-0.7220121
C	-4.0566046	0.1671546	-0.3702610
C	-3.1322232	-2.4331429	-0.3857089
C	4.0818385	-1.4557762	0.1437867
N	5.2253777	-1.6392311	0.0666163
H	-1.4962377	2.2323444	-1.7266454
H	-2.3677842	1.8993209	0.7576280
H	-0.1432336	1.3515219	2.2179840
H	-0.5388666	3.0535730	1.9993952
H	1.7063312	1.5184404	0.6706816
H	1.5740416	3.2624772	0.9249414
H	-1.9387628	-0.5400710	1.5739157
H	0.0008952	-0.5250186	-1.7250897
H	2.4123882	-0.9231568	-1.8783234
H	2.6096000	-1.5224331	2.3853856
H	0.1829906	-1.1234585	2.5523994

H	-3.9179313	1.1991893	-0.6921933
H	-4.8531118	-0.2945704	-0.9565253
H	-4.2800032	0.1083344	0.6971564
H	-2.2670675	-3.0947679	-0.4564210
H	-3.8706470	-2.6976336	-1.1458115
H	-3.5670538	-2.4667228	0.6151777

la_sy_tr_8_ts2.log

E = -1109.611967
H = -1109.308086
G = -1109.373435

NImag=1

C	2.3312247	1.4011231	-1.0508765
C	2.4147113	0.1393627	-0.2321727
C	1.9715607	2.5117058	-0.2682478
O	1.7491100	3.6947179	-0.6224340
C	1.1494010	-0.4326202	-0.7864858
C	-0.2407814	-0.0307033	-0.4451178
C	-0.7034926	0.1413029	0.8691110
C	-2.0397108	0.4311174	1.1179993
C	-2.9344238	0.5436354	0.0484859
C	-2.4967472	0.3620071	-1.2698529
C	-1.1609829	0.0706511	-1.5028710
C	1.8840181	2.0716296	1.1986529
C	2.4616799	0.6477067	1.2246388
S	1.1687607	-2.6574066	-0.3286428
C	1.2075088	-2.7685242	1.4716432
C	-0.5338716	-3.1680758	-0.6421306
C	-4.3178983	0.8398249	0.3076965
N	-5.4321708	1.0774497	0.5160962
H	2.4889018	1.4283061	-2.1236360
H	3.2528419	-0.5287868	-0.4624869
H	1.2547260	-0.6525425	-1.8479956
H	-0.0321586	0.0385110	1.7119999
H	-2.3905808	0.5623589	2.1361779
H	-3.1973522	0.4462662	-2.0939596
H	-0.8164989	-0.0777251	-2.5226182
H	2.4474562	2.7649800	1.8310051
H	0.8371947	2.1225599	1.5234817
H	1.9747167	-0.0232013	1.9372613
H	3.5186753	0.6917776	1.5045951
H	1.0688353	-3.8143011	1.7558771
H	2.1880764	-2.4279330	1.8085666
H	0.4173120	-2.1564562	1.9118312
H	-0.6355459	-4.2249159	-0.3858883
H	-0.7354257	-3.0299101	-1.7064738
H	-1.2251180	-2.5666239	-0.0458572

la_sy_tr_9.log

E = -1109.625757
H = -1109.320223
G = -1109.385434

NImag=0

C	4.8259797	2.2496661	1.5213599
C	4.5526894	1.3341054	2.6783675
C	3.8306759	0.1267578	2.0167644
C	3.2760182	0.6537086	0.6867522
C	4.0908370	1.9267364	0.3915357
O	3.9965271	2.5131371	-0.7313664
C	3.6723110	1.8941173	3.8367195

C	2.2308629	2.2241206	3.5509221
C	1.8337470	3.0683659	2.5020344
C	0.4856880	3.3029839	2.2590116
C	-0.4798166	2.6937770	3.0689583
C	-0.1027870	1.8533323	4.1218897
C	1.2485311	1.6282606	4.3545307
S	4.5952075	3.2935896	4.6339773
C	3.7350060	3.4595353	6.2094887
C	4.0883820	4.8286334	3.8370255
C	-1.8756488	2.9367343	2.8164464
N	-2.9989653	3.1322866	2.6135409
H	5.4707110	3.1233532	1.5909280
H	5.4635332	0.9873028	3.1881962
H	3.0654377	-0.3096721	2.6691686
H	4.5773722	-0.6506420	1.8272224
H	2.2113216	0.9170606	0.7488913
H	3.3812592	-0.0670449	-0.1316478
H	3.7010646	1.1641890	4.6559734
H	2.5773714	3.5295311	1.8623718
H	0.1802907	3.9520246	1.4448772
H	-0.8575069	1.3853152	4.7449308
H	1.5469808	0.9728055	5.1682008
H	3.9195342	2.5524898	6.7870567
H	4.1638051	4.3228963	6.7219623
H	2.6672399	3.6066116	6.0339300
H	4.3921123	4.7909411	2.7907200
H	4.6311718	5.6223338	4.3554850
H	3.0120558	4.9691560	3.9415750

1a_sy_tr_9_ts1.log

E = -1109.600799

H = -1109.297691

G = -1109.361047

NImag=1

C	1.2116656	-2.0295943	-0.6772944
C	1.6057777	-1.6590411	0.6096098
C	0.5806317	-2.1768718	1.6125432
C	-0.6452629	-2.5309317	0.7577251
C	-0.1217678	-2.5504610	-0.6802091
O	-0.7774504	-2.9935439	-1.6359754
C	1.3958917	0.4609445	0.9747268
C	0.0281725	0.7324752	0.5921217
C	-0.4056279	0.6994488	-0.7510290
C	-1.7516304	0.8121441	-1.0718432
C	-2.7030676	0.9520566	-0.0534556
C	-2.2943544	0.9995652	1.2925567
C	-0.9516528	0.8935235	1.6012995
S	2.7400626	1.2864736	0.2057403
C	2.1596523	2.8743410	-0.4414205
C	3.2033008	0.4855540	-1.3506466
C	-4.0932340	1.0637970	-0.3842518
N	-5.2187682	1.1550329	-0.6500022
H	1.8055598	-1.9406359	-1.5797410
H	2.6485578	-1.6079373	0.9110057
H	0.3621504	-1.4610206	2.4099567
H	0.9930588	-3.0744890	2.0883170
H	-1.4396607	-1.7785372	0.8312953
H	-1.0851532	-3.5006317	1.0094818
H	1.5945801	0.5105050	2.0439679
H	0.3107760	0.5690145	-1.5542618
H	-2.0715711	0.7777028	-2.1086288

H	-3.0334323	1.1227072	2.0780662
H	-0.6359202	0.9306429	2.6403729
H	1.8011741	3.4590059	0.4070180
H	3.0178206	3.3674599	-0.9028150
H	1.3651534	2.7216819	-1.1732208
H	3.5893545	-0.5069210	-1.1192255
H	4.0057588	1.1011394	-1.7638892
H	2.3672749	0.4352592	-2.0473758

la_sy_tr_prod_1.log
E = -631.741910
H = -631.520098
G = -631.572454

NImag=0

C	0.0623270	3.5059294	0.3623326
C	0.7667342	2.2199024	0.6217071
C	-0.2715857	1.2402404	1.1068657
C	-1.6362385	1.9263271	1.0971122
C	-1.3384105	3.4286366	0.9566510
O	0.5171619	4.4484187	-0.2564090
C	0.7240980	1.7736756	2.0875530
C	1.8279051	0.9175943	2.5934942
C	2.4221924	-0.0799026	1.8052725
C	3.4440611	-0.8708208	2.3121015
C	3.8870374	-0.6698057	3.6262315
C	3.3071141	0.3218648	4.4261549
C	2.2858129	1.1056927	3.9047918
H	0.3674611	2.5056709	2.8085762
H	1.6325296	1.9510103	0.0263542
H	-0.1998590	0.1926550	0.8315956
C	4.9445938	-1.4862533	4.1555053
N	5.7972310	-2.1445362	4.5825391
H	-2.2013596	1.5740150	0.2293299
H	-2.2140250	1.6924818	1.9955009
H	-1.3199600	3.9403154	1.9264992
H	-2.0460661	3.9607575	0.3180313
H	2.0906937	-0.2458724	0.7841887
H	3.9000933	-1.6407517	1.6982767
H	3.6558984	0.4736655	5.4424649
H	1.8337595	1.8761894	4.5224791

lb.log
E = -308.557006
H = -308.422842
G = -308.461468

NImag=0

C	0.9410857	-0.1810061	-0.9842478
C	0.3069281	1.1024825	-0.5168417
C	0.9799174	1.3813106	0.8345731
C	1.9519666	0.2294843	1.0350312
C	1.8551464	-0.6778843	-0.1346915
O	2.6876428	0.0744531	1.9961803
C	2.6856480	-1.9134113	-0.2449537
H	0.6673646	-0.6454213	-1.9286709
H	-0.7783352	0.9848443	-0.4281113
H	0.4791643	1.9032809	-1.2438658
H	1.5343998	2.3243404	0.8500373
H	0.2723866	1.4019390	1.6688251
H	2.4738838	-2.4487804	-1.1734938
H	3.7520327	-1.6653176	-0.2193115

H 2.4923674 -2.5850142 0.5982408

1b_sy_c_1.log

E = -1148.923877

H = -1148.588789

G = -1148.656831

NImag=0

C	-0.1096670	3.5505088	-0.1169639
C	0.2246127	4.9415297	0.3553389
C	-1.2151742	3.5516332	-0.9498290
O	-1.7424528	2.5903036	-1.5995589
C	1.3118448	5.6995189	-0.4684578
C	1.8656876	6.9174090	0.2241412
C	2.4757634	6.8133644	1.4817428
C	2.9704112	7.9431607	2.1200122
C	2.8446666	9.1920391	1.4982055
C	2.2339327	9.3119905	0.2449865
C	1.7529900	8.1704187	-0.3865294
C	-1.7774133	4.9813223	-1.0262899
C	-1.1058693	5.7077831	0.1465923
S	2.7067641	4.5441142	-0.8809613
C	2.1437648	3.8429887	-2.4494717
C	3.9835328	5.6589387	-1.5025325
C	3.3514636	10.3666683	2.1569405
N	3.7594615	11.3123964	2.6864083
C	0.6573473	2.3139709	0.2569112
H	0.5488578	4.9701137	1.4052691
H	0.9136538	5.9764680	-1.4521224
H	2.5739367	5.8460674	1.9684050
H	3.4485313	7.8652463	3.0906962
H	2.1428756	10.2852063	-0.2258363
H	1.2821807	8.2524679	-1.3620371
H	-1.5151217	5.4320913	-1.9947902
H	-2.8709045	4.9776964	-0.9601921
H	-1.7134127	5.5948154	1.0503268
H	-0.9589924	6.7812468	-0.0233009
H	2.9221099	3.1603837	-2.7956462
H	1.2105350	3.3118681	-2.2583662
H	1.9933726	4.6577953	-3.1607189
H	4.7266348	5.0336041	-2.0020481
H	4.4390262	6.1700014	-0.6538042
H	3.5417108	6.3704360	-2.2034513
H	-0.0233210	1.4549936	0.3114287
H	1.4533552	2.0147871	-0.4488091
H	1.1405054	2.4182520	1.2376121

1b_sy_c_1_ts1.log

E = -1148.898970

H = -1148.567032

G = -1148.636707

NImag=1

C	2.4457628	-0.8872201	0.9640706
C	1.1452102	-1.1355726	0.5105333
C	3.3887603	-1.4035998	0.0213027
O	4.6291905	-1.3244736	0.0670062
C	0.2393053	0.4573275	-0.6175052
C	-1.1690124	0.2562049	-0.3748395
C	-1.8113084	0.6454882	0.8270233
C	-3.1383936	0.3328253	1.0679031
C	-3.8743819	-0.3924372	0.1175785

C	-3.2569426	-0.7979458	-1.0787697
C	-1.9332120	-0.4766675	-1.3164347
C	2.6180780	-2.0585577	-1.1245715
C	1.1889163	-2.1857812	-0.5850360
S	0.9563047	1.8978194	0.1055024
C	2.5484397	1.9602711	-0.7369639
C	0.1528576	3.3201915	-0.6792974
C	-5.2462748	-0.7156631	0.3645708
N	-6.3589638	-0.9786482	0.5645097
C	2.8494711	-0.1078681	2.1800294
H	0.2965644	-1.0993429	1.1935120
H	0.5687602	0.3463584	-1.6511658
H	-1.2646423	1.1991263	1.5869887
H	-3.6120235	0.6445775	1.9937889
H	-3.8253401	-1.3546939	-1.8174965
H	-1.4684478	-0.7815062	-2.2499980
H	2.6516081	-1.3766454	-1.9863111
H	3.0751210	-3.0038681	-1.4295686
H	1.0396691	-3.1707107	-0.1256633
H	0.4131668	-2.0574573	-1.3444698
H	3.0460765	2.8789025	-0.4218323
H	3.1319373	1.0918901	-0.4328465
H	2.3759227	1.9599969	-1.8153655
H	0.6802693	4.2225752	-0.3610820
H	-0.8801283	3.3493444	-0.3277865
H	0.1924519	3.1993350	-1.7635007
H	3.5808814	-0.6626104	2.7801741
H	3.3240584	0.8529805	1.9305575
H	1.9851856	0.1063712	2.8173282

1b_sy_c_2.log

E = -1148.924549

H = -1148.589610

G = -1148.657559

NImag=0

C	-0.1181276	3.5158573	-0.4805544
C	0.3706521	4.7407468	0.2513557
C	-1.4088672	3.6884722	-0.9570986
O	-2.1480121	2.8924806	-1.6228272
C	1.2788265	5.6944191	-0.5798443
C	1.8632288	6.8706538	0.1589999
C	2.4333811	6.7334936	1.4317856
C	2.9534364	7.8391180	2.0950331
C	2.8996949	9.0963196	1.4829744
C	2.3267993	9.2524208	0.2153545
C	1.8141457	8.1378947	-0.4362856
C	-1.9061833	5.0860688	-0.5499821
C	-0.9377567	5.5165783	0.5575613
S	2.5713731	4.6967491	-1.4521808
C	3.6773418	5.9340645	-2.1529606
C	3.6075369	4.0223171	-0.1420782
C	3.4345900	10.2430614	2.1681932
N	3.8657272	11.1657841	2.7194035
C	0.6287485	2.2145035	-0.5493103
H	0.9111204	4.4938249	1.1763033
H	0.6972908	6.0563038	-1.4374898
H	2.4700063	5.7655452	1.9212061
H	3.3942960	7.7329937	3.0806035
H	2.2852884	10.2328744	-0.2472725
H	1.3654699	8.2507803	-1.4194702
H	-1.8756949	5.7644089	-1.4145653

H	-2.9474598	5.0420907	-0.2128809
H	-1.3142095	5.1806678	1.5292421
H	-0.7886709	6.6010086	0.6178088
H	4.4671318	5.3872704	-2.6722981
H	3.1050503	6.5254633	-2.8703268
H	4.0961452	6.5627633	-1.3654041
H	4.3525763	3.3929889	-0.6332292
H	2.9792588	3.4122855	0.5092237
H	4.0919851	4.8282881	0.4115654
H	1.0628919	1.9353566	0.4227394
H	-0.0722022	1.4223398	-0.8382209
H	1.4556908	2.1739426	-1.2778731

1b_sy_c_2_r.log

E = -1148.920525
H = -1148.585339
G = -1148.653822

NImag=0

C	-1.2848058	-0.0563248	-2.0638075
C	-1.6458716	-0.5696615	-0.6993975
C	-2.3348666	0.5917665	-2.6877919
O	-2.3755564	1.1868506	-3.8162166
C	-0.7703530	0.1267319	0.3783707
C	-0.6794943	1.6301485	0.3833433
C	-1.8118073	2.4564494	0.3651831
C	-1.6788812	3.8382630	0.3519739
C	-0.3985653	4.4072429	0.3604486
C	0.7423077	3.6000141	0.3823283
C	0.5914333	2.2172883	0.3934256
C	-3.5791679	0.5273445	-1.7907410
C	-3.1869814	-0.3870346	-0.6181246
S	-1.1655490	-0.5787870	2.0638384
C	0.3783440	-0.3126988	2.9572136
C	-2.2212031	0.6097592	2.9157888
C	-0.2565120	5.8392870	0.3511242
N	-0.1417657	6.9916625	0.3459650
C	0.1076602	-0.1606464	-2.6041940
H	-1.3991852	-1.6373319	-0.5717157
H	0.2455013	-0.2680967	0.2521580
H	-2.8083847	2.0296751	0.3706893
H	-2.5568672	4.4753454	0.3362437
H	1.7296654	4.0495045	0.3886021
H	1.4743446	1.5836916	0.4020754
H	-3.8525153	1.5431245	-1.4747337
H	-4.4343084	0.1357072	-2.3538757
H	-3.6481764	-1.3710770	-0.7425736
H	-3.5310402	-0.0111006	0.3516581
H	0.2094373	-0.6154299	3.9924020
H	1.1386930	-0.9481448	2.5008603
H	0.6576513	0.7416593	2.9035235
H	-2.3724185	0.2048575	3.9188844
H	-3.1785619	0.6705330	2.3979096
H	-1.7287570	1.5820344	2.9629533
H	0.5029493	-1.1869320	-2.5596779
H	0.1210160	0.1578296	-3.6523436
H	0.8356029	0.4716390	-2.0667682

1b_sy_c_2_ts1.log

E = -1148.895924
H = -1148.563325

G = -1148.631604
 NImag=1

C	-2.8723733	-0.5318961	-0.7283389
C	-1.5019576	-0.7896359	-0.8460252
C	-3.4725795	-1.5056967	0.1331540
O	-4.6614114	-1.5763183	0.4892739
C	-0.3257522	0.2974262	0.5941871
C	1.0908125	0.0979089	0.3604136
C	1.8151805	0.7513678	-0.6641537
C	3.1473711	0.4556477	-0.9069136
C	3.8022993	-0.5192574	-0.1403323
C	3.1020186	-1.1947513	0.8739734
C	1.7758696	-0.8858293	1.1158388
C	-2.3957541	-2.4944782	0.5775261
C	-1.2095256	-2.1924515	-0.3438638
S	-1.0418245	1.8976142	0.6165798
C	0.0842508	3.0134033	1.4921603
C	-0.9593926	2.6366497	-1.0384067
C	5.1773724	-0.8276996	-0.3935959
N	6.2917911	-1.0778031	-0.5985040
C	-3.6509741	0.6061655	-1.3166888
H	-0.9014839	-0.3851615	-1.6605117
H	-0.7212492	-0.2131308	1.4718877
H	1.3323722	1.4904794	-1.2930020
H	3.6841847	0.9710042	-1.6973378
H	3.6070536	-1.9480455	1.4706532
H	1.2451728	-1.4023721	1.9112381
H	-2.1474871	-2.2876295	1.6270284
H	-2.7580900	-3.5247179	0.5203888
H	-1.2115185	-2.8693729	-1.2069728
H	-0.2351876	-2.2893879	0.1409937
H	-0.3259311	4.0231395	1.4164988
H	0.1122557	2.6942283	2.5350118
H	1.0776361	2.9652282	1.0419257
H	-1.7657339	3.3708987	-1.0917427
H	-1.1170492	1.8574577	-1.7833928
H	0.0036766	3.1269226	-1.1846302
H	-3.2228941	0.9484972	-2.2646858
H	-4.6822149	0.2893053	-1.5067767
H	-3.7136682	1.4789301	-0.6491470

lb_sy_c_2_ts2.log
 E = -1148.909187
 H = -1148.575707
 G = -1148.644906
 NImag=1

C	-2.3228010	-1.2188327	0.6054854
C	-2.2662542	0.1118711	-0.1050192
C	-1.9634708	-2.2660688	-0.2564761
O	-1.8424154	-3.4890058	0.0175698
C	-1.0167100	0.5602086	0.5835288
C	0.3610509	0.0742632	0.3159382
C	0.9222632	-0.0218617	-0.9682411
C	2.2447175	-0.4129315	-1.1363943
C	3.0285807	-0.7056539	-0.0144157
C	2.4942715	-0.5992197	1.2759383
C	1.1736464	-0.2034345	1.4292609
C	-1.7404505	-1.7152098	-1.6668044
C	-2.2269760	-0.2580129	-1.6017089
S	-0.8665198	2.7968763	0.3485041
C	0.8390958	3.1567539	0.8169618

C	-0.7697668	3.0562354	-1.4339033
C	4.3973815	-1.1103016	-0.1889555
N	5.5000038	-1.4363012	-0.3293071
C	-2.6886396	-1.4072475	2.0468257
H	-3.0843977	0.8047324	0.1335180
H	-1.1902250	0.6811402	1.6533197
H	0.3379171	0.2185909	-1.8472917
H	2.6716651	-0.4854890	-2.1311691
H	3.1094047	-0.8217807	2.1414740
H	0.7577255	-0.1094981	2.4286589
H	-0.6784086	-1.8056700	-1.9290662
H	-2.2986314	-2.3113674	-2.3961925
H	-3.2572113	-0.2025089	-1.9665477
H	-1.6394535	0.4364103	-2.2082942
H	1.0316312	4.2189220	0.6496624
H	0.9499324	2.9284124	1.8790075
H	1.5299803	2.5499145	0.2260315
H	-0.5393125	4.1082040	-1.6174110
H	-1.7452601	2.8182043	-1.8614119
H	0.0054160	2.4240551	-1.8721303
H	-3.2231889	-0.5342740	2.4397247
H	-3.3441808	-2.2788250	2.1646419
H	-1.8227245	-1.5805507	2.7040948

1b_sy_c_3.log

E = -1148.921817

H = -1148.586512

G = -1148.654561

NImag=0

C	-0.0377793	4.0317006	0.1574978
C	-0.1426716	5.4343737	-0.3913466
C	-0.8377039	3.1268754	-0.5256362
O	-1.0207241	1.8855993	-0.3102842
C	1.1930443	6.0926063	-0.8812633
C	1.8413242	7.1043647	0.0333209
C	2.0465453	6.8493471	1.3945523
C	2.6483110	7.8008127	2.2089334
C	3.0440754	9.0254551	1.6580442
C	2.8402951	9.2993010	0.3014078
C	2.2426493	8.3346441	-0.5010740
C	-1.5756981	3.8373566	-1.6639187
C	-1.1679960	5.3145555	-1.5656859
S	2.4110090	4.7400440	-1.2267488
C	1.7940788	4.0607167	-2.7802131
C	3.8171093	5.6817841	-1.8626289
C	3.6621898	10.0165651	2.4986265
N	4.1601897	10.8143819	3.1743380
C	0.6298043	3.6816761	1.4536085
H	-0.5205011	6.1452545	0.3615853
H	1.0513224	6.5674128	-1.8582554
H	1.7338598	5.9063555	1.8288934
H	2.8078907	7.6021508	3.2634726
H	3.1476192	10.2528524	-0.1149341
H	2.0842151	8.5408644	-1.5557647
H	-1.3182065	3.3837931	-2.6304994
H	-2.6541420	3.6912780	-1.5306901
H	-2.0318556	5.9530348	-1.3610969
H	-0.7316594	5.6728106	-2.5036652
H	2.5773632	3.4096427	-3.1736026
H	0.9025143	3.4764206	-2.5552991
H	1.5821171	4.8757321	-3.4755253

H	4.5051267	4.9574218	-2.3038320
H	4.3003645	6.1820572	-1.0223595
H	3.4833817	6.4025060	-2.6120032
H	0.4103319	2.6326639	1.6822558
H	1.7264218	3.7872579	1.4521582
H	0.2608838	4.2894310	2.2956324

lb_sy_c_3_r.log

E = -1148.923673

H = -1148.588625

G = -1148.657351

NImag=0

C	-0.6444809	-1.9559132	0.4666766
C	-1.2501709	-0.6840997	0.9972015
C	-1.3700789	-2.4827698	-0.5865902
O	-1.1326381	-3.5021422	-1.3175949
C	-0.3451320	0.5295179	0.6386158
C	-0.0210361	0.7088818	-0.8269189
C	-0.9642722	1.1735691	-1.7516496
C	-0.6340743	1.2992680	-3.0958986
C	0.6544303	0.9585887	-3.5214202
C	1.6125368	0.5042433	-2.6079383
C	1.2693468	0.3914233	-1.2663937
C	-2.6188459	-1.6183323	-0.8225285
C	-2.6720657	-0.6657465	0.3809995
S	-1.0804728	2.1175568	1.2447256
C	-1.2172451	1.8328944	3.0191118
C	0.3468872	3.2185791	1.1858356
C	1.0009730	1.0881031	-4.9118616
N	1.2805797	1.1932071	-6.0307978
C	0.6600389	-2.4903918	0.9721004
H	-1.3056200	-0.6816273	2.0959583
H	0.5901710	0.4404492	1.2042086
H	-1.9683171	1.4414955	-1.4362321
H	-1.3664989	1.6579128	-3.8113825
H	2.6114997	0.2507310	-2.9467078
H	2.0112161	0.0492648	-0.5506029
H	-2.5189092	-1.0868636	-1.7786854
H	-3.5134147	-2.2469523	-0.8998826
H	-3.3646292	-1.0578008	1.1324247
H	-3.0282360	0.3393948	0.1256448
H	-1.3658444	2.8101127	3.4829411
H	-2.0905350	1.2045964	3.1962888
H	-0.3035010	1.3622691	3.3877020
H	0.0515052	4.1598622	1.6531606
H	0.5934143	3.3865776	0.1361010
H	1.1816195	2.7590529	1.7188581
H	0.8474129	-3.4757955	0.5311097
H	1.5269807	-1.8568578	0.7212895
H	0.6730564	-2.6057023	2.0666144

lb_sy_c_3_ts2.log

E = -1148.911075

H = -1148.577826

G = -1148.647641

NImag=1

C	1.8770632	1.6697625	0.4935085
C	2.0921592	0.5468124	-0.4948306
C	1.0652049	2.6697916	-0.0632617
O	0.6217682	3.7069399	0.4956130

C	1.1144112	-0.3507200	0.1858223
C	-0.3708218	-0.1950743	0.1156166
C	-1.0870628	-0.3104663	-1.0843504
C	-2.4742011	-0.2241142	-1.0910582
C	-3.1585986	-0.0280971	0.1136180
C	-2.4609204	0.0709708	1.3246261
C	-1.0763472	-0.0257785	1.3161723
C	0.7755859	2.3378232	-1.5315259
C	1.6975609	1.1496334	-1.8538104
S	1.3554781	-2.4221708	-0.5695763
C	3.0181461	-2.7184021	0.0691550
C	0.3779805	-3.2606310	0.6963004
C	-4.5942319	0.0594051	0.1084179
N	-5.7504719	0.1291016	0.1047008
C	2.4216875	1.7067264	1.8893270
H	3.0944023	0.1024882	-0.4969498
H	1.4424468	-0.6248858	1.1917037
H	-0.5681965	-0.4840596	-2.0214119
H	-3.0258585	-0.3143122	-2.0209515
H	-3.0006553	0.2154214	2.2546113
H	-0.5270492	0.0419615	2.2513414
H	-0.2896072	2.1012443	-1.6503918
H	0.9810748	3.2094802	-2.1613997
H	2.6166369	1.5173486	-2.3203767
H	1.2605916	0.4176152	-2.5394312
H	3.1781902	-3.7952539	0.1528518
H	3.7317435	-2.2997240	-0.6419153
H	3.1353698	-2.2425624	1.0468729
H	0.6299899	-4.3228872	0.6944393
H	-0.6767345	-3.1351014	0.4437595
H	0.5859042	-2.8234858	1.6770755
H	3.0456744	2.5955359	2.0547450
H	1.6329713	1.7352705	2.6550959
H	3.0468444	0.8301858	2.0947693

lb_sy_c_4.log

E = -1148.922023

H = -1148.586950

G = -1148.655541

NImag=0

C	-0.0528697	3.9675345	0.1857919
C	-0.1920543	5.4289565	-0.1598039
C	-0.7840467	3.1558454	-0.6690407
O	-0.8678437	1.8858402	-0.7105106
C	1.0863359	6.1009278	-0.7797523
C	1.7736696	7.1132774	0.1034459
C	2.0497497	8.3901873	-0.3952832
C	2.6766748	9.3423386	0.4009393
C	3.0393554	9.0048244	1.7090991
C	2.7704134	7.7297983	2.2232274
C	2.1342118	6.7932572	1.4190298
C	-1.5406319	4.0291393	-1.6804583
C	-1.3938292	5.4585468	-1.1447243
S	2.3312072	4.7903072	-1.2033967
C	1.6958853	4.0590748	-2.7271009
C	3.6513391	5.8060314	-1.9110931
C	3.6939331	9.9813040	2.5390841
N	4.2215417	10.7671475	3.2063462
C	0.6794937	3.4646399	1.3936544
H	-0.4202528	6.0462578	0.7217019
H	0.8633277	6.5677672	-1.7454745

H	1.7712130	8.6416413	-1.4146242
H	2.8877585	10.3342262	0.0153975
H	3.0547215	7.4830068	3.2406802
H	1.9162453	5.8083525	1.8228362
H	-1.1127561	3.9031486	-2.6845146
H	-2.5863253	3.7081210	-1.7432871
H	-2.2890956	5.7313096	-0.5771580
H	-1.2708629	6.2103091	-1.9315097
H	2.5603660	3.6682244	-3.2679986
H	1.0237110	3.2468805	-2.4543622
H	1.1898098	4.8262331	-3.3174050
H	4.3650181	5.1181806	-2.3686106
H	4.1364534	6.3526503	-1.1016547
H	3.2407156	6.4895539	-2.6577161
H	0.3369967	3.9502758	2.3208342
H	0.4976508	2.3885184	1.4953176
H	1.7724703	3.6015645	1.3617936

1b_sy_c_5.log

E = -1148.924316

H = -1148.589569

G = -1148.658191

NImag=0

C	-0.4850573	4.8535952	-1.0172849
C	0.7760951	4.1597537	-0.5839507
C	-1.2050362	5.3426606	0.0590641
O	-2.2763110	6.0347637	0.0841048
C	2.0203264	5.0476316	-0.9127062
C	2.0990342	6.3187876	-0.1043424
C	2.7332451	6.4001686	1.1408281
C	2.6941091	7.5766364	1.8801726
C	2.0018642	8.6818152	1.3734405
C	1.3672277	8.6185392	0.1271611
C	1.4288245	7.4408808	-0.6070797
C	-0.4904676	4.9441532	1.3603150
C	0.5637715	3.9143504	0.9283854
S	3.5853337	4.0845133	-0.7080983
C	3.4256347	2.8372584	-2.0021554
C	4.7926326	5.1876815	-1.4704763
C	1.9513326	9.9003147	2.1365620
N	1.9114870	10.8817934	2.7502224
C	-0.8010383	5.1131840	-2.4572330
H	0.9328859	3.2134001	-1.1220322
H	2.0044860	5.2925178	-1.9816662
H	3.2602592	5.5467570	1.5592379
H	3.1878979	7.6372591	2.8441085
H	0.8386340	9.4835899	-0.2593831
H	0.9468115	7.3865064	-1.5786284
H	-0.0392626	5.8411052	1.8090175
H	-1.2013372	4.5422507	2.0911501
H	0.1671580	2.9020641	1.0550877
H	1.4906404	3.9692049	1.5117549
H	4.4299717	2.4506729	-2.1864402
H	2.7861614	2.0353515	-1.6345807
H	3.0137431	3.2970097	-2.9032093
H	5.7279749	4.6319554	-1.5587443
H	4.9302344	6.0445842	-0.8094994
H	4.4267163	5.4990900	-2.4511281
H	-1.7971377	5.5623780	-2.5378520
H	-0.0962100	5.8078134	-2.9460753
H	-0.7970353	4.1972083	-3.0671466

1b_sy_c_5_ts1.log

E = -1148.903091

H = -1148.570933

G = -1148.639735

NImag=1

C	-0.4535551	2.3935070	-0.2859195
C	-1.2829413	1.5794448	0.4921484
C	0.8386085	2.5079302	0.3161762
O	1.8151790	3.1686170	-0.0813504
C	-1.3985310	-0.3183394	-0.4377620
C	-0.0392796	-0.8069423	-0.3907173
C	0.4581365	-1.7121757	0.5797130
C	1.8088263	-1.9889071	0.6762374
C	2.7189392	-1.3647008	-0.1968686
C	2.2482799	-0.4874877	-1.1841614
C	0.8925224	-0.2194281	-1.2803486
C	0.8443693	1.7066166	1.6201133
C	-0.6229334	1.3009959	1.8337300
S	-2.5996513	-1.3441923	0.3366507
C	-4.0679317	-0.3017766	0.4138819
C	-3.1352373	-2.5297081	-0.9260388
C	4.1198193	-1.6431485	-0.0917555
N	5.2548558	-1.8689779	-0.0056120
C	-0.8197413	3.0069582	-1.6006443
H	-2.3629830	1.6902376	0.4392894
H	-1.7552550	0.0261566	-1.4095776
H	-0.2172609	-2.1986491	1.2777429
H	2.1720593	-2.6819179	1.4287051
H	2.9488804	-0.0179644	-1.8680572
H	0.5346261	0.4525360	-2.0538583
H	1.5041057	0.8384638	1.4968320
H	1.2492898	2.3136871	2.4359075
H	-1.0951896	1.9303072	2.5969927
H	-0.7366809	0.2609159	2.1594933
H	-4.9166110	-0.9633042	0.5968242
H	-3.9574904	0.3905267	1.2488299
H	-4.1897520	0.2303726	-0.5320775
H	-3.9497586	-3.1271108	-0.5107404
H	-2.2782233	-3.1668053	-1.1517362
H	-3.4587810	-1.9825133	-1.8138468
H	-0.1679538	3.8591828	-1.8194563
H	-0.7147835	2.2995747	-2.4375944
H	-1.8579508	3.3585272	-1.6103764

1b_sy_c_6.log

E = -1148.922539

H = -1148.587482

G = -1148.655652

NImag=0

C	-0.2493888	3.7174249	-0.9019009
C	0.3992397	4.7998595	-0.0727252
C	-1.6209947	3.6780977	-0.6941971
O	-2.4775240	2.8288638	-1.1049292
C	1.4449246	5.6987397	-0.7712153
C	1.9400053	6.8643801	0.0465673
C	2.2880992	6.7216607	1.3968516
C	2.7268709	7.8170026	2.1310980
C	2.8140781	9.0695199	1.5119998
C	2.4616550	9.2306823	0.1672923

C	2.0275765	8.1257886	-0.5547814
C	-2.0301801	4.8166702	0.2465386
C	-0.7926961	5.7111370	0.3340525
S	2.8560204	4.6743249	-1.4193464
C	4.0566760	5.9018596	-1.9651472
C	3.6876313	4.0191067	0.0382270
C	3.2641213	10.2067682	2.2701165
N	3.6267577	11.1221938	2.8797055
C	0.4826864	2.5448991	-1.4964113
H	0.8796067	4.3894796	0.8342532
H	1.0126734	6.0666851	-1.7103458
H	2.2080419	5.7566811	1.8879161
H	2.9952865	7.7077619	3.1765922
H	2.5268719	10.2073963	-0.3003747
H	1.7493908	8.2429276	-1.5985250
H	-2.9187740	5.3460143	-0.1149598
H	-2.2890950	4.3807287	1.2216747
H	-0.6424837	6.1665942	1.3174098
H	-0.8756421	6.5279390	-0.3942539
H	4.9103291	5.3470778	-2.3600028
H	3.5964019	6.4886951	-2.7624760
H	4.3591421	6.5349386	-1.1294712
H	4.5166326	3.4117013	-0.3316202
H	2.9830092	3.3877112	0.5812099
H	4.0590816	4.8345108	0.6607182
H	-0.2331380	1.7243533	-1.6287685
H	0.9450789	2.7236263	-2.4772186
H	1.2859272	2.1751984	-0.8372525

1b_sy_c_7.log

E = -1148.921669

H = -1148.586444

G = -1148.654366

NImag=0

C	-0.1604845	4.0842685	0.1977398
C	-0.4139770	5.4974656	-0.2790347
C	-0.6539894	3.1389235	-0.6928547
O	-0.6083640	1.8682218	-0.6271922
C	0.8033130	6.2957588	-0.8478893
C	1.6216054	7.1434835	0.0906765
C	1.8941963	6.7510965	1.4063833
C	2.6319614	7.5699684	2.2528700
C	3.1024289	8.8004509	1.7805381
C	2.8326402	9.2146613	0.4715024
C	2.0926460	8.3843205	-0.3612924
C	-1.3343350	3.8485514	-1.8701362
C	-1.4807974	5.2986561	-1.3946271
S	1.8346816	5.0908828	-1.8228208
C	2.9213504	6.1970782	-2.7488875
C	3.0338448	4.3620989	-0.6959818
C	3.8640500	9.6539898	2.6537871
N	4.4776003	10.3408891	3.3557909
C	0.3663122	3.6959467	1.5479926
H	-0.8101882	6.1525018	0.5124114
H	0.4545942	6.9527088	-1.6532792
H	1.5263215	5.8034360	1.7795523
H	2.8404855	7.2623972	3.2721966
H	3.1925575	10.1749770	0.1177302
H	1.8696850	8.7078592	-1.3744671
H	-0.7193392	3.7576714	-2.7761325
H	-2.2976299	3.3752326	-2.0893251

H	-2.4684671	5.4331836	-0.9419808
H	-1.3906538	6.0362882	-2.1999757
H	3.5576992	5.5648035	-3.3712865
H	2.2977974	6.8298373	-3.3830987
H	3.5297012	6.7962218	-2.0690760
H	3.7972196	3.9023266	-1.3282308
H	2.5208444	3.5999605	-0.1119992
H	3.4802132	5.1311303	-0.0625277
H	0.1018997	2.6480689	1.7327976
H	1.4588584	3.7656619	1.6778712
H	-0.0756817	4.3008211	2.3540559

1b_sy_c_7_ts1.log

E = -1148.895968
H = -1148.563438
G = -1148.631432

NImag=1

C	1.5611500	-1.6913985	0.0092895
C	1.3676407	-0.9589186	-1.1711473
C	2.9125412	-1.5686878	0.4454231
O	3.4254804	-2.0378934	1.4789642
C	0.3979716	0.8895813	-0.9485825
C	-0.9712462	0.5834666	-0.5718436
C	-1.4606033	0.5662906	0.7529145
C	-2.7493708	0.1449239	1.0380512
C	-3.5944087	-0.2851493	0.0041177
C	-3.1310282	-0.2809584	-1.3213075
C	-1.8455671	0.1506305	-1.5974213
C	3.6824008	-0.7178695	-0.5658204
C	2.7231291	-0.5838484	-1.7549224
S	1.3976173	1.9900842	-0.0185955
C	0.4117219	3.4419599	0.4439983
C	1.6992014	1.2562915	1.6217066
C	-4.9256790	-0.7235595	0.2997508
N	-6.0039631	-1.0789000	0.5385576
C	0.5098190	-2.4030889	0.8071531
H	0.5546650	-1.2066546	-1.8530070
H	0.5316259	1.1669291	-1.9928504
H	-0.8328754	0.8739176	1.5818746
H	-3.1058482	0.1416207	2.0633115
H	-3.7834329	-0.6094899	-2.1243559
H	-1.4967680	0.1600806	-2.6265960
H	3.9081720	0.2555853	-0.1082102
H	4.6402114	-1.1816885	-0.8190470
H	2.9729957	-1.3116356	-2.5358845
H	2.7352365	0.4056356	-2.2214978
H	1.0396669	4.0680129	1.0820502
H	0.1686437	3.9697888	-0.4794108
H	-0.4934528	3.1368896	0.9707416
H	2.7563910	1.3943732	1.8523151
H	1.4582476	0.1940579	1.5815583
H	1.0812297	1.7670817	2.3614307
H	0.8332002	-3.4151493	1.0798229
H	0.2823454	-1.8858375	1.7507282
H	-0.4271534	-2.4858706	0.2450395

1b_sy_c_8.log

E = -1148.920771
H = -1148.585698
G = -1148.655049

NImag=0

C	-0.5764671	5.1679314	-0.8436362
C	0.7239314	4.4104764	-0.7380518
C	-1.5197481	4.6594669	0.0357304
O	-2.7627270	4.9216239	0.1432769
C	1.9734514	5.3050663	-0.9497200
C	2.1080715	6.5337321	-0.0757861
C	2.4902473	6.4759992	1.2716744
C	2.5826754	7.6356180	2.0328737
C	2.2956632	8.8708323	1.4430247
C	1.9377690	8.9497211	0.0928010
C	1.8575054	7.7827943	-0.6565899
C	-0.8693928	3.5640445	0.8929594
C	0.6343735	3.7086589	0.6346551
S	3.5104052	4.2977487	-0.7329842
C	3.3511290	3.0342376	-2.0088098
C	4.7506577	5.3743363	-1.4776664
C	2.3888467	10.0733895	2.2275287
N	2.4642749	11.0415805	2.8583938
C	-0.9238604	5.9882868	-2.0492406
H	0.7924198	3.6523339	-1.5406896
H	2.0039796	5.6166151	-2.0010208
H	2.7366423	5.5310593	1.7454851
H	2.8780266	7.5852410	3.0754905
H	1.7358196	9.9133297	-0.3630214
H	1.6012416	7.8437804	-1.7096792
H	-1.1360670	3.6575704	1.9515675
H	-1.2482847	2.5911146	0.5488850
H	1.1767926	2.7562382	0.6539872
H	1.0625777	4.3494530	1.4098976
H	4.3429607	2.5942813	-2.1335141
H	2.6535270	2.2750541	-1.6543149
H	3.0067275	3.4906983	-2.9388705
H	5.6796218	4.8041764	-1.5363027
H	4.8843005	6.2345969	-0.8197096
H	4.4155522	5.6830781	-2.4699398
H	-2.0015368	6.1882700	-2.0481510
H	-0.4146533	6.9604473	-2.1101396
H	-0.6855537	5.4588174	-2.9874932

1b_sy_c_9.log

E = -1148.922391

H = -1148.587417

G = -1148.654605

NImag=0

C	-0.4253966	4.7333598	-0.9051177
C	0.9328230	4.2048771	-0.5388273
C	-1.1192773	5.2034491	0.1973048
O	-2.2585343	5.7719534	0.2680995
C	2.0352537	5.2038082	-1.0219693
C	2.1032239	6.4834494	-0.2281859
C	2.9122423	6.6430828	0.9019713
C	2.8634329	7.8146710	1.6485470
C	1.9868486	8.8355657	1.2646137
C	1.1758648	8.6946923	0.1319524
C	1.2464887	7.5234332	-0.6113329
C	-0.2741454	4.9638134	1.4566268
C	0.8582591	4.0339915	0.9987406
S	3.7322437	4.4685391	-1.1993732
C	3.8610513	3.1252115	0.0007334
C	3.5334554	3.5278833	-2.7248371

C	1.9275155	10.0483298	2.0361775
N	1.8804232	11.0255535	2.6561387
C	-0.8654901	4.8852898	-2.3274436
H	1.1528852	3.2477690	-1.0358281
H	1.8254578	5.4522393	-2.0695472
H	3.5883638	5.8564064	1.2273991
H	3.4926437	7.9368900	2.5237017
H	0.5065836	9.4966903	-0.1615509
H	0.6284950	7.4087051	-1.4969971
H	0.1054080	5.9298087	1.8216181
H	-0.8800237	4.5318217	2.2612257
H	0.5968975	2.9917482	1.2106235
H	1.8051968	4.2358794	1.5094026
H	4.7736828	2.5845742	-0.2595290
H	3.9638891	3.5552711	0.9971401
H	2.9932930	2.4677161	-0.0645644
H	4.4465369	2.9460084	-2.8627621
H	3.4211806	4.2453585	-3.5389385
H	2.6631974	2.8736282	-2.6510095
H	-0.7773494	3.9523027	-2.9040736
H	-1.9155525	5.1967597	-2.3545802
H	-0.2927682	5.6456691	-2.8870491

lb_sy_c_9_ts1.log

E = -1148.900072

H = -1148.568033

G = -1148.636649

NImag=1

C	-0.6933572	2.3233104	-0.1666663
C	-1.4067588	1.3430051	0.5254866
C	0.5825435	2.5389118	0.4453778
O	1.4683068	3.3425065	0.1039352
C	-1.3027144	-0.4491859	-0.6316175
C	0.0835931	-0.8270909	-0.5686742
C	0.5927265	-1.8051572	0.3212579
C	1.9529099	-1.9969183	0.4742288
C	2.8596139	-1.2037436	-0.2537702
C	2.3791768	-0.2419389	-1.1562294
C	1.0156462	-0.0626743	-1.3140639
C	0.6940822	1.6385506	1.6766458
C	-0.6981212	1.0051747	1.8274270
S	-2.4773812	-1.7167376	-0.2139021
C	-3.0685163	-1.4162908	1.4742083
C	-3.9178596	-1.1629075	-1.1442093
C	4.2687502	-1.3902146	-0.0852161
N	5.4111787	-1.5428933	0.0520848
C	-1.1312883	2.9899566	-1.4317910
H	-2.4933780	1.3069418	0.4770966
H	-1.6361023	0.0289485	-1.5510983
H	-0.0849899	-2.4154845	0.9150658
H	2.3261934	-2.7496863	1.1615972
H	3.0804167	0.3589054	-1.7275902
H	0.6494439	0.6735722	-2.0229966
H	1.4750973	0.8881303	1.4986141
H	0.9981803	2.2268918	2.5482491
H	-1.2528096	1.4522568	2.6610833
H	-0.6459171	-0.0705083	2.0167415
H	-3.9114647	-2.0948793	1.6235520
H	-2.2664394	-1.6781736	2.1650634
H	-3.3800332	-0.3793741	1.6001532
H	-4.7656057	-1.7804361	-0.8437522

H	-3.7018784	-1.3095715	-2.2031900
H	-4.1039249	-0.1096255	-0.9246499
H	-2.2152755	3.1491914	-1.4527151
H	-0.6392280	3.9612701	-1.5471341
H	-0.8767578	2.3943011	-2.3223220

lb_sy_c_prod_1.log

E = -671.038631

H = -670.787707

G = -670.843098

NImag=0

C	0.9753701	-0.2892521	-1.7831079
C	0.3332128	0.3834398	-2.9549733
C	-0.9038337	-0.4440584	-3.2764940
C	-1.0297047	-1.5829293	-2.2669126
C	0.3084901	-1.6294763	-1.5101889
O	1.8591860	0.2029735	-1.1069993
C	0.2609663	-0.4663913	-4.2146577
C	1.1102007	-1.6733223	-4.4601521
C	2.4987008	-1.6188670	-4.2839849
C	3.2918289	-2.7316126	-4.5344363
C	2.6872145	-3.9184158	-4.9685088
C	1.3016077	-3.9882963	-5.1582589
C	0.5236439	-2.8644185	-4.9041572
H	0.1318258	0.1526102	-5.1020289
C	0.4291569	1.8821231	-3.0585780
H	-1.8053231	0.0644369	-3.6035881
C	3.4994494	-5.0769878	-5.2253740
N	4.1539440	-6.0101692	-5.4325757
H	-1.8422633	-1.3465553	-1.5743452
H	-1.2713443	-2.5355395	-2.7476886
H	0.9727321	-2.4268554	-1.8643085
H	0.1894048	-1.7594068	-0.4317691
H	2.9608768	-0.6956894	-3.9442189
H	4.3672047	-2.6892013	-4.3955895
H	0.8460743	-4.9126920	-5.4983177
H	-0.5516948	-2.9106524	-5.0507356
H	1.4679343	2.1951050	-3.2048330
H	-0.1595957	2.2411456	-3.9073124
H	0.0533350	2.3623547	-2.1496049

lb_sy_tr_.log

E = -1148.921184

H = -1148.586210

G = -1148.654353

NImag=0

C	-0.3129241	3.0392955	1.2494343
C	0.6638731	2.3323639	0.3465333
C	-0.9726087	2.1613211	2.0891008
O	-1.9270359	2.3667395	2.9115554
C	1.9372974	3.1627123	0.0765385
C	2.8919139	2.6918094	-0.9893109
C	3.3561152	1.3701901	-1.0482981
C	4.2193693	0.9695831	-2.0600191
C	4.6268689	1.8981936	-3.0257402
C	4.1767733	3.2213418	-2.9811856
C	3.3130408	3.6072096	-1.9624305
C	-0.4227628	0.7475981	1.8554111
C	0.8484232	0.9513356	1.0214334
S	2.7947713	3.5364002	1.6979275

C	4.2608596	2.4850894	1.7749739
C	3.5813199	5.1130500	1.3109103
C	5.5182614	1.4850650	-4.0776121
N	6.2358141	1.1534657	-4.9238541
C	-0.6931187	4.4744875	1.0497439
H	0.2599279	2.1971287	-0.6765468
H	1.6066184	4.1722226	-0.1948667
H	3.0571448	0.6460475	-0.2987750
H	4.5782741	-0.0532353	-2.1045673
H	4.4971812	3.9327448	-3.7349364
H	2.9533546	4.6318664	-1.9258501
H	-0.2346424	0.2272583	2.8014376
H	-1.1746357	0.1603583	1.3094756
H	1.0210224	0.1487523	0.2990641
H	1.7161410	0.9752746	1.6937260
H	4.7880737	2.7817110	2.6845634
H	3.9473902	1.4438262	1.8568836
H	4.8880758	2.6452302	0.8967603
H	4.2027360	5.3827424	2.1669135
H	2.7910423	5.8534592	1.1772664
H	4.1888104	5.0145521	0.4086900
H	-1.5572646	4.7095801	1.6810049
H	0.0988081	5.1962788	1.3116422
H	-0.9721093	4.6959504	0.0064026

lb_sy_tr_1.log

E = -1148.924233

H = -1148.588877

G = -1148.656122

NImag=0

C	-0.3334372	3.0032956	1.0602151
C	0.6291887	2.4434486	0.0551395
C	-0.5043046	2.1561570	2.1399197
O	-1.0885284	2.3694672	3.2547841
C	2.0100594	3.1732365	0.0980941
C	2.9720770	2.7225844	-0.9749975
C	3.7831251	1.5853934	-0.8635669
C	4.5886475	1.1836517	-1.9219997
C	4.5782245	1.9195403	-3.1124141
C	3.7735812	3.0571397	-3.2412820
C	2.9826211	3.4529188	-2.1700139
C	0.2029272	0.8229582	1.8567016
C	0.6790355	0.9326570	0.3988816
S	2.7641336	2.9890422	1.7838503
C	4.3736330	3.7801915	1.5514533
C	1.9803789	4.2704257	2.7936549
C	5.4090777	1.5064838	-4.2115161
N	6.0781231	1.1744326	-5.0966708
C	-0.8415824	4.4099848	0.9913712
H	0.3177168	2.5945945	-0.9912818
H	1.8456629	4.2524032	-0.0028715
H	3.8103899	1.0011365	0.0527274
H	5.2205275	0.3067332	-1.8292992
H	3.7763154	3.6251729	-4.1656396
H	2.3625043	4.3402941	-2.2608626
H	1.0312210	0.6874444	2.5663133
H	-0.4833256	-0.0173646	2.0128721
H	-0.0211781	0.4142441	-0.2628676
H	1.6609476	0.4802999	0.2317528
H	4.7927609	3.9312999	2.5478711
H	5.0174591	3.1134299	0.9789312

H	4.2375865	4.7349298	1.0385920
H	2.6271476	4.3946358	3.6654171
H	0.9927860	3.9172932	3.0934132
H	1.9277696	5.1974611	2.2198139
H	-0.0424492	5.1684595	0.9771143
H	-1.4534178	4.5969832	0.0963541
H	-1.4647054	4.6158404	1.8690449

lb_sy_tr_1_r.log

E = -1148.921115
H = -1148.586023
G = -1148.653804

NImag=0

C	1.6118996	-1.7002628	1.5982012
C	1.1356288	-1.1390371	0.2756527
C	2.9716678	-1.5035777	1.7787406
O	3.7134778	-1.8052437	2.7709824
C	0.4372807	0.2313377	0.4915010
C	-0.6277344	0.2048052	1.5612591
C	-1.7375419	-0.6409246	1.4429554
C	-2.6976545	-0.6853004	2.4448146
C	-2.5409761	0.1219329	3.5790977
C	-1.4375665	0.9728326	3.7082906
C	-0.4906566	1.0150587	2.6908096
C	3.5452415	-0.8153772	0.5332770
C	2.4541724	-1.0000976	-0.5265060
S	-0.4715661	0.8354566	-1.0426090
C	-1.1385030	2.4105605	-0.4613091
C	0.7872518	1.4564339	-2.1783345
C	-3.5293430	0.0778842	4.6239734
N	-4.3255939	0.0435807	5.4642276
C	0.7430623	-2.4158978	2.5917259
H	0.4168768	-1.7993020	-0.2363222
H	1.1750266	1.0139675	0.7064653
H	-1.8485231	-1.2849525	0.5739832
H	-3.5574435	-1.3413392	2.3593010
H	-1.3296659	1.5934824	4.5917201
H	0.3688560	1.6732891	2.7791965
H	3.7390116	0.2458640	0.7463291
H	4.5014453	-1.2645771	0.2433634
H	2.6201661	-1.9381592	-1.0664623
H	2.4446953	-0.1964986	-1.2650929
H	-1.5256399	2.9327665	-1.3381759
H	-1.9514978	2.2032247	0.2345423
H	-0.3437675	2.9876511	0.0167366
H	0.2686110	2.1421512	-2.8521469
H	1.1860831	0.6198793	-2.7499708
H	1.5673764	1.9794293	-1.6218378
H	0.1886812	-1.7604336	3.2830030
H	-0.0085462	-3.0502466	2.1004791
H	1.3729528	-3.0643475	3.2130438

lb_sy_tr_1_ts1.log

E = -1148.899282
H = -1148.567516
G = -1148.637808

NImag=1

C	2.4784079	-1.3523923	0.6451956
C	1.1231581	-1.3034930	0.3081665
C	3.2785283	-1.3406877	-0.5373745

O	4.5202011	-1.3112675	-0.6162506
C	0.2381710	0.6221810	0.6252657
C	-1.1666752	0.3731691	0.3947290
C	-1.8383636	0.6276689	-0.8263919
C	-3.1594461	0.2573534	-1.0116209
C	-3.8627203	-0.3870732	0.0187931
C	-3.2188127	-0.6527935	1.2390849
C	-1.9002595	-0.2769450	1.4193711
C	2.3551728	-1.3278524	-1.7558987
C	0.9534252	-1.5658052	-1.1787313
S	0.9898847	1.8191396	-0.4219107
C	0.3447958	3.4342073	0.0981328
C	2.6545406	1.9502889	0.2596883
C	-5.2292340	-0.7664861	-0.1713416
N	-6.3372945	-1.0756010	-0.3255578
C	3.0470881	-1.2396794	2.0241083
H	0.3554689	-1.6527670	0.9980433
H	0.5308781	0.7777992	1.6642421
H	-1.3267155	1.1250370	-1.6464640
H	-3.6557725	0.4670236	-1.9541527
H	-3.7606908	-1.1475834	2.0392061
H	-1.4131246	-0.4768297	2.3700762
H	2.4390165	-0.3465466	-2.2428770
H	2.6642838	-2.0779089	-2.4898164
H	0.6464030	-2.6090629	-1.3167010
H	0.1788864	-0.9441635	-1.6386120
H	0.8789862	4.2076325	-0.4589536
H	-0.7172085	3.4585267	-0.1523359
H	0.4948265	3.5448726	1.1740055
H	3.1114571	2.8291091	-0.1989125
H	3.2187029	1.0571657	-0.0050463
H	2.5857934	2.0699504	1.3427746
H	3.3370187	-0.2050663	2.2647225
H	2.3242554	-1.5600865	2.7819010
H	3.9489465	-1.8517648	2.1324027

lb_sy_tr_1_ts2.log
E = -1148.915553
H = -1148.582477
G = -1148.651428

NImag=1

C	1.6400902	-1.7423139	-0.4190227
C	1.7014355	-0.3568958	-1.0266317
C	2.7389299	-1.9409814	0.4326087
O	3.0113348	-2.9403807	1.1504672
C	0.8174465	0.3146616	-0.0263543
C	-0.6365460	0.0185996	0.0030661
C	-1.3685361	-0.1481886	-1.1815623
C	-2.7319479	-0.4015935	-1.1357766
C	-3.3725533	-0.4941013	0.1076353
C	-2.6564303	-0.3292503	1.2987186
C	-1.2926994	-0.0682425	1.2369668
C	3.6495438	-0.7040718	0.3737552
C	3.1761110	0.0488303	-0.8760231
S	0.8472845	2.4946924	-0.4507233
C	-0.7618279	3.1082718	0.0926698
C	1.8504195	3.0065753	0.9621351
C	-4.7850333	-0.7627977	0.1586448
N	-5.9222776	-0.9783283	0.1989761
C	0.5878867	-2.7740542	-0.6884362
H	1.3247994	-0.2664824	-2.0511584

H	1.2624234	0.4144238	0.9647708
H	-0.8740696	-0.0760713	-2.1456893
H	-3.3017603	-0.5300056	-2.0500510
H	-3.1639552	-0.4050139	2.2545500
H	-0.7253852	0.0630949	2.1545175
H	3.5191970	-0.1084962	1.2890826
H	4.7019539	-0.9994981	0.3284184
H	3.7166611	-0.3163851	-1.7551976
H	3.3269619	1.1333601	-0.8264054
H	-0.7266151	4.1999980	0.1042634
H	-1.5138073	2.7743646	-0.6246841
H	-0.9924491	2.7262919	1.0899124
H	1.8721813	4.0972550	1.0048755
H	2.8635341	2.6273020	0.8166642
H	1.4243119	2.5987833	1.8822809
H	-0.3211722	-2.6734495	-0.0743518
H	0.2624969	-2.7643586	-1.7364869
H	1.0025286	-3.7662004	-0.4752215

lb_sy_tr_2.log

E = -1148.926530

H = -1148.591736

G = -1148.660045

NImag=0

C	0.5769079	2.0912138	1.4237520
C	0.6764736	3.4849524	0.8753410
C	0.0914631	1.1966273	0.4839511
O	-0.0567588	-0.0669262	0.5652957
C	2.1057618	3.9798948	0.4675736
C	2.7903879	3.1214462	-0.5609297
C	3.2035614	1.8150216	-0.2638640
C	3.7505667	1.0101336	-1.2561675
C	3.8895405	1.5171992	-2.5538863
C	3.5009564	2.8270781	-2.8592324
C	2.9583186	3.6220954	-1.8566819
C	-0.2562901	1.9577148	-0.8038225
C	-0.2079867	3.4364419	-0.4002242
S	3.2065914	4.0781939	1.9452931
C	4.5583738	5.0781126	1.2938200
C	2.3651521	5.2929929	2.9773683
C	4.4514912	0.6848515	-3.5843939
N	4.9040107	0.0159213	-4.4145898
C	1.0772467	1.6798859	2.7768611
H	0.2969417	4.2567846	1.5612082
H	2.0431791	5.0159706	0.1129270
H	3.0944589	1.4173011	0.7401748
H	4.0657778	-0.0036292	-1.0324561
H	3.6253444	3.2120241	-3.8658430
H	2.6510823	4.6391157	-2.0835760
H	0.4858022	1.7124110	-1.5781886
H	-1.2361676	1.6536554	-1.1889722
H	-1.2106784	3.7808244	-0.1280477
H	0.1596246	4.0973368	-1.1937781
H	5.2199737	5.3151790	2.1290033
H	5.0926908	4.4741964	0.5585765
H	4.1547019	5.9861108	0.8408745
H	3.0916058	5.6297235	3.7196754
H	1.5297991	4.8006375	3.4751494
H	2.0266070	6.1264343	2.3579147
H	2.1545912	1.4366304	2.8109052
H	0.9089714	2.4536937	3.5394973

H 0.5537258 0.7747489 3.1069917

1b_sy_tr_2_ts1.log

E = -1148.903732

H = -1148.571642

G = -1148.639159

NImag=1

C	-1.0222047	2.0212971	-0.2165148
C	-1.3668445	1.3374753	0.9516050
C	0.3223193	2.5079696	-0.1287382
O	0.9518545	3.1662062	-0.9753193
C	-1.2243692	-0.8001314	0.6924437
C	0.1621845	-0.9732901	0.3259737
C	0.6663624	-0.5457353	-0.9257026
C	2.0276708	-0.5539972	-1.1874557
C	2.9291545	-0.9819046	-0.2025774
C	2.4495821	-1.4306297	1.0430877
C	1.0911809	-1.4274490	1.2942806
C	0.8932131	2.1367969	1.2405100
C	-0.3020127	1.5616982	2.0143821
S	-2.3734046	-1.2444187	-0.5608953
C	-2.6984806	-3.0092360	-0.3046375
C	-3.9484436	-0.5783325	0.0090061
C	4.3362172	-0.9800450	-0.4704157
N	5.4766445	-0.9793746	-0.6851022
C	-1.8645219	2.1769720	-1.4444260
H	-2.3990311	1.2237757	1.2739495
H	-1.5275658	-1.2126537	1.6567694
H	-0.0133117	-0.1949637	-1.6967226
H	2.4012956	-0.2124851	-2.1479876
H	3.1485159	-1.7795265	1.7969795
H	0.7225335	-1.7741035	2.2558962
H	1.6965177	1.4025865	1.1008288
H	1.3334162	3.0184303	1.7170710
H	-0.6859653	2.2898310	2.7385091
H	-0.0600622	0.6520778	2.5723414
H	-3.4748724	-3.3218217	-1.0065189
H	-1.7679430	-3.5403141	-0.5125987
H	-3.0141667	-3.1670357	0.7287876
H	-4.7314458	-1.0744705	-0.5674209
H	-3.9682179	0.4925714	-0.1916980
H	-4.0658168	-0.7844141	1.0751555
H	-1.8242121	1.2919576	-2.0990322
H	-2.9190838	2.3526475	-1.2033666
H	-1.5064773	3.0236166	-2.0395117

1b_sy_tr_3.log

E = -1148.915723

H = -1148.580576

G = -1148.648427

NImag=0

C	-0.3842836	2.7972979	1.0526171
C	0.7339550	2.1582898	0.2793447
C	-0.5403155	2.2558624	2.3116676
O	-1.3091643	2.6087905	3.2687790
C	1.8713173	3.1454477	-0.0757093
C	2.8635743	2.7152518	-1.1443445
C	3.0653859	1.3693983	-1.4677246
C	3.9688766	1.0099090	-2.4630803
C	4.6799591	2.0049224	-3.1403087

C	4.4848831	3.3573403	-2.8341849
C	3.5766490	3.7001976	-1.8424171
C	0.4517124	1.1006373	2.4934931
C	1.0916078	0.8941216	1.1128110
S	2.9268198	3.8643860	1.2793883
C	1.8615647	4.4397465	2.6199293
C	3.8417180	2.5175434	2.0531639
C	5.6167154	1.6356092	-4.1685443
N	6.3711729	1.3387187	-4.9953836
C	-1.1254542	3.9945852	0.5442957
H	0.4125407	1.8533432	-0.7331148
H	1.3984351	4.0721624	-0.4279388
H	2.5129823	0.5877322	-0.9595604
H	4.1208999	-0.0343110	-2.7149981
H	5.0322858	4.1234178	-3.3729966
H	3.4125207	4.7501317	-1.6134856
H	1.1824905	1.3728532	3.2703166
H	-0.0601559	0.2027476	2.8583368
H	0.6420917	0.0264019	0.6196314
H	2.1653949	0.6972923	1.1645464
H	2.5188473	5.0070512	3.2834479
H	1.1114149	5.1022268	2.1839821
H	1.3947992	3.6072601	3.1429467
H	4.6047875	2.9929035	2.6726085
H	4.3211948	1.9394579	1.2600966
H	3.1859811	1.8977441	2.6626814
H	-1.9732009	4.2071296	1.2049305
H	-0.5143067	4.9132735	0.5066262
H	-1.5195964	3.8494264	-0.4727492

1b_sy_tr_3_r.log

E = -1148.919162

H = -1148.584340

G = -1148.652944

NImag=0

C	1.5454229	-1.6403671	1.5847429
C	0.9735786	-1.2286563	0.2467258
C	2.8766853	-1.2734549	1.7034500
O	3.6778605	-1.4153151	2.6847637
C	0.1499276	0.0808530	0.3984621
C	-0.8954230	0.0138561	1.4850962
C	-1.9406753	-0.9146146	1.4120016
C	-2.8631643	-1.0189301	2.4437329
C	-2.7349248	-0.1853602	3.5630859
C	-1.6990661	0.7513875	3.6455455
C	-0.7875522	0.8485522	2.5994586
C	3.3287059	-0.6133002	0.3924272
C	2.2411005	-1.0074002	-0.6125050
S	-0.7777214	0.6465467	-1.1467375
C	0.3002677	1.8887790	-1.8867953
C	-0.6841487	-0.7012908	-2.3420849
C	-3.6840340	-0.2918621	4.6391862
N	-4.4484919	-0.3771140	5.5050670
C	0.7841320	-2.3820664	2.6446596
H	0.3112245	-1.9943630	-0.1836379
H	0.8284202	0.9216340	0.5843097
H	-2.0302215	-1.5785633	0.5546496
H	-3.6718201	-1.7405777	2.3936408
H	-1.6122901	1.3918480	4.5170636
H	0.0242082	1.5681516	2.6560863
H	3.3924584	0.4768736	0.5224950

H	4.3258407	-0.9614964	0.1020937
H	2.5004319	-1.9608735	-1.0853070
H	2.1166056	-0.2732216	-1.4136536
H	-0.1846616	2.2175450	-2.8081300
H	0.3597882	2.7213459	-1.1835739
H	1.2880691	1.4783831	-2.0937431
H	-1.1423876	-0.3182718	-3.2565269
H	-1.2773630	-1.5321310	-1.9576183
H	0.3482100	-0.9993566	-2.5236980
H	1.4943105	-2.9083108	3.2940446
H	0.1648284	-1.7504025	3.3019456
H	0.1066156	-3.1328593	2.2129685

lb_sy_tr_3_ts2.log
E = -1148.912492
H = -1148.579358
G = -1148.648567

NImag=1

C	-1.2260315	1.7987809	-0.5673865
C	-1.5668820	0.3599324	-0.8979302
C	-2.2194127	2.3513376	0.2582055
O	-2.2663275	3.5021857	0.7684399
C	-0.7509592	-0.2547307	0.2006378
C	0.7345685	-0.1335092	0.1627826
C	1.4443009	-0.3219369	-1.0309102
C	2.8278326	-0.2138413	-1.0519534
C	3.5118755	0.0878648	0.1335215
C	2.8167056	0.2731459	1.3343541
C	1.4320438	0.1545112	1.3410192
C	-3.3403429	1.3208331	0.4537029
C	-3.0822172	0.2825696	-0.6448401
S	-0.8909945	-2.4648358	0.2547567
C	-2.3104147	-2.7584003	1.3303412
C	-1.5704788	-2.8638628	-1.3692308
C	4.9451143	0.2083451	0.1156498
N	6.0993030	0.3050581	0.1011739
C	-0.0459605	2.5695425	-1.0761048
H	-1.2664946	0.0198579	-1.8946437
H	-1.1743172	-0.1155614	1.1965186
H	0.9159343	-0.5497554	-1.9524917
H	3.3795144	-0.3580203	-1.9750279
H	3.3570914	0.5078769	2.2454961
H	0.8825455	0.2992370	2.2670618
H	-3.2748333	0.8825088	1.4598713
H	-4.3208566	1.7995285	0.3736866
H	-3.5878919	0.5860636	-1.5675626
H	-3.4365871	-0.7196357	-0.3896874
H	-2.5801025	-3.8149902	1.2720073
H	-1.9978335	-2.5177998	2.3483371
H	-3.1586349	-2.1358374	1.0419322
H	-1.7964620	-3.9321089	-1.3939492
H	-0.8015707	-2.6396167	-2.1112681
H	-2.4718888	-2.2826058	-1.5692985
H	-0.3097682	3.6330798	-1.1163767
H	0.8573844	2.4932594	-0.4506885
H	0.2412397	2.2563377	-2.0873850

lb_sy_tr_4.log
E = -1148.914301
H = -1148.578938

G = -1148.646534
NImag=0

C	-0.3812296	2.9020121	1.0895343
C	0.7299444	2.2362183	0.3276439
C	-0.7239153	2.2330445	2.2441480
O	-1.5827744	2.5324364	3.1417166
C	1.8576715	3.2162415	-0.0755389
C	2.8419795	2.7667978	-1.1332619
C	3.2469698	1.4318260	-1.2458008
C	4.1639449	1.0541517	-2.2197301
C	4.6870455	2.0218044	-3.0849167
C	4.2905016	3.3602494	-2.9871411
C	3.3672619	3.7210396	-2.0134985
C	0.1204143	0.9606665	2.3679655
C	1.1085253	0.9936072	1.1885882
S	2.8977246	3.9877439	1.2880488
C	2.0664475	3.7973396	2.8824619
C	4.3306721	2.9149207	1.5235501
C	5.6410352	1.6341941	-4.0902961
N	6.4092659	1.3224327	-4.8987383
C	-0.9873370	4.1995996	0.6543029
H	0.3998272	1.9056611	-0.6762389
H	1.3691728	4.1210240	-0.4528088
H	2.8527068	0.6768065	-0.5756345
H	4.4763490	0.0191233	-2.3099393
H	4.6965158	4.1010626	-3.6677664
H	3.0467545	4.7570835	-1.9389557
H	0.6254681	0.9413436	3.3435299
H	-0.5315899	0.0787962	2.3393706
H	1.0514889	0.0818519	0.5875905
H	2.1398180	1.0563932	1.5467900
H	2.7440156	4.2639228	3.6020505
H	1.1212759	4.3374789	2.8437792
H	1.9152151	2.7451878	3.1204605
H	4.8676439	3.3295780	2.3796587
H	4.9551719	2.9841373	0.6323177
H	4.0307040	1.8859713	1.7209039
H	-1.8987885	4.3878383	1.2321294
H	-0.3298837	5.0743790	0.8088515
H	-1.2571132	4.2073350	-0.4128266

lb_sy_tr_4_r.log
E = -1148.918291
H = -1148.582759
G = -1148.650342
NImag=0

C	1.2614220	-0.9640783	-1.3354748
C	1.4270065	-0.7000405	0.1506347
C	1.4011778	-2.3148114	-1.6237826
O	1.4572301	-2.9019268	-2.7538680
C	0.4007966	0.3158915	0.6860224
C	0.4448671	1.6945633	0.0625193
C	1.6508047	2.3885978	-0.0900473
C	1.6688765	3.6469679	-0.6793077
C	0.4682713	4.2158065	-1.1202265
C	-0.7463246	3.5375774	-0.9650226
C	-0.7489324	2.2829953	-0.3686558
C	1.5941331	-3.0978393	-0.3228578
C	1.2320353	-2.1028265	0.7802752
S	0.4660977	0.6640186	2.5321115
C	-0.2339091	-0.7738615	3.3702527

C	2.2028845	0.5518306	3.0022491
C	0.4823530	5.5151892	-1.7383724
N	0.4935564	6.5612382	-2.2352009
C	1.3810188	0.0777310	-2.4119744
H	2.4334381	-0.3077196	0.3851007
H	-0.6100181	-0.0965070	0.5794973
H	2.5892283	1.9439627	0.2275298
H	2.6032497	4.1836757	-0.8056411
H	-1.6704511	3.9888702	-1.3104341
H	-1.6864763	1.7470967	-0.2496986
H	0.9847078	-4.0079454	-0.2971380
H	2.6457817	-3.4113766	-0.2614545
H	1.8206900	-2.2436449	1.6924276
H	0.1745410	-2.2289075	1.0417173
H	-0.3600213	-0.4780214	4.4139583
H	-1.2096014	-0.9745018	2.9241383
H	0.4263499	-1.6351746	3.2898521
H	2.2313373	0.7021834	4.0836698
H	2.7426812	1.3603312	2.5074188
H	2.6113439	-0.4230757	2.7366156
H	1.4622909	-0.4413146	-3.3740126
H	0.5348873	0.7748248	-2.4854515
H	2.2816578	0.7024852	-2.2943931

lb_sy_tr_4_ts1.log

E = -1148.894302

H = -1148.561688

G = -1148.631712

NImag=1

C	2.6758670	-1.0549260	0.7248279
C	1.2890146	-1.2021237	0.5794684
C	3.3376189	-1.2740178	-0.5180643
O	4.5553555	-1.1800788	-0.7660981
C	0.2542995	0.6143741	0.8910972
C	-1.1284382	0.3530949	0.5455048
C	-1.7259662	0.6227716	-0.7080233
C	-3.0288721	0.2386289	-0.9814150
C	-3.7801430	-0.4474238	-0.0152226
C	-3.2051245	-0.7427425	1.2317065
C	-1.9085295	-0.3439196	1.5017258
C	2.3066459	-1.7064336	-1.5622502
C	0.9617589	-1.7062237	-0.8186776
S	1.1651475	1.9664568	0.2415800
C	1.6561295	1.5986516	-1.4616458
C	0.0509013	3.3724498	-0.0174213
C	-5.1254725	-0.8459519	-0.3008451
N	-6.2156275	-1.1692854	-0.5320022
C	3.3721906	-0.6330023	1.9803784
H	0.6690466	-1.5517153	1.4043603
H	0.4528867	0.6239530	1.9612300
H	-1.1753765	1.1325875	-1.4910424
H	-3.4690678	0.4628659	-1.9480925
H	-3.7826522	-1.2734715	1.9822869
H	-1.4764579	-0.5618047	2.4747619
H	2.3321524	-1.0250160	-2.4202937
H	2.5725764	-2.7002527	-1.9375860
H	0.5404505	-2.7146005	-0.7452131
H	0.2046189	-1.0890059	-1.3131586
H	1.8782053	2.5609145	-1.9284214
H	2.5658047	1.0019994	-1.4156882
H	0.8681762	1.0810778	-2.0068153

H	0.6718852	4.2156555	-0.3269678
H	-0.4192115	3.5874649	0.9436114
H	-0.6992935	3.1507456	-0.7755767
H	4.4239991	-0.9358004	1.9576581
H	3.3552014	0.4590207	2.1173676
H	2.9071220	-1.0736972	2.8698191

lb_sy_tr_5_r.log

E = -1148.923961
H = -1148.588857
G = -1148.656632

NImag=0

C	-1.5707574	-1.5738446	0.9452287
C	-1.4729548	-0.6857225	-0.2759604
C	-1.9389326	-2.8650775	0.6002318
O	-2.2289786	-3.8582067	1.3463122
C	-0.2504711	0.2534845	-0.2381717
C	-0.2520015	1.3311538	0.8123380
C	-1.4013047	2.0766142	1.1045823
C	-1.3753127	3.0531677	2.0932825
C	-0.1898173	3.2844538	2.8002117
C	0.9669473	2.5468712	2.5215843
C	0.9268458	1.5781820	1.5271584
C	-2.0516752	-2.9687187	-0.9258971
C	-1.3806142	-1.6964077	-1.4466326
S	0.0030618	0.9754854	-1.9482322
C	-1.4275938	2.0300763	-2.2366391
C	1.2929269	2.2110970	-1.7186155
C	-0.1611703	4.2910058	3.8283730
N	-0.1376881	5.1018308	4.6548785
C	-1.6375395	-1.0634581	2.3551694
H	-2.3701477	-0.0510116	-0.3946702
H	0.6565005	-0.3561097	-0.1394034
H	-2.3306560	1.8888551	0.5761716
H	-2.2662299	3.6279532	2.3234248
H	1.8788630	2.7308478	3.0796947
H	1.8176885	0.9954670	1.3094834
H	-1.5894942	-3.8856123	-1.3078648
H	-3.1165307	-3.0063286	-1.1956710
H	-1.8278245	-1.3129927	-2.3708834
H	-0.3227265	-1.9044060	-1.6524692
H	-1.2749796	2.4919153	-3.2144333
H	-2.3175894	1.3994329	-2.2617607
H	-1.4979150	2.7945425	-1.4612488
H	1.4745387	2.6561856	-2.6992496
H	2.1919724	1.6972730	-1.3728305
H	0.9681775	2.9689460	-1.0037506
H	-1.8982929	-1.9008535	3.0125432
H	-0.7000350	-0.6294547	2.7316930
H	-2.4073844	-0.2852456	2.4874272

lb_sy_tr_5_ts2.log

E = -1148.916502
H = -1148.583232
G = -1148.651337

NImag=1

C	-1.9549600	-1.3957038	0.3647215
C	-1.8050702	0.0704164	0.7137119
C	-3.0572902	-1.5786002	-0.4842335
O	-3.4762913	-2.6418079	-1.0167176

C	-0.7990996	0.4202694	-0.3381224
C	0.5923681	-0.0804229	-0.2682002
C	1.2372918	-0.2954847	0.9591885
C	2.5588639	-0.7201803	0.9958722
C	3.2442682	-0.9396781	-0.2058062
C	2.6138017	-0.7364524	-1.4396487
C	1.2943177	-0.3049949	-1.4610943
C	-3.7640481	-0.2302301	-0.6908339
C	-3.1888785	0.6719691	0.4099855
S	-0.5199618	2.6370011	-0.2743888
C	-0.3807811	2.8817446	1.5068482
C	1.1924279	2.9355694	-0.7608350
C	4.6121819	-1.3834751	-0.1718888
N	5.7139268	-1.7395917	-0.1446765
C	-1.0999999	-2.5127602	0.8782556
H	-1.4500311	0.2761354	1.7289446
H	-1.2099544	0.4297845	-1.3467864
H	0.7057364	-0.1428843	1.8931524
H	3.0586871	-0.8871168	1.9441713
H	3.1540578	-0.9159340	-2.3631848
H	0.7966914	-0.1386292	-2.4126705
H	-3.5428277	0.1513537	-1.6971227
H	-4.8494221	-0.3514739	-0.6240477
H	-3.7994840	0.5920549	1.3149501
H	-3.1487274	1.7308183	0.1285267
H	-0.0489313	3.9059759	1.6901786
H	-1.3684302	2.7349357	1.9475036
H	0.3365006	2.1741711	1.9303224
H	1.4201011	3.9891799	-0.5828605
H	1.2842870	2.7165011	-1.8261698
H	1.8676669	2.3003277	-0.1817677
H	-1.6587722	-3.4512305	0.7852859
H	-0.1517531	-2.6541589	0.3362552
H	-0.8401381	-2.3797722	1.9365388

lb_sy_tr_6.log

E = -1148.922404
H = -1148.587237
G = -1148.655817

NImag=0

C	-0.4427177	2.9984483	0.9896016
C	0.5828799	2.1929634	0.2434882
C	-0.7552441	2.4661450	2.2278373
O	-1.5598966	2.8878312	3.1235384
C	1.8824874	3.0063293	0.0199705
C	2.8466267	2.5526060	-1.0451948
C	3.0147714	1.1985596	-1.3602532
C	3.9094181	0.8099586	-2.3501379
C	4.6439336	1.7852009	-3.0348382
C	4.4789958	3.1435381	-2.7416066
C	3.5766559	3.5162966	-1.7528697
C	0.0601149	1.1851059	2.4459419
C	0.7406901	0.8988907	1.0969436
S	2.6983669	3.1900558	1.6924877
C	4.2689435	2.3076955	1.5718463
C	3.2866570	4.8934033	1.6581088
C	5.5721734	1.3860808	-4.0596638
N	6.3197746	1.0649388	-4.8836932
C	-1.0468720	4.2441273	0.4157343
H	0.2631001	1.9405765	-0.7814372
H	1.6032392	4.0435886	-0.1961232

H	2.4461146	0.4358660	-0.8388856
H	4.0386272	-0.2390259	-2.5950337
H	5.0439660	3.8916776	-3.2875563
H	3.4302437	4.5700141	-1.5312705
H	0.7854306	1.3468563	3.2556007
H	-0.5949129	0.3669232	2.7667106
H	0.2388141	0.0743057	0.5818591
H	1.7859896	0.5904604	1.2196738
H	4.7727643	2.4578724	2.5291894
H	4.0546090	1.2469863	1.4328152
H	4.8706127	2.7011320	0.7507339
H	3.8649591	5.0544670	2.5700796
H	2.4086151	5.5417015	1.6528076
H	3.9054729	5.0577128	0.7740773
H	-1.8418706	4.6006083	1.0800924
H	-0.3322399	5.0747349	0.2966436
H	-1.4903934	4.0787671	-0.5783178

1b_sy_tr_prod_1.log
E = -671.039596
H = -670.788521
G = -670.845627

NImag=0

C	-3.1452560	-0.7590050	-0.0781470
C	-1.8711700	-0.2884290	0.5449480
C	-1.8370700	1.2081440	0.3473350
C	-3.1369950	1.6609060	-0.3146510
C	-3.7798010	0.3778060	-0.8688830
O	-3.6182160	-1.8705880	0.0623520
C	-0.9455400	0.3675930	-0.5051760
C	0.5287960	0.2654640	-0.3278670
C	1.2275560	0.8988810	0.7101830
C	2.6053170	0.7653770	0.8275760
C	3.3065110	-0.0084580	-0.1050400
C	2.6279960	-0.6451250	-1.1518920
C	1.2511610	-0.5025350	-1.2538970
H	-1.2513220	0.2304650	-1.5405250
C	-1.3266910	-1.0525690	1.7204530
H	-1.3929780	1.8375460	1.1120540
C	4.7324180	-0.1473180	0.0102360
N	5.8819520	-0.2591840	0.1034430
H	-3.7858650	2.1054230	0.4453260
H	-2.9586530	2.4111340	-1.0900310
H	-3.5570990	0.2227160	-1.9310820
H	-4.8652220	0.3463450	-0.7543740
H	0.7005060	1.5072830	1.4378320
H	3.1390700	1.2602700	1.6324070
H	3.1775860	-1.2398530	-1.8742740
H	0.7223610	-0.9911450	-2.0674680
H	-2.1030330	-1.1692260	2.4826660
H	-0.9963000	-2.0512450	1.4163570
H	-0.4803800	-0.5351200	2.1771430

1c.log
E = -308.559579
H = -308.425580
G = -308.464111

NImag=0

C	0.3297897	2.7547113	-0.4777871
C	0.1859692	1.3235732	-0.0151384

C	1.6248330	0.8144503	0.1311831
C	2.5022090	1.9978936	-0.2608035
C	1.6195122	3.1195829	-0.6111258
O	3.7239190	1.9940491	-0.2744543
C	-0.8750075	3.5925889	-0.7328009
H	-0.3947711	0.7525874	-0.7483110
H	-0.3742435	1.2918277	0.9261265
H	1.8711657	0.5113978	1.1531215
H	1.8505322	-0.0297889	-0.5269938
H	1.9857755	4.0904004	-0.9282400
H	-0.6101827	4.6000056	-1.0604750
H	-1.5028940	3.1209103	-1.4974909
H	-1.4823077	3.6602092	0.1771918

lc_sy_c_1.log

E = -1148.925402

H = -1148.590753

G = -1148.657742

NImag=0

C	1.3411580	1.3092101	0.1497184
C	-0.1107655	1.6954085	0.2786822
C	2.1579660	2.3226025	-0.3276446
O	3.4130480	2.3459245	-0.5227253
C	-0.6040921	1.8808739	1.7534227
C	-0.9390128	0.6661513	2.5812683
C	-0.1193184	-0.4709516	2.6244356
C	-0.4757330	-1.5720211	3.3912716
C	-1.6658566	-1.5417846	4.1295099
C	-2.4962287	-0.4175395	4.1000570
C	-2.1251872	0.6768535	3.3264229
C	1.2943780	3.5601000	-0.6174202
C	-0.1551204	3.0858358	-0.4426623
S	0.6408787	2.9736582	2.6016799
C	-0.3225447	3.5999539	3.9931048
C	1.7916726	1.9054812	3.4864598
C	-2.0393568	-2.6819040	4.9242509
N	-2.3400481	-3.5990527	5.5642264
C	-1.0928412	0.7170548	-0.3851013
H	1.7171096	0.3216610	0.4042038
H	-1.4879191	2.5308113	1.7488522
H	0.8030321	-0.5021055	2.0559824
H	0.1592663	-2.4512640	3.4198993
H	-3.4179602	-0.4036868	4.6720246
H	-2.7706595	1.5505879	3.2957215
H	1.5666465	4.3663637	0.0759152
H	1.4974515	3.9279206	-1.6292870
H	-0.6212745	2.9404812	-1.4224599
H	-0.7809162	3.8078157	0.0963768
H	0.3512293	4.2008660	4.6070441
H	-1.1191103	4.2286127	3.5913561
H	-0.7301606	2.7695551	4.5736472
H	2.4712720	2.5766645	4.0168127
H	2.3390517	1.3227955	2.7455732
H	1.2536700	1.2692091	4.1905952
H	-1.0013040	-0.2924545	0.0281929
H	-2.1344324	1.0428654	-0.2603114
H	-0.8752881	0.6633465	-1.4559956

lc_sy_c_1_r.log

E = -1148.919706

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H =      -1148.584816
G =      -1148.651394
NImag=0
C      0.9100290      -2.0681442      -0.1124747
C      1.6182623      -0.8903078      -0.7340456
C      1.2969790      -2.3266734      1.1925565
O      0.8810596      -3.1918499      2.0246720
C      0.5462073      0.2453894      -0.8382096
C      -0.0888268      0.7787793      0.4246112
C      0.6217806      1.4355505      1.4381986
C      -0.0333943      1.9273223      2.5618538
C      -1.4173587      1.7650826      2.6807374
C      -2.1460881      1.1140803      1.6791426
C      -1.4768741      0.6341875      0.5610024
C      2.4062441      -1.3339689      1.5772932
C      2.7883276      -0.6409048      0.2631114
S      1.0387130      1.6374881      -2.0102085
C      -0.2722714      2.8541602      -1.7856248
C      2.4465698      2.5193132      -1.3154531
C      -2.0976057      2.2742403      3.8418951
N      -2.6451238      2.6852476      4.7759673
C      2.1607393      -1.1785487      -2.1425306
H      0.0983031      -2.5800875      -0.6265655
H      -0.2570251      -0.1763897      -1.4556608
H      1.6945730      1.5677437      1.3753305
H      0.5246866      2.4329232      3.3428444
H      -3.2195331      0.9907149      1.7765654
H      -2.0406331      0.1330316      -0.2206391
H      2.0185832      -0.6383014      2.3327286
H      3.2502401      -1.8628616      2.0340652
H      3.6724021      -1.1305064      -0.1601528
H      3.0498722      0.4146739      0.3779923
H      -0.0689941      3.6671603      -2.4855476
H      -1.2185776      2.3733636      -2.0417335
H      -0.2798959      3.2185785      -0.7568707
H      2.6071608      3.3790971      -1.9705141
H      3.3164670      1.8629408      -1.3574209
H      2.2387098      2.8542481      -0.2989883
H      1.3491324      -1.3293245      -2.8647579
H      2.8131143      -0.3790605      -2.5203753
H      2.7573596      -2.0944687      -2.1081822

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lc_sy_c_1_ts1.log
E =      -1148.896350
H =      -1148.564287
G =      -1148.631598
NImag=1
C      1.6828389      -1.6855179      0.5566277
C      1.5105754      -1.3031232      -0.7799045
C      2.9705113      -1.3098649      1.0424574
O      3.4579104      -1.4769110      2.1727819
C      0.3892545      0.5833558      -0.9647045
C      -0.9719930      0.3361528      -0.5195032
C      -1.3259676      0.2121056      0.8428251
C      -2.6190054      -0.1190514      1.2226606
C      -3.5985227      -0.3497402      0.2473967
C      -3.2676966      -0.2494726      -1.1148913
C      -1.9780102      0.0888956      -1.4831911
C      3.7210315      -0.6067617      -0.0940482
C      2.8615448      -0.8643097      -1.3360034
S      1.3029818      1.9307765      -0.3058049

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C	0.1968716	3.3667332	-0.2315732
C	1.5767141	1.7053307	1.4743211
C	-4.9345802	-0.6891325	0.6385508
N	-6.0165884	-0.9634996	0.9544056
C	0.5752118	-2.0472716	-1.6927494
H	0.9352239	-2.1948048	1.1574014
H	0.5011861	0.6798992	-2.0447262
H	-0.5829198	0.3539264	1.6187636
H	-2.8723825	-0.2094119	2.2744524
H	-4.0269011	-0.4272811	-1.8701024
H	-1.7286196	0.1731214	-2.5374344
H	3.8020212	0.4621075	0.1472655
H	4.7413463	-0.9917663	-0.1761179
H	3.2654750	-1.7060600	-1.9135950
H	2.7893491	-0.0126601	-2.0187872
H	0.7383165	4.1768239	0.2631981
H	-0.0471046	3.6448688	-1.2579760
H	-0.7036513	3.1032272	0.3270318
H	2.4742910	2.2738263	1.7252307
H	1.7311769	0.6470995	1.6818439
H	0.7194140	2.0866231	2.0309295
H	-0.3873068	-2.2467946	-1.2132661
H	0.4017205	-1.5210078	-2.6360065
H	1.0384090	-3.0142787	-1.9267603

lc_sy_c_1_ts2.log

E = -1148.912371

H = -1148.579141

G = -1148.645823

NImag=1

C	-1.9350499	1.6885012	-0.9651083
C	-2.2146823	0.4423489	-0.1613666
C	-1.4047592	2.7262067	-0.1837300
O	-1.0085211	3.8659673	-0.5327527
C	-1.0264408	-0.3003274	-0.7143567
C	0.4073820	-0.0496264	-0.3958499
C	0.9167865	0.0407919	0.9086772
C	2.2804900	0.1972447	1.1281557
C	3.1548051	0.2567523	0.0376972
C	2.6687372	0.1531328	-1.2719475
C	1.3060208	-0.0059327	-1.4751655
C	-1.3720290	2.2705546	1.2807399
C	-2.1413350	0.9407867	1.3025038
S	-1.2502539	-2.4898158	-0.2817302
C	0.3901693	-3.1739929	-0.5972238
C	-1.3042991	-2.6202547	1.5172160
C	4.5659958	0.4179939	0.2636398
N	5.7026699	0.5477962	0.4444707
C	-3.5273986	-0.2704413	-0.4730560
H	-2.0876969	1.7377273	-2.0392042
H	-1.1650362	-0.4900411	-1.7792033
H	0.2592709	-0.0188953	1.7668016
H	2.6670656	0.2673435	2.1394279
H	3.3526251	0.1946238	-2.1131785
H	0.9239751	-0.0929174	-2.4884744
H	-0.3276091	2.1759425	1.6023321
H	-1.8324620	3.0325750	1.9178970
H	-3.1737139	1.1253134	1.6179577
H	-1.7336366	0.1928682	1.9888913
H	0.3753127	-4.2360343	-0.3421318
H	0.6040619	-3.0578699	-1.6615753

H	1.1416903	-2.6520005	0.0003049
H	-1.2985126	-3.6800184	1.7824104
H	-2.2337838	-2.1643060	1.8628975
H	-0.4421910	-2.1209555	1.9640077
H	-3.5538565	-0.6234625	-1.5101195
H	-3.6945820	-1.1303863	0.1879721
H	-4.3569682	0.4281515	-0.3274713

lc_sy_c_2.log

E = -1148.922955
H = -1148.588371
G = -1148.655814

NImag=0

C	1.8388101	2.1306118	0.0529412
C	0.8140302	1.1429075	0.5504057
C	1.2647976	3.1756312	-0.6541173
O	1.7707873	4.2556624	-1.0887840
C	0.2861605	1.5711318	1.9770352
C	-0.5556616	0.5717931	2.7309608
C	-0.0163387	-0.5756458	3.3304913
C	-0.8364233	-1.4902981	3.9759904
C	-2.2183738	-1.2634475	4.0191751
C	-2.7733758	-0.1224334	3.4319580
C	-1.9363818	0.7900179	2.7987810
C	-0.2338633	2.8646356	-0.8313340
C	-0.3645214	1.3911183	-0.4271633
S	1.7356333	2.1457394	2.9989889
C	1.7240379	3.9337923	2.7150920
C	1.0918916	2.1557630	4.6898304
C	-3.0745127	-2.2112039	4.6812934
N	-3.7637635	-2.9743750	5.2140831
C	1.2970621	-0.3059054	0.5267795
H	2.8833874	2.0972547	0.3582093
H	-0.2949289	2.4918915	1.8550170
H	1.0534211	-0.7660331	3.3018579
H	-0.4154037	-2.3752935	4.4412350
H	-3.8437282	0.0486926	3.4776393
H	-2.3614514	1.6831673	2.3493491
H	-0.8171479	3.5284062	-0.1762687
H	-0.5585691	3.0630344	-1.8581662
H	-0.2084089	0.7495878	-1.3019291
H	-1.3377447	1.1288529	0.0055347
H	2.4587435	4.3640443	3.3989953
H	2.0044373	4.1128712	1.6772721
H	0.7238561	4.3164636	2.9297483
H	1.7807489	2.7708723	5.2727471
H	1.0916834	1.1381011	5.0781777
H	0.0878057	2.5851083	4.7021801
H	2.1178416	-0.4743372	1.2353551
H	0.4981681	-1.0207962	0.7511362
H	1.6780949	-0.5254834	-0.4751976

lc_sy_c_2_r.log

E = -1148.920616
H = -1148.585903
G = -1148.652602

NImag=0

C	0.7123625	-0.7070645	2.1392081
C	1.3324911	-0.8065688	0.7692339
C	1.4912976	-0.0068089	3.0466513

O	1.2657959	0.3233519	4.2523055
C	0.5526498	0.1947413	-0.1538883
C	0.6868372	1.6539725	0.2260040
C	1.8054374	2.4245187	-0.1150476
C	1.9034919	3.7512312	0.2858105
C	0.8723728	4.3160775	1.0442079
C	-0.2585721	3.5647998	1.3839123
C	-0.3467806	2.2435141	0.9625654
C	2.8079475	0.3887739	2.3543750
C	2.8059947	-0.3935476	1.0340590
S	0.9966416	0.0425974	-1.9808520
C	-0.0579534	-1.3033467	-2.5774336
C	0.0751340	1.4156249	-2.7179030
C	0.9698916	5.6879693	1.4666105
N	1.0481799	6.7926740	1.8054549
C	1.2624623	-2.2183337	0.1773154
H	-0.3024926	-1.0492378	2.3339252
H	-0.5074538	-0.0847555	-0.1396725
H	2.6172175	2.0039679	-0.7024899
H	2.7715004	4.3444228	0.0182586
H	-1.0574774	4.0140497	1.9643220
H	-1.2241058	1.6565652	1.2169529
H	2.8198505	1.4767301	2.2074038
H	3.6650691	0.1409067	2.9904376
H	3.3814589	-1.3172786	1.1586831
H	3.2594286	0.1425412	0.1926534
H	-0.1472608	-1.1580857	-3.6558115
H	0.4233555	-2.2568232	-2.3737707
H	-1.0362616	-1.2372238	-2.0970877
H	0.0694349	1.2406592	-3.7953961
H	0.5923500	2.3481668	-2.4984838
H	-0.9418571	1.4231609	-2.3192740
H	0.2298518	-2.5187926	-0.0355250
H	1.8583746	-2.3208690	-0.7397919
H	1.6736469	-2.9215139	0.9071394

lc_sy_c_2_ts1.log

E = -1148.898837

H = -1148.567259

G = -1148.635293

NImag=1

C	2.7020068	-0.7826992	1.0611490
C	1.4057117	-1.2016382	0.7199553
C	3.6279062	-1.1035167	0.0267698
O	4.8409340	-0.8381919	-0.0447149
C	0.4109362	0.4108088	-0.4062713
C	-1.0194801	0.2579040	-0.3107215
C	-1.8019639	0.7747257	0.7533938
C	-3.1530996	0.4970437	0.8558293
C	-3.7825193	-0.3107385	-0.1058562
C	-3.0324551	-0.8239483	-1.1789289
C	-1.6840824	-0.5375302	-1.2790547
C	2.8594036	-1.8240058	-1.0851832
C	1.5138152	-2.1726000	-0.4445495
S	1.0926398	1.8680255	0.3416826
C	2.6438453	2.0745624	-0.5583701
C	0.1957111	3.2724951	-0.3748177
C	-5.1796904	-0.5981567	-0.0009678
N	-6.3135029	-0.8325778	0.0839484
C	0.3488585	-1.4329397	1.7603471
H	2.9615398	-0.2234035	1.9556958

H	0.8330635	0.2738020	-1.4018195
H	-1.3441554	1.3875399	1.5264683
H	-3.7302940	0.9002335	1.6823194
H	-3.5182482	-1.4365697	-1.9323254
H	-1.1168107	-0.9273501	-2.1196289
H	2.7337496	-1.1162535	-1.9165914
H	3.4189098	-2.6841567	-1.4626405
H	1.5375536	-3.1871640	-0.0237354
H	0.6583667	-2.1227140	-1.1240804
H	3.0095773	3.0756823	-0.3219970
H	3.3556143	1.3266602	-0.2134662
H	2.4450174	1.9764081	-1.6278904
H	0.6922043	4.1844637	-0.0356247
H	-0.8297989	3.2509528	-0.0049133
H	0.2183245	3.1916960	-1.4631168
H	0.2120132	-0.5604433	2.4082732
H	-0.6144817	-1.7014135	1.3197107
H	0.6752843	-2.2683194	2.3922632

lc_sy_c_2_ts1_rot2.log

E = -1148.899003

H = -1148.567242

G = -1148.633884

NImag=1

C	0.4909261	-2.4458573	-0.7629758
C	1.2796460	-1.7752439	0.1845480
C	-0.8367987	-2.6600283	-0.2920212
O	-1.7820949	-3.2428813	-0.8526127
C	1.3279388	0.2753174	-0.4713982
C	-0.0504103	0.7042809	-0.3301271
C	-0.5515326	1.3899762	0.8033181
C	-1.9041505	1.6320310	0.9573385
C	-2.8097729	1.1909539	-0.0235115
C	-2.3360886	0.5360910	-1.1692259
C	-0.9776172	0.3083438	-1.3214459
C	-0.9398509	-2.0844792	1.1254815
C	0.5011142	-1.7065850	1.4941274
S	2.4865314	1.3602846	0.3389485
C	4.0692165	0.9577165	-0.4315535
C	2.2496288	2.9973198	-0.4165249
C	-4.2128877	1.4326308	0.1379299
N	-5.3487199	1.6283155	0.2705764
C	2.7656384	-2.0016313	0.2804871
H	0.8372569	-2.7586473	-1.7441372
H	1.6549556	0.1057973	-1.4986360
H	0.1208867	1.7260219	1.5891670
H	-2.2705006	2.1537867	1.8358465
H	-3.0348509	0.2127585	-1.9346535
H	-0.6149254	-0.1825515	-2.2184415
H	-1.6172237	-1.2223539	1.1113590
H	-1.3740645	-2.8310649	1.7980390
H	0.9364310	-2.4482744	2.1764311
H	0.5919199	-0.7316934	1.9852545
H	4.7171494	1.8199353	-0.2636887
H	4.4969350	0.0808584	0.0487660
H	3.9163057	0.7925728	-1.5000125
H	3.0144710	3.6654130	-0.0147289
H	1.2577392	3.3550515	-0.1374029
H	2.3377470	2.8997662	-1.5006220
H	3.2711551	-1.8373065	-0.6754649
H	3.2223607	-1.3717647	1.0508735

H 2.9361068 -3.0449168 0.5762798

1c_sy_c_2_ts2.log

E = -1148.913310

H = -1148.580235

G = -1148.646798

NImag=1

C	-1.6013231	1.8809414	-0.9277175
C	-2.0350758	0.8704699	0.1068010
C	-0.7297365	2.8451578	-0.3973771
O	-0.1214514	3.7771270	-0.9791991
C	-1.0992313	-0.1898188	-0.4076550
C	0.3876843	-0.1489021	-0.2289956
C	0.9945667	-0.1995639	1.0333797
C	2.3787639	-0.2304598	1.1542851
C	3.1706426	-0.2167219	0.0011967
C	2.5819605	-0.1838064	-1.2696909
C	1.1980168	-0.1603869	-1.3735756
C	-0.5993972	2.6112347	1.1148293
C	-1.6577635	1.5477078	1.4436310
S	-1.5276925	-2.1698550	0.5098407
C	-2.9070142	-2.7577144	-0.5028958
C	-0.2102180	-3.1495477	-0.2505981
C	4.6035756	-0.2472212	0.1225643
N	5.7574415	-0.2721367	0.2202968
C	-3.4964361	0.4449773	0.0582764
H	-1.8837362	1.8089936	-1.9737897
H	-1.3819139	-0.5226708	-1.4096845
H	0.3922365	-0.2359306	1.9348810
H	2.8440976	-0.2708838	2.1334900
H	3.2040042	-0.1810644	-2.1585453
H	0.7335376	-0.1399544	-2.3554358
H	0.4242476	2.2891161	1.3414314
H	-0.7655129	3.5504481	1.6523518
H	-2.5655508	2.0411749	1.8067674
H	-1.3597802	0.8305869	2.2150734
H	-2.9188053	-3.8486689	-0.4549110
H	-3.8361297	-2.3666614	-0.0901176
H	-2.7797272	-2.4290059	-1.5375140
H	-0.4519046	-4.2063972	-0.1202193
H	0.7277479	-2.9238058	0.2584673
H	-0.1339410	-2.9058155	-1.3137455
H	-3.7443476	-0.0315689	-0.8966117
H	-3.7425756	-0.2493730	0.8718439
H	-4.1297386	1.3302210	0.1723413

1c_sy_c_3.log

E = -1148.915104

H = -1148.580177

G = -1148.646643

NImag=0

C	1.4315546	1.5204157	0.4240442
C	-0.0553497	1.7539857	0.5029960
C	2.0959636	2.4068265	-0.4032103
O	3.3219419	2.4674701	-0.7385167
C	-0.6890561	1.9064420	1.9241577
C	-1.0310886	0.6460445	2.6978576
C	-0.1514825	-0.4419025	2.7738294
C	-0.4980751	-1.5829066	3.4851061
C	-1.7383039	-1.6386985	4.1332409

C	-2.6267487	-0.5607405	4.0717362
C	-2.2647368	0.5741798	3.3547530
C	1.0880868	3.4282261	-0.9537736
C	-0.2558642	3.0906623	-0.2936716
S	0.2028979	2.9688942	3.1820384
C	1.6570320	2.0471075	3.7234934
C	0.9984266	4.3629306	2.3534802
C	-2.1035943	-2.8207684	4.8684710
N	-2.3978227	-3.7718826	5.4599152
C	-0.8699703	0.6426102	-0.1981880
H	1.9168450	0.6503817	0.8591703
H	-1.6183335	2.4795492	1.8158703
H	0.8092314	-0.4052029	2.2715619
H	0.1822470	-2.4262199	3.5384284
H	-3.5859441	-0.6141684	4.5755954
H	-2.9532059	1.4131506	3.3002300
H	1.4262401	4.4493064	-0.7329782
H	1.0534582	3.3367833	-2.0461871
H	-1.0569231	2.9595500	-1.0280949
H	-0.5857697	3.8966423	0.3661715
H	2.2120020	2.7356529	4.3648487
H	1.3226266	1.1937541	4.3131853
H	2.2490050	1.7446102	2.8602078
H	1.5715246	4.8638811	3.1373771
H	0.2253726	5.0364551	1.9846110
H	1.6526629	4.0030763	1.5603316
H	-0.6203491	-0.3524038	0.1810131
H	-1.9531155	0.7930732	-0.0892808
H	-0.6277851	0.6660321	-1.2656202

1c_sy_c_3_r.log

E = -1148.910035

H = -1148.575025

G = -1148.641647

NImag=0

C	0.9000976	-1.8209347	0.4645413
C	1.4381115	-0.9609061	-0.6503773
C	1.7413913	-1.9305574	1.5552351
O	1.6035883	-2.5641906	2.6495366
C	0.4111876	0.1920543	-0.8994625
C	-0.2326730	0.8717948	0.2914120
C	0.4874630	1.2118947	1.4452319
C	-0.1339182	1.8683984	2.4969522
C	-1.4937999	2.1970153	2.3984672
C	-2.2259146	1.8694681	1.2549968
C	-1.5874307	1.2081261	0.2094631
C	3.0216915	-1.1300741	1.2753058
C	2.8455646	-0.5207723	-0.1268021
S	0.8842451	1.6532488	-2.0362472
C	1.5732535	2.9436341	-0.9760966
C	2.3402071	1.2448999	-3.0274645
C	-2.1403076	2.8809078	3.4867133
N	-2.6593822	3.4331549	4.3624678
C	1.5503473	-1.7821201	-1.9487169
H	-0.0740958	-2.3006971	0.3903771
H	-0.3962357	-0.2325120	-1.5062186
H	1.5405502	0.9705061	1.5291123
H	0.4240204	2.1284595	3.3903613
H	-3.2778864	2.1255971	1.1870703
H	-2.1553547	0.9455374	-0.6793390
H	3.1599483	-0.3703396	2.0561278

H	3.8894947	-1.7973390	1.3340815
H	3.6115147	-0.8898413	-0.8169026
H	2.9571872	0.5671296	-0.1038042
H	1.9432550	3.7111021	-1.6591978
H	0.7656511	3.3536669	-0.3698464
H	2.3831730	2.5609444	-0.3551303
H	2.6813964	2.1996620	-3.4342871
H	2.0264173	0.5978898	-3.8452602
H	3.1203126	0.7861887	-2.4206586
H	0.5727992	-2.1957612	-2.2222855
H	1.9328498	-1.2214608	-2.8060836
H	2.2317460	-2.6199646	-1.7729325

lc_sy_c_3_ts1.log

E = -1148.889646
H = -1148.557444
G = -1148.623554

NImag=1

C	1.5747659	-1.6365646	0.6638236
C	1.2531990	-1.3234196	-0.6635955
C	2.9506671	-1.3991673	0.9377729
O	3.5596489	-1.4950798	2.0174604
C	0.2964891	0.6523346	-0.7828058
C	-1.1046570	0.4608235	-0.4398336
C	-1.5303477	0.3916762	0.9060073
C	-2.8511814	0.1214245	1.2321676
C	-3.7897706	-0.0969230	0.2143392
C	-3.3904994	-0.0329049	-1.1330949
C	-2.0730251	0.2443832	-1.4475026
C	3.6376302	-0.9702721	-0.3640668
C	2.5507779	-1.0943277	-1.4368111
S	0.9775914	2.0185953	0.1406387
C	2.0117200	1.4835040	1.5396058
C	2.2623518	2.6581860	-0.9492842
C	-5.1542703	-0.3798177	0.5454747
N	-6.2599327	-0.6092799	0.8121921
C	0.1493601	-2.0326976	-1.3982878
H	0.8619310	-1.9759432	1.4101417
H	0.4919473	0.8596721	-1.8351954
H	-0.8169317	0.5344110	1.7143175
H	-3.1589063	0.0699085	2.2719081
H	-4.1217013	-0.1896657	-1.9200651
H	-1.7726575	0.3024176	-2.4899280
H	4.0260870	0.0504636	-0.2611394
H	4.5014243	-1.6154437	-0.5529570
H	2.7198037	-1.9829446	-2.0582371
H	2.4943500	-0.2399518	-2.1162998
H	2.1785890	2.3961137	2.1161786
H	1.4580236	0.7606782	2.1389182
H	2.9597877	1.0705204	1.2023340
H	2.7864381	3.4444271	-0.4028576
H	1.7747613	3.0767948	-1.8304575
H	2.9502606	1.8564078	-1.2214761
H	-0.7508869	-2.1449623	-0.7883782
H	-0.1144205	-1.5356081	-2.3370010
H	0.5161563	-3.0373727	-1.6443017

lc_sy_c_4_ts1.log

E = -1148.894568
H = -1148.562896

G = -1148.631059
NImag=1

C	-1.8659563	-1.3123399	-0.9061477
C	-1.3843108	-1.3144192	0.4123934
C	-3.2817681	-1.1561594	-0.9592443
O	-4.0235561	-1.0859248	-1.9540835
C	-0.2919386	0.5881083	0.7562856
C	1.0972347	0.3652855	0.4148733
C	2.0298576	0.0885045	1.4442771
C	3.3411330	-0.2447045	1.1619619
C	3.7772825	-0.3052178	-0.1739390
C	2.8764706	-0.0231425	-1.2122870
C	1.5631959	0.3075372	-0.9218212
C	-3.8219449	-1.1927773	0.4757446
C	-2.5748034	-1.2209584	1.3736528
S	-1.0896821	1.7188664	-0.3410256
C	-2.6439185	2.0775857	0.4879065
C	-0.2530098	3.3055008	-0.0845662
C	5.1356058	-0.6423964	-0.4730063
N	6.2372702	-0.9165198	-0.7143731
C	-0.2407664	-2.1896527	0.8441055
H	-1.2468574	-1.4522372	-1.7878600
H	-0.4827953	0.8579646	1.7963853
H	1.7007874	0.1358356	2.4786729
H	4.0391632	-0.4520909	1.9672290
H	3.2113582	-0.0678795	-2.2439964
H	0.8865966	0.5068865	-1.7490499
H	-4.5039699	-0.3583192	0.6678584
H	-4.4129692	-2.1093786	0.5822033
H	-2.5661011	-2.0976959	2.0309388
H	-2.5053643	-0.3432544	2.0227711
H	-3.0518766	2.9750416	0.0192508
H	-3.3250406	1.2458060	0.3254748
H	-2.4602399	2.2441785	1.5513205
H	-0.7669663	4.0582389	-0.6863125
H	0.7762311	3.1934532	-0.4302135
H	-0.2806082	3.5611866	0.9762328
H	0.5843528	-2.1842059	0.1266499
H	0.1430454	-1.9128618	1.8310454
H	-0.6247022	-3.2161550	0.9095873

lc_sy_c_4_ts2.log
E = -1148.909111
H = -1148.575939
G = -1148.642648
NImag=1

C	-1.1530508	2.0741009	-0.8902502
C	-1.8249131	1.0128455	-0.0557922
C	-0.2444268	2.8454660	-0.1481540
O	0.5270439	3.7577236	-0.5335734
C	-0.9797336	-0.0937050	-0.6366504
C	0.4934748	-0.2416151	-0.3852837
C	1.0227868	-0.4810418	0.8897278
C	2.3894242	-0.6622374	1.0693160
C	3.2415223	-0.6154573	-0.0389063
C	2.7280991	-0.3984522	-1.3244306
C	1.3613614	-0.2231914	-1.4870053
C	-0.3210382	2.4147861	1.3225944
C	-1.5148648	1.4497146	1.3959351
S	-1.5827281	-2.1654779	-0.1004282
C	-2.2258806	-2.1104411	1.5871232

C	-3.1024610	-2.4662703	-1.0325625
C	4.6559201	-0.8026570	0.1409022
N	5.7953012	-0.9538182	0.2851409
C	-3.3144782	0.8312395	-0.3226815
H	-1.3222777	2.1731720	-1.9583138
H	-1.2250762	-0.2557112	-1.6885670
H	0.3726976	-0.5330725	1.7566602
H	2.7936206	-0.8434175	2.0597790
H	3.3946253	-0.3710720	-2.1800989
H	0.9575576	-0.0547094	-2.4811673
H	0.6290182	1.9490112	1.6109463
H	-0.4515996	3.2952351	1.9601547
H	-2.3987414	1.9877476	1.7549558
H	-1.3639782	0.6029712	2.0723615
H	-2.7303161	-3.0591966	1.7845890
H	-1.3811368	-2.0033559	2.2693256
H	-2.9226862	-1.2806226	1.7109374
H	-3.3692727	-3.5188224	-0.9168908
H	-2.8939760	-2.2581969	-2.0841661
H	-3.9122030	-1.8313046	-0.6738781
H	-3.4967364	0.4947314	-1.3495248
H	-3.7772305	0.1168003	0.3664890
H	-3.8153850	1.7950005	-0.1863651

lc_sy_c_5.log

E = -1148.916494

H = -1148.581659

G = -1148.647842

NImag=0

C	1.6363932	2.4614638	0.1832845
C	0.8288928	1.3058920	0.7201168
C	0.8927663	3.3117277	-0.6195572
O	1.1973738	4.4225471	-1.1558775
C	0.1515411	1.6505483	2.1042666
C	-0.6560457	0.5541141	2.7685938
C	-0.0531004	-0.5200392	3.4365143
C	-0.8247970	-1.5128315	4.0256420
C	-2.2206832	-1.4363969	3.9434110
C	-2.8399857	-0.3697976	3.2834568
C	-2.0526487	0.6202536	2.7071825
C	-0.5113071	2.7014444	-0.7877036
C	-0.3452711	1.2599145	-0.3019246
S	1.2069559	2.4018605	3.4405863
C	2.9037322	1.8026859	3.3182739
C	1.3934638	4.1327915	2.9637732
C	-3.0259141	-2.4630524	4.5493912
N	-3.6741212	-3.2896084	5.0372706
C	1.5626564	-0.0378313	0.7553731
H	2.6560980	2.6734919	0.4923644
H	-0.5209614	2.4973141	1.9197445
H	1.0287609	-0.5984500	3.4977314
H	-0.3543094	-2.3421544	4.5431069
H	-3.9222624	-0.3154328	3.2306472
H	-2.5291059	1.4568886	2.2032189
H	-1.2306669	3.2655737	-0.1757646
H	-0.8492001	2.7714266	-1.8269694
H	-0.0185317	0.6257020	-1.1340279
H	-1.2570374	0.8134620	0.1106544
H	3.4693935	2.4061681	4.0322837
H	2.9232579	0.7591155	3.6327681
H	3.2959274	1.9295604	2.3111427

H	1.9215003	4.6193661	3.7868592
H	0.3890820	4.5501409	2.8710255
H	1.9391023	4.2102376	2.0251901
H	2.3567469	-0.0734539	1.5077850
H	0.8787194	-0.8725024	0.9452000
H	2.0264853	-0.2001403	-0.2223335

lc_sy_c_5_r.log

E = -1148.915963

H = -1148.581153

G = -1148.647960

NImag=0

C	0.9112473	0.0600323	2.1235955
C	1.4002876	-0.5071108	0.8149380
C	1.7715133	0.9892211	2.6851688
O	1.6603389	1.6931203	3.7368744
C	0.5127802	0.1449887	-0.3016055
C	0.5690941	1.6589937	-0.3831608
C	1.5987527	2.3387228	-1.0433241
C	1.6290733	3.7286605	-1.0747192
C	0.6159876	4.4506217	-0.4364142
C	-0.4296586	3.7876547	0.2180001
C	-0.4485524	2.3991167	0.2313998
C	3.0153161	1.1014533	1.7895204
C	2.8884086	-0.0527518	0.7851633
S	0.6327103	-0.4544531	-2.0876006
C	2.3182171	-0.9899763	-2.4560607
C	-0.2617444	-2.0225852	-2.1315747
C	0.6427093	5.8887585	-0.4616482
N	0.6637368	7.0466026	-0.4821156
C	1.2581381	-2.0341015	0.7687861
H	-0.0780543	-0.1763701	2.5114062
H	-0.5236112	-0.1494425	-0.0941093
H	2.4017294	1.7993335	-1.5372134
H	2.4316521	4.2496764	-1.5857746
H	-1.2163381	4.3556312	0.7032955
H	-1.2590465	1.8794864	0.7332729
H	3.0164332	2.0859514	1.3028129
H	3.9286555	1.0399871	2.3918269
H	3.4941556	-0.9027726	1.1191581
H	3.2455135	0.2093283	-0.2151953
H	2.2509720	-1.5068211	-3.4164354
H	2.9468010	-0.1056641	-2.5649480
H	2.7042775	-1.6588389	-1.6881485
H	-0.3936405	-2.2650111	-3.1879075
H	-1.2359030	-1.8585738	-1.6676710
H	0.2922998	-2.8082584	-1.6216778
H	0.2028901	-2.3326619	0.7782316
H	1.7405562	-2.4973022	-0.0984166
H	1.7325001	-2.4510306	1.6619436

lc_sy_c_5_ts1.log

E = -1148.894166

H = -1148.562279

G = -1148.629198

NImag=1

C	2.8326082	-0.5207285	0.9167136
C	1.4640554	-0.8259304	1.0054134
C	3.4808471	-1.3358720	-0.0567657
O	4.6660217	-1.3092458	-0.4314358

C	0.3770611	0.3593536	-0.4744244
C	-1.0636452	0.2017872	-0.3914386
C	-1.8738091	1.0277235	0.4249233
C	-3.2359446	0.8118166	0.5455622
C	-3.8398775	-0.2551044	-0.1382688
C	-3.0585135	-1.0919826	-0.9530808
C	-1.7002675	-0.8604991	-1.0779796
C	2.4399473	-2.3016602	-0.6305878
C	1.2489521	-2.1688729	0.3208258
S	0.8806927	2.0690803	-0.5687434
C	1.4850154	2.6404445	1.0410119
C	2.4334266	1.9544270	-1.4778915
C	-5.2467019	-0.4859818	-0.0097162
N	-6.3873143	-0.6733072	0.0938248
C	0.6268281	-0.5198045	2.2152643
H	3.3447294	0.2629296	1.4646953
H	0.8389370	-0.1391292	-1.3261762
H	-1.4307793	1.8433858	0.9918073
H	-3.8380929	1.4593111	1.1754097
H	-3.5267912	-1.9080245	-1.4947333
H	-1.1109858	-1.4945546	-1.7346601
H	2.1852271	-1.9715465	-1.6470433
H	2.8445799	-3.3147860	-0.7054887
H	1.2952583	-2.9379077	1.1037793
H	0.2709659	-2.2587273	-0.1574261
H	1.8797449	3.6445631	0.8694750
H	0.6318957	2.6985554	1.7179233
H	2.2574470	1.9814844	1.4298309
H	2.8736511	2.9529900	-1.4999388
H	2.1939926	1.6280092	-2.4911512
H	3.0928523	1.2417951	-0.9799314
H	0.7532853	0.5083870	2.5631797
H	-0.4350998	-0.7046671	2.0312541
H	0.9456545	-1.1874799	3.0264067

lc_sy_c_6.log

E = -1148.921623

H = -1148.586977

G = -1148.653379

NImag=0

C	1.0489909	0.9305622	0.1528182
C	-0.1935683	1.7432156	0.3946836
C	2.1150918	1.6780703	-0.3209811
O	3.3045784	1.3407951	-0.6139196
C	-0.5290955	2.0052050	1.9119105
C	-0.8839069	0.7541935	2.6790201
C	0.0637340	-0.2347329	2.9762490
C	-0.3117128	-1.3924718	3.6458420
C	-1.6491441	-1.5671288	4.0216957
C	-2.6049866	-0.5850567	3.7392752
C	-2.2129765	0.5715965	3.0756150
C	1.6576277	3.1429537	-0.4586016
C	0.1291717	3.0751436	-0.3428777
S	0.8822920	2.8455752	2.7915872
C	0.5357272	4.6104100	2.5808737
C	0.3909706	2.7090637	4.5284420
C	-2.0426507	-2.7649359	4.7150692
N	-2.3600752	-3.7289514	5.2729817
C	-1.4698932	1.1094908	-0.1853327
H	1.0972296	-0.1376507	0.3470783
H	-1.3566995	2.7200730	1.9942033

H	1.1032902	-0.1021297	2.6927743
H	0.4227963	-2.1559733	3.8795326
H	-3.6374693	-0.7262033	4.0408840
H	-2.9492725	1.3395850	2.8564555
H	2.1381980	3.7445494	0.3264551
H	1.9893547	3.5624633	-1.4143801
H	-0.2947013	2.9981109	-1.3495878
H	-0.3448854	3.9455844	0.1246404
H	1.1202729	5.1249663	3.3463563
H	0.8695198	4.9290928	1.5956380
H	-0.5314686	4.7907119	2.7230083
H	1.0471381	3.3816193	5.0843109
H	0.5499713	1.6829423	4.8580097
H	-0.6543770	3.0043814	4.6397965
H	-1.6527545	0.1139923	0.2321316
H	-2.3572105	1.7284809	0.0035887
H	-1.3491069	1.0027061	-1.2673461

lc_sy_c_6_ts1.log

E = -1148.897410

H = -1148.565715

G = -1148.633398

NImag=1

C	-1.2461312	-1.8119074	-0.4180235
C	-1.2949255	-1.2742021	0.8750905
C	-2.5031488	-1.6919248	-1.0824339
O	-2.8171538	-2.0425581	-2.2319134
C	-0.4641590	0.7622053	0.8045371
C	0.9119511	0.5123992	0.4374508
C	1.3046995	0.1678857	-0.8783654
C	2.6143265	-0.1823852	-1.1692725
C	3.5801539	-0.1936002	-0.1531699
C	3.2166791	0.1551709	1.1607881
C	1.9095204	0.5029572	1.4430791
C	-3.5028647	-1.0579394	-0.1052225
C	-2.7571252	-1.0262464	1.2354653
S	-1.4046640	1.5994617	-0.4455589
C	-2.6902356	2.4282580	0.5119306
C	-0.4501746	3.0710180	-0.9162058
C	4.9347316	-0.5452245	-0.4543429
N	6.0332706	-0.8309710	-0.6960190
C	-0.3860238	-1.7483674	1.9744564
H	-0.3651866	-2.2512628	-0.8751590
H	-0.6132490	1.2455062	1.7714998
H	0.5785950	0.1683804	-1.6871560
H	2.8952851	-0.4462380	-2.1842524
H	3.9666577	0.1570680	1.9458268
H	1.6352023	0.7734734	2.4590516
H	-3.7865528	-0.0648080	-0.4748567
H	-4.4199635	-1.6536851	-0.0725878
H	-3.0787823	-1.8672688	1.8636645
H	-2.9035226	-0.1213850	1.8313175
H	-3.2186512	3.0904906	-0.1761927
H	-3.3791913	1.6850403	0.9087862
H	-2.2215735	2.9972846	1.3169918
H	-1.0813978	3.6742020	-1.5723745
H	0.4370166	2.7408886	-1.4580068
H	-0.1751620	3.6215140	-0.0146083
H	0.6386536	-1.8957656	1.6230136
H	-0.3745711	-1.0623057	2.8275355
H	-0.7605212	-2.7180223	2.3270805

lc_sy_c_prod_1.log

E = -671.038738

H = -670.787963

G = -670.843261

NImag=0

C	1.6936520	1.8414329	0.0037070
C	2.2435918	0.5831733	0.5777069
C	2.3281145	0.7775098	2.0878848
C	1.8020819	2.1793797	2.4106225
C	1.6712078	2.9251208	1.0733858
O	1.2714755	1.9713156	-1.1304201
C	3.5869137	0.6995688	1.2901389
C	4.5303906	1.8412971	1.0793786
C	4.8780511	2.2572341	-0.2117983
C	5.7706970	3.3041238	-0.4052955
C	6.3249538	3.9453353	0.7100418
C	5.9960375	3.5359285	2.0083344
C	5.1025181	2.4853684	2.1830485
H	4.0900583	-0.2643509	1.3587606
H	1.9857918	-0.3604695	0.1091018
C	1.9826741	-0.3334482	3.0459832
C	7.2438947	5.0350132	0.5186711
N	7.9840512	5.9127276	0.3641449
H	0.8162682	2.0698018	2.8740989
H	2.4472255	2.6995317	3.1258877
H	2.5037222	3.6137129	0.8854419
H	0.7459988	3.4998884	0.9867487
H	4.4403719	1.7589467	-1.0726951
H	6.0375351	3.6285095	-1.4059582
H	6.4355390	4.0384606	2.8638422
H	4.8430029	2.1610140	3.1869292
H	2.3724785	-1.2928635	2.6930170
H	2.4142657	-0.1326754	4.0332277
H	0.8971367	-0.4203871	3.1611629

lc_sy_tr_1.log

E = -1148.923894

H = -1148.589048

G = -1148.656063

NImag=0

C	-4.0354345	2.8916809	1.0467227
C	-2.9572919	2.2839033	1.9105991
C	-3.5634581	3.2766930	-0.2005342
O	-4.1242841	3.9224761	-1.1379580
C	-3.5125815	1.1178774	2.7738214
C	-2.5149628	0.3940183	3.6471828
C	-2.6452575	0.5121645	5.0353663
C	-1.7287340	-0.0861031	5.8923708
C	-0.6715773	-0.8244816	5.3506553
C	-0.5335512	-0.9650949	3.9642932
C	-1.4525785	-0.3537153	3.1211073
C	-2.0969362	2.8272016	-0.3135918
C	-1.8956263	1.8601692	0.8590133
S	-4.4139601	-0.0766309	1.6592659
C	-4.5588736	-1.5521426	2.6987048
C	-6.1367992	0.4635536	1.7510880
C	0.2798998	-1.4538098	6.2277534
N	1.0453150	-1.9606461	6.9337210
C	-2.3507973	3.2976486	2.9024848

H	-4.9819609	3.2300246	1.4653450
H	-4.3089560	1.5155078	3.4137698
H	-3.4706499	1.0841146	5.4493675
H	-1.8307021	0.0120672	6.9680075
H	0.2855041	-1.5474286	3.5556473
H	-1.3375724	-0.4800957	2.0493625
H	-1.8898435	2.3700396	-1.2872659
H	-1.4551973	3.7150334	-0.2293444
H	-0.8810059	1.8700320	1.2720364
H	-2.0986535	0.8432209	0.5042749
H	-5.2737693	-2.2085287	2.1987118
H	-3.5872519	-2.0422890	2.7529096
H	-4.9177542	-1.2758179	3.6924548
H	-6.7399754	-0.3605716	1.3638497
H	-6.2440970	1.3446355	1.1225269
H	-6.3943211	0.6763886	2.7904871
H	-1.5374755	2.8677531	3.4999869
H	-1.9483357	4.1472465	2.3409516
H	-3.1184933	3.6788053	3.5864548

lc_sy_tr_1_r.log

E = -1148.921621
H = -1148.586761
G = -1148.654206

NImag=0

C	1.4177504	-1.2479294	-0.9055370
C	1.4389255	-0.7208568	0.5130660
C	1.3207411	-2.6298215	-0.9678989
O	1.3821111	-3.4200002	-1.9600026
C	0.4856644	0.5098986	0.5884286
C	0.7600719	1.5969327	-0.4301450
C	-0.1299352	1.7400085	-1.5005171
C	0.0840181	2.7020016	-2.4798999
C	1.1983828	3.5428721	-2.3793371
C	2.0887620	3.4247423	-1.3064387
C	1.8650647	2.4531582	-0.3377609
C	1.1727803	-3.1665566	0.4633546
C	0.8692753	-1.9296180	1.3158953
S	0.4844878	1.3835254	2.2383518
C	-0.8745995	2.5484750	2.0003004
C	-0.3041552	0.2361260	3.3845510
C	1.4255698	4.5473466	-3.3842301
N	1.6080315	5.3561498	-4.1927429
C	2.8613046	-0.3889838	0.9974796
H	1.6736639	-0.6233547	-1.7581150
H	-0.5457422	0.1603046	0.4702031
H	-0.9951293	1.0871213	-1.5687347
H	-0.6046198	2.8065932	-3.3116948
H	2.9440908	4.0879576	-1.2328906
H	2.5605490	2.3794538	0.4930851
H	0.3906776	-3.9308954	0.5264796
H	2.1170786	-3.6465564	0.7544649
H	1.3007910	-1.9914390	2.3204456
H	-0.2161823	-1.8227594	1.4220527
H	-1.0954305	2.9802508	2.9782360
H	-0.5398850	3.3290886	1.3165557
H	-1.7422987	2.0175021	1.6027070
H	-0.5961802	0.8335453	4.2510941
H	0.4262507	-0.5127285	3.6869448
H	-1.1781436	-0.2175276	2.9143843
H	2.8886871	0.0328614	2.0125766

H	3.4442085	-1.3159289	1.0141916
H	3.3688862	0.3031573	0.3193024

```
lc_sy_tr_1_ts1.log
E = -1148.897964
H = -1148.565952
G = -1148.633780
```

```
NImag=1
C 2.8346526 -1.0399998 0.4001838
C 1.5777417 -1.0941355 1.0344458
C 2.7840663 -1.6165800 -0.9021598
O 3.6923674 -1.7395765 -1.7420430
C 0.4902460 0.7796770 0.7371030
C -0.8940456 0.5423352 0.3966945
C -1.8338754 0.4001649 1.4479000
C -3.1512900 0.0611597 1.2002217
C -3.5891361 -0.1357068 -0.1209628
C -2.6819547 0.0173468 -1.1822024
C -1.3632358 0.3483296 -0.9260351
C 1.3499991 -2.1045597 -1.1406142
C 0.7164943 -2.0770163 0.2528743
S 1.4770395 1.5835923 -0.4964230
C 0.6157102 3.1192599 -0.9291145
C 2.7770116 2.2866507 0.5364068
C -4.9527565 -0.4791017 -0.3846112
N -6.0592986 -0.7577330 -0.5972653
C 1.4342707 -1.0634422 2.5321967
H 3.7321350 -0.6024661 0.8257200
H 0.6466460 1.2680273 1.6989122
H -1.5075419 0.5617023 2.4714361
H -3.8524956 -0.0444872 2.0224325
H -3.0177249 -0.1280227 -2.2043266
H -0.6842104 0.4384677 -1.7709218
H 0.8548096 -1.4040752 -1.8256274
H 1.3467254 -3.0897433 -1.6153850
H 0.8341425 -3.0545795 0.7400909
H -0.3495514 -1.8395144 0.2657734
H 1.3016120 3.7167748 -1.5342837
H -0.2662281 2.8635297 -1.5175133
H 0.3354595 3.6468408 -0.0158718
H 3.4870984 2.7918199 -0.1199164
H 3.2656857 1.4697238 1.0635009
H 2.3210431 2.9884607 1.2375994
H 0.3915459 -0.9332102 2.8383020
H 1.7863966 -2.0221209 2.9350535
H 2.0369991 -0.2670071 2.9787589
```

```
lc_sy_tr_1_ts2.log
E = -1148.913277
H = -1148.580291
G = -1148.648062
```

```
NImag=1
C -1.6144344 -1.7534542 0.2905110
C -1.7301211 -0.3795066 0.9122088
C -2.5904460 -1.9654843 -0.6972656
O -2.7607953 -2.9481945 -1.4604368
C -0.7362605 0.2410626 -0.0350402
C 0.7173702 -0.1263679 -0.0002620
C 1.3030031 -0.6461522 -1.1625499
C 2.6535561 -0.9651114 -1.1992882
```

C	3.4374648	-0.7464503	-0.0594974
C	2.8748608	-0.2070090	1.1025367
C	1.5199058	0.1030191	1.1254300
C	-3.5032257	-0.7283914	-0.7408720
C	-3.1760782	0.0255568	0.5524073
S	-0.5343019	2.4290447	0.2354647
C	0.7010794	2.7435293	-1.0485029
C	-1.9934215	3.0479856	-0.6363936
C	4.8390063	-1.0698220	-0.0873933
N	5.9673195	-1.3301716	-0.1100313
C	-1.4282958	-0.2715600	2.3994636
H	-0.7963836	-2.4321026	0.5097629
H	-1.1176661	0.3315753	-1.0537936
H	0.6869470	-0.8089220	-2.0424920
H	3.1016571	-1.3758120	-2.0979208
H	3.4951321	-0.0263626	1.9741145
H	1.1015371	0.5498087	2.0212264
H	-3.2663771	-0.1403802	-1.6391380
H	-4.5541184	-1.0224838	-0.8161896
H	-3.8188347	-0.3425755	1.3594813
H	-3.3184158	1.1075769	0.4895810
H	0.7200720	3.8168514	-1.2474130
H	1.6752988	2.4236402	-0.6761348
H	0.4404928	2.1935318	-1.9570918
H	-1.7413426	4.0186764	-1.0686300
H	-2.8015741	3.1750034	0.0837238
H	-2.2866667	2.3490511	-1.4253617
H	-1.3787102	0.7728511	2.7322697
H	-2.2293666	-0.7685697	2.9557341
H	-0.4908187	-0.7666108	2.6646368

lc_sy_tr_2.log

E = -1148.923706

H = -1148.588934

G = -1148.655727

NImag=0

C	-3.9676715	3.1181334	1.3164904
C	-2.8566371	2.4742771	2.0972583
C	-3.8845706	2.8864610	-0.0445004
O	-4.7340293	3.1050178	-0.9663416
C	-3.4073233	1.1863064	2.8133587
C	-2.4220294	0.4081620	3.6553960
C	-1.4460430	-0.4354854	3.1077868
C	-0.5292284	-1.0837190	3.9259582
C	-0.5823678	-0.8853471	5.3103607
C	-1.5579985	-0.0564931	5.8755908
C	-2.4744385	0.5758889	5.0447032
C	-2.5439670	2.1962753	-0.3461289
C	-1.7945979	2.1966855	0.9951232
S	-4.1989358	0.0442748	1.5739152
C	-4.6260000	-1.3698054	2.6189570
C	-5.8720844	0.6850917	1.3041703
C	0.3684680	-1.5502321	6.1611127
N	1.1340570	-2.0851156	6.8459787
C	-2.2771887	3.3561989	3.2132007
H	-4.8564372	3.5105174	1.8084884
H	-4.2456273	1.4952900	3.4492027
H	-1.3995487	-0.6159059	2.0376017
H	0.2209085	-1.7402639	3.4981049
H	-1.5997298	0.0819319	6.9508709
H	-3.2384711	1.2142972	5.4790131

H	-2.7353896	1.1854207	-0.7306979
H	-2.0018214	2.7343036	-1.1319095
H	-1.0836487	3.0294594	1.0184766
H	-1.2113308	1.2887413	1.1708123
H	-5.2874835	-2.0046580	2.0269696
H	-3.7173571	-1.9168987	2.8669869
H	-5.1328674	-1.0150601	3.5193184
H	-6.4705718	-0.1745031	0.9926420
H	-5.8296975	1.4356397	0.5140019
H	-6.2522744	1.1012390	2.2390812
H	-1.3906618	2.9087061	3.6776684
H	-1.9886271	4.3201984	2.7837535
H	-3.0180771	3.5427701	4.0001249

lc_sy_tr_2_r.log

E = -1148.921327

H = -1148.586649

G = -1148.653883

NImag=0

C	1.5385609	-1.4697057	-0.8533844
C	1.3330854	-1.1648585	0.6103224
C	0.6131607	-2.3699647	-1.3592634
O	0.4309198	-2.7978258	-2.5411350
C	0.4861842	0.1610365	0.7139364
C	0.8601103	1.2521764	-0.2676110
C	2.0403963	1.9966310	-0.1541596
C	2.3562243	2.9685799	-1.0973124
C	1.4805765	3.2031179	-2.1627299
C	0.2904368	2.4757198	-2.2828913
C	-0.0122241	1.5107694	-1.3311536
C	-0.2859778	-2.8288055	-0.1993355
C	0.4586589	-2.3712431	1.0580617
S	0.5378385	0.9916667	2.3874813
C	-0.7553969	2.2376733	2.1987336
C	-0.2929888	-0.1453009	3.5122860
C	1.8024246	4.2081250	-3.1406669
N	2.0602012	5.0173773	-3.9280463
C	2.6330921	-1.0801590	1.4162975
H	2.2400909	-0.9084161	-1.4668537
H	-0.5724299	-0.0882289	0.5725485
H	2.7278750	1.8329254	0.6699256
H	3.2726043	3.5426918	-1.0096809
H	-0.3850615	2.6681847	-3.1097262
H	-0.9333737	0.9414892	-1.4182180
H	-1.2697939	-2.3474601	-0.2959319
H	-0.4521381	-3.9109529	-0.2306281
H	1.1388931	-3.1629440	1.3922209
H	-0.2077787	-2.1409625	1.8930280
H	-0.9555532	2.6442737	3.1920456
H	-0.3742088	3.0238367	1.5461454
H	-1.6501579	1.7732173	1.7784498
H	-0.4753088	0.4164226	4.4309618
H	0.3772250	-0.9795437	3.7201999
H	-1.2334590	-0.4819284	3.0722017
H	2.4616818	-0.9665675	2.4958750
H	3.1922786	-2.0096799	1.2733907
H	3.2742565	-0.2578669	1.0824101

lc_sy_tr_3.log

E = -1148.922800

```

H =      -1148.588229
G =      -1148.655927
NImag=0
C      -3.4610439      2.0874590      0.6519687
C      -3.8090695      2.5397471      2.0447883
C      -2.1439757      2.3285765      0.2998657
O      -1.4996368      2.0365176      -0.7559101
C      -3.9835121      1.3744874      3.0808963
C      -2.7646768      0.6282986      3.5627437
C      -1.8154766      0.0668315      2.6952804
C      -0.7012253      -0.5924474      3.1996706
C      -0.5290676      -0.7002173      4.5846882
C      -1.4666966      -0.1511439      5.4654368
C      -2.5757124      0.5060298      4.9465744
C      -1.4468876      3.0464403      1.4693947
C      -2.5705661      3.3971523      2.4547225
S      -5.2917696      0.2112702      2.4342141
C      -4.4624747      -1.1615783      1.6119102
C      -5.8283779      -0.6101980      3.9466889
C      0.6239847      -1.3844749      5.1074121
N      1.5516242      -1.9356409      5.5280790
C      -5.0870135      3.3926101      2.1114410
H      -4.1812931      1.5888681      0.0038061
H      -4.4999624      1.7718242      3.9642803
H      -1.9422522      0.1518648      1.6216573
H      0.0332741      -1.0224270      2.5266161
H      -1.3265376      -0.2380748      6.5376513
H      -3.3047392      0.9376461      5.6269655
H      -0.6912148      2.3790707      1.9040670
H      -0.9161829      3.9330766      1.1044730
H      -2.8465602      4.4510079      2.3440033
H      -2.2944716      3.2496185      3.5052871
H      -5.2610052      -1.8329046      1.2877682
H      -3.9307357      -0.7685583      0.7450348
H      -3.7907217      -1.6693697      2.3050766
H      -6.5453737      -1.3810251      3.6580222
H      -6.3154451      0.1357710      4.5765992
H      -4.9681612      -1.0548144      4.4515594
H      -5.2688970      3.7680751      3.1266374
H      -4.9801259      4.2498291      1.4404065
H      -5.9753211      2.8361020      1.7902234

```

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lc_sy_tr_3_r.log
E =      -1148.921652
H =      -1148.587062
G =      -1148.653689
NImag=0
C      -1.5934229      -1.6190026      -0.1787860
C      -2.1743283      -0.3410941      -0.7337003
C      -1.0954243      -2.4592533      -1.1645715
O      -0.4845546      -3.5688008      -1.0788841
C      -1.0565524      0.7548916      -0.6750194
C      -0.2135045      0.8962133      0.5690581
C      -0.7541532      0.9362681      1.8618246
C      0.0704400      1.0610210      2.9720851
C      1.4566897      1.1509017      2.7954213
C      2.0159308      1.1136400      1.5147014
C      1.1762106      0.9863833      0.4141498
C      -1.3733888      -1.8105335      -2.5331975
C      -2.3932514      -0.7098965      -2.2283118
S      -1.7264250      2.4245779      -1.2272583

```


C	-2.2248081	3.3014059	0.2677685
C	-0.2279679	3.3336889	-1.6492491
C	2.3138151	1.2802704	3.9437488
N	3.0037552	1.3861385	4.8678613
C	-3.5010760	0.0952442	-0.1002042
H	-1.4579509	-1.7815128	0.8878096
H	-0.3738976	0.5498815	-1.5086787
H	-1.8242503	0.8662164	2.0164303
H	-0.3529724	1.0876543	3.9705216
H	3.0912431	1.1777452	1.3858302
H	1.6081863	0.9445927	-0.5821055
H	-0.4328752	-1.4084930	-2.9357966
H	-1.7412582	-2.5492990	-3.2529684
H	-3.4083370	-1.1093243	-2.3288185
H	-2.3208602	0.1598905	-2.8939066
H	-2.6088581	4.2688542	-0.0625878
H	-3.0198920	2.7351690	0.7543908
H	-1.3666236	3.4326146	0.9284772
H	-0.5346306	4.3409881	-1.9376845
H	0.2391585	2.8295345	-2.4969693
H	0.4430023	3.3679048	-0.7887996
H	-3.9530774	0.9490346	-0.6243028
H	-4.2075338	-0.7368365	-0.1758802
H	-3.4139242	0.3530435	0.9585099

lc_sy_tr_3_ts1.log

E = -1148.900288

H = -1148.568122

G = -1148.634394

NImag=1

C	-1.3627875	-1.7996573	0.8256942
C	-1.6851826	-1.4349335	-0.4894281
C	-0.0833898	-2.4272607	0.9039935
O	0.4971526	-2.8889335	1.9014282
C	-1.1809235	0.6384173	-0.8586239
C	0.2316733	0.7559975	-0.5498189
C	0.7356969	0.7254335	0.7682324
C	2.1015371	0.6857149	1.0128929
C	3.0034739	0.6709095	-0.0586477
C	2.5271451	0.7205622	-1.3812938
C	1.1652965	0.7674096	-1.6132915
C	0.4975472	-2.5098665	-0.5107954
C	-0.6558642	-2.0722716	-1.4223676
S	-2.3535718	1.6922349	-0.0782134
C	-2.7494573	1.1344226	1.5988861
C	-1.5262995	3.2503955	0.3347492
C	4.4138714	0.6207749	0.1938593
N	5.5552969	0.5803923	0.3962878
C	-3.1065025	-1.3663175	-0.9933813
H	-1.9917564	-1.6340170	1.6941694
H	-1.4131751	0.6992317	-1.9213794
H	0.0605275	0.7135360	1.6158104
H	2.4730523	0.6521811	2.0323406
H	3.2286008	0.7264814	-2.2097603
H	0.7984023	0.8078457	-2.6352972
H	1.3686424	-1.8473863	-0.5779595
H	0.8431552	-3.5287819	-0.7114643
H	-1.1350144	-2.9452847	-1.8843498
H	-0.3512445	-1.4082478	-2.2368631
H	-3.4001294	1.9108545	2.0084636
H	-3.3012664	0.1982312	1.5360453

H	-1.8587414	1.0279098	2.2161283
H	-2.2700574	3.9017606	0.7984742
H	-1.1742141	3.6871496	-0.6008488
H	-0.6942019	3.0687598	1.0168273
H	-3.1725599	-0.8730409	-1.9677097
H	-3.4763009	-2.3931484	-1.1117967
H	-3.7797302	-0.8623716	-0.2939312

lc_sy_tr_3_ts2.log

E = -1148.913536
H = -1148.580520
G = -1148.647973

NImag=1

C	-1.8158607	-1.6405567	0.6048841
C	-1.9676553	-0.1484731	0.7701176
C	-2.6909623	-2.1608608	-0.3640032
O	-2.8002735	-3.3357179	-0.7921526
C	-0.8621514	0.1940795	-0.1891786
C	0.5685070	-0.2006935	-0.0684903
C	1.2138210	-0.4718416	1.1491126
C	2.5652553	-0.7840937	1.1811146
C	3.2973969	-0.8219549	-0.0128876
C	2.6735832	-0.5608700	-1.2374829
C	1.3185516	-0.2570705	-1.2547385
C	-3.5625418	-1.0133093	-0.8966472
C	-3.3326561	0.1342241	0.0931154
S	-0.7243727	2.4364245	-0.1955790
C	0.6245985	2.7903279	0.9492383
C	0.0820269	2.8353538	-1.7599140
C	4.6994976	-1.1395411	0.0210603
N	5.8292299	-1.3938540	0.0487895
C	-1.9198927	0.4554647	2.1702500
H	-1.0413060	-2.2170086	1.0996072
H	-1.1964592	0.1476326	-1.2274438
H	0.6669567	-0.4564857	2.0827251
H	3.0559804	-0.9971526	2.1250266
H	3.2426109	-0.6026765	-2.1601877
H	0.8275893	-0.0687205	-2.2058417
H	-3.2376740	-0.7632691	-1.9152199
H	-4.6102235	-1.3221859	-0.9597380
H	-4.0982289	0.1088712	0.8758270
H	-3.3620951	1.1291935	-0.3663666
H	0.7895461	3.8699087	0.9666936
H	0.3239866	2.4497962	1.9423418
H	1.5332043	2.2742045	0.6294392
H	0.2234589	3.9171589	-1.8132547
H	-0.5749238	2.5115898	-2.5695471
H	1.0473486	2.3284855	-1.8268728
H	-2.1114955	1.5358832	2.1358661
H	-2.7122189	0.0000261	2.7726558
H	-0.9752075	0.2974036	2.6924911

lc_sy_tr_4.log

E = -1148.915933
H = -1148.581276
G = -1148.648386

NImag=0

C	-4.0897519	2.8415424	1.2324843
C	-2.9942999	2.2339570	2.0675226
C	-3.7321423	3.0444960	-0.0861227

O	-4.3658900	3.5843812	-1.0492228
C	-3.5094401	1.0702406	2.9774069
C	-2.4603900	0.3669978	3.8154046
C	-1.6080425	-0.6132524	3.2925039
C	-0.6358361	-1.2065023	4.0893121
C	-0.5111353	-0.8160543	5.4268263
C	-1.3611331	0.1548736	5.9691145
C	-2.3313125	0.7332837	5.1610166
C	-2.3049261	2.5103676	-0.2938910
C	-1.9225408	1.8056943	1.0182823
S	-4.5569986	-0.2602342	2.1994052
C	-6.1989279	0.4713456	2.0423161
C	-4.1332322	-0.4952384	0.4587428
C	0.4933567	-1.4282948	6.2550992
N	1.3017982	-1.9209901	6.9221562
C	-2.3842040	3.2695722	3.0379095
H	-5.0106318	3.2106598	1.6801977
H	-4.2501144	1.5057835	3.6602810
H	-1.6920957	-0.9397258	2.2599882
H	0.0201137	-1.9676486	3.6805152
H	-1.2645210	0.4442433	7.0102272
H	-2.9971890	1.4835413	5.5779857
H	-2.2688230	1.8389330	-1.1612190
H	-1.6438163	3.3566912	-0.5203560
H	-0.9187635	2.0703330	1.3669533
H	-1.9163883	0.7250921	0.8677789
H	-6.8661903	-0.3431932	1.7525272
H	-6.4872942	0.8541088	3.0227833
H	-6.1805303	1.2629412	1.2949736
H	-4.9201868	-1.1469324	0.0705483
H	-3.1739312	-1.0089434	0.3953105
H	-4.1291284	0.4636468	-0.0589201
H	-1.5454737	2.8693291	3.6193102
H	-2.0130648	4.1118600	2.4448690
H	-3.1409226	3.6521949	3.7332791

lc_sy_tr_4_r.log

E = -1148.914135

H = -1148.579039

G = -1148.645211

NImag=0

C	-1.9251226	-1.1837545	-1.8047201
C	-1.2105946	-0.8930963	-0.4976648
C	-3.2383095	-1.5867053	-1.6072724
O	-4.1005216	-2.0331609	-2.4255199
C	-0.3527343	0.3871165	-0.6966823
C	0.7835134	0.2461182	-1.6877981
C	1.9636702	-0.4419195	-1.3787270
C	2.9753912	-0.5706487	-2.3222733
C	2.8041767	-0.0083320	-3.5926476
C	1.6332198	0.6857338	-3.9160179
C	0.6339740	0.8128226	-2.9584159
C	-3.5530413	-1.4754134	-0.1061774
C	-2.4074035	-0.6285005	0.4548137
S	0.3801157	1.2953467	0.7840893
C	-1.0007199	2.2002831	1.5174614
C	0.7708558	0.1669880	2.1378373
C	3.8477245	-0.1411307	-4.5744293
N	4.6876815	-0.2477189	-5.3645726
C	-0.3913771	-2.1140468	-0.0408233
H	-1.3847723	-1.3221390	-2.7385858

H	-1.0286472	1.1717602	-1.0545743
H	2.1058466	-0.8922071	-0.4001527
H	3.8893234	-1.1033046	-2.0815254
H	1.5129811	1.1229403	-4.9016406
H	-0.2750524	1.3556700	-3.2003660
H	-4.5387149	-1.0308063	0.0676424
H	-3.5708428	-2.4859866	0.3244400
H	-2.1663123	-0.8469074	1.5018807
H	-2.6957865	0.4259200	0.3825423
H	-0.5556951	2.9132805	2.2145400
H	-1.5138868	2.7375203	0.7181747
H	-1.6723525	1.5202283	2.0398859
H	1.0819064	0.8160297	2.9606447
H	1.6066104	-0.4668408	1.8415189
H	-0.1045546	-0.4164544	2.4216993
H	0.2136514	-1.9462871	0.8555249
H	-1.0905804	-2.9276672	0.1806094
H	0.2687943	-2.4634377	-0.8402868

lc_sy_tr_4_ts1.log

E = -1148.890393

H = -1148.558271

G = -1148.625290

NImag=1

C	2.7660741	-0.9322796	0.8323180
C	1.4014941	-1.2343231	0.7045648
C	3.4713118	-1.1373795	-0.3844156
O	4.6712944	-0.9242042	-0.6373167
C	0.2501397	0.6349363	0.7700012
C	-1.1483448	0.4298491	0.4326623
C	-1.6280340	0.5266009	-0.8952930
C	-2.9527821	0.2653880	-1.2073169
C	-3.8471159	-0.1174132	-0.1970353
C	-3.3962675	-0.2238791	1.1307126
C	-2.0754311	0.0500308	1.4339400
C	2.5018259	-1.7203130	-1.4150239
C	1.1497395	-1.8015285	-0.6908693
S	0.9413263	2.0438361	-0.0755871
C	2.2250613	2.5856896	1.0664996
C	1.9678334	1.5218218	-1.4805180
C	-5.2151967	-0.3939842	-0.5158262
N	-6.3243951	-0.6180348	-0.7729659
C	0.6239783	-1.8339435	1.8458046
H	3.2392458	-0.5980722	1.7511406
H	0.4481760	0.7900483	1.8297447
H	-0.9554135	0.8037663	-1.7038691
H	-3.2989564	0.3496134	-2.2327459
H	-4.0911338	-0.5065239	1.9154724
H	-1.7409256	-0.0137590	2.4655383
H	2.4910777	-1.0949428	-2.3140153
H	2.8669175	-2.7071736	-1.7189970
H	0.8087519	-2.8386304	-0.5875248
H	0.3511681	-1.2620741	-1.2108440
H	2.7926973	3.3744570	0.5694596
H	1.7330306	2.9806793	1.9563190
H	2.8640936	1.7359033	1.3118587
H	2.1796754	2.4365692	-2.0385073
H	1.3716882	0.8487124	-2.0977558
H	2.8933428	1.0573716	-1.1455089
H	-0.4463237	-1.8957262	1.6366694
H	0.9896464	-2.8593240	1.9871439

H 0.7798898 -1.2902257 2.7820802

lc_sy_tr_4_ts2.log

E = -1148.909209

H = -1148.576233

G = -1148.644509

NImag=1

C	-1.3286938	-1.8480868	0.4879336
C	-1.5367756	-0.4144808	0.9179255
C	-2.3315729	-2.2846122	-0.3927870
O	-2.4538499	-3.3820031	-0.9913770
C	-0.6509925	0.1522086	-0.1689298
C	0.8335354	-0.0786864	-0.1541926
C	1.6530562	0.4400155	0.8564232
C	3.0238667	0.2142973	0.8412951
C	3.5853825	-0.5299689	-0.2030310
C	2.7837832	-1.0345492	-1.2339689
C	1.4150936	-0.7991625	-1.2046356
C	-3.3537164	-1.1472686	-0.5529213
C	-3.0305224	-0.1857604	0.5963105
S	-0.6438685	2.3546957	-0.4011983
C	-1.9306666	2.5158561	-1.6572719
C	-1.4534097	3.1281449	1.0167908
C	5.0039276	-0.7678877	-0.2228842
N	6.1461048	-0.9594902	-0.2386386
C	-1.1577465	-0.1064382	2.3600489
H	-0.4442306	-2.4181880	0.7535433
H	-1.0804150	0.0174956	-1.1618717
H	1.2283786	1.0410364	1.6552453
H	3.6573146	0.6149822	1.6256856
H	3.2303307	-1.6016706	-2.0439117
H	0.7841628	-1.1896650	-1.9980814
H	-3.2184755	-0.6774356	-1.5379950
H	-4.3759888	-1.5349611	-0.5189356
H	-3.5980049	-0.4755236	1.4875226
H	-3.2731130	0.8585276	0.3789556
H	-2.1133759	3.5781353	-1.8321165
H	-1.5524793	2.0573526	-2.5731962
H	-2.8499264	2.0204791	-1.3389487
H	-1.6830210	4.1597735	0.7399610
H	-0.7455302	3.1260022	1.8471063
H	-2.3673800	2.5998589	1.2907063
H	-1.1958958	0.9632824	2.5897591
H	-1.8650338	-0.6208782	3.0185024
H	-0.1578139	-0.4771996	2.6013337

lc_sy_tr_5_ts1.log

E = -1148.897964

H = -1148.565952

G = -1148.633778

NImag=1

C	2.8346468	-1.0401197	0.4018099
C	1.5778777	-1.0925651	1.0364897
C	2.7835210	-1.6192040	-0.8993996
O	3.6915664	-1.7441709	-1.7392687
C	0.4910122	0.7810656	0.7357664
C	-0.8934996	0.5435715	0.3963632
C	-1.3632591	0.3470537	-0.9257934
C	-2.6822036	0.0160752	-1.1807997
C	-3.5890524	-0.1344561	-0.1189154

C	-3.1506370	0.0649262	1.2017022
C	-1.8329964	0.4039142	1.4482028
C	1.3492122	-2.1071116	-1.1365504
C	0.7160718	-2.0766417	0.2570434
S	1.4776101	1.5821628	-0.4997586
C	0.6165799	3.1172272	-0.9351801
C	2.7782121	2.2869325	0.5311079
C	-4.9529052	-0.4778468	-0.3813637
N	-6.0596343	-0.7564714	-0.5930512
C	1.4347911	-1.0589010	2.5342128
H	3.7323943	-0.6021046	0.8262876
H	0.6479673	1.2712888	1.6965317
H	-0.6845129	0.4351961	-1.7711142
H	-3.0184078	-0.1312414	-2.2025023
H	-3.8515784	-0.0387667	2.0243870
H	-1.5062234	0.5674121	2.4712875
H	0.8541035	-1.4077706	-1.8227903
H	1.3454549	-3.0932098	-1.6094146
H	0.8334928	-3.0533034	0.7461194
H	-0.3498847	-1.8387298	0.2697576
H	1.3024090	3.7133165	-1.5418343
H	-0.2656882	2.8605941	-1.5226907
H	0.3368808	3.6467207	-0.0228751
H	3.4879478	2.7908979	-0.1265225
H	3.2671553	1.4709135	1.0593591
H	2.3226906	2.9900167	1.2313142
H	0.3921983	-0.9276368	2.8403248
H	1.7866125	-2.0169437	2.9388447
H	2.0379674	-0.2618535	2.9790739

lc_sy_tr_6.log

E = -1148.922026

H = -1148.587246

G = -1148.653756

NImag=0

C	-3.9204538	3.3569098	1.4750009
C	-2.7599005	2.5165820	1.9405601
C	-4.1938231	3.2343259	0.1228694
O	-5.1070832	3.7494770	-0.5951365
C	-3.2948209	1.3232462	2.8129832
C	-2.3468417	0.4962336	3.6484925
C	-1.1666948	-0.0653860	3.1397869
C	-0.3166230	-0.7941122	3.9610404
C	-0.6440010	-0.9687332	5.3113588
C	-1.8151772	-0.4164958	5.8388445
C	-2.6555260	0.3100107	5.0025897
C	-3.1599574	2.2729114	-0.4890973
C	-2.0860170	2.1152088	0.5955786
S	-4.4425606	0.2640831	1.8003913
C	-3.4800775	-1.1469014	1.2188943
C	-5.4178017	-0.5453923	3.0831016
C	0.2379854	-1.7201199	6.1647941
N	0.9478079	-2.3251976	6.8511899
C	-1.7840477	3.2815531	2.8495550
H	-4.5241977	3.9324313	2.1750470
H	-4.0240397	1.7754863	3.4962965
H	-0.8955452	0.0630324	2.0984669
H	0.5964398	-1.2240500	3.5631466
H	-2.0599193	-0.5524907	6.8869139
H	-3.5630170	0.7473276	5.4101362
H	-3.6544139	1.3234260	-0.7452204

H	-2.7586886	2.6768257	-1.4248666
H	-1.2796053	2.8337353	0.4121606
H	-1.6192550	1.1269909	0.6078522
H	-4.1904211	-1.7940874	0.6997391
H	-2.7290922	-0.7915787	0.5124100
H	-3.0244403	-1.6740602	2.0584866
H	-6.0766133	-1.2567390	2.5811244
H	-6.0107788	0.2224706	3.5828095
H	-4.7604696	-1.0604674	3.7866395
H	-0.8813094	2.7024759	3.0744957
H	-1.4828076	4.2052693	2.3467629
H	-2.2605116	3.5516990	3.8002019

lc_sy_tr_6_ts1.log
E = -1148.893354
H = -1148.561559
G = -1148.629891

NImag=1

C	-2.8280209	-1.2669792	-0.9069104
C	-1.6165525	-1.4994992	-0.2529954
C	-3.8246389	-0.7903334	-0.0019734
O	-5.0035660	-0.4785578	-0.2325270
C	-0.3499626	0.2764771	-0.6946477
C	1.0712515	0.1783021	-0.3917165
C	1.6043222	0.2605788	0.9166665
C	2.9504366	0.0400264	1.1623830
C	3.8131958	-0.2934331	0.1074527
C	3.3069926	-0.4060066	-1.1975549
C	1.9641982	-0.1693114	-1.4345972
C	-3.2048078	-0.7294885	1.3992034
C	-1.8441053	-1.4215805	1.2497388
S	-1.2939508	1.6909107	-0.2570331
C	-0.9577165	2.1482816	1.4580531
C	-0.5205205	3.1266833	-1.0554539
C	5.2027661	-0.5290599	0.3632775
N	6.3283660	-0.7198175	0.5700306
C	-0.5797256	-2.4594897	-0.7627250
H	-2.9930524	-1.3917393	-1.9730127
H	-0.5736631	0.1403469	-1.7538927
H	0.9559827	0.4611964	1.7614729
H	3.3368577	0.1068557	2.1746591
H	3.9713971	-0.6671368	-2.0154463
H	1.5815502	-0.2491424	-2.4484436
H	-3.1243422	0.3218962	1.7024770
H	-3.8637289	-1.2165642	2.1239864
H	-1.8924825	-2.4508685	1.6297692
H	-1.0167252	-0.9305841	1.7718483
H	-1.6675525	2.9419460	1.7007564
H	-1.1334167	1.2886907	2.1040523
H	0.0648111	2.5153587	1.5572471
H	-1.0513596	4.0246049	-0.7296767
H	-0.6311988	2.9957895	-2.1330374
H	0.5340084	3.1724121	-0.7753539
H	0.3565461	-2.3853524	-0.2020707
H	-0.9666280	-3.4789498	-0.6360725
H	-0.3702868	-2.3088145	-1.8262030

lc_sy_tr_7_ts1.log
E = -1148.900280
H = -1148.568550

G = -1148.635478
NImag=1

C	-0.9909988	1.9345408	-0.9141201
C	-1.4457985	1.6076080	0.3696998
C	0.3581104	2.4012560	-0.8953207
O	1.0582211	2.8030319	-1.8400862
C	-1.2675876	-0.5598356	0.6416608
C	0.1406391	-0.7872067	0.4344778
C	0.7458307	-0.7215864	-0.8431938
C	2.1241105	-0.7772510	-0.9860427
C	2.9410970	-0.9111518	0.1445826
C	2.3605062	-1.0165731	1.4236849
C	0.9876059	-0.9596941	1.5583102
C	0.8442562	2.3976014	0.5583173
C	-0.4094451	2.0789737	1.3852575
S	-2.3330382	-1.2034914	-0.6247653
C	-1.8441188	-2.9310903	-0.8929181
C	-3.8641772	-1.5129577	0.2814065
C	4.3648589	-0.9646516	-0.0023571
N	5.5186170	-1.0068116	-0.1190882
C	-2.8988076	1.7351900	0.7486335
H	-1.5831126	1.8518635	-1.8212527
H	-1.6516094	-0.8307148	1.6261670
H	0.1368297	-0.6126587	-1.7361685
H	2.5740845	-0.7096849	-1.9717642
H	2.9945309	-1.1441876	2.2955533
H	0.5418762	-1.0401314	2.5459904
H	1.6324640	1.6435064	0.6680249
H	1.2844451	3.3694481	0.8032154
H	-0.8025881	2.9874028	1.8596451
H	-0.2394003	1.3500949	2.1839406
H	-2.5836674	-3.3799299	-1.5598160
H	-0.8638326	-2.9375726	-1.3707985
H	-1.8124926	-3.4464401	0.0688852
H	-4.5335530	-2.0426194	-0.3984699
H	-4.3065954	-0.5617811	0.5699297
H	-3.6377836	-2.1219137	1.1585680
H	-3.1422947	1.1970445	1.6694304
H	-3.1144968	2.7989018	0.9141490
H	-3.5599151	1.4006404	-0.0574031

lc_sy_tr_8.log
E = -1148.912723
H = -1148.577920
G = -1148.644372
NImag=0

C	-3.9869112	3.2101524	1.4142195
C	-2.8575935	2.3529129	1.9250370
C	-4.0578913	3.2841488	0.0395171
O	-4.8716886	3.8981239	-0.7234586
C	-3.3799677	1.3741539	3.0115556
C	-2.3981607	0.5540228	3.8206898
C	-1.2566204	-0.0212850	3.2467727
C	-0.3959905	-0.7950500	4.0136897
C	-0.6813979	-1.0045208	5.3690390
C	-1.8146852	-0.4358108	5.9583314
C	-2.6634437	0.3419376	5.1784081
C	-2.9109001	2.4504626	-0.5537889
C	-2.2815607	1.6969366	0.6302883
S	-4.7339150	0.1438243	2.5060507
C	-5.4449773	0.4941399	0.8777466

C	-3.9031781	-1.4207441	2.1501214
C	0.2056505	-1.8114367	6.1648879
N	0.9187880	-2.4619229	6.8046041
C	-1.7784896	3.2069252	2.6296401
H	-4.6545799	3.7343179	2.0965898
H	-3.9601315	1.9815837	3.7145285
H	-1.0313102	0.1313794	2.1971046
H	0.4894683	-1.2380857	3.5703121
H	-2.0238991	-0.5994951	7.0101137
H	-3.5434018	0.7903816	5.6320928
H	-3.2928865	1.7764807	-1.3311905
H	-2.1959727	3.1238623	-1.0436518
H	-1.1879009	1.7509961	0.6243382
H	-2.5335335	0.6327893	0.5789432
H	-6.1229359	-0.3456668	0.7023099
H	-5.9974202	1.4288169	0.9355574
H	-4.6754254	0.5360805	0.1083393
H	-4.6842805	-2.0846956	1.7739392
H	-3.5051243	-1.8195885	3.0829060
H	-3.1177337	-1.2920308	1.4047708
H	-0.9129237	2.6237241	2.9629382
H	-1.4276859	3.9635306	1.9204312
H	-2.1997896	3.7282489	3.4978758

lc_sy_tr_8_ts1.log

E = -1148.883946

H = -1148.551841

G = -1148.619500

NImag=1

C	-2.6500529	-1.4377487	-0.7492045
C	-1.3862910	-1.4772570	-0.1554454
C	-3.6509163	-1.0488558	0.1853898
O	-4.8655294	-0.8637651	-0.0035682
C	-0.2804504	0.3857351	-0.7681297
C	1.1493937	0.2961698	-0.4729389
C	1.6854564	0.5585430	0.8094695
C	3.0288841	0.3586496	1.0870948
C	3.8859044	-0.1294637	0.0896069
C	3.3784793	-0.4090231	-1.1904438
C	2.0394081	-0.1906606	-1.4607858
C	-2.9841722	-0.8583315	1.5512669
C	-1.5447121	-1.3465476	1.3518167
S	-0.9275119	2.0481778	-0.5193155
C	-2.6743206	1.9164481	-0.9600684
C	-1.0781198	2.3872216	1.2496802
C	5.2729143	-0.3440107	0.3755280
N	6.3965118	-0.5183241	0.6065479
C	-0.2888779	-2.3643856	-0.6716412
H	-2.8485994	-1.6266610	-1.8001861
H	-0.4839126	0.2269378	-1.8318137
H	1.0385836	0.8887137	1.6153556
H	3.4174754	0.5641541	2.0797548
H	4.0414749	-0.7821091	-1.9650214
H	1.6572442	-0.3975936	-2.4565537
H	-3.0455560	0.2026468	1.8252018
H	-3.5306807	-1.4147736	2.3186434
H	-1.4112464	-2.3467956	1.7853129
H	-0.7778095	-0.7037566	1.7944762
H	-3.0463939	2.9396539	-1.0374585
H	-2.7434106	1.4195992	-1.9290291
H	-3.2225846	1.3652545	-0.1978912

H	-1.8356564	3.1691516	1.3437281
H	-0.1231434	2.7676841	1.6107036
H	-1.3794881	1.4896647	1.7892659
H	0.6500810	-2.2196744	-0.1317632
H	-0.6051789	-3.4042177	-0.5183390
H	-0.1112241	-2.2240004	-1.7424115

lc_sy_tr_prod_1.log

E = -671.038783
H = -670.787834
G = -670.844292

NImag=0

C	-0.1030284	5.6164365	-2.1849774
C	-0.6565214	4.2372230	-2.1381219
C	-1.9038539	4.2832338	-1.2734879
C	-2.0944312	5.7265074	-0.8001384
C	-0.7713512	6.4503900	-1.0980215
O	0.7131385	6.0282815	-2.9873539
C	-0.6681608	3.6173290	-0.7468922
C	-0.6219936	2.1339448	-0.5760397
C	-0.0722338	1.2725879	-1.5307157
C	-0.0530792	-0.1028996	-1.3208906
C	-0.5901383	-0.6260350	-0.1399463
C	-1.1404741	0.2227312	0.8305292
C	-1.1513053	1.5917458	0.6050673
H	-0.1282331	4.1555405	0.0311084
H	-0.5661977	3.5968851	-3.0089111
C	-3.1338436	3.4796447	-1.6048228
C	-0.5757719	-2.0464413	0.0825021
N	-0.5648290	-3.1908905	0.2625167
H	-2.9051833	6.1766464	-1.3832586
H	-2.3760649	5.7685048	0.2568349
H	-0.1028265	6.4688450	-0.2288068
H	-0.8968495	7.4799809	-1.4385661
H	0.3530459	1.6727521	-2.4454459
H	0.3766641	-0.7677400	-2.0630912
H	-1.5542262	-0.1923159	1.7438532
H	-1.5791314	2.2552486	1.3517898
H	-3.7440298	3.3283290	-0.7065006
H	-3.7432650	4.0090365	-2.3443620
H	-2.8779254	2.4968979	-2.0107508

2a.log

E = -308.554827
H = -308.419756
G = -308.456691

NImag=0

C	3.6391555	-0.3862233	3.2290148
C	2.8534666	-0.4470892	2.1412401
C	3.2381499	-1.1660487	0.8817345
C	4.3388605	-2.1952123	1.1326634
C	5.4823789	-1.5770955	1.9375493
C	4.9938210	-0.9770690	3.2374751
O	5.6975202	-0.9370554	4.2382934
H	3.3244173	0.1272806	4.1338772
H	1.8850277	0.0501172	2.1594927
H	2.3501901	-1.6380780	0.4490800
H	3.5749463	-0.4184588	0.1479580
H	3.9184199	-3.0391255	1.6935176
H	4.7165377	-2.5895305	0.1851136

H	6.2731834	-2.2979345	2.1606222
H	5.9345229	-0.7540779	1.3642691

2a_sy_c_1.log

E = -1148.926606
H = -1148.590629
G = -1148.658355

NImag=0

C	-0.5813965	2.3217067	6.4659612
C	-1.2197563	1.5773935	5.3251893
C	-0.1262868	1.7447232	7.6391969
O	0.5221751	2.3542663	8.5567218
C	-0.2312685	1.2549236	4.1593314
C	-0.9011403	1.0050481	2.8327065
C	-0.7085430	-0.2188829	2.1838863
C	-1.3335110	-0.4836880	0.9705292
C	-2.1513064	0.4961467	0.3966861
C	-2.3499157	1.7288047	1.0316905
C	-1.7280292	1.9744096	2.2489625
C	-0.4573666	0.2721179	7.9067415
C	-1.8296219	0.2448849	5.7892798
C	-0.8528039	-0.5347044	6.6699464
S	0.9891880	2.6473619	3.9681986
C	1.8155903	2.1997801	2.4248161
C	2.3107665	2.2125929	5.1244842
C	-2.7961822	0.2346187	-0.8629228
N	-3.3141734	0.0235883	-1.8769799
H	-0.3772101	3.3841905	6.3219714
H	-2.0182196	2.1854849	4.8793281
H	0.4050489	0.4025758	4.4193502
H	-0.0669587	-0.9708340	2.6345799
H	-1.1882146	-1.4346020	0.4687082
H	-2.9848178	2.4799465	0.5738628
H	-1.8859030	2.9320497	2.7390997
H	0.4085385	-0.1796041	8.4043292
H	-1.2763272	0.2567945	8.6406829
H	-2.1385459	-0.3595291	4.9267614
H	-2.7350847	0.4705279	6.3665208
H	0.0486702	-0.7832495	6.0940460
H	-1.2993976	-1.4911282	6.9651544
H	1.1332995	2.3915038	1.5963292
H	2.6911536	2.8464185	2.3394656
H	2.1123488	1.1490688	2.4573213
H	1.9829777	2.4766549	6.1292356
H	3.1850341	2.7971611	4.8290680
H	2.5139897	1.1422780	5.0431597

2a_sy_c_10.log

E = -1148.926757
H = -1148.590852
G = -1148.658008

NImag=0

C	0.3691311	1.5607026	6.5507733
C	-0.5354928	1.3084066	5.3679309
C	0.2126293	1.0147732	7.8163056
O	0.9766152	1.2339381	8.8168995
C	0.2506133	1.0233088	4.0655009
C	-0.5783004	0.8162005	2.8244466
C	-1.6651806	1.6446200	2.5117125
C	-2.4130262	1.4223513	1.3617234

C	-2.0751169	0.3595149	0.5157108
C	-0.9994226	-0.4827382	0.8183194
C	-0.2595339	-0.2467703	1.9705918
C	-0.9630475	0.0628421	8.0602607
C	-1.4591753	0.1032170	5.6080559
C	-2.0624346	0.1640714	7.0073450
S	1.5371779	2.3484826	3.8174056
C	0.6101405	3.8839562	3.6605738
C	2.0870615	2.1016371	2.1202338
C	-2.8483395	0.1265681	-0.6752950
N	-3.4701259	-0.0607817	-1.6341175
H	1.1742184	2.2883862	6.4424400
H	-1.1830435	2.1776432	5.1597550
H	0.8918291	0.1484118	4.2300534
H	-1.9480303	2.4593688	3.1708546
H	-3.2554024	2.0620540	1.1204378
H	-0.7503620	-1.3079131	0.1595772
H	0.5762300	-0.8973352	2.2128371
H	-0.5707310	-0.9638213	8.0960656
H	-1.3536307	0.2801778	9.0609584
H	-0.8738602	-0.8232493	5.5090593
H	-2.2466010	0.0747456	4.8471312
H	-2.7973048	-0.6389156	7.1352610
H	-2.6029262	1.1136406	7.1239579
H	0.1128388	4.0783925	4.6124469
H	1.3472936	4.6656124	3.4640505
H	-0.1037341	3.8176985	2.8381625
H	2.5289004	1.1052491	2.0550563
H	2.8516641	2.8575431	1.9294998
H	1.2508791	2.2124109	1.4279184

2a_sy_c_10_ts1.log

E = -1148.892092

H = -1148.558524

G = -1148.626848

NImag=1

C	2.8071381	-0.1624232	0.8991350
C	1.4849250	-0.6172026	0.8690810
C	3.8343932	-0.7477476	0.0928480
O	4.9922272	-0.2969323	0.0100283
C	0.3084279	0.5140817	-0.5567188
C	-1.0922900	0.2124539	-0.3638870
C	-1.8612221	0.7135169	0.7140438
C	-3.1712459	0.3089792	0.9138016
C	-3.7589426	-0.6274656	0.0495388
C	-3.0130462	-1.1521707	-1.0198393
C	-1.7100358	-0.7339728	-1.2194863
C	3.4544657	-2.0045334	-0.6770437
C	1.1762776	-2.0244847	0.3691018
C	2.4453139	-2.8385613	0.1105752
S	0.9545294	2.1371974	-0.4194750
C	0.8349725	2.7244139	1.2930192
C	-0.2159424	3.2744738	-1.1996521
C	-5.1111206	-1.0485451	0.2597870
N	-6.2069303	-1.3902727	0.4303745
H	3.0678959	0.7370578	1.4542982
H	0.8160711	-0.2542066	1.6482595
H	0.7549688	0.0965497	-1.4578154
H	-1.4276289	1.4124687	1.4203553
H	-3.7427404	0.7068819	1.7467463
H	-3.4662827	-1.8743956	-1.6918767

H	-1.1458263	-1.1306036	-2.0591385
H	3.0145143	-1.7018272	-1.6391453
H	4.3698005	-2.5624345	-0.8953778
H	0.5909326	-1.9890106	-0.5558953
H	0.5432034	-2.5263883	1.1092022
H	2.1924666	-3.7556026	-0.4316775
H	2.8977848	-3.1388537	1.0635469
H	1.1081260	1.9172085	1.9716220
H	1.5542610	3.5407264	1.3836335
H	-0.1711886	3.0891340	1.4988357
H	-0.2218170	3.0525296	-2.2678311
H	0.1450189	4.2910646	-1.0267157
H	-1.2091466	3.1374927	-0.7675034

2a_sy_c_11.log

E = -1148.926589

H = -1148.590810

G = -1148.659620

NImag=0

C	-0.3699221	2.0971172	6.6041904
C	-1.0022136	1.3538036	5.4577149
C	0.0735837	1.5242397	7.7844217
O	0.6496211	2.1493380	8.7393346
C	-0.0341390	1.1102584	4.2581072
C	-0.7263855	0.7395192	2.9717344
C	-1.7139204	1.5654170	2.4182511
C	-2.3597866	1.2009855	1.2438843
C	-2.0211643	-0.0070754	0.6213143
C	-1.0395638	-0.8437358	1.1641973
C	-0.3950263	-0.4609740	2.3349619
C	-0.1756187	0.0286931	8.0119842
C	-1.5457628	-0.0136827	5.9017475
C	-0.5230073	-0.7649229	6.7531537
S	0.9908806	2.6409160	3.9858734
C	1.7191547	2.3450394	2.3593615
C	2.4532334	2.3374408	5.0040584
C	-2.6904870	-0.3916495	-0.5931112
N	-3.2286097	-0.7012908	-1.5707171
H	-0.2266468	3.1730188	6.4897386
H	-1.8384679	1.9379689	5.0495959
H	0.7115625	0.3497207	4.5122012
H	-1.9802713	2.5045931	2.8960079
H	-3.1203048	1.8414903	0.8100078
H	-0.7862255	-1.7770708	0.6724078
H	0.3703653	-1.1024101	2.7626153
H	0.7133867	-0.3858141	8.5013634
H	-0.9939938	-0.0522457	8.7422246
H	-1.8433853	-0.6131258	5.0324001
H	-2.4503022	0.1607752	6.4980566
H	0.3890085	-0.9416409	6.1673093
H	-0.9126805	-1.7539460	7.0201515
H	0.9496699	2.4897140	1.6008330
H	2.5066100	3.0907296	2.2321617
H	2.1323510	1.3350485	2.3164812
H	2.1501687	2.4099271	6.0478920
H	3.1778676	3.1149392	4.7524942
H	2.8470214	1.3459914	4.7705954

2a_sy_c_1_r.log

E = -1148.923134

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H =      -1148.587459
G =      -1148.655454
NImag=0
C      0.5793097      -0.8223337      1.8855036
C      1.3173665      -0.5175606      0.6073124
C      1.0573726      -0.6210982      3.1699163
O      0.4558348      -0.9588199      4.2473051
C      0.4464882      0.4447923      -0.2673168
C      0.4248293      1.8910081      0.1603704
C     -0.5880658      2.2984924      1.0362612
C     -0.6120296      3.5940525      1.5396319
C      0.3783328      4.4998625      1.1442960
C      1.3835407      4.1151415      0.2490691
C      1.4027493      2.8132219      -0.2338967
C      2.4336412      0.0287421      3.3371301
C      2.7522699      -0.0193405      0.8506151
C      2.8880368      0.8256923      2.1183086
S      0.9746864      0.3530594      -2.0445424
C     -0.3487267      1.2686165      -2.8614859
C      0.5142517      -1.3347434      -2.4864986
C      0.3553000      5.8461522      1.6510464
N      0.3366411      6.9302582      2.0580959
H     -0.3926328      -1.3067562      1.7795265
H      1.3902487      -1.4368975      0.0081038
H     -0.5768681      0.0526224      -0.2849182
H     -1.3598482      1.5933025      1.3285223
H     -1.3926344      3.9057912      2.2256391
H      2.1425501      4.8274320      -0.0567528
H      2.2028105      2.5261961      -0.9112662
H      2.3906932      0.6668979      4.2271099
H      3.1590756      -0.7678531      3.5591965
H      3.1324818      0.5251709      -0.0238676
H      3.3941996      -0.9024687      0.9622374
H      2.2836412      1.7366293      2.0404786
H      3.9303012      1.1464462      2.2332413
H     -0.2169816      2.3278963      -2.6377865
H     -0.2400305      1.0996738      -3.9343759
H     -1.3139799      0.9046947      -2.5031659
H      1.2933567      -2.0119990      -2.1386335
H      0.4622889      -1.3652291      -3.5765902
H     -0.4541606      -1.5767074      -2.0438622

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2a_sy_c_1_ts1.log
E =      -1148.899474
H =      -1148.566666
G =      -1148.634534
NImag=1
C     -2.2401339      -0.6879148      -1.3008255
C     -1.1237222      -1.0915044      -0.5613571
C     -3.5847567      -0.9240257      -0.8721663
O     -4.5843120      -0.5732246      -1.5278734
C     -0.1591596      0.5107346      0.5822793
C      1.2390395      0.2625293      0.3365722
C      1.9760332      -0.5007312      1.2761249
C      3.2881224      -0.8669766      1.0390855
C      3.9214009      -0.4780073      -0.1544337
C      3.2121217      0.2754673      -1.1032325
C      1.8961839      0.6324114      -0.8635799
C     -3.7995692      -1.7071237      0.4196212
C     -1.3163170      -2.0447650      0.5924871
C     -2.5928282      -1.7065367      1.3573446

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S	-0.8511379	1.9425307	-0.1728968
C	0.0082849	3.3683304	0.5417348
C	-2.4196827	2.0729250	0.7016037
C	5.2816847	-0.8471837	-0.4007757
N	6.3849983	-1.1475269	-0.6001502
H	-2.1092146	-0.1679375	-2.2475815
H	-0.1838656	-1.1812249	-1.1046363
H	-0.4911346	0.4191892	1.6159669
H	1.4987694	-0.7938212	2.2071740
H	3.8354354	-1.4469197	1.7759103
H	3.6977970	0.5735545	-2.0274230
H	1.3694035	1.2048362	-1.6236311
H	-4.6922132	-1.3062336	0.9110590
H	-4.0397997	-2.7376470	0.1206279
H	-0.4419277	-2.0373763	1.2511947
H	-1.3942943	-3.0616255	0.1790926
H	-2.4818691	-0.7129438	1.8110993
H	-2.7506829	-2.4170124	2.1753400
H	1.0382726	3.3475165	0.1808857
H	-0.4910293	4.2728660	0.1865475
H	-0.0235868	3.3001679	1.6304848
H	-3.0318969	1.2170921	0.4200373
H	-2.8970924	2.9991604	0.3777697
H	-2.2251442	2.0867727	1.7761448

2a_sy_c_1_ts1_rot1.log

E = -1148.899949

H = -1148.566782

G = -1148.634443

NImag=1

C	-0.4195008	-2.3698302	0.8896562
C	-1.2951444	-1.7444793	-0.0053181
C	0.8854380	-2.8293252	0.5363326
O	1.6599527	-3.3855790	1.3418650
C	-1.4379830	0.3052177	0.5608398
C	-0.1203222	0.8846261	0.4136474
C	0.8722516	0.4930369	1.3448930
C	2.2003520	0.8500448	1.1751270
C	2.5781240	1.6420215	0.0808788
C	1.6022896	2.0826809	-0.8315185
C	0.2821208	1.7072740	-0.6677388
C	1.2946841	-2.7455607	-0.9290366
C	-0.9428876	-1.7149023	-1.4768334
C	0.5680068	-1.6537446	-1.7102878
S	-2.7197827	1.1449334	-0.3106611
C	-3.3132263	2.4405157	0.8095488
C	-4.1191467	0.0127288	-0.2288517
C	3.9475960	2.0216024	-0.0936979
N	5.0574605	2.3287477	-0.2374375
H	-0.7315620	-2.5343070	1.9196122
H	-2.3550514	-1.8384998	0.2162543
H	-1.7531518	0.0898666	1.5820408
H	0.5849698	-0.1006745	2.2061042
H	2.9491461	0.5256269	1.8914664
H	1.8909770	2.7112312	-1.6682594
H	-0.4415543	2.0438429	-1.4045041
H	2.3804664	-2.6117117	-0.9730841
H	1.0771575	-3.7304297	-1.3677066
H	-1.4431683	-0.8811974	-1.9851813
H	-1.3425673	-2.6358051	-1.9274643
H	0.9506032	-0.6780643	-1.3967027

H	0.7810700	-1.7500391	-2.7804435
H	-2.4999252	3.1582411	0.9298088
H	-4.1766400	2.9235325	0.3470040
H	-3.5793001	1.9881079	1.7669880
H	-3.9581214	-0.7891134	-0.9499935
H	-5.0035815	0.5867313	-0.5117464
H	-4.2208429	-0.3770398	0.7861462

2a_sy_c_1_ts2.log

E = -1148.908680
H = -1148.574519
G = -1148.642389

NImag=1

C	-2.2182228	1.0276322	-0.9426473
C	-2.1714642	0.0067287	0.1680920
C	-2.0378300	2.4132704	-0.7699593
O	-2.0856489	3.2482992	-1.7122707
C	-0.9528319	-0.6392586	-0.4047833
C	0.4627778	-0.1920539	-0.2298086
C	1.2190117	0.0950456	-1.3734976
C	2.5629513	0.4328866	-1.2745838
C	3.1671590	0.4624832	-0.0124538
C	2.4335709	0.1539572	1.1399409
C	1.0896958	-0.1754381	1.0244544
C	-1.8791849	2.9546737	0.6479941
C	-2.1094235	0.6112513	1.5721837
C	-1.3487501	1.9380583	1.6548996
S	-0.7978595	-2.7156646	0.4834872
C	0.4845480	-3.3428186	-0.6237577
C	-2.2591921	-3.4214205	-0.3080074
C	4.5606993	0.8003935	0.1016642
N	5.6829080	1.0717821	0.1936814
H	-2.4923797	0.6813726	-1.9359645
H	-3.0069351	-0.7029138	0.1198780
H	-1.1336661	-1.0565320	-1.3965730
H	0.7431265	0.0603347	-2.3494041
H	3.1419881	0.6649808	-2.1622133
H	2.9160712	0.1660894	2.1115232
H	0.5310610	-0.4304210	1.9199762
H	-1.2306823	3.8359547	0.6041931
H	-2.8725745	3.3111556	0.9566974
H	-1.6988330	-0.1190050	2.2806190
H	-3.1462319	0.7944180	1.8805597
H	-0.2815807	1.7879664	1.4739207
H	-1.4374075	2.3354891	2.6722510
H	1.4477174	-2.9727303	-0.2669473
H	0.4788695	-4.4341738	-0.5927934
H	0.3014347	-2.9926968	-1.6437551
H	-3.1291877	-3.1658842	0.2986207
H	-2.1515222	-4.5073904	-0.3483834
H	-2.3703846	-3.0166379	-1.3178578

2a_sy_c_2.log

E = -1148.921443
H = -1148.585409
G = -1148.653822

NImag=0

C	-0.0681873	2.1641864	6.5031665
C	-0.8547424	1.8601691	5.2530703
C	-0.0376180	1.3737299	7.6406299

O	0.6148287	1.6398848	8.7087323
C	0.0045860	1.2710401	4.0928779
C	-0.7643556	0.9009137	2.8434532
C	-1.6173273	1.8184433	2.2159729
C	-2.3356915	1.4525823	1.0847605
C	-2.2050212	0.1536029	0.5782655
C	-1.3595570	-0.7745034	1.1962739
C	-0.6426253	-0.3921460	2.3241030
C	-0.8790670	0.0927654	7.6781032
C	-1.9876984	0.8626121	5.5621468
C	-1.4598304	-0.3449933	6.3335435
S	1.4027854	2.3513782	3.5120287
C	2.7275674	2.1389888	4.7184237
C	0.8937290	4.0592609	3.7820203
C	-2.9520420	-0.2307839	-0.5898351
N	-3.5534329	-0.5396771	-1.5301555
H	0.5078293	3.0871857	6.5428562
H	-1.3185172	2.7761178	4.8590258
H	0.5559587	0.3944937	4.4515284
H	-1.7394832	2.8224123	2.6121037
H	-2.9969845	2.1616540	0.5978421
H	-1.2682823	-1.7789358	0.7963778
H	0.0143869	-1.1074274	2.8110514
H	-0.2608975	-0.6995211	8.1164027
H	-1.6945464	0.2743539	8.3931935
H	-2.5007815	0.5473617	4.6475044
H	-2.7265615	1.3884685	6.1802473
H	-0.6899859	-0.8554024	5.7389248
H	-2.2637310	-1.0743461	6.4851406
H	2.9837505	1.0777874	4.7281570
H	3.5733570	2.7209095	4.3454490
H	2.4086581	2.4746137	5.7029422
H	0.0548561	4.2698994	3.1169671
H	1.7494764	4.6737436	3.4931945
H	0.6298978	4.2288776	4.8251098

2a_sy_c_2_r.log

E = -1148.920176

H = -1148.584224

G = -1148.650347

NImag=0

C	2.1736510	-0.9958060	0.2413450
C	0.9434504	-0.3845043	0.8629977
C	2.5322606	-2.3331332	0.2775757
O	3.6204130	-2.8213258	-0.1853738
C	0.1341918	0.3596500	-0.2530690
C	-0.7737783	-0.5014119	-1.0933787
C	-2.0883387	-0.8062646	-0.7220677
C	-2.8541855	-1.6820182	-1.4813262
C	-2.2972833	-2.2646285	-2.6258311
C	-0.9899557	-1.9581314	-3.0198359
C	-0.2409531	-1.0709677	-2.2563072
C	1.5775106	-3.3215091	0.9509429
C	0.1191892	-1.4067661	1.6671805
C	0.1443271	-2.8116105	1.0630301
S	-0.8008738	1.8625402	0.3325208
C	0.5540461	3.0287075	0.5668406
C	-1.2969876	1.5939970	2.0484188
C	-3.0837966	-3.1766844	-3.4128661
N	-3.7175255	-3.9105822	-4.0462330
H	2.8701397	-0.3003557	-0.2300187

H	1.2502228	0.4096718	1.5594867
H	0.8616540	0.8468009	-0.9116986
H	-2.5344792	-0.3801859	0.1726023
H	-3.8720774	-1.9179877	-1.1899389
H	-0.5721341	-2.4044285	-3.9161446
H	0.7701081	-0.8202409	-2.5615151
H	1.6169716	-4.2574277	0.3819091
H	1.9755354	-3.5479668	1.9511532
H	-0.9153066	-1.0697795	1.7960692
H	0.5529318	-1.4590194	2.6745869
H	-0.3171484	-2.8077034	0.0684351
H	-0.4563581	-3.4847011	1.6863425
H	0.9463208	3.2784560	-0.4199140
H	0.1311675	3.9187428	1.0365665
H	1.3261258	2.5864654	1.1988061
H	-2.1274726	0.8881809	2.0704827
H	-1.6388531	2.5680586	2.4054584
H	-0.4547938	1.2431412	2.6457011

2a_sy_c_2_ts1.log

E = -1148.893432

H = -1148.560378

G = -1148.627927

NImag=1

C	-2.8144514	-0.3460521	-0.7680793
C	-1.4496029	-0.4233064	-1.0530501
C	-3.5368046	-1.3972752	-0.1164660
O	-4.7507704	-1.3211191	0.1523131
C	-0.3019309	0.6770354	0.4709068
C	1.1109115	0.3953133	0.3620772
C	1.9436616	1.0528574	-0.5755710
C	3.2750112	0.7021079	-0.7281208
C	3.8209090	-0.3341553	0.0453586
C	3.0115561	-1.0083462	0.9787453
C	1.6871151	-0.6462716	1.1322768
C	-2.8017250	-2.6978690	0.1861231
C	-0.7657480	-1.7635357	-0.9402657
C	-1.2841492	-2.5428516	0.2648463
S	-0.6927975	2.4064143	0.3773761
C	-2.1717552	2.5110131	1.4026753
C	-1.4040931	2.8035860	-1.2448374
C	5.1937336	-0.7035589	-0.1148569
N	6.3075920	-1.0036360	-0.2442234
H	-3.3887534	0.5444030	-1.0113930
H	-1.0401905	0.2430697	-1.8103401
H	-0.8123238	0.2567655	1.3341587
H	1.5405516	1.8410008	-1.2075320
H	3.8966918	1.2199344	-1.4521555
H	3.4351919	-1.8047791	1.5829538
H	1.0719650	-1.1640018	1.8629811
H	-3.2159095	-3.1146997	1.1094987
H	-3.0623021	-3.3960599	-0.6225875
H	0.3205432	-1.6501497	-0.9081870
H	-0.9942896	-2.3217273	-1.8608383
H	-1.0192333	-2.0040651	1.1831971
H	-0.8040767	-3.5254815	0.3209658
H	-1.8659348	2.3479496	2.4368607
H	-2.5852117	3.5142435	1.2848063
H	-2.8843033	1.7502037	1.0790267
H	-0.6495889	2.5924685	-2.0043735
H	-1.6076551	3.8766237	-1.2220224

H -2.3197784 2.2438461 -1.4288177

2a_sy_c_2_ts2.log

E = -1148.905568

H = -1148.571121

G = -1148.638389

NImag=1

C	-1.5869383	1.8114931	-0.8007265
C	-1.8936245	0.6725863	0.1416609
C	-0.8685953	2.9721793	-0.4627735
O	-0.6202709	3.9032869	-1.2760537
C	-1.0206793	-0.2741427	-0.6249294
C	0.4607191	-0.3981120	-0.4387335
C	1.0090708	-0.9664810	0.7184933
C	2.3838175	-1.0894138	0.8657884
C	3.2253732	-0.6426931	-0.1605625
C	2.6945856	-0.0895926	-1.3314258
C	1.3153265	0.0189301	-1.4659015
C	-0.4532134	3.1744103	0.9909028
C	-1.5472410	0.9739260	1.6036985
C	-0.3290236	1.8834377	1.7941342
S	-1.6828432	-2.4186179	-0.2269027
C	-3.1217663	-2.3828958	-1.3167570
C	-2.5134549	-2.3763044	1.3780994
C	4.6511808	-0.7647579	-0.0128254
N	5.7990309	-0.8632168	0.1064436
H	-1.9997725	1.7576557	-1.8050561
H	-2.9387583	0.3482118	0.0741644
H	-1.3306108	-0.3829268	-1.6634561
H	0.3614740	-1.3108794	1.5204069
H	2.8056022	-1.5268829	1.7643954
H	3.3550475	0.2469252	-2.1235919
H	0.8948362	0.4464588	-2.3711615
H	0.4878026	3.7344915	1.0008554
H	-1.2127255	3.8289893	1.4424276
H	-1.4160061	0.0427760	2.1655289
H	-2.4218697	1.4779451	2.0340268
H	0.5889696	1.3688426	1.4982943
H	-0.2245340	2.1134026	2.8605168
H	-2.7597396	-2.4076069	-2.3461538
H	-3.7357472	-3.2655960	-1.1262041
H	-3.7041587	-1.4742029	-1.1448913
H	-1.7508830	-2.3219702	2.1573472
H	-3.0819542	-3.3020069	1.4930648
H	-3.1830483	-1.5160592	1.4401027

2a_sy_c_3.log

E = -1148.925093

H = -1148.589305

G = -1148.656159

NImag=0

C	-1.1566765	1.8499804	6.1174168
C	-1.1968286	0.4701344	5.5065555
C	-0.4634871	2.1752769	7.2725005
O	-0.4012859	3.3390042	7.7960606
C	-0.2596781	0.3008958	4.2613038
C	-0.9116902	0.4868250	2.9163956
C	-1.8949789	1.4657375	2.7149872
C	-2.4910468	1.6227190	1.4709317
C	-2.1044934	0.7885714	0.4138720

C	-1.1309318	-0.1981397	0.5987217
C	-0.5416314	-0.3411970	1.8500364
C	0.2715462	1.0656540	8.0377539
C	-0.8818925	-0.6095655	6.5523813
C	0.3937997	-0.2843788	7.3247920
S	1.1980881	1.4432951	4.4748322
C	0.7929574	2.9907127	3.6440085
C	2.3573595	0.7639450	3.2649434
C	-2.7225422	0.9440611	-0.8763791
N	-3.2189367	1.0695109	-1.9151321
H	-1.6913721	2.6546555	5.6132240
H	-2.2002461	0.2609736	5.1129716
H	0.2364597	-0.6778864	4.2742776
H	-2.1994231	2.1118494	3.5329859
H	-3.2513090	2.3807300	1.3145173
H	-0.8458748	-0.8449160	-0.2242826
H	0.2083657	-1.1124690	2.0036900
H	1.2609803	1.4537173	8.3084880
H	-0.2719419	0.9350807	8.9844491
H	-0.8051361	-1.5919324	6.0711159
H	-1.7243812	-0.6554521	7.2540122
H	1.2494442	-0.2755367	6.6358552
H	0.6059747	-1.0772420	8.0511082
H	-0.0193258	3.4649420	4.1934031
H	1.6961501	3.6027933	3.7011688
H	0.5245097	2.8015044	2.6034426
H	2.6104804	-0.2515412	3.5750705
H	3.2497746	1.3921270	3.2970725
H	1.9220200	0.7733601	2.2638482

2a_sy_c_3_r.log

E = -1148.917886

H = -1148.581593

G = -1148.647668

NImag=0

C	-0.0929033	-2.1141182	-0.5184608
C	1.0409150	-1.1336722	-0.6929308
C	-0.0838254	-3.2396897	0.2898588
O	-1.0130294	-4.1160008	0.3526339
C	0.4691688	0.3018097	-0.4958737
C	0.0217496	0.7717505	0.8644998
C	0.8933991	0.8950386	1.9555239
C	0.4263069	1.3233340	3.1917595
C	-0.9301197	1.6329120	3.3454009
C	-1.8154791	1.5189887	2.2691687
C	-1.3305859	1.0947402	1.0375715
C	1.1442984	-3.4863282	1.1694071
C	2.2846136	-1.5116831	0.1326898
C	1.9549054	-2.2244377	1.4449159
S	1.5537859	1.5521968	-1.3759378
C	2.6927801	2.3135313	-0.2032938
C	0.3990296	2.9173564	-1.6101427
C	-1.4173087	2.0773034	4.6243674
N	-1.8091816	2.4362735	5.6532498
H	-0.9600578	-1.9670266	-1.1645586
H	1.3596289	-1.1220461	-1.7481589
H	-0.3958606	0.3555228	-1.1684035
H	1.9459189	0.6534290	1.8551166
H	1.1045115	1.4160210	4.0334175
H	-2.8653451	1.7606699	2.3967390
H	-2.0142607	1.0072979	0.1978639

H	0.7946143	-3.9387393	2.1042887
H	1.7743499	-4.2394009	0.6733636
H	2.9267522	-0.6398921	0.3078583
H	2.8795584	-2.2027880	-0.4780769
H	1.3768606	-1.5716959	2.1073217
H	2.8855410	-2.4684439	1.9709787
H	3.3810096	1.5548484	0.1699373
H	3.2487353	3.0565929	-0.7797882
H	2.1413527	2.7930529	0.6064664
H	-0.3855357	2.5770399	-2.2877865
H	0.9570136	3.7372433	-2.0664099
H	-0.0139011	3.2196111	-0.6453636

2a_sy_c_3_ts1.log

E = -1148.896107
H = -1148.562624
G = -1148.630074

NImag=1

C	2.7886824	-0.1302909	0.9681289
C	1.4877927	-0.6336082	0.8904054
C	3.9123155	-0.7638953	0.3467846
O	5.0701511	-0.3091799	0.4091461
C	0.2717597	0.4374529	-0.5863820
C	-1.1276642	0.1645357	-0.3525113
C	-1.8901005	0.7633203	0.6788560
C	-3.2035481	0.3886591	0.9145265
C	-3.8022734	-0.6117245	0.1346647
C	-3.0627266	-1.2338802	-0.8866693
C	-1.7562367	-0.8482593	-1.1211480
C	3.6895889	-2.1048161	-0.3423123
C	1.2758774	-2.0263790	0.3490213
C	2.2470806	-2.3348755	-0.7872077
S	0.9457761	2.0511297	-0.5194799
C	0.8332125	2.7080308	1.1702731
C	-0.2032532	3.1748747	-1.3506776
C	-5.1581111	-0.9995783	0.3810949
N	-6.2570963	-1.3146536	0.5804926
H	2.9947301	0.7901913	1.5114010
H	0.7666118	-0.3120159	1.6419429
H	0.6883866	-0.0192837	-1.4817823
H	-1.4534831	1.5233190	1.3168154
H	-3.7697250	0.8635239	1.7098768
H	-3.5232696	-2.0075806	-1.4932104
H	-1.1943616	-1.3254944	-1.9199190
H	4.3881780	-2.1754453	-1.1818478
H	3.9839244	-2.8781178	0.3820756
H	0.2376849	-2.1663673	0.0337933
H	1.4493019	-2.7288199	1.1781494
H	2.0225186	-1.6852243	-1.6425800
H	2.1161051	-3.3669310	-1.1285398
H	0.9858922	1.8987041	1.8831913
H	1.6320562	3.4451705	1.2690143
H	-0.1357421	3.1839196	1.3223399
H	-0.2104341	2.9080134	-2.4085014
H	0.1753638	4.1913071	-1.2203240
H	-1.1998780	3.0747409	-0.9164969

2a_sy_c_3_ts2.log

E = -1148.905715
H = -1148.571199

G = -1148.638639
NImag=1

C	2.5678574	-0.3489705	-1.0304433
C	2.1502242	0.7259662	-0.0574051
C	2.9334044	-1.6621523	-0.6804526
O	3.3045087	-2.5323223	-1.5136040
C	0.7868484	0.8635340	-0.6604988
C	-0.4228979	0.0401853	-0.3986831
C	-0.9358151	-0.1769548	0.8892638
C	-2.1191604	-0.8807263	1.0713476
C	-2.8063022	-1.3734063	-0.0445361
C	-2.3196769	-1.1545694	-1.3389430
C	-1.1408054	-0.4408609	-1.5048509
C	2.9792130	-2.0320608	0.7986353
C	2.2951451	0.3197878	1.4122685
C	2.0760561	-1.1727697	1.6770754
S	0.0677135	2.9801914	-0.1540420
C	-0.6651493	3.0359238	1.4953806
C	-1.4365319	3.0229688	-1.1511759
C	-4.0318086	-2.1031145	0.1415323
N	-5.0188301	-2.6903005	0.2912689
H	2.6927914	-0.0619242	-2.0717568
H	2.6885622	1.6695921	-0.2175345
H	0.8474680	1.1745521	-1.7034048
H	-0.4205092	0.2139182	1.7596227
H	-2.5132827	-1.0442506	2.0688330
H	-2.8630333	-1.5345408	-2.1975824
H	-0.7606713	-0.2577568	-2.5060050
H	2.7222648	-3.0925195	0.8911944
H	4.0269094	-1.9324409	1.1172493
H	1.6403804	0.9334680	2.0432192
H	3.3236535	0.5654670	1.7046547
H	1.0374596	-1.4567905	1.4885653
H	2.2689034	-1.3799870	2.7357035
H	0.1183370	2.8304770	2.2268460
H	-1.0640515	4.0397303	1.6603203
H	-1.4678255	2.3001000	1.5783649
H	-1.1519058	2.8912908	-2.1972851
H	-1.9202464	3.9938435	-1.0246062
H	-2.1131722	2.2221519	-0.8406221

2a_sy_c_4.log
E = -1148.927681
H = -1148.591490
G = -1148.658100
NImag=0

C	-0.0609164	2.0605921	6.6182832
C	-0.8863728	1.6808975	5.4143000
C	0.0150540	1.3373043	7.7987704
O	0.6808150	1.6773765	8.8354056
C	-0.0349122	1.1274090	4.2320766
C	-0.7603486	0.8978665	2.9320371
C	-1.6640873	1.8344070	2.4112581
C	-2.3247317	1.5879396	1.2136056
C	-2.0860187	0.3904259	0.5296382
C	-1.1945609	-0.5599897	1.0401604
C	-0.5385368	-0.2977207	2.2364706
C	-0.7953058	0.0418885	7.9217257
C	-1.9476027	0.6256545	5.7708942
C	-1.3470523	-0.5034409	6.6056016
S	1.4579615	2.2109978	4.0228995

C	0.8044333	3.8410171	3.6217078
C	2.1190068	1.7144826	2.4212115
C	-2.7699494	0.1320424	-0.7096444
N	-3.3199674	-0.0750771	-1.7074991
H	0.4864654	3.0039982	6.5838663
H	-1.4128935	2.5646219	5.0281757
H	0.4484149	0.1955982	4.5487903
H	-1.8699208	2.7601269	2.9387486
H	-3.0237309	2.3134918	0.8112337
H	-1.0212577	-1.4879365	0.5053836
H	0.1539961	-1.0316507	2.6393144
H	-0.1597148	-0.7003154	8.4186322
H	-1.6235833	0.2493717	8.6148538
H	-2.4238897	0.2322989	4.8651903
H	-2.7310537	1.1244049	6.3556314
H	-0.5445899	-0.9972875	6.0413732
H	-2.1055114	-1.2709285	6.7979323
H	0.2308351	4.1998873	4.4776017
H	1.6710365	4.4861257	3.4630859
H	0.1936429	3.7950576	2.7188379
H	2.4079553	0.6638039	2.4903102
H	3.0047041	2.3290337	2.2475589
H	1.3784880	1.8701250	1.6347771

2a_sy_c_5.log

E = -1148.925303

H = -1148.589480

G = -1148.656483

NImag=0

C	-0.9242131	1.8211136	5.9910981
C	-0.6481889	0.4968461	5.3114693
C	-0.8013657	2.0613027	7.3517233
O	-1.0337321	3.1766756	7.9302869
C	0.1341143	0.6266212	3.9689497
C	-0.7183181	0.6381984	2.7211942
C	-0.3814165	-0.1991307	1.6526396
C	-1.1515665	-0.2170075	0.4950344
C	-2.2686098	0.6203411	0.4069718
C	-2.6189152	1.4643880	1.4684095
C	-1.8434223	1.4667944	2.6203796
C	-0.3405335	0.9131731	8.2565211
C	0.0926502	-0.4819775	6.2345581
C	-0.5151190	-0.4689475	7.6318361
S	1.1211423	2.1971343	3.9617868
C	2.0958260	1.9723955	2.4558065
C	2.4119126	1.9036296	5.1873471
C	-3.0703452	0.6134514	-0.7881151
N	-3.7147786	0.6082990	-1.7502817
H	-1.3346906	2.6320595	5.3901704
H	-1.5875603	0.0002866	5.0128884
H	0.8856709	-0.1662654	3.8760803
H	0.4884996	-0.8453063	1.7283315
H	-0.8925115	-0.8695124	-0.3320748
H	-3.4898005	2.1062910	1.3881983
H	-2.1233372	2.1158426	3.4447078
H	0.7179624	1.0773308	8.5090284
H	-0.8997591	0.9974819	9.1952140
H	1.1511460	-0.2003860	6.3094858
H	0.0590660	-1.4857649	5.7942103
H	-0.0493512	-1.2390431	8.2574060
H	-1.5843034	-0.7137658	7.5647925

H	1.4406482	2.1304787	1.5983564
H	2.8732932	2.7391730	2.4683899
H	2.5377412	0.9740214	2.4370547
H	1.9542383	1.9793507	6.1734685
H	3.1520912	2.6950237	5.0507075
H	2.8596362	0.9219033	5.0208685

2a_sy_c_5_r.log

E = -1148.924186
H = -1148.588407
G = -1148.656302

NImag=0

C	-0.6103672	-1.7959147	-0.0356493
C	-1.2813310	-0.5847314	0.5716426
C	-1.2400925	-2.7384428	-0.8296817
O	-0.6834284	-3.7639534	-1.3558598
C	-0.2770076	0.5984478	0.5389113
C	0.2042884	1.0437606	-0.8235997
C	1.4850311	0.6536774	-1.2329324
C	1.9703811	1.0067504	-2.4856746
C	1.1684954	1.7756755	-3.3370797
C	-0.1056316	2.1912343	-2.9366154
C	-0.5804800	1.8234178	-1.6826555
C	-2.7365171	-2.5632966	-1.1187736
C	-2.6216144	-0.2824630	-0.1002067
C	-3.4402369	-1.5675759	-0.1986162
S	-0.9733185	2.0840311	1.3969191
C	0.5213007	3.0589354	1.6589398
C	-1.2796063	1.4775608	3.0665896
C	1.6640182	2.1522326	-4.6344260
N	2.0625921	2.4556962	-5.6785589
H	0.4413931	-1.9561627	0.2047841
H	-1.4829231	-0.7472754	1.6440233
H	0.5898689	0.3230582	1.1513969
H	2.1059705	0.0654858	-0.5638268
H	2.9606309	0.6965374	-2.8021828
H	-0.7156101	2.7949104	-3.6002009
H	-1.5703340	2.1573949	-1.3858122
H	-2.8443572	-2.2463623	-2.1662593
H	-3.1980698	-3.5550927	-1.0478260
H	-2.4564684	0.0993269	-1.1155815
H	-3.1741196	0.4861745	0.4577427
H	-4.4491057	-1.3487459	-0.5661193
H	-3.5514561	-2.0006802	0.8050947
H	0.8591506	3.4180515	0.6854403
H	0.2485990	3.9048612	2.2924243
H	1.2815856	2.4380721	2.1371549
H	-2.2140305	0.9156625	3.0615359
H	-1.3839055	2.3593399	3.7023799
H	-0.4419530	0.8580053	3.3933422

2a_sy_c_5_ts1.log

E = -1148.894081
H = -1148.561051
G = -1148.629270

NImag=1

C	-1.8478431	-0.9615970	-1.0637918
C	-1.1420860	-1.1326784	0.1337060
C	-3.2763681	-0.9631888	-1.1399285
O	-3.9135612	-0.7164921	-2.1825329

C	-0.0619808	0.6600892	0.7537677
C	1.3070751	0.3423235	0.4289100
C	2.0939580	-0.3187162	1.4043931
C	3.3754831	-0.7549693	1.1246194
C	3.9230963	-0.5483495	-0.1539836
C	3.1582991	0.0909752	-1.1417147
C	1.8733130	0.5224312	-0.8563317
C	-4.0496875	-1.3751813	0.1122045
C	-1.9184206	-1.4335887	1.4063970
C	-3.2056544	-2.1956546	1.0862175
S	-0.8133479	1.9171975	-0.2152997
C	-0.0127660	3.4706667	0.2593466
C	-2.3967386	2.1155488	0.6131355
C	5.2523475	-0.9896091	-0.4477424
N	6.3305184	-1.3480819	-0.6845698
H	-1.3053167	-0.8570926	-2.0018489
H	-0.1526626	-1.5783146	0.0603228
H	-0.2948257	0.7774319	1.8117029
H	1.6779289	-0.4795620	2.3954022
H	3.9631041	-1.2530515	1.8896717
H	3.5760982	0.2451038	-2.1318625
H	1.3057757	1.0071476	-1.6467223
H	-4.4120438	-0.4654666	0.6135646
H	-4.9364365	-1.9230170	-0.2223082
H	-2.1996649	-0.5002386	1.9082574
H	-1.2833615	-1.9882987	2.1045204
H	-3.7650364	-2.3890572	2.0078761
H	-2.9649679	-3.1679610	0.6393479
H	1.0215443	3.4229887	-0.0865593
H	-0.5357008	4.2867150	-0.2445814
H	-0.0540836	3.5843737	1.3439042
H	-2.9914012	1.2255803	0.4121034
H	-2.8823050	2.9919844	0.1808840
H	-2.2296480	2.2488564	1.6840059

2a_sy_c_5_ts2.log

E = -1148.908244

H = -1148.574162

G = -1148.642383

NImag=1

C	-2.2302794	-0.6512024	1.1075459
C	-2.2006532	0.4282170	0.0489486
C	-1.8777171	-1.9836961	0.8432269
O	-1.7378324	-2.8810118	1.7189845
C	-0.8385129	0.8815001	0.4782117
C	0.4310387	0.1223003	0.2143763
C	1.1174134	-0.4146107	1.3134010
C	2.3097577	-1.1046659	1.1473730
C	2.8436346	-1.2459215	-0.1401920
C	2.1924805	-0.6899228	-1.2453898
C	0.9951193	-0.0059970	-1.0624518
C	-1.7088555	-2.3627240	-0.6267680
C	-2.3761570	-0.0491507	-1.4086027
C	-2.6471139	-1.5521041	-1.5228448
S	-0.3748952	2.8268827	-0.4710732
C	1.0364406	3.2641753	0.5678648
C	-1.6724286	3.7847613	0.3397218
C	4.0802079	-1.9571613	-0.3242027
N	5.0762838	-2.5296087	-0.4715868
H	-2.4363678	-0.3552779	2.1328556
H	-2.9196290	1.2195295	0.2825075

H	-0.8484530	1.3176359	1.4788558
H	0.6963905	-0.3037750	2.3083836
H	2.8268599	-1.5283427	2.0018863
H	2.6221902	-0.7877110	-2.2368145
H	0.5202425	0.4389374	-1.9298456
H	-0.6638521	-2.2012578	-0.9294511
H	-1.9062852	-3.4360512	-0.7138034
H	-1.4897390	0.1967743	-1.9989886
H	-3.2025273	0.5073284	-1.8616690
H	-2.5481316	-1.8617745	-2.5692663
H	-3.6817850	-1.7616218	-1.2249590
H	1.9093386	2.7284577	0.1901083
H	1.2093262	4.3398427	0.4979103
H	0.8377596	2.9784227	1.6046904
H	-2.5996432	3.6320732	-0.2147826
H	-1.4014636	4.8419972	0.3097043
H	-1.7910548	3.4540511	1.3754014

2a_sy_c_6.log

E = -1148.917717
H = -1148.581746
G = -1148.648975

NImag=0

C	-0.8508452	1.8451888	5.8216966
C	-0.7109166	0.4163931	5.3502793
C	-0.6755426	2.2772059	7.1240169
O	-0.7495652	3.4930741	7.5210225
C	0.0373042	0.2291850	4.0093263
C	-0.7773152	0.4173547	2.7413775
C	-1.9668482	1.1537550	2.7333394
C	-2.6888231	1.3142827	1.5556500
C	-2.2159680	0.7349931	0.3735793
C	-1.0320392	-0.0118846	0.3666770
C	-0.3235802	-0.1665145	1.5509807
C	-0.3523768	1.2341280	8.1991077
C	-0.1004629	-0.5004565	6.4226653
C	-0.6989571	-0.1956015	7.7906090
S	1.5813191	1.2443482	3.7169854
C	2.4934005	1.3622498	5.2679930
C	1.0886354	2.9639986	3.4720831
C	-2.9584646	0.9026730	-0.8477482
N	-3.5549024	1.0378576	-1.8311118
H	-1.1250689	2.6017130	5.0888617
H	-1.6984764	-0.0228909	5.1145837
H	0.4690022	-0.7798135	3.9753798
H	-2.3427228	1.6035748	3.6459327
H	-3.6119560	1.8841914	1.5510900
H	-0.6798819	-0.4678850	-0.5525629
H	0.5885731	-0.7576332	1.5496826
H	0.7204391	1.3042584	8.4361489
H	-0.8897264	1.5270848	9.1084228
H	0.9854551	-0.3618663	6.4801322
H	-0.2727242	-1.5454565	6.1384876
H	-0.3308809	-0.9120065	8.5340955
H	-1.7904483	-0.3141688	7.7438884
H	2.8840747	0.3731764	5.5090919
H	3.3215845	2.0452123	5.0633513
H	1.8400263	1.7519427	6.0494917
H	0.2597987	2.9865365	2.7619523
H	1.9586414	3.4582955	3.0343102
H	0.8091388	3.4128041	4.4232309

2a_sy_c_6_ts1.log

E = -1148.885578
H = -1148.552370
G = -1148.619405

NImag=1

C	1.7547173	-0.7935901	1.2435310
C	1.0783080	-1.2189056	0.0985101
C	3.1689308	-0.6152968	1.2821871
O	3.7568968	0.0145269	2.1863814
C	0.0319372	0.3891422	-0.9047714
C	-1.3634492	0.2375960	-0.5594903
C	-2.0456886	1.0437966	0.3819222
C	-3.3581296	0.7787671	0.7393288
C	-4.0331400	-0.3164425	0.1798369
C	-3.3716381	-1.1428112	-0.7463080
C	-2.0653678	-0.8683456	-1.1036347
C	3.9905521	-1.2594267	0.1714661
C	1.8884085	-1.8118269	-1.0504204
C	3.2254387	-2.3641449	-0.5538314
S	0.6757883	2.0363735	-0.7138206
C	2.2232945	1.9270496	-1.6289907
C	1.3359454	2.2874551	0.9679226
C	-5.3868798	-0.5934294	0.5521533
N	-6.4850487	-0.8187169	0.8527096
H	1.1894322	-0.4580204	2.1107329
H	0.0827480	-1.6359510	0.2376752
H	0.2954371	0.0653397	-1.9098067
H	-1.5578472	1.9004985	0.8390749
H	-3.8661274	1.4178642	1.4549097
H	-3.8921075	-1.9905446	-1.1812881
H	-1.5630095	-1.5070104	-1.8258545
H	4.2774319	-0.4740011	-0.5434534
H	4.9181257	-1.6288966	0.6212259
H	2.1066235	-1.0480710	-1.8046568
H	1.2984967	-2.5863878	-1.5516395
H	3.8088743	-2.7430356	-1.3998416
H	3.0548196	-3.2050672	0.1290606
H	1.9830337	1.7720745	-2.6818483
H	2.7435102	2.8774597	-1.4974909
H	2.8165627	1.1025515	-1.2308218
H	0.5789032	1.9877678	1.6930093
H	1.5044062	3.3642760	1.0344730
H	2.2616488	1.7360645	1.1264384

2a_sy_c_9.log

E = -1148.924544
H = -1148.588654
G = -1148.656358

NImag=0

C	-0.0630772	1.8945615	6.5845285
C	-0.7929091	1.3730758	5.3726913
C	-0.1103681	1.3469574	7.8572567
O	0.4881947	1.8109353	8.8869686
C	0.0999246	1.2595451	4.1099973
C	-0.6723969	0.9437016	2.8545171
C	-1.7285228	1.7615436	2.4306002
C	-2.4498497	1.4431684	1.2874228
C	-2.1167263	0.2903606	0.5648292
C	-1.0673348	-0.5371798	0.9785668

C	-0.3483498	-0.2010834	2.1203349
C	-0.9525968	0.0846429	8.0719966
C	-1.3827576	-0.0268606	5.6120872
C	-2.0150851	-0.1212261	6.9962581
S	1.0531751	2.8484203	3.8593022
C	1.5624751	2.7718329	2.1287812
C	2.6418443	2.4705755	4.6330804
C	-2.8616240	-0.0454180	-0.6197030
N	-3.4606592	-0.3158089	-1.5731961
H	0.4409554	2.8589576	6.4991406
H	-1.6258931	2.0416471	5.0940995
H	0.8847162	0.5116765	4.2704896
H	-1.9903895	2.6590526	2.9848387
H	-3.2642081	2.0775485	0.9535581
H	-0.8191504	-1.4277585	0.4108514
H	0.4697723	-0.8362535	2.4476684
H	-0.2806435	-0.7851730	8.1073189
H	-1.4076951	0.1670524	9.0654608
H	-0.5775219	-0.7733220	5.5396700
H	-2.1136027	-0.2624219	4.8302462
H	-2.5089125	-1.0920995	7.1178590
H	-2.7931463	0.6485844	7.0923723
H	0.6994647	2.9907545	1.4999043
H	2.3201881	3.5480755	2.0008712
H	1.9768009	1.7861676	1.9078017
H	2.4675804	2.3067752	5.6956998
H	3.2853489	3.3387717	4.4776736
H	3.0621798	1.5814210	4.1592556

2a_sy_c_9_ts1.log

E = -1148.894657

H = -1148.561813

G = -1148.630731

NImag=1

C	-2.4900798	-0.5104926	-1.1655669
C	-1.1962198	-0.8746999	-0.7790837
C	-3.6426133	-0.9032373	-0.4150835
O	-4.7879322	-0.4575341	-0.6195496
C	-0.2456883	0.6161498	0.4854114
C	1.1552236	0.3330930	0.3080598
C	1.8752242	0.6965493	-0.8582511
C	3.1903630	0.3060116	-1.0432594
C	3.8376284	-0.4718795	-0.0702113
C	3.1438468	-0.8490137	1.0938235
C	1.8332409	-0.4496775	1.2768093
C	-3.4091446	-1.9136655	0.6975789
C	-0.9821490	-2.1031806	0.0985451
C	-2.2806567	-2.8770831	0.3343117
S	-0.8418786	2.1106719	-0.2363297
C	0.0675037	3.4601407	0.5598119
C	-2.4345818	2.3018794	0.5849982
C	5.1975168	-0.8734955	-0.2604119
N	6.3006324	-1.2002479	-0.4146851
H	-2.6373120	0.2122412	-1.9664690
H	-0.4049803	-0.6725513	-1.5007704
H	-0.6507685	0.4809669	1.4880753
H	1.3987528	1.2905755	-1.6346211
H	3.7237651	0.5976369	-1.9428699
H	3.6448206	-1.4442611	1.8511038
H	1.3101148	-0.7314120	2.1863357
H	-3.1431246	-1.3574775	1.6100528

H	-4.3513553	-2.4337987	0.8938541
H	-0.5639801	-1.8166360	1.0696353
H	-0.2340393	-2.7471281	-0.3771231
H	-2.1324350	-3.6170284	1.1275558
H	-2.5591262	-3.4257544	-0.5735795
H	1.1059034	3.3986862	0.2291466
H	-0.3733876	4.4026897	0.2270034
H	-0.0038177	3.3495109	1.6432970
H	-3.0969754	1.5112298	0.2326745
H	-2.8282952	3.2781082	0.2968015
H	-2.2839152	2.2447919	1.6650486

2a_sy_c_prod_1.log

E = -671.036095
H = -670.784080
G = -670.838777

NImag=0

C	-0.5955795	0.9277681	2.8648940
C	-1.5914813	-0.1904406	2.6250791
C	-1.5771761	0.9920245	1.7032720
C	-1.1877736	0.9170118	0.2619826
C	-0.0740113	1.6019923	-0.2363427
C	0.2631291	1.5254578	-1.5832309
C	-0.5310791	0.7607631	-2.4456253
C	-1.6629644	0.0865435	-1.9671721
C	-1.9836747	0.1721749	-0.6189903
H	-2.3779655	1.7068910	1.8819322
H	-0.7852996	1.6412256	3.6606704
H	-2.4259102	-0.2207727	3.3197357
C	-1.0804550	-1.5567337	2.2019001
C	0.2814398	-1.5444057	1.4983545
C	1.3111628	-0.7150353	2.2637833
C	0.8621242	0.6737498	2.6602029
O	1.6771630	1.5477418	2.9143196
C	-0.1860659	0.6713740	-3.8388130
N	0.0918064	0.5987763	-4.9611645
H	0.5391220	2.1975467	0.4336437
H	1.1313474	2.0510487	-1.9672179
H	-2.2743143	-0.4977431	-2.6472034
H	-2.8545099	-0.3542318	-0.2382736
H	-0.9989535	-2.1701840	3.1076250
H	-1.8242647	-2.0411777	1.5581801
H	0.1898520	-1.1685285	0.4758101
H	0.6458614	-2.5730388	1.4169804
H	2.2585098	-0.6322519	1.7236735
H	1.5305606	-1.2083461	3.2233944

2a_sy_c_prod_2.log

E = -671.035810
H = -670.783692
G = -670.838268

NImag=0

C	-0.5327941	0.9223185	2.7729639
C	-1.5550621	-0.1888973	2.5667913
C	-1.5481913	0.9924349	1.6426196
C	-1.1814280	0.9195767	0.1942006
C	-0.1185589	1.6688591	-0.3238179
C	0.1811327	1.6384981	-1.6808181
C	-0.5976510	0.8492022	-2.5355335
C	-1.6728592	0.1024007	-2.0376589

C	-1.9568267	0.1446765	-0.6781694
H	-2.3333599	1.7206352	1.8358266
H	-0.6863187	1.6289913	3.5818159
H	-2.3622510	-0.1889378	3.2922200
C	-1.0716090	-1.5683161	2.1249229
C	0.4030448	-1.8096500	2.4475036
C	1.2671526	-0.6832327	1.8699652
C	0.9076300	0.6375405	2.5134361
O	1.7663732	1.4274298	2.8775561
C	-0.2931581	0.8072935	-3.9405691
N	-0.0479657	0.7732811	-5.0722545
H	0.4812857	2.2851623	0.3402250
H	1.0073832	2.2185872	-2.0786283
H	-2.2727592	-0.5016076	-2.7106033
H	-2.7909847	-0.4306046	-0.2862524
H	-1.6881934	-2.3230523	2.6209527
H	-1.2201347	-1.6986586	1.0466711
H	0.7270773	-2.7710092	2.0373230
H	0.5444940	-1.8544614	3.5345244
H	1.0960404	-0.6108575	0.7869507
H	2.3351919	-0.8513029	2.0301367

2a_sy_tr_1.log

E = -1148.924672

H = -1148.588809

G = -1148.656669

NImag=0

C	-4.2101160	4.1734095	-5.0594072
C	-4.0567295	5.6655694	-5.1924850
C	-3.2054370	3.2773440	-4.7375941
O	-3.3617619	2.0206405	-4.5573393
C	-5.2377787	6.3799135	-4.4852218
C	-5.2220183	7.8859027	-4.5981759
C	-6.0638229	8.4782948	-5.5451048
C	-6.0473630	9.8533566	-5.7508800
C	-5.1851674	10.6466308	-4.9873188
C	-4.3443614	10.0710084	-4.0263452
C	-4.3636777	8.6950832	-3.8416714
C	-1.7811444	3.8192967	-4.5803581
C	-2.6815171	6.1508351	-4.7174203
C	-1.5874192	5.2013273	-5.1985619
S	-5.3031885	5.8482540	-2.6984414
C	-6.5495166	6.9811145	-2.0348999
C	-6.3022210	4.3389296	-2.6985891
C	-5.1650063	12.0714053	-5.1870774
N	-5.1486057	13.2181587	-5.3479161
H	-5.2083013	3.7680969	-5.2303985
H	-4.1812850	6.0017150	-6.2388342
H	-6.1784857	5.9988889	-4.8987622
H	-6.7366100	7.8569189	-6.1290671
H	-6.6981783	10.3096437	-6.4893116
H	-3.6834257	10.6970064	-3.4363096
H	-3.7048881	8.2600531	-3.0944057
H	-1.5365693	3.8492822	-3.5083605
H	-1.1030912	3.0862954	-5.0326886
H	-2.4937208	7.1687349	-5.0745857
H	-2.6484531	6.1814756	-3.6181881
H	-0.6011937	5.6056199	-4.9436723
H	-1.6297923	5.1269102	-6.2939868
H	-6.8322659	6.5911921	-1.0554617
H	-6.1069276	7.9701152	-1.9223039

H	-7.4123525	7.0086221	-2.7043003
H	-6.7010505	4.2392462	-1.6865016
H	-5.6485762	3.5048114	-2.9438066
H	-7.1104803	4.4401971	-3.4254471

2a_sy_tr_10.log

E = -1148.913664
H = -1148.577636
G = -1148.645527

NImag=0

C	-4.1815011	4.3737093	-5.4340312
C	-3.8812657	5.7868507	-4.9848347
C	-3.3974190	3.2635063	-5.1898097
O	-3.6865944	2.0567196	-5.5107072
C	-5.2033588	6.5121193	-4.6128176
C	-5.2307877	8.0237618	-4.7404316
C	-4.2963905	8.8570689	-4.1109702
C	-4.3397917	10.2337457	-4.2963178
C	-5.3295090	10.7874278	-5.1162246
C	-6.2751411	9.9718421	-5.7461604
C	-6.2173736	8.5971509	-5.5525874
C	-2.0641198	3.4675079	-4.4633911
C	-2.7479689	5.8202128	-3.9521512
C	-1.6041431	4.9218416	-4.4201958
S	-6.0565286	6.1085800	-3.0059307
C	-5.7952729	4.3603201	-2.6326175
C	-5.1597446	6.9151543	-1.6630094
C	-5.3755314	12.2124956	-5.3127121
N	-5.4130149	13.3589379	-5.4712176
H	-5.1163566	4.2188669	-5.9753322
H	-3.5422137	6.4105914	-5.8344685
H	-5.9618987	6.1272833	-5.3029976
H	-3.5317133	8.4449355	-3.4632033
H	-3.6138542	10.8768226	-3.8102080
H	-7.0392909	10.4098958	-6.3793981
H	-6.9455625	7.9588541	-6.0450276
H	-2.1706352	3.0772492	-3.4397408
H	-1.3200060	2.8328582	-4.9588611
H	-2.3846435	6.8397915	-3.7954152
H	-3.0924050	5.4387045	-2.9836082
H	-0.7420548	5.0358483	-3.7532402
H	-1.2809619	5.2424321	-5.4202435
H	-6.3304907	4.1885253	-1.6955824
H	-6.2471817	3.7790036	-3.4359700
H	-4.7365443	4.1298603	-2.5312230
H	-5.5758256	6.4916445	-0.7458231
H	-5.3854549	7.9808084	-1.7024708
H	-4.0887497	6.7291721	-1.7198687

2a_sy_tr_10_ts1.log

E = -1148.891534
H = -1148.558019
G = -1148.624931

NImag=1

C	-2.7091206	-0.6530816	-1.1471456
C	-1.3366440	-0.9013305	-1.0007176
C	-3.6806037	-1.0047028	-0.1614643
O	-4.8900805	-0.7087564	-0.2461938
C	-0.1760749	0.9061307	-0.9555911
C	1.1661624	0.5366298	-0.5649450

C	1.6840421	0.5933955	0.7500239
C	2.9432875	0.0997616	1.0495890
C	3.7306556	-0.4833593	0.0452944
C	3.2381550	-0.5569129	-1.2688716
C	1.9855800	-0.0507825	-1.5626253
C	-3.2162925	-1.8560092	1.0188295
C	-0.8539192	-1.6458219	0.2323241
C	-1.9252382	-2.6188338	0.7281874
S	-1.1226254	2.1578701	-0.1751523
C	-1.6613539	1.6031939	1.4570334
C	-0.0319702	3.5295213	0.2806482
C	5.0298433	-0.9964779	0.3580997
N	6.0829705	-1.4129772	0.6114513
H	-3.0795969	-0.1927485	-2.0611869
H	-0.7625365	-1.0765707	-1.9084835
H	-0.3030440	1.0776838	-2.0220004
H	1.1032416	1.0206531	1.5589859
H	3.3212259	0.1583479	2.0655702
H	3.8454946	-1.0035698	-2.0500693
H	1.6166833	-0.1015797	-2.5835159
H	-3.0681756	-1.1971240	1.8872663
H	-4.0397048	-2.5305044	1.2745694
H	0.0847622	-2.1640226	0.0125886
H	-0.6364842	-0.9388463	1.0432334
H	-1.5733282	-3.1329432	1.6289779
H	-2.1124398	-3.3856576	-0.0334108
H	-2.2115853	2.4423416	1.8885310
H	-2.3389710	0.7646377	1.3064508
H	-0.8247775	1.3290169	2.0972716
H	-0.6533125	4.2874898	0.7628161
H	0.3889798	3.9237752	-0.6456482
H	0.7577317	3.1944129	0.9534393

2a_sy_tr_1_r.log

E = -1148.925066

H = -1148.589005

G = -1148.657470

NImag=0

C	1.8443049	-0.9129101	2.0041180
C	1.2174319	-0.7724747	0.6342328
C	3.1482950	-1.3161774	2.2516639
O	3.6837356	-1.4232523	3.4069871
C	0.3942096	0.5313478	0.6230198
C	-0.7162773	0.5664362	1.6455424
C	-0.8341548	1.6739896	2.4899491
C	-1.8487394	1.7371353	3.4385711
C	-2.7600136	0.6799677	3.5326267
C	-2.6563206	-0.4347233	2.6910201
C	-1.6323423	-0.4875489	1.7542238
C	4.0432243	-1.6697847	1.0592857
C	2.2767639	-0.7836741	-0.4721652
C	3.2751066	-1.9128880	-0.2362347
S	-0.3956855	0.7793926	-1.0683025
C	-1.6724733	2.0206275	-0.7651750
C	0.7982516	1.8244295	-1.9356013
C	-3.8171265	0.7375843	4.5073334
N	-4.6685695	0.7848506	5.2908198
H	1.2106664	-0.7273923	2.8705973
H	0.5105561	-1.5926884	0.4146824
H	1.0499717	1.4008422	0.7464526
H	-0.1229347	2.4908142	2.4070225

H	-1.9370845	2.5936699	4.0985027
H	-3.3695299	-1.2478433	2.7761431
H	-1.5555680	-1.3566875	1.1069928
H	4.7652109	-0.8521854	0.9199987
H	4.6270295	-2.5531566	1.3422772
H	1.8045598	-0.9056917	-1.4560219
H	2.8150230	0.1759370	-0.4739477
H	3.9622791	-1.9938451	-1.0858656
H	2.7293199	-2.8643775	-0.1734391
H	-2.0207030	2.3453735	-1.7479467
H	-2.4912128	1.5522311	-0.2188038
H	-1.2486388	2.8578255	-0.2070564
H	0.2859802	2.2103042	-2.8193825
H	1.6481380	1.2154423	-2.2379665
H	1.1063618	2.6404902	-1.2792870

2a_sy_tr_1_ts1.log

E = -1148.894884

H = -1148.561941

G = -1148.629917

NImag=1

C	2.5089921	-0.9531831	1.1861884
C	1.1510482	-1.0530930	0.8658936
C	3.5499187	-1.1769120	0.2349093
O	4.7528945	-0.9320738	0.4574038
C	0.2052440	0.8826240	0.7080233
C	-1.1719904	0.5560317	0.4365857
C	-1.9765491	0.1245420	1.5226377
C	-3.2684851	-0.3270238	1.3300452
C	-3.8155108	-0.3591298	0.0351164
C	-3.0437270	0.0729566	-1.0554566
C	-1.7495864	0.5223946	-0.8573294
C	3.1446481	-1.7633916	-1.1114526
C	0.7398932	-1.7146919	-0.4427191
C	1.8613800	-2.5849554	-1.0102096
S	1.0613423	1.7909277	-0.5325893
C	0.2811426	3.4280544	-0.6031465
C	2.5977134	2.2406924	0.2977086
C	-5.1541285	-0.8206779	-0.1691926
N	-6.2398460	-1.1964848	-0.3346743
H	2.8057294	-0.5928518	2.1694151
H	0.4576323	-1.1764866	1.6962382
H	0.4293738	1.2664355	1.7024393
H	-1.5643591	0.1535669	2.5276248
H	-3.8652973	-0.6534760	2.1762646
H	-3.4661209	0.0563905	-2.0554208
H	-1.1834233	0.8493625	-1.7260512
H	2.9959788	-0.9296772	-1.8149634
H	3.9855060	-2.3544988	-1.4872510
H	-0.1741430	-2.2971965	-0.2877670
H	0.4934629	-0.9569991	-1.1978380
H	1.5707835	-2.9694035	-1.9935202
H	2.0322078	-3.4497748	-0.3576333
H	0.8601192	4.0455002	-1.2937679
H	-0.7340134	3.2958160	-0.9813070
H	0.2704239	3.8573317	0.4004752
H	3.0772090	2.9988212	-0.3243555
H	3.2305208	1.3571651	0.3697498
H	2.3640062	2.6393973	1.2869657

2a_sy_tr_1_ts2.log

E = -1148.913683
H = -1148.579607
G = -1148.647659

NImag=1

C	1.6110087	-1.5577314	-0.1835140
C	1.5981881	-0.1649622	-0.7661704
C	2.7258286	-2.1488637	0.4418038
O	2.7149833	-3.2956142	0.9651953
C	0.5421871	0.3364134	0.1546413
C	-0.8616263	-0.1332595	0.0639501
C	-1.6330754	-0.2083804	1.2315559
C	-2.9651809	-0.5959743	1.1772177
C	-3.5357411	-0.9033108	-0.0642105
C	-2.7792289	-0.8288246	-1.2414604
C	-1.4466159	-0.4463699	-1.1720261
C	4.0519719	-1.3883654	0.4212950
C	2.9236410	0.5858848	-0.5765676
C	4.1190179	-0.3518851	-0.6990318
S	0.2259836	2.5259323	-0.4336092
C	-1.3433879	2.9246009	0.3679432
C	1.3489719	3.3784610	0.6993744
C	-4.9167265	-1.3006525	-0.1320836
N	-6.0288370	-1.6195345	-0.1868392
H	0.7285183	-2.1768638	-0.3155637
H	1.2844346	-0.1286816	-1.8175129
H	0.8860218	0.5526480	1.1668747
H	-1.1794484	0.0341499	2.1885233
H	-3.5614676	-0.6599658	2.0812093
H	-3.2360627	-1.0687861	-2.1958545
H	-0.8640152	-0.3861268	-2.0861265
H	4.1921290	-0.8921205	1.3921088
H	4.8469759	-2.1357784	0.3295611
H	2.9836754	1.4107031	-1.2961910
H	2.9491079	1.0283401	0.4286341
H	5.0528643	0.2175697	-0.6422392
H	4.1039550	-0.8549934	-1.6746982
H	-1.5002900	4.0034266	0.3012781
H	-2.1414175	2.4064823	-0.1670395
H	-1.3231269	2.6102718	1.4142647
H	1.0248909	4.4179108	0.7870264
H	2.3531541	3.3471021	0.2760502
H	1.3346675	2.8962820	1.6797997

2a_sy_tr_2.log

E = -1148.921535
H = -1148.585676
G = -1148.652694

NImag=0

C	-4.3219715	4.2955947	-5.5007276
C	-4.0548579	5.7674288	-5.3435710
C	-3.4782851	3.2709244	-5.1165246
O	-3.7285699	2.0198767	-5.2296592
C	-5.1351531	6.4692130	-4.4527678
C	-5.1536448	7.9758513	-4.5928808
C	-4.2975078	8.8255592	-3.8808234
C	-4.3222540	10.1981469	-4.0982440
C	-5.2074577	10.7283766	-5.0434220
C	-6.0702431	9.8930757	-5.7619824
C	-6.0409732	8.5244875	-5.5264753
C	-2.1165209	3.6323803	-4.5140173

C	-2.5978189	6.0598355	-4.9548545
C	-2.0360468	5.0499878	-3.9539909
S	-5.0311442	6.0605111	-2.6512370
C	-6.5290609	6.8655021	-2.0422724
C	-5.5553648	4.3358767	-2.5271477
C	-5.2351727	12.1480056	-5.2751852
N	-5.2577858	13.2906731	-5.4624001
H	-5.2957936	4.0187311	-5.9086364
H	-4.2385247	6.2866107	-6.2989385
H	-6.1127051	6.0728735	-4.7510451
H	-3.6042625	8.4306431	-3.1429329
H	-3.6613198	10.8547490	-3.5424524
H	-6.7575575	10.3143169	-6.4880285
H	-6.7137298	7.8713888	-6.0751670
H	-1.8954050	2.8926655	-3.7358058
H	-1.3549882	3.4972690	-5.2959734
H	-1.9963045	5.9991530	-5.8706732
H	-2.4862554	7.0835608	-4.5818562
H	-2.5844156	5.0992190	-3.0039806
H	-0.9987788	5.3107648	-3.7136705
H	-6.6812871	6.5178712	-1.0187372
H	-6.3678086	7.9437259	-2.0461083
H	-7.3728123	6.5885527	-2.6781396
H	-5.8273924	4.1856845	-1.4795427
H	-4.7195035	3.6963696	-2.8051115
H	-6.4111226	4.1687442	-3.1838169

2a_sy_tr_2_r.log

E = -1148.925047

H = -1148.589056

G = -1148.656087

NImag=0

C	1.4912981	-2.4540527	1.5947413
C	0.8205261	-1.7581572	0.4333202
C	2.8582844	-2.4667833	1.8304833
O	3.4370506	-3.0641002	2.8005519
C	0.1058459	-0.4984139	0.9869505
C	-0.9634206	-0.8194024	2.0032174
C	-1.9787786	-1.7403341	1.7155511
C	-2.9614786	-2.0210447	2.6560169
C	-2.9247205	-1.3780873	3.8997923
C	-1.9154154	-0.4576590	4.2015486
C	-0.9431981	-0.1812262	3.2467654
C	3.7869510	-1.7512899	0.8407251
C	1.8273145	-1.4482120	-0.6792214
C	3.0874525	-0.7918346	-0.1215358
S	-0.7104849	0.4815520	-0.4084235
C	-1.9318215	1.5178501	0.4273604
C	0.5256442	1.7519165	-0.7671645
C	-3.9387143	-1.6673130	4.8790919
N	-4.7552517	-1.8991161	5.6668977
H	0.8508208	-2.9693130	2.3098194
H	0.0357639	-2.3948677	0.0007567
H	0.8242729	0.2084068	1.4140388
H	-2.0130820	-2.2435835	0.7530822
H	-3.7509240	-2.7314864	2.4348305
H	-1.8965530	0.0325072	5.1692859
H	-0.1564905	0.5334671	3.4706361
H	4.5528032	-1.2301813	1.4265445
H	4.3130473	-2.5311294	0.2711621
H	2.1021644	-2.4022386	-1.1467532

H	1.3754381	-0.8466146	-1.4778824
H	2.8251542	0.1365312	0.4045682
H	3.7607687	-0.5068732	-0.9381406
H	-2.2776388	2.2415996	-0.3136833
H	-2.7630063	0.8877305	0.7446498
H	-1.4687145	2.0231139	1.2772004
H	0.0475325	2.4762548	-1.4295478
H	1.3719381	1.2916373	-1.2757700
H	0.8344108	2.2247127	0.1671843

2a_sy_tr_2_ts1.log

E = -1148.897692
H = -1148.564630
G = -1148.631837

NImag=1

C	2.4549308	-1.0899638	1.2194891
C	1.1489902	-1.1744998	0.7225821
C	3.6126537	-1.2901605	0.4121237
O	4.7792610	-1.1852472	0.8436503
C	0.1861768	0.7401115	0.6259981
C	-1.2112881	0.4305485	0.3913338
C	-1.8424250	0.4886572	-0.8750589
C	-3.1516081	0.0734489	-1.0464138
C	-3.8806683	-0.4269066	0.0447297
C	-3.2759135	-0.5006765	1.3095874
C	-1.9688164	-0.0765993	1.4751796
C	3.4128043	-1.7269874	-1.0364634
C	0.9263057	-1.7609971	-0.6501507
C	2.0437051	-1.3698488	-1.6126011
S	0.8885664	1.8891169	-0.5073863
C	0.3009661	3.5210180	0.0243003
C	2.6090493	2.0214099	0.0148052
C	-5.2347561	-0.8564366	-0.1313929
N	-6.3320987	-1.2058775	-0.2743281
H	2.6209825	-0.8189969	2.2603831
H	0.3580448	-1.3833614	1.4431741
H	0.4329721	1.0282011	1.6484553
H	-1.3034409	0.8608319	-1.7422255
H	-3.6169482	0.1313373	-2.0254427
H	-3.8383100	-0.8831575	2.1558724
H	-1.5137155	-0.1229655	2.4608696
H	4.2240985	-1.2978671	-1.6334691
H	3.5495851	-2.8178993	-1.0545458
H	0.9073018	-2.8554067	-0.5391463
H	-0.0529427	-1.4706060	-1.0433872
H	1.9950638	-0.2902074	-1.8069128
H	1.9005975	-1.8618029	-2.5802649
H	0.7901689	4.2775466	-0.5938370
H	-0.7781212	3.5449697	-0.1378913
H	0.5403285	3.6578401	1.0809093
H	2.9920920	2.9437358	-0.4258534
H	3.1650420	1.1688324	-0.3712608
H	2.6581597	2.0610829	1.1048167

2a_sy_tr_2_ts2.log

E = -1148.917918
H = -1148.583518
G = -1148.650050

NImag=1

C	-1.4893781	-1.7318877	0.5734075
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C	-1.5559464	-0.3120164	1.0830370
C	-2.4966676	-2.3347998	-0.1967195
O	-2.4448933	-3.5206693	-0.6287708
C	-0.6483477	0.2457980	0.0351223
C	0.7979152	-0.1075908	0.0366319
C	1.5156119	-0.2380188	1.2344819
C	2.8771137	-0.5083746	1.2123232
C	3.5309961	-0.6501412	-0.0187941
C	2.8287065	-0.5199544	-1.2231021
C	1.4681497	-0.2447548	-1.1859678
C	-3.7843173	-1.5541926	-0.4734354
C	-2.9736260	0.2558177	1.0763730
C	-3.7045350	-0.0463484	-0.2309274
S	-0.5220581	2.4508822	0.3661173
C	0.9940058	2.9381615	-0.4871715
C	-1.7312496	3.0159419	-0.8537518
C	4.9412099	-0.9322894	-0.0451363
N	6.0769429	-1.1586546	-0.0665551
H	-0.6071868	-2.3212420	0.8081333
H	-1.1198837	-0.2020758	2.0813578
H	-1.0774546	0.3181581	-0.9639295
H	1.0148443	-0.1221018	2.1909087
H	3.4351213	-0.6087275	2.1373283
H	3.3457553	-0.6333157	-2.1701149
H	0.9134022	-0.1398382	-2.1143579
H	-4.0898160	-1.7703295	-1.5029243
H	-4.5539339	-1.9955190	0.1756825
H	-3.5175862	-0.2104927	1.9073973
H	-2.9589397	1.3338508	1.2800795
H	-3.1920461	0.4384184	-1.0711248
H	-4.7116678	0.3836737	-0.1998046
H	1.0270596	4.0290898	-0.5301669
H	1.8442046	2.5688334	0.0893604
H	1.0083250	2.5195810	-1.4961611
H	-1.6047797	4.0916632	-0.9939431
H	-2.7313313	2.8156947	-0.4666395
H	-1.5769812	2.4909677	-1.7997045

2a_sy_tr_3.log

E = -1148.926550
H = -1148.591050
G = -1148.659311

NImag=0

C	-3.4780180	5.0912317	-3.9021639
C	-4.7252325	5.1302290	-4.7463592
C	-2.1908062	4.9308419	-4.3890148
O	-1.1254437	4.9128296	-3.6822500
C	-5.7742048	6.1817488	-4.2919846
C	-5.3971178	7.6297719	-4.4779274
C	-4.3599263	8.2291497	-3.7506203
C	-4.0127173	9.5550478	-3.9850258
C	-4.7090500	10.2883220	-4.9522888
C	-5.7545906	9.7058420	-5.6784148
C	-6.0935663	8.3811298	-5.4315336
C	-1.9990596	4.7675555	-5.9018314
C	-4.4023951	5.3766350	-6.2256246
C	-3.2811107	4.4391199	-6.6649519
S	-6.1717903	5.9372811	-2.5032579
C	-7.7299188	6.8337363	-2.3742011
C	-6.7496953	4.2316463	-2.4626095
C	-4.3508244	11.6601048	-5.1978386

N	-4.0630758	12.7642329	-5.3962753
H	-3.5801646	5.1645171	-2.8176337
H	-5.2794045	4.1753508	-4.7129460
H	-6.7213056	5.9839232	-4.8079617
H	-3.8175904	7.6642119	-2.9996780
H	-3.2088847	10.0203111	-3.4243315
H	-6.2923514	10.2859267	-6.4210550
H	-6.9034814	7.9210679	-5.9906810
H	-1.5620834	5.7001155	-6.2874283
H	-1.2425859	3.9883022	-6.0508067
H	-5.3046343	5.2348171	-6.8334052
H	-4.0674808	6.4133522	-6.3662323
H	-3.1182884	4.5219002	-7.7455412
H	-3.5797785	3.4008935	-6.4646564
H	-8.1278523	6.6479898	-1.3748107
H	-7.5114362	7.8963907	-2.4936996
H	-8.4203449	6.4832922	-3.1438597
H	-7.2482134	4.0930999	-1.5012012
H	-5.8778765	3.5789420	-2.5246243
H	-7.4416992	4.0569399	-3.2889741

2a_sy_tr_3_ts1.log

E = -1148.899940

H = -1148.566917

G = -1148.633875

NImag=1

C	0.9684119	-1.9303112	-0.7626120
C	1.3915854	-1.5581098	0.5192593
C	-0.3835468	-2.2926879	-1.0558143
O	-0.8015681	-2.5526197	-2.2019365
C	1.4346140	0.5900036	0.6737527
C	0.0684930	0.9628533	0.4030776
C	-0.4954965	0.8959863	-0.8950519
C	-1.8542701	1.0828573	-1.0956735
C	-2.6973968	1.3413723	-0.0055649
C	-2.1586936	1.4317885	1.2913449
C	-0.8025653	1.2488330	1.4844726
C	-1.3307761	-2.4196863	0.1330296
C	0.5336043	-1.8966570	1.7301984
C	-0.5882735	-2.8790967	1.3873225
S	2.5811291	1.0775236	-0.5707187
C	3.0390868	2.7779249	-0.1525850
C	4.1128882	0.2345882	-0.1306668
C	-4.1018432	1.5299028	-0.2135867
N	-5.2401461	1.6820840	-0.3801753
H	1.6608423	-1.8750455	-1.6019492
H	2.4603877	-1.5823483	0.7130975
H	1.8198900	0.8050650	1.6717564
H	0.1323059	0.6904913	-1.7556298
H	-2.2709272	1.0182438	-2.0962559
H	-2.8088109	1.6498918	2.1329143
H	-0.3904337	1.3267416	2.4868617
H	-1.7990976	-1.4401505	0.3130417
H	-2.1275924	-3.1162972	-0.1454940
H	1.1791883	-2.3068424	2.5143204
H	0.0781228	-0.9926384	2.1491050
H	-1.2773503	-2.9647416	2.2344672
H	-0.1673328	-3.8763754	1.2090834
H	3.8091543	3.1053316	-0.8546000
H	2.1426941	3.3899156	-0.2664724
H	3.4033294	2.8086299	0.8762191

H	4.9222234	0.7716384	-0.6286271
H	4.0699446	-0.7872306	-0.5069564
H	4.2451732	0.2563879	0.9530750

2a_sy_tr_4.log

E = -1148.926753
H = -1148.591069
G = -1148.658092

NImag=0

C	-3.6336712	4.8112574	-3.9449967
C	-4.8969102	4.9593018	-4.7454041
C	-2.3449661	5.0017666	-4.4174652
O	-1.2744273	4.8303003	-3.7399226
C	-5.8631995	6.0859545	-4.2413155
C	-5.4058921	7.5028492	-4.4605986
C	-4.3419099	8.0603493	-3.7377261
C	-3.8861607	9.3396103	-4.0329642
C	-4.5013476	10.0696020	-5.0568342
C	-5.5786773	9.5331331	-5.7724626
C	-6.0277867	8.2550636	-5.4635717
C	-2.1555801	5.4063928	-5.8829922
C	-4.6287877	5.1513706	-6.2507960
C	-3.3950415	6.0054226	-6.5432083
S	-6.1578569	5.8720225	-2.4332050
C	-7.6755054	6.8223096	-2.2236670
C	-6.7963680	4.1901795	-2.3277743
C	-4.0298012	11.3930380	-5.3676304
N	-3.6502139	12.4581644	-5.6182739
H	-3.7284220	4.4786668	-2.9086382
H	-5.5134240	4.0521182	-4.6597255
H	-6.8486365	5.9428558	-4.7002880
H	-3.8543115	7.4927739	-2.9516947
H	-3.0585136	9.7707227	-3.4795265
H	-6.0554465	10.1132880	-6.5554219
H	-6.8618096	7.8303221	-6.0150570
H	-1.3144644	6.1080040	-5.9247239
H	-1.8354470	4.5078966	-6.4309771
H	-4.4672832	4.1559373	-6.6838373
H	-5.5171194	5.5685711	-6.7425282
H	-3.5432636	7.0289145	-6.1812673
H	-3.2524325	6.0757855	-7.6282380
H	-8.0050837	6.6841556	-1.1924106
H	-7.4342848	7.8725764	-2.3970243
H	-8.4302252	6.4687618	-2.9288392
H	-7.2463909	4.0902388	-1.3379895
H	-5.9572118	3.5001407	-2.4238279
H	-7.5399265	4.0285821	-3.1108763

2a_sy_tr_4_ts1.log

E = -1148.900930
H = -1148.567901
G = -1148.634998

NImag=1

C	1.5466171	-1.8595412	-0.3610340
C	1.5422521	-1.2527939	0.8957534
C	0.4963540	-2.7120161	-0.8306579
O	0.4903700	-3.2247446	-1.9665455
C	1.2197464	0.9068279	0.6935965
C	-0.1674289	1.0481752	0.3426007
C	-0.6711007	0.7272924	-0.9444196

C	-2.0338214	0.7062424	-1.1930689
C	-2.9429725	1.0152774	-0.1697207
C	-2.4643908	1.3671270	1.1077349
C	-1.1057124	1.3868508	1.3519052
C	-0.5881292	-3.1107892	0.1614462
C	0.4751395	-1.6199352	1.9011732
C	-0.8349133	-2.0752851	1.2559648
S	2.3523785	1.3209059	-0.5844843
C	2.5353441	3.1200512	-0.4979832
C	3.9577604	0.8196857	0.0649080
C	-4.3499078	0.9936879	-0.4291956
N	-5.4917306	0.9755871	-0.6376924
H	2.3864397	-1.7101489	-1.0390848
H	2.4975927	-0.9905069	1.3444862
H	1.5336015	1.3169056	1.6545097
H	0.0088963	0.4777177	-1.7531705
H	-2.4028375	0.4447961	-2.1802890
H	-3.1669853	1.6247359	1.8943672
H	-0.7417030	1.6565387	2.3394613
H	-1.5033819	-3.3262792	-0.3987836
H	-0.2574968	-4.0590058	0.6101960
H	0.8850658	-2.4425438	2.5063145
H	0.2992528	-0.7875310	2.5917981
H	-1.3571929	-1.2180321	0.8221745
H	-1.4953224	-2.4914576	2.0245731
H	3.2928540	3.4217684	-1.2246561
H	1.5692461	3.5539847	-0.7621233
H	2.8249062	3.4044426	0.5154182
H	4.7131560	1.3489360	-0.5191590
H	4.0745966	-0.2549041	-0.0774832
H	4.0260778	1.0923128	1.1200768

2a_sy_tr_5.log

E = -1148.918379

H = -1148.582503

G = -1148.648866

NImag=0

C	-4.3509031	4.2505243	-5.0405182
C	-4.2199080	5.7450212	-5.1716258
C	-3.3378764	3.3830673	-4.6780187
O	-3.4594481	2.1196179	-4.5042666
C	-5.4204861	6.4913733	-4.5208943
C	-5.3380045	7.9946909	-4.6601641
C	-5.8910892	8.5751283	-5.8065858
C	-5.7863135	9.9425760	-6.0312071
C	-5.1257115	10.7406516	-5.0906927
C	-4.5692967	10.1752021	-3.9372007
C	-4.6740750	8.8052647	-3.7324218
C	-1.9398167	3.9708033	-4.4574197
C	-2.8534896	6.2855747	-4.7224826
C	-1.7394785	5.3260539	-5.1312558
S	-5.8646441	6.0879327	-2.7594288
C	-6.8042452	4.5497937	-2.8683068
C	-4.4180559	5.5121902	-1.8424916
C	-5.0187026	12.1584049	-5.3093745
N	-4.9325733	13.2998643	-5.4855238
H	-5.3315709	3.8252087	-5.2569640
H	-4.3471108	6.0573912	-6.2255846
H	-6.3310593	6.1433675	-5.0231095
H	-6.4096898	7.9507484	-6.5286132
H	-6.2166632	10.3908143	-6.9205886

H	-4.0576911	10.8026741	-3.2151639
H	-4.2218154	8.3788022	-2.8404120
H	-1.7639815	4.0627285	-3.3741377
H	-1.2165269	3.2351905	-4.8275449
H	-2.6888557	7.2776151	-5.1571229
H	-2.8166536	6.4110984	-3.6343433
H	-0.7644830	5.7516897	-4.8671987
H	-1.7492750	5.2000787	-6.2226577
H	-7.2370874	4.3890771	-1.8785936
H	-7.5995883	4.6945613	-3.6013756
H	-6.1410854	3.7346468	-3.1542846
H	-4.8219128	5.1171806	-0.9068328
H	-3.7720610	6.3637676	-1.6283488
H	-3.9068712	4.7352243	-2.4108441

2a_sy_tr_5_r.log

E = -1148.920812

H = -1148.584600

G = -1148.651445

NImag=0

C	-1.3008208	-1.4251547	0.4440657
C	-1.1013901	-0.6990068	-0.8739974
C	-1.2614791	-2.7997899	0.6257256
O	-1.4091109	-3.4016290	1.7437702
C	-0.1368148	0.4709918	-0.6001904
C	-0.5853656	1.4295661	0.4859298
C	0.3475243	1.8935104	1.4187654
C	-0.0302400	2.7838514	2.4165056
C	-1.3593005	3.2190954	2.4741808
C	-2.3034330	2.7662943	1.5453437
C	-1.9116250	1.8720615	0.5563059
C	-1.0284305	-3.6916382	-0.5965104
C	-0.5595839	-1.6417952	-1.9546429
C	-1.2874983	-2.9823415	-1.9204745
S	0.2682309	1.6182594	-2.0333063
C	1.3816911	0.7298565	-3.1436734
C	-1.2377653	1.7585603	-3.0141826
C	-1.7617216	4.1415435	3.5025818
N	-2.0856970	4.8850933	4.3292200
H	-1.5318155	-0.8231951	1.3210931
H	-2.0459813	-0.2679954	-1.2480469
H	0.8571139	0.0788246	-0.3528307
H	1.3766676	1.5488075	1.3671058
H	0.6913259	3.1383647	3.1449368
H	-3.3312588	3.1086926	1.6037084
H	-2.6511486	1.5116853	-0.1528600
H	0.0074501	-4.0593674	-0.5632809
H	-1.6735855	-4.5707278	-0.4859790
H	-0.6737726	-1.1949369	-2.9469072
H	0.5150726	-1.8105720	-1.7890114
H	-0.9667697	-3.6036020	-2.7643786
H	-2.3653275	-2.8076077	-2.0435777
H	1.8037108	1.4850167	-3.8098387
H	2.1749273	0.2938154	-2.5336483
H	0.8529449	-0.0319861	-3.7126685
H	-0.9879795	2.4041813	-3.8591907
H	-1.9951084	2.2434415	-2.3959367
H	-1.5717946	0.7807387	-3.3605843

2a_sy_tr_5_ts1.log

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E =      -1148.890742
H =      -1148.557679
G =      -1148.625569
NImag=1
C        -2.4909495      -0.6907134      -1.2026692
C        -1.1149317      -0.8230473      -0.9869273
C        -3.4775905      -1.1929019      -0.2998848
O        -4.7003697      -0.9798387      -0.4248032
C        -0.1320331       1.0735407      -0.6773456
C         1.2418889       0.7224834      -0.4143170
C         2.0404490       0.2566570      -1.4894208
C         3.3190784      -0.2255059      -1.2801350
C         3.8558797      -0.2513598       0.0192757
C         3.0869254       0.2118708       1.0996734
C         1.8025363       0.6812575       0.8855961
C        -2.9961557      -2.0758880       0.8465774
C        -0.6231679      -1.6662903       0.1787752
C        -1.6500988      -2.7357903       0.5534625
S        -0.8563790       2.2375530       0.4524250
C        -2.1600399       2.9422005      -0.5737289
C        -1.8728995       1.3318130       1.6509299
C         5.1808027      -0.7442569       0.2392106
N         6.2558757      -1.1442557       0.4171071
H        -2.8516836      -0.1754698      -2.0909157
H        -0.4752747      -0.8253334      -1.8679121
H        -0.3566158       1.4142692      -1.6855062
H         1.6385189       0.2885160      -2.4984998
H         3.9154503      -0.5765982      -2.1168218
H         3.5006008       0.1933139       2.1032466
H         1.2261547       1.0129900       1.7465955
H        -2.9126707      -1.4520734       1.7496540
H        -3.7799863      -2.8140979       1.0435638
H         0.3435030      -2.1154528      -0.0709750
H        -0.4517572      -1.0370535       1.0603615
H        -1.3008083      -3.2976375       1.4262927
H        -1.7623376      -3.4503444      -0.2710802
H        -2.7700278       3.5845202       0.0635913
H        -1.6817201       3.5324688      -1.3562632
H        -2.7535353       2.1302930      -0.9983189
H        -2.3639710       2.0919826       2.2623341
H        -1.2104071       0.7312863       2.2752387
H        -2.6041151       0.7188739       1.1286406

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2a_sy_tr_5_ts2.log
E =      -1148.911014
H =      -1148.576728
G =      -1148.644645
NImag=1
C        -1.3514452      -1.6350753       0.4169622
C        -1.5123989      -0.1544876       0.6804743
C        -2.3433227      -2.4558737      -0.1473265
O        -2.1827922      -3.6782228      -0.4172624
C        -0.5181799       0.2588543      -0.3560798
C         0.9310210      -0.0573841      -0.2112973
C         1.7206865      -0.1687889      -1.3642391
C         3.0809399      -0.4252151      -1.2702650
C         3.6639427      -0.5642705      -0.0038856
C         2.8912428      -0.4458563       1.1578380
C         1.5300504      -0.1917040       1.0490892
C        -3.7267596      -1.8484588      -0.3741389
C        -2.9228694       0.3827859       0.3782989

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C	-3.9990812	-0.6802235	0.5707976
S	-0.2611376	2.4955683	-0.4115506
C	-1.7851179	3.2456856	-1.0341931
C	-0.3717192	2.9145853	1.3414209
C	5.0729890	-0.8315041	0.1042293
N	6.2078846	-1.0461235	0.1915977
H	-0.4217171	-2.1094021	0.7155499
H	-1.1985064	0.1318809	1.6910779
H	-0.8921563	0.1898955	-1.3774776
H	1.2586589	-0.0570351	-2.3414520
H	3.6903047	-0.5191361	-2.1628996
H	3.3555931	-0.5547588	2.1322880
H	0.9346687	-0.1091460	1.9530159
H	-3.8063992	-1.5069391	-1.4162465
H	-4.4573013	-2.6536745	-0.2451292
H	-3.1223204	1.2603665	1.0025468
H	-2.9683964	0.7152523	-0.6669895
H	-4.9863461	-0.2465475	0.3775185
H	-3.9986772	-1.0364297	1.6090535
H	-1.6257257	4.3236438	-1.1102294
H	-1.9776273	2.8355050	-2.0275491
H	-2.6210275	3.0346723	-0.3675897
H	-0.3091807	4.0003125	1.4426823
H	0.4786822	2.4560046	1.8501109
H	-1.3101629	2.5490028	1.7626359

2a_sy_tr_6.log

E = -1148.923445

H = -1148.587634

G = -1148.654919

NImag=0

C	-3.6109143	4.8200047	-3.9900418
C	-4.6859364	5.0427006	-5.0239341
C	-2.2624953	4.6614081	-4.2589746
O	-1.3432616	4.4861352	-3.3856457
C	-5.7565100	6.1000590	-4.6485844
C	-5.3753216	7.5567641	-4.6390504
C	-4.1902233	8.0204508	-4.0477858
C	-3.8698472	9.3714399	-4.0788282
C	-4.7404989	10.2736491	-4.7032190
C	-5.9252363	9.8287499	-5.2983716
C	-6.2321168	8.4731255	-5.2623248
C	-1.8053993	4.7019653	-5.7223236
C	-4.1026258	5.4162235	-6.3931796
C	-2.9339439	4.4952958	-6.7305481
S	-6.5510786	5.5775460	-3.0414362
C	-5.8210640	6.5812915	-1.7328557
C	-8.1698969	6.3605360	-3.1607534
C	-4.4096485	11.6738501	-4.7361529
N	-4.1434622	12.8006424	-4.7628324
H	-3.9135516	4.7143420	-2.9464832
H	-5.2837979	4.1255071	-5.1781811
H	-6.6042905	5.9709062	-5.3326157
H	-3.5179148	7.3163446	-3.5692369
H	-2.9522075	9.7295340	-3.6238310
H	-6.5912009	10.5346967	-5.7832078
H	-7.1471188	8.1211725	-5.7312851
H	-1.3174016	5.6715516	-5.9014086
H	-1.0277417	3.9383780	-5.8394719
H	-4.8885394	5.3637174	-7.1566478
H	-3.7338180	6.4504458	-6.3715818

H	-2.5815620	4.6883833	-7.7502200
H	-3.2740124	3.4509059	-6.7008093
H	-6.3237296	6.2782687	-0.8116344
H	-4.7573135	6.3522623	-1.6683169
H	-5.9906505	7.6397770	-1.9360715
H	-8.6790601	6.1891782	-2.2103439
H	-8.7164914	5.8746977	-3.9703459
H	-8.0505172	7.4299935	-3.3461648

2a_sy_tr_6_ts1.log

E = -1148.897008

H = -1148.563466

G = -1148.629291

NImag=1

C	-1.0275562	-1.8345340	0.8588135
C	-1.5045802	-1.6195708	-0.4448617
C	0.3223359	-2.2023225	1.1441324
O	0.7763814	-2.3421489	2.2984732
C	-1.4573828	0.4279626	-0.9626670
C	-0.1121741	0.8410274	-0.6192264
C	0.3280625	0.9574026	0.7169314
C	1.6636675	1.1932512	1.0130284
C	2.5989074	1.3069325	-0.0233999
C	2.1849238	1.2013681	-1.3630880
C	0.8503821	0.9742119	-1.6472479
C	1.2166175	-2.4993901	-0.0531445
C	-0.7085592	-2.1695142	-1.6279367
C	0.4062497	-3.1218940	-1.1903638
S	-2.8602222	1.2296741	-0.2574599
C	-3.2472125	0.5612818	1.3801458
C	-2.3869276	2.9128809	0.2083927
C	3.9795640	1.5443327	0.2832443
N	5.0965959	1.7365611	0.5293643
H	-1.6755368	-1.6681462	1.7152821
H	-2.5850078	-1.6508575	-0.5756581
H	-1.6643133	0.3906139	-2.0313343
H	-0.3734093	0.8552987	1.5368979
H	1.9888267	1.2757703	2.0454255
H	2.9104485	1.3033152	-2.1640108
H	0.5296343	0.8986409	-2.6827063
H	1.6779639	-1.5590798	-0.3911268
H	2.0227476	-3.1592183	0.2818037
H	-1.3985868	-2.6715198	-2.3148544
H	-0.2455873	-1.3563561	-2.1976405
H	1.0509203	-3.3508295	-2.0459193
H	-0.0235706	-4.0701293	-0.8445459
H	-4.0870430	1.1595459	1.7411378
H	-3.5663173	-0.4737899	1.2592425
H	-2.4026363	0.6429723	2.0633403
H	-3.2752030	3.3940791	0.6228827
H	-2.0725955	3.4243393	-0.7025025
H	-1.5807049	2.8945435	0.9429033

2a_sy_tr_6_ts2.log

E = -1148.914344

H = -1148.580011

G = -1148.647923

NImag=1

C	-1.2052307	1.7176808	-0.7164619
C	-1.4666325	0.2472923	-0.9434762

C	-2.0712646	2.5564005	0.0023978
O	-1.8540783	3.7825642	0.2158427
C	-0.5930115	-0.2050576	0.1892715
C	0.8843562	0.0176617	0.1119380
C	1.5725130	-0.0347479	-1.1081254
C	2.9513834	0.1285920	-1.1463039
C	3.6535610	0.3426397	0.0462060
C	2.9806388	0.3878746	1.2740397
C	1.6033175	0.2202116	1.2975735
C	-3.4113863	2.0020311	0.4950736
C	-2.9506069	-0.0952868	-0.8222957
C	-3.5666319	0.4796282	0.4513403
C	5.0806653	0.5162981	0.0100106
N	6.2302403	0.6559327	-0.0188191
H	-0.2835410	2.1468941	-1.0985201
H	-1.0820407	-0.0997602	-1.9074873
H	1.0356446	-0.1957602	-2.0378641
H	3.4843756	0.0921412	-2.0905828
H	3.5341890	0.5543037	2.1922293
H	1.0725404	0.2529782	2.2452014
H	-3.5782705	2.3854937	1.5076307
H	-4.1770498	2.4700975	-0.1394735
H	-3.1135413	-1.1754916	-0.8815783
H	-3.4514141	0.3438024	-1.6945938
H	-3.0973872	0.0251150	1.3329195
H	-4.6274003	0.2108757	0.5021871
H	-1.0025266	-0.0210879	1.1813125
S	-0.5093478	-2.3986755	0.4400505
C	-2.0751445	-2.8804988	1.2024210
H	-2.1006995	-2.4343822	2.1985908
H	-2.9271347	-2.5422635	0.6127338
H	-2.0893100	-3.9689133	1.2931099
C	-0.7209708	-2.9836744	-1.2536459
H	-0.7661016	-4.0746273	-1.2395421
H	-1.6291994	-2.5731120	-1.6971013
H	0.1560523	-2.6655190	-1.8216086

2a_sy_tr_7.log

E = -1148.919293

H = -1148.583180

G = -1148.649629

NImag=0

C	-3.6469772	5.0473076	-3.8477273
C	-4.7049972	5.1297813	-4.9174559
C	-2.2866987	4.9206075	-4.0771391
O	-1.3832014	4.8698272	-3.1719977
C	-5.8339119	6.1722923	-4.7120611
C	-5.4609208	7.6366695	-4.7205170
C	-4.4412129	8.1588822	-3.9115148
C	-4.1062255	9.5058529	-3.9856946
C	-4.7962011	10.3415243	-4.8715746
C	-5.8181857	9.8369283	-5.6828530
C	-6.1415862	8.4879981	-5.5999126
C	-1.7927946	4.8347902	-5.5256367
C	-4.0938268	5.4181015	-6.2989072
C	-2.8906632	4.5113192	-6.5360283
S	-6.9587654	5.8732301	-3.2511423
C	-6.8678309	4.0984266	-2.9466381
C	-6.1870388	6.5463487	-1.7667638
C	-4.4498633	11.7362739	-4.9477215
N	-4.1714419	12.8587213	-5.0089224

H	-3.9580590	5.0468640	-2.8046154
H	-5.2494506	4.1751861	-5.0252471
H	-6.5608073	6.0132317	-5.5175666
H	-3.9024927	7.5108314	-3.2300584
H	-3.3154094	9.9102583	-3.3625673
H	-6.3462829	10.4923711	-6.3673268
H	-6.9289776	8.0877353	-6.2325079
H	-1.3200291	5.7944715	-5.7811950
H	-0.9969668	4.0814597	-5.5530748
H	-4.8560325	5.2817866	-7.0757958
H	-3.7580477	6.4632683	-6.3456599
H	-2.5214901	4.6321261	-7.5608919
H	-3.2009251	3.4628099	-6.4281492
H	-7.5238455	3.9035071	-2.0958413
H	-7.2543085	3.5898737	-3.8311165
H	-5.8423188	3.7978650	-2.7283397
H	-6.8154464	6.2071787	-0.9396017
H	-6.2305162	7.6339157	-1.8313979
H	-5.1654503	6.1904771	-1.6468388

2a_sy_tr_8.log

E = -1148.922771
H = -1148.586861
G = -1148.653553

NImag=0

C	-3.7286421	4.6068540	-4.0583300
C	-4.8743157	4.8506639	-4.9994381
C	-2.3937447	4.8447464	-4.3345887
O	-1.4189392	4.6276640	-3.5345423
C	-5.8607830	5.9861770	-4.5769871
C	-5.3808374	7.4105014	-4.5987645
C	-4.2461193	7.8429046	-3.8935288
C	-3.8084789	9.1566180	-4.0022476
C	-4.5058778	10.0518441	-4.8229533
C	-5.6410269	9.6396816	-5.5286263
C	-6.0712947	8.3235314	-5.4062882
C	-2.0096066	5.3650938	-5.7250611
C	-4.4091520	5.0855399	-6.4482090
C	-3.1540196	5.9516947	-6.5520676
S	-6.6288559	5.4988131	-2.9534765
C	-5.6910178	6.2573514	-1.6137747
C	-8.0981692	6.5424926	-2.9267964
C	-4.0510655	11.4121048	-4.9392405
N	-3.6855403	12.5070181	-5.0332887
H	-3.9637613	4.1831310	-3.0797387
H	-5.5289200	3.9652360	-5.0254026
H	-6.7456598	5.9107916	-5.2221337
H	-3.6883163	7.1448535	-3.2804067
H	-2.9285094	9.4892085	-3.4615774
H	-6.1752710	10.3406280	-6.1612380
H	-6.9493912	7.9957555	-5.9558889
H	-1.2116519	6.1049599	-5.5898104
H	-1.5540303	4.5208070	-6.2631068
H	-4.1873484	4.1012913	-6.8804915
H	-5.2256803	5.5167917	-7.0418955
H	-3.3702168	6.9714881	-6.2168353
H	-2.8558579	6.0302798	-7.6044416
H	-6.2139835	5.9765745	-0.6965378
H	-4.6857380	5.8361152	-1.6129409
H	-5.6775329	7.3416727	-1.7293704
H	-8.5738753	6.4048924	-1.9538435

H	-8.7648928	6.2014182	-3.7201972
H	-7.8102764	7.5859105	-3.0722337

2a_sy_tr_9.log

E = -1148.919112
H = -1148.582921
G = -1148.648765

NImag=0

C	-3.7475695	4.8220659	-3.8861570
C	-4.8710971	4.9586428	-4.8740773
C	-2.4102319	5.0733220	-4.1423116
O	-1.4550810	4.9149119	-3.3053975
C	-5.9300793	6.0749653	-4.5999297
C	-5.4664428	7.5086048	-4.6630252
C	-6.0337754	8.3466705	-5.6311460
C	-5.5839842	9.6507431	-5.7986919
C	-4.5553649	10.1266424	-4.9779878
C	-3.9852887	9.3072818	-3.9963974
C	-4.4413318	8.0037697	-3.8426691
C	-1.9964080	5.5342750	-5.5437830
C	-4.3566380	5.1302851	-6.3194277
C	-3.1345783	6.0414931	-6.4279135
S	-6.9456582	5.8505035	-3.0559608
C	-7.0819472	4.0636313	-2.8581076
C	-5.9607163	6.2972656	-1.6119449
C	-4.0795714	11.4747405	-5.1428937
N	-3.6966886	12.5595882	-5.2761503
H	-3.9869975	4.4377146	-2.8946688
H	-5.4771008	4.0416767	-4.8838329
H	-6.7292122	5.9486693	-5.3405076
H	-6.8261857	7.9686437	-6.2708828
H	-6.0206754	10.2942147	-6.5550557
H	-3.1880782	9.6883884	-3.3668075
H	-3.9760846	7.3637053	-3.1032667
H	-1.2251240	6.3042840	-5.4236689
H	-1.5008205	4.6782985	-6.0251426
H	-4.0765579	4.1331051	-6.6829267
H	-5.1646514	5.4893461	-6.9698312
H	-3.3975292	7.0656978	-6.1429457
H	-2.8092193	6.0858920	-7.4742256
H	-7.7330745	3.9024511	-1.9967466
H	-7.5555438	3.6635797	-3.7563501
H	-6.1006796	3.6184973	-2.6908226
H	-6.5360328	5.9408180	-0.7539190
H	-5.8932643	7.3846075	-1.5746283
H	-4.9784158	5.8284077	-1.6452987

2a_sy_tr_9_ts1.log

E = -1148.895747
H = -1148.562509
G = -1148.630080

NImag=1

C	-1.4397388	-2.0056348	0.1216147
C	-1.6869965	-1.3520789	-1.0894821
C	-0.3148822	-2.8612992	0.3428319
O	-0.1039240	-3.4448925	1.4247873
C	-1.2015566	0.7637680	-0.9596796
C	0.0820835	0.8884958	-0.2968395
C	1.2158325	1.2807251	-1.0466940
C	2.4797988	1.3034677	-0.4877974

C	2.6499389	0.9328402	0.8590432
C	1.5435595	0.5467678	1.6254066
C	0.2784934	0.5213520	1.0518858
C	0.5968327	-3.1683602	-0.8384099
C	-0.8657884	-1.7332159	-2.3036826
C	0.5689270	-2.1066034	-1.9345389
S	-2.6210172	1.5518683	-0.2762875
C	-3.3617914	0.5622664	1.0474465
C	-2.0693205	2.9680495	0.7064649
C	3.9558224	0.9586048	1.4496281
N	5.0136437	0.9806074	1.9251725
H	-2.1247699	-1.8949049	0.9584656
H	-2.7173449	-1.0838788	-1.3177173
H	-1.1984385	1.0590278	-2.0079730
H	1.0852947	1.5645681	-2.0876627
H	3.3382119	1.6109051	-1.0769123
H	1.6791079	0.2596756	2.6635641
H	-0.5604088	0.2029636	1.6602218
H	1.6105801	-3.3251171	-0.4560661
H	0.2575749	-4.1332295	-1.2431590
H	-1.3591838	-2.6030938	-2.7634004
H	-0.8819301	-0.9338586	-3.0503189
H	1.0996239	-1.2156055	-1.5855793
H	1.1005017	-2.4666858	-2.8220047
H	-4.1734332	1.1767952	1.4443705
H	-3.7786769	-0.3458772	0.6132617
H	-2.6427902	0.3369899	1.8341356
H	-2.9617111	3.4510301	1.1099902
H	-1.5452944	3.6479181	0.0331550
H	-1.4131210	2.6360095	1.5126672

2a_sy_tr_prod_1.log

E = -671.042180

H = -670.789954

G = -670.845110

NImag=0

C	0.5915044	-1.4513059	2.0663000
C	0.4870547	-1.9850483	0.6640185
C	0.6445637	-0.5052074	0.8604211
C	-0.4823243	0.4359548	0.6340155
C	-1.8164743	0.0817151	0.8876728
C	-2.8476395	0.9802840	0.6528018
C	-2.5526112	2.2573625	0.1566391
C	-1.2278851	2.6291203	-0.1007578
C	-0.2068136	1.7185105	0.1398569
H	1.6172559	-0.0809042	0.6308342
H	-0.3059806	-1.3730711	2.6735951
H	-0.5055733	-2.3142706	0.3660300
C	1.6405578	-2.7954055	0.1031882
C	2.9960435	-2.3562832	0.6600817
C	3.0035628	-2.3670324	2.1895331
C	1.8394452	-1.6602898	2.8528889
O	1.8906454	-1.3334100	4.0284982
C	-3.6172701	3.1908381	-0.0880807
N	-4.4758676	3.9435346	-0.2856523
H	-2.0603692	-0.9039898	1.2736787
H	-3.8775740	0.7007477	0.8498861
H	-1.0057497	3.6197407	-0.4841184
H	0.8222944	2.0037766	-0.0585156
H	1.4729880	-3.8500160	0.3555211
H	1.6407050	-2.7204458	-0.9895827

H	3.2553510	-1.3588905	0.2896433
H	3.7747418	-3.0321812	0.2950068
H	3.9320782	-1.9613988	2.6009647
H	2.9270409	-3.4062342	2.5429316

2a_sy_tr_prod_3.log

E = -671.041285
H = -670.788923
G = -670.843842

NImag=0

C	1.3192449	-0.6700549	1.9647143
C	0.3991653	-1.8145631	1.6046674
C	0.4935873	-0.6403074	0.6765049
C	-0.6045402	0.3494124	0.5356714
C	-0.8304809	0.9381371	-0.7164495
C	-1.8524569	1.8606063	-0.9011284
C	-2.6673631	2.2069202	0.1830539
C	-2.4556853	1.6300822	1.4425232
C	-1.4308159	0.7095751	1.6113245
H	1.0510876	-0.8163052	-0.2402569
H	1.0129314	0.0253576	2.7407802
H	-0.5104738	-1.8597960	2.1976865
C	0.9915450	-3.1556189	1.1741983
C	2.4745131	-3.2920056	1.5230782
C	3.2648143	-2.0568364	1.0687917
C	2.7898841	-0.8437863	1.8343426
O	3.5633235	-0.0603603	2.3640070
C	-3.7278905	3.1599921	0.0046510
N	-4.5833694	3.9281899	-0.1394944
H	-0.1960301	0.6669580	-1.5552702
H	-2.0208640	2.3112770	-1.8737969
H	-3.0915803	1.9050687	2.2777311
H	-1.2795565	0.2724886	2.5942913
H	0.4263275	-3.9592712	1.6543388
H	0.8635192	-3.2766322	0.0919554
H	2.8891021	-4.1895867	1.0546923
H	2.5902830	-3.4094991	2.6077132
H	3.1032293	-1.8893965	-0.0049388
H	4.3386493	-2.1667455	1.2372178

2b.log

E = -347.855437
H = -347.690745
G = -347.731078

NImag=0

C	0.8952271	0.2843500	-0.4020630
C	0.0039541	1.2924400	-0.4367416
C	-1.4655308	1.1422791	-0.1700155
C	-1.9264668	-0.3022852	-0.3443040
C	-0.9969251	-1.2454835	0.4154540
C	0.4455706	-1.0786348	-0.0080732
O	1.2321354	-2.0160804	0.0166274
C	2.3556171	0.4575947	-0.7062614
H	0.3646031	2.2939571	-0.6722376
H	-1.6722655	1.4836877	0.8555092
H	-2.0222695	1.8138900	-0.8317698
H	-2.9559419	-0.4230907	0.0048668
H	-1.9098068	-0.5591918	-1.4107904
H	-1.0368662	-1.0151381	1.4905999
H	-1.2731020	-2.2959648	0.2926920

H	2.5745812	1.4975140	-0.9606988
H	2.9719227	0.1675969	0.1510585
H	2.6577623	-0.1786401	-1.5444497

2b_sy_c_1.log

E = -1188.221650
H = -1187.856160
G = -1187.925979

NImag=0

C	-3.5134020	0.0827856	-2.3470084
C	-4.5565140	-0.2039919	-1.2942134
C	-3.7000925	-0.1701248	-3.6942045
O	-2.8341971	0.1010192	-4.6018838
C	-5.3913110	1.0304912	-0.8133668
C	-5.9714991	0.8679584	0.5688985
C	-5.1407912	0.6540852	1.6770170
C	-5.6853794	0.4941940	2.9446222
C	-7.0763716	0.5381164	3.1033515
C	-7.9183940	0.7460748	2.0052613
C	-7.3579307	0.9159661	0.7442658
C	-4.9753133	-0.8674870	-4.1737195
C	-5.5740009	-1.2579585	-1.7620739
C	-6.1106374	-0.9251921	-3.1535523
S	-4.3742303	2.5839672	-0.8403153
C	-4.4977046	3.1188099	-2.5630936
C	-5.5082682	3.7735650	-0.0929399
C	-7.6462920	0.3671975	4.4135220
N	-8.1052397	0.2299067	5.4678973
C	-2.1736294	0.6309662	-1.9126977
H	-4.0550330	-0.5855387	-0.3930940
H	-6.1936924	1.2516407	-1.5252361
H	-4.0608241	0.6151296	1.5557366
H	-5.0450044	0.3343207	3.8057084
H	-8.9941970	0.7779849	2.1419819
H	-8.0022815	1.0845604	-0.1141027
H	-5.3055546	-0.3704759	-5.0938676
H	-4.6852648	-1.8874272	-4.4669110
H	-5.0649332	-2.2294079	-1.7937114
H	-6.3968545	-1.3481042	-1.0411425
H	-6.6323112	0.0407824	-3.1302044
H	-6.8585581	-1.6681602	-3.4538760
H	-4.1277184	4.1459074	-2.5967058
H	-3.8795374	2.4578683	-3.1703516
H	-5.5445996	3.0728713	-2.8717421
H	-5.0839897	4.7636208	-0.2723238
H	-5.5549430	3.5806384	0.9792579
H	-6.4939171	3.6846348	-0.5550735
H	-2.0426880	0.5594399	-0.8252540
H	-1.3542233	0.0745071	-2.3871672
H	-1.9973764	1.6866581	-2.1863874

2b_sy_c_10.log

E = -1188.216412
H = -1187.851205
G = -1187.921139

NImag=0

C	-4.9541890	0.3712281	-2.7642100
C	-4.0517811	0.9576228	-1.7044311
C	-5.2469402	-0.9775055	-2.8880706
O	-5.9853550	-1.4845346	-3.8078429

C	-4.8742215	1.9964012	-0.8607025
C	-5.7141159	1.4093807	0.2416870
C	-5.2345418	1.2008372	1.5391814
C	-6.0199605	0.5594185	2.4889411
C	-7.2992267	0.1153626	2.1336848
C	-7.7980151	0.3273078	0.8429714
C	-7.0051079	0.9809617	-0.0920876
C	-4.6229242	-1.9721805	-1.9078383
C	-3.3297769	-0.0991484	-0.8515827
C	-4.1710612	-1.3491428	-0.5926573
S	-3.8990215	3.4411853	-0.2135426
C	-2.2082600	2.8928046	0.1046705
C	-3.6517215	4.3835630	-1.7312337
C	-8.1146783	-0.5554491	3.1106943
N	-8.7711406	-1.0950452	3.8976917
C	-5.5196252	1.3435802	-3.7677239
H	-3.2814462	1.5623371	-2.2113140
H	-5.5379070	2.5302473	-1.5496983
H	-4.2355046	1.5174674	1.8274643
H	-5.6458245	0.3965397	3.4941174
H	-8.7950510	-0.0115104	0.5816188
H	-7.3870205	1.1584567	-1.0934722
H	-5.3599311	-2.7636926	-1.7294338
H	-3.7689931	-2.4517040	-2.4097005
H	-2.4248684	-0.4001314	-1.3958427
H	-2.9901095	0.3254783	0.0998541
H	-5.0511644	-1.0991628	0.0108604
H	-3.5825374	-2.0660908	-0.0074087
H	-1.6319938	3.8070160	0.2635144
H	-2.1978572	2.2935490	1.0150601
H	-1.8159361	2.3370788	-0.7474397
H	-3.0105621	5.2305417	-1.4799212
H	-4.6291148	4.7403744	-2.0600095
H	-3.1825694	3.7552469	-2.4901593
H	-5.7026077	0.8362255	-4.7202660
H	-6.4816363	1.7956275	-3.4678121
H	-4.8305009	2.1814583	-3.9514105

2b_sy_c_10_ts1.log

E = -1188.195169

H = -1187.832421

G = -1187.902587

NImag=1

C	-0.9086611	2.1972605	-0.2774376
C	-1.4243817	1.1872251	0.5481588
C	0.3444176	2.8330733	-0.0106425
O	0.8492801	3.6827046	-0.7775852
C	-1.2663181	-0.5900646	-0.5922068
C	0.1234120	-0.9679894	-0.5612319
C	0.6468407	-1.9714344	0.2888029
C	2.0105587	-2.1624140	0.4137710
C	2.9026545	-1.3427818	-0.3024209
C	2.4052862	-0.3554282	-1.1686911
C	1.0387931	-0.1802139	-1.3036456
C	1.0258289	2.5682550	1.3259469
C	-0.7767473	0.8905701	1.8831259
C	0.7219812	1.1941077	1.9129608
S	-2.4311779	-1.8973732	-0.2428905
C	-3.0144973	-1.7114440	1.4624743
C	-3.8810963	-1.2914202	-1.1255077
C	4.3149644	-1.5277101	-0.1609228

N	5.4600310	-1.6782505	-0.0452374
C	-1.6325259	2.5653591	-1.5435749
H	-2.5082224	1.0650773	0.5339338
H	-1.6033811	-0.1135408	-1.5113708
H	-0.0200523	-2.5986114	0.8769309
H	2.3977217	-2.9342484	1.0717082
H	3.0960442	0.2636624	-1.7334602
H	0.6567806	0.5739703	-1.9850429
H	2.1026578	2.7137604	1.1913075
H	0.6825161	3.3545852	2.0143659
H	-1.2897337	1.5102027	2.6341800
H	-0.9491090	-0.1500748	2.1748268
H	1.2658970	0.4339658	1.3445439
H	1.0848650	1.1353457	2.9451295
H	-3.8494691	-2.4075855	1.5703375
H	-2.2064800	-2.0092810	2.1316332
H	-3.3375143	-0.6879288	1.6542731
H	-4.7217431	-1.9358832	-0.8641926
H	-3.6702500	-1.3625051	-2.1932887
H	-4.0746870	-0.2575500	-0.8317712
H	-1.6410946	3.6485581	-1.7045510
H	-1.1564004	2.1233761	-2.4333999
H	-2.6694590	2.2114908	-1.5192570

2b_sy_c_11.log

E = -1188.216023

H = -1187.850815

G = -1187.921224

NImag=0

C	-3.6309458	0.2629151	-2.6547152
C	-4.3543469	-0.0539326	-1.3648196
C	-4.1982293	-0.0424499	-3.8815393
O	-3.7223160	0.2693496	-5.0293781
C	-5.3633326	1.0558505	-0.9287224
C	-5.9694651	0.9115975	0.4452110
C	-5.1960271	0.5326018	1.5505786
C	-5.7769834	0.3960546	2.8058635
C	-7.1472732	0.6359044	2.9585782
C	-7.9368207	1.0056361	1.8636186
C	-7.3409847	1.1399425	0.6157328
C	-5.4634772	-0.9055228	-3.8424671
C	-5.1759317	-1.3851366	-1.3874444
C	-5.3071797	-1.9982085	-2.7844521
S	-4.5833234	2.7203797	-1.1694396
C	-5.8320819	3.8628806	-0.5508072
C	-3.3468902	2.8501108	0.1349259
C	-7.7520863	0.4953517	4.2566445
N	-8.2383639	0.3836422	5.3017180
C	-2.2828191	0.9363860	-2.5993609
H	-3.6049367	-0.1247210	-0.5653365
H	-6.1635329	1.1025085	-1.6784431
H	-4.1339082	0.3367496	1.4412863
H	-5.1778909	0.1029250	3.6614930
H	-8.9994749	1.1823338	1.9925267
H	-7.9474985	1.4233081	-0.2403158
H	-6.3550291	-0.2986788	-3.6216901
H	-5.6033912	-1.3355494	-4.8396597
H	-4.7179364	-2.1046281	-0.7005804
H	-6.1868037	-1.2008415	-1.0022666
H	-6.1556451	-2.6928574	-2.7955387
H	-4.4116020	-2.5836695	-3.0257262

H	-5.4182050	4.8671277	-0.6633673
H	-6.7191690	3.7575619	-1.1785214
H	-6.0593141	3.6550009	0.4960149
H	-2.8494925	3.8119755	-0.0064782
H	-2.6279568	2.0394501	0.0066738
H	-3.8270876	2.8057381	1.1138906
H	-1.6926829	0.6544423	-3.4792114
H	-2.3018799	2.0418916	-2.5968654
H	-1.7203847	0.6361800	-1.7040094

2b_sy_c_12.log

E = -1188.216527
H = -1187.851196
G = -1187.922003

NImag=0

C	-5.4529100	-0.2260347	-2.5081252
C	-4.6736725	1.0526319	-2.2933912
C	-4.8654965	-1.4757626	-2.6210348
O	-5.4976705	-2.5822319	-2.7823119
C	-5.4017313	1.9210282	-1.2205393
C	-5.8550378	1.3051281	0.0815030
C	-5.0916529	0.3792558	0.8058504
C	-5.5661918	-0.1521319	1.9989452
C	-6.8190512	0.2439112	2.4816593
C	-7.5981814	1.1633692	1.7728591
C	-7.1108593	1.6809849	0.5781762
C	-3.3370602	-1.5782173	-2.5897898
C	-3.1746167	0.8385285	-2.0347941
C	-2.6360631	-0.2683003	-2.9332967
S	-4.4180039	3.4827335	-0.9457838
C	-5.6384708	4.6206978	-0.2641718
C	-3.4072621	3.1900079	0.5181775
C	-7.3117759	-0.3036734	3.7179279
N	-7.7083418	-0.7424158	4.7136168
C	-6.9337977	-0.0733120	-2.7360688
H	-4.7447804	1.6846651	-3.2006669
H	-6.2883424	2.3451886	-1.7054494
H	-4.1196522	0.0598766	0.4515365
H	-4.9724416	-0.8707738	2.5538267
H	-8.5713779	1.4606050	2.1490382
H	-7.7224348	2.3818988	0.0154233
H	-3.0169167	-1.9223301	-1.5944886
H	-3.0591914	-2.3697670	-3.2952035
H	-2.6265497	1.7738593	-2.2107737
H	-2.9808777	0.5465199	-0.9979838
H	-1.5506297	-0.3583659	-2.8104250
H	-2.8223198	-0.0109859	-3.9849757
H	-5.1154273	5.5551821	-0.0510107
H	-6.4021749	4.7869822	-1.0255951
H	-6.0696795	4.2058389	0.6485611
H	-2.8777105	4.1253449	0.7119094
H	-2.6906649	2.3988737	0.2962657
H	-4.0453992	2.9259562	1.3631720
H	-7.3342300	-1.0032653	-3.1501600
H	-7.5158574	0.1508970	-1.8259147
H	-7.1540945	0.7418026	-3.4448937

2b_sy_c_13.log

E = -1188.214075
H = -1187.848722

G = -1187.918435
NImag=0

C	-5.1719817	0.3626939	-2.7051099
C	-4.2028225	0.8806693	-1.6600567
C	-5.3051051	-0.9781974	-3.0339881
O	-6.1214347	-1.4425246	-3.9094320
C	-4.9258189	1.9552480	-0.7773801
C	-5.7510499	1.4037976	0.3581205
C	-5.2582520	1.2396795	1.6570278
C	-6.0451589	0.6616797	2.6455103
C	-7.3388089	0.2315409	2.3272773
C	-7.8455497	0.3864834	1.0322200
C	-7.0503082	0.9771646	0.0573308
C	-4.3978478	-2.0093577	-2.3561622
C	-3.5853507	-0.2394116	-0.8162699
C	-3.1592843	-1.3986856	-1.7098008
S	-3.8515656	3.3395491	-0.1720930
C	-2.1826930	2.7084462	0.0997477
C	-3.6027122	4.2670195	-1.6977883
C	-8.1580302	-0.3713182	3.3445729
N	-8.8177071	-0.8568144	4.1634692
C	-5.9042885	1.3905780	-3.5285104
H	-3.3833495	1.4249547	-2.1644063
H	-5.5936038	2.5322592	-1.4261919
H	-4.2485137	1.5478202	1.9171308
H	-5.6617908	0.5373373	3.6526982
H	-8.8516123	0.0548219	0.7977442
H	-7.4410734	1.1135504	-0.9467784
H	-4.9809371	-2.5572135	-1.6010007
H	-4.1231693	-2.7409892	-3.1248996
H	-2.7426102	0.1333010	-0.2245671
H	-4.3309550	-0.6206980	-0.1072330
H	-2.6141399	-2.1477216	-1.1239939
H	-2.4723740	-1.0346025	-2.4864649
H	-1.5727285	3.5876157	0.3194299
H	-2.1930662	2.0457518	0.9652779
H	-1.8147311	2.2014668	-0.7928277
H	-2.9195201	5.0851665	-1.4623598
H	-4.5713618	4.6666136	-2.0024421
H	-3.1790497	3.6178133	-2.4657588
H	-6.1993128	0.9478447	-4.4847015
H	-6.8276077	1.7832677	-3.0669980
H	-5.2719232	2.2680997	-3.7373423

2b_sy_c_1_ts1.log
E = -1188.197351
H = -1187.835076
G = -1187.906244
NImag=1

C	2.2751903	-0.6482451	1.0657354
C	1.0555849	-1.0253798	0.4799162
C	3.5286307	-1.0150100	0.4836580
O	4.6249757	-0.6666308	0.9733134
C	0.0539283	0.5106745	-0.6438502
C	-1.3462567	0.2603693	-0.3711050
C	-1.9685215	0.6132981	0.8513312
C	-3.2817649	0.2638674	1.1174954
C	-4.0197552	-0.4664836	0.1728017
C	-3.4204722	-0.8402711	-1.0420195
C	-2.1107537	-0.4797718	-1.3046218
C	3.5416438	-1.9190698	-0.7436032

C	1.0491138	-2.0777890	-0.6028614
C	2.2395034	-1.8942445	-1.5385246
S	0.6776737	2.0334350	-0.0036408
C	2.3127648	2.1147928	-0.7556054
C	-0.1466287	3.3429012	-0.9468599
C	-5.3779610	-0.8276604	0.4453938
N	-6.4789584	-1.1209746	0.6656357
C	2.3080147	0.2044233	2.3085319
H	0.1903839	-1.0321423	1.1454613
H	0.3544858	0.3948455	-1.6860623
H	-1.4161581	1.1671470	1.6066582
H	-3.7418038	0.5485298	2.0587675
H	-3.9909877	-1.4017064	-1.7754465
H	-1.6598667	-0.7581317	-2.2531822
H	4.3979453	-1.6309035	-1.3620455
H	3.7401729	-2.9394602	-0.3844695
H	1.1149139	-3.0626742	-0.1167562
H	0.1029336	-2.0621510	-1.1530612
H	2.1445440	-0.9290300	-2.0537878
H	2.2477125	-2.6714911	-2.3098939
H	2.7245241	3.0979574	-0.5214304
H	2.9303729	1.3322735	-0.3159965
H	2.2139453	1.9808939	-1.8350957
H	0.3188717	4.2948891	-0.6806985
H	-1.1975478	3.3464625	-0.6518896
H	-0.0421505	3.1357806	-2.0137181
H	1.2997803	0.3405435	2.7152652
H	2.9325342	-0.2479840	3.0884477
H	2.7312894	1.2035684	2.1256030

2b_sy_c_2.log

E = -1188.221040

H = -1187.855708

G = -1187.925393

NImag=0

C	-3.6086826	-0.0656490	-2.0767893
C	-4.9668080	-0.3540228	-1.4792871
C	-3.3710984	-0.0673833	-3.4443788
O	-2.2328682	0.1152792	-4.0028303
C	-5.7340166	0.9142246	-0.9467330
C	-6.1672762	0.8272232	0.4941824
C	-7.5137316	1.0048984	0.8258220
C	-7.9349833	0.9174878	2.1486724
C	-6.9913953	0.6606011	3.1486979
C	-5.6375861	0.4835630	2.8325828
C	-5.2350525	0.5606359	1.5063214
C	-4.5292917	-0.3481461	-4.4109089
C	-5.8977452	-1.0993309	-2.4441144
C	-5.9303462	-0.4026090	-3.8004846
S	-4.6786508	2.4281723	-1.1719208
C	-5.0523303	2.9533017	-2.8582358
C	-5.6565563	3.6729683	-0.2926575
C	-7.4166135	0.5729906	4.5205947
N	-7.7587865	0.5032193	5.6247804
C	-2.4576307	0.0179108	-1.1086769
H	-4.8204868	-0.9886137	-0.5933976
H	-6.6113954	1.1316342	-1.5659405
H	-8.2378827	1.2121525	0.0430390
H	-8.9803060	1.0503455	2.4068009
H	-4.9175077	0.2829544	3.6187671
H	-4.1867502	0.4108226	1.2589079

H	-4.4831086	0.4008712	-5.2120529
H	-4.2962040	-1.3111999	-4.8877353
H	-5.5203757	-2.1223559	-2.5669803
H	-6.9063796	-1.1740897	-2.0164969
H	-6.3270867	0.6139192	-3.6783674
H	-6.6209482	-0.9174141	-4.4782839
H	-4.6237054	3.9514297	-2.9736929
H	-4.5687478	2.2558627	-3.5413786
H	-6.1350776	2.9788805	-2.9999616
H	-5.2330399	4.6444030	-0.5558980
H	-5.5474510	3.5044570	0.7793232
H	-6.7040941	3.6150247	-0.5964969
H	-1.5286669	0.1984941	-1.6572673
H	-2.5592088	0.8189260	-0.3591100
H	-2.3366268	-0.9154389	-0.5338146

2b_sy_c_3.log

E = -1188.216998
H = -1187.851814
G = -1187.921815

NImag=0

C	-3.9869875	-0.1377382	-1.9535187
C	-5.4811875	0.0171011	-1.7671814
C	-3.3870595	-0.3371282	-3.1918877
O	-2.1269511	-0.4685051	-3.3796907
C	-5.8964420	1.3006016	-0.9511333
C	-6.1680397	1.0596496	0.5181631
C	-5.1963131	1.1343326	1.5220255
C	-5.5192985	0.8456385	2.8431027
C	-6.8264144	0.4663975	3.1656926
C	-7.8100170	0.3837771	2.1731022
C	-7.4746770	0.6871404	0.8602930
C	-4.2716657	-0.4658909	-4.4358549
C	-6.2868871	0.0144487	-3.0797540
C	-5.6864208	-0.9324660	-4.1075256
S	-4.6131129	2.6057918	-1.1567523
C	-4.7890045	3.1137779	-2.8786518
C	-5.4323421	4.0116139	-0.3651096
C	-7.1645453	0.1659547	4.5311030
N	-7.4376239	-0.0753959	5.6304635
C	-3.1495043	-0.3313820	-0.7136079
H	-5.8578984	-0.8124759	-1.1430591
H	-6.8016174	1.7381357	-1.3894893
H	-4.1734797	1.4196174	1.2929548
H	-4.7639976	0.9106799	3.6191445
H	-8.8232389	0.0947437	2.4319408
H	-8.2368900	0.6353184	0.0876041
H	-4.3138814	0.4988149	-4.9648473
H	-3.7650048	-1.1674928	-5.1078263
H	-7.3295534	-0.2399200	-2.8536797
H	-6.3003582	1.0211351	-3.5154978
H	-6.3118221	-0.9602102	-5.0076080
H	-5.6556886	-1.9535153	-3.7034277
H	-4.2035020	4.0300338	-2.9842739
H	-4.3704635	2.3252512	-3.5035344
H	-5.8412099	3.2992138	-3.1030464
H	-4.8499574	4.8994867	-0.6190012
H	-5.4150525	3.8583615	0.7144603
H	-6.4562291	4.1025513	-0.7331786
H	-2.2594302	-0.9177602	-0.9670600
H	-2.7801785	0.5950846	-0.2434673

H -3.7083524 -0.8710727 0.0658145

2b_sy_c_3_ts1.log

E = -1188.192173

H = -1187.829663

G = -1187.900576

NImag=1

C	-1.8059625	-1.0354718	-0.8048010
C	-1.1164129	-1.0385796	0.4200153
C	-3.2356682	-1.0214503	-0.8605867
O	-3.8755334	-0.9163086	-1.9292488
C	-0.0029804	0.7690358	0.7738735
C	1.3670340	0.4193859	0.4718526
C	1.9458320	0.5155572	-0.8159585
C	3.2307346	0.0616020	-1.0626435
C	3.9826180	-0.5206776	-0.0300748
C	3.4232086	-0.6435223	1.2533384
C	2.1420042	-0.1816080	1.4938880
C	-4.0174401	-1.2414328	0.4333922
C	-1.8952374	-1.1383572	1.7227045
C	-3.1893605	-1.9253931	1.5180655
S	-0.7445205	1.9559272	-0.2942759
C	-2.3344765	2.2347047	0.4986357
C	0.0629857	3.5351808	0.0730896
C	5.3102270	-0.9906527	-0.2840991
N	6.3869170	-1.3722894	-0.4892363
C	-1.0437240	-1.0833021	-2.1040596
H	-0.1429953	-1.5293247	0.4158287
H	-0.2129701	0.9986201	1.8186615
H	1.3865798	0.9491976	-1.6413527
H	3.6582399	0.1524506	-2.0564074
H	4.0007094	-1.0967527	2.0531549
H	1.7180493	-0.2755218	2.4901810
H	-4.3759586	-0.2689866	0.8020839
H	-4.9078537	-1.8224774	0.1719075
H	-1.2640029	-1.5899172	2.4949946
H	-2.1684753	-0.1396555	2.0831058
H	-3.7512380	-1.9763220	2.4572169
H	-2.9603611	-2.9549168	1.2168300
H	-2.7997547	3.0837363	-0.0050878
H	-2.9404516	1.3415421	0.3545681
H	-2.1791002	2.4473399	1.5583114
H	-0.4468079	4.3151460	-0.4971708
H	1.1018767	3.4551595	-0.2522592
H	0.0058031	3.7276501	1.1459343
H	-1.5377136	-1.7430388	-2.8262982
H	-0.9598886	-0.1004907	-2.5890646
H	-0.0230974	-1.4495710	-1.9398172

2b_sy_c_3_ts2.log

E = -1188.204776

H = -1187.841034

G = -1187.912026

NImag=1

C	-1.8193658	-1.3798949	0.7532001
C	-2.0692576	-0.3165142	-0.2994635
C	-0.9748546	-2.4689311	0.4933008
O	-0.6168836	-3.3082813	1.3709570
C	-1.0050863	0.5771954	0.2612948
C	0.4686841	0.3256196	0.1273766

C	1.1615649	0.4425780	-1.0852822
C	2.5352046	0.2314755	-1.1408104
C	3.2299753	-0.0946432	0.0279656
C	2.5582319	-0.1927150	1.2540508
C	1.1894074	0.0310813	1.2940734
C	-0.5231757	-2.6827236	-0.9486240
C	-1.9357637	-0.7502248	-1.7742331
C	-1.5976639	-2.2345430	-1.9403043
S	-1.1881629	2.5855514	-0.6041588
C	-2.8195661	2.9742208	0.0630440
C	-0.1454587	3.4566736	0.5854575
C	4.6498993	-0.3170679	-0.0275850
N	5.7935123	-0.4957006	-0.0719376
C	-2.4050955	-1.2098573	2.1295034
H	-3.0423462	0.1570190	-0.1275510
H	-1.2550312	0.9246115	1.2666710
H	0.6441940	0.7118936	-1.9994271
H	3.0667566	0.3217497	-2.0823510
H	3.1061356	-0.4374186	2.1580000
H	0.6609120	-0.0418227	2.2407292
H	0.4140906	-2.1387052	-1.1341260
H	-0.3016575	-3.7487976	-1.0645672
H	-2.8769209	-0.5316921	-2.2886371
H	-1.1741145	-0.1491315	-2.2788330
H	-1.2799152	-2.4239056	-2.9718997
H	-2.4994725	-2.8351884	-1.7695798
H	-2.9427416	4.0589388	0.0795112
H	-3.5679160	2.5336572	-0.5975127
H	-2.9178391	2.5675311	1.0737463
H	-0.3631566	4.5251266	0.5321040
H	0.8963195	3.2812515	0.3103889
H	-0.3391190	3.0797177	1.5937598
H	-2.9617436	-2.1038764	2.4402200
H	-1.6440719	-1.0408689	2.9060619
H	-3.0991847	-0.3613976	2.1603111

2b_sy_c_4.log

E = -1188.219190

H = -1187.853859

G = -1187.924424

NImag=0

C	-5.0664049	0.3524385	-2.7872666
C	-4.0198442	0.8655255	-1.8274500
C	-5.4086261	-0.9832036	-2.9270669
O	-6.2493944	-1.4411265	-3.7826414
C	-4.6700557	1.9228619	-0.8677890
C	-5.5203169	1.3512925	0.2362304
C	-5.0075890	0.9725330	1.4830221
C	-5.8252442	0.3663891	2.4284242
C	-7.1694122	0.1255895	2.1199032
C	-7.6977542	0.5030733	0.8801145
C	-6.8713416	1.1215994	-0.0504428
C	-4.7200951	-2.0272926	-2.0451165
C	-3.2492460	-0.2405197	-1.0901587
C	-4.1123175	-1.4605350	-0.7675531
S	-3.3715244	3.0242742	-0.1425523
C	-2.7869269	3.9231487	-1.5942860
C	-4.3771376	4.3049207	0.6358393
C	-8.0195423	-0.5057702	3.0937195
N	-8.7039873	-1.0131513	3.8782835
C	-5.6922139	1.3777317	-3.6968956

H	-3.2882387	1.4484433	-2.4099770
H	-5.2732270	2.6109984	-1.4708828
H	-3.9604941	1.1278968	1.7307022
H	-5.4273239	0.0736350	3.3942836
H	-8.7429130	0.3188135	0.6548231
H	-7.2750387	1.4289112	-1.0108589
H	-5.4627013	-2.7989699	-1.8115412
H	-3.9411572	-2.5191617	-2.6470764
H	-2.4302877	-0.5672110	-1.7435832
H	-2.7759608	0.1510723	-0.1794956
H	-4.9180013	-1.1903872	-0.0758394
H	-3.5010967	-2.2169346	-0.2605540
H	-2.2870050	4.8190226	-1.2204342
H	-2.0700187	3.2994790	-2.1272735
H	-3.6373296	4.1883980	-2.2260012
H	-3.7033588	5.1205413	0.9046827
H	-4.8279545	3.8845692	1.5354406
H	-5.1398049	4.6427465	-0.0690983
H	-6.0500700	0.8951773	-4.6117862
H	-6.5593034	1.9025959	-3.2591205
H	-4.9721400	2.1608856	-3.9796279

2b_sy_c_4_ts1.log

E = -1188.199021
H = -1187.836473
G = -1187.906695

NImag=1

C	-0.6325909	2.2872677	-0.3976377
C	-1.3219549	1.4521828	0.4963375
C	0.6865099	2.7647517	-0.1270127
O	1.3309984	3.4722354	-0.9330981
C	-1.3834591	-0.4457713	-0.4031651
C	-0.0271687	-0.9487520	-0.3983362
C	0.4676840	-1.9265534	0.4990281
C	1.8168421	-2.2210900	0.5649502
C	2.7266293	-1.5424382	-0.2662290
C	2.2563132	-0.5935766	-1.1863097
C	0.9015061	-0.3132459	-1.2592820
C	1.2823192	2.5187810	1.2541321
C	-0.7829021	1.2211768	1.8911594
C	0.7447153	1.2735586	1.9528735
S	-2.5747394	-1.5028542	0.3583588
C	-4.0616355	-0.4859609	0.4222146
C	-3.0711857	-2.6875049	-0.9206253
C	4.1255803	-1.8384221	-0.1903972
N	5.2592335	-2.0784836	-0.1272403
C	-1.2609005	2.6474895	-1.7162886
H	-2.4077601	1.5025790	0.4346898
H	-1.7571757	-0.0974246	-1.3674311
H	-0.2052193	-2.4533501	1.1696272
H	2.1787531	-2.9704936	1.2619915
H	2.9562952	-0.0845917	-1.8422402
H	0.5435600	0.4092067	-1.9853282
H	2.3714156	2.4740226	1.1485506
H	1.0587133	3.4128593	1.8546928
H	-1.1977160	2.0105468	2.5354525
H	-1.1499413	0.2695534	2.2967457
H	1.1682495	0.3856039	1.4750029
H	1.0714859	1.2561619	2.9984995
H	-4.9000928	-1.1652189	0.5867919
H	-3.9775107	0.2011666	1.2645030

H	-4.1797273	0.0514152	-0.5214014
H	-3.8763727	-3.3060856	-0.5183602
H	-2.1986415	-3.3040550	-1.1440168
H	-3.3981652	-2.1385522	-1.8060141
H	-1.1176794	3.7070756	-1.9547935
H	-0.8263628	2.0819191	-2.5554853
H	-2.3366953	2.4388140	-1.7064129

2b_sy_c_5.log

E = -1188.221139
H = -1187.855618
G = -1187.925414

NImag=0

C	-3.6237595	0.3051451	-2.6817488
C	-4.3003233	0.0199433	-1.3581821
C	-4.0301923	-0.2788810	-3.8732032
O	-3.4599130	-0.0994194	-5.0081008
C	-5.3289445	1.1076067	-0.9113271
C	-5.9328023	0.9343734	0.4584207
C	-5.1482740	0.6177129	1.5762826
C	-5.7358746	0.4400545	2.8227386
C	-7.1231862	0.5740867	2.9548711
C	-7.9219536	0.8818286	1.8480072
C	-7.3193836	1.0605147	0.6084824
C	-5.1877903	-1.2837199	-3.8824062
C	-5.0448539	-1.3274235	-1.3760758
C	-5.9777637	-1.4203091	-2.5808582
S	-4.5963734	2.7909804	-1.1448713
C	-5.8837250	3.8890406	-0.5259354
C	-3.3632590	2.9613193	0.1581564
C	-7.7345199	0.3871554	4.2440147
N	-8.2261403	0.2374931	5.2818330
C	-2.3422628	1.1060308	-2.6774254
H	-3.5316693	-0.0276523	-0.5716747
H	-6.1311629	1.1534977	-1.6568680
H	-4.0733768	0.4979185	1.4820869
H	-5.1293318	0.1947321	3.6882003
H	-8.9967070	0.9777657	1.9608355
H	-7.9328353	1.2961884	-0.2570006
H	-5.8519730	-1.0257502	-4.7160191
H	-4.7386442	-2.2528311	-4.1449476
H	-4.2908252	-2.1218923	-1.4403428
H	-5.5988522	-1.4842549	-0.4431232
H	-6.7442669	-0.6369565	-2.5189619
H	-6.5179841	-2.3739319	-2.5629809
H	-5.4979718	4.9063045	-0.6210844
H	-6.7610598	3.7657468	-1.1639976
H	-6.1144969	3.6601401	0.5158288
H	-2.8723567	3.9230061	-0.0048953
H	-2.6381988	2.1530470	0.0507661
H	-3.8450318	2.9365312	1.1369827
H	-1.7123953	0.7839771	-3.5144050
H	-2.4592071	2.1973044	-2.7926649
H	-1.7766580	0.9511769	-1.7473067

2b_sy_c_5_r.log

E = -1188.213091
H = -1187.847494
G = -1187.917522

NImag=0

C	-0.4506052	0.0009408	-2.2408040
C	-1.3186268	-0.2284875	-1.0227283
C	-0.9112882	0.5251576	-3.4397886
O	-0.2202964	0.6204705	-4.5172264
C	-0.6147515	0.3952247	0.2215899
C	-0.4877196	1.8910327	0.3552042
C	-1.5919021	2.7461937	0.4764180
C	-1.4166731	4.1200742	0.5807985
C	-0.1217588	4.6521010	0.5621205
C	0.9928220	3.8160413	0.4449689
C	0.7999115	2.4427167	0.3488009
C	-2.3613054	1.0022907	-3.5365771
C	-2.7949707	0.1501780	-1.2291803
C	-2.9947263	1.3223145	-2.1891557
S	-1.2220372	-0.4366688	1.7846162
C	0.1760609	-0.1535779	2.8883947
C	-2.4612525	0.5931523	2.5951036
C	0.0637497	6.0752944	0.6685807
N	0.2130291	7.2203595	0.7555232
C	0.9488268	-0.5583675	-2.1726588
H	-1.2963226	-1.3078094	-0.7852720
H	0.3993225	-0.0216646	0.2216503
H	-2.6014183	2.3497734	0.4880018
H	-2.2739453	4.7783917	0.6740378
H	1.9926342	4.2368907	0.4325212
H	1.6629040	1.7881619	0.2613492
H	-2.3735300	1.8814808	-4.1909081
H	-2.9432394	0.2231208	-4.0516332
H	-3.2994406	-0.7229331	-1.6622380
H	-3.2940800	0.3402761	-0.2705432
H	-2.5369350	2.2337784	-1.7913303
H	-4.0665064	1.5262957	-2.3004124
H	-0.1087557	-0.5229630	3.8753023
H	1.0224373	-0.7253936	2.5049794
H	0.4033627	0.9140873	2.9244397
H	-2.7014624	0.0742689	3.5261316
H	-3.3513264	0.6439086	1.9678110
H	-2.0554675	1.5834806	2.8047563
H	1.3256438	-0.7224605	-3.1867261
H	1.6777379	0.0959374	-1.6656039
H	0.9753529	-1.5197126	-1.6351712

2b_sy_c_5_ts1.log

E = -1188.191937

H = -1187.829090

G = -1187.900443

NImag=1

C	-2.8424388	-0.2790982	-0.6322645
C	-1.4895141	-0.5016927	-0.9270171
C	-3.6122797	-1.2477941	0.0889555
O	-4.8120364	-1.0667336	0.3869500
C	-0.2149079	0.4983180	0.5079882
C	1.1939753	0.2040512	0.3120822
C	1.9647166	0.7451466	-0.7423582
C	3.2786467	0.3527853	-0.9470715
C	3.8637980	-0.6088594	-0.1101099
C	3.1131004	-1.1750414	0.9346307
C	1.8061501	-0.7705356	1.1372018
C	-2.9866327	-2.5964301	0.4299304
C	-0.9158522	-1.8913434	-0.7826470
C	-1.4607934	-2.5913430	0.4573981

S	-0.7912826	2.1577560	0.5627833
C	0.3903069	3.1166575	1.5466316
C	-0.5404972	2.9633888	-1.0420907
C	5.2202476	-1.0162524	-0.3239375
N	6.3191039	-1.3463770	-0.4965614
C	-3.5414591	0.9930937	-1.0396723
H	-1.0533583	0.0815364	-1.7395907
H	-0.6498549	0.0296198	1.3893610
H	1.5292714	1.4627313	-1.4287387
H	3.8543173	0.7800719	-1.7623531
H	3.5647706	-1.9194073	1.5830851
H	1.2323741	-1.2059515	1.9510632
H	-3.4069153	-2.9293715	1.3843017
H	-3.3409634	-3.3038943	-0.3341386
H	-1.2107706	-2.4581768	-1.6785570
H	0.1773275	-1.8646455	-0.7782908
H	-1.1103467	-2.0669490	1.3550776
H	-1.0773373	-3.6154897	0.5179748
H	0.0859893	4.1651595	1.5049729
H	0.3339226	2.7478343	2.5719458
H	1.3957041	2.9882165	1.1405961
H	-1.2399500	3.8012000	-1.0781838
H	-0.7694034	2.2572831	-1.8394988
H	0.4847807	3.3260070	-1.1242267
H	-4.5095222	0.7736509	-1.5047020
H	-3.7545357	1.6561636	-0.1894389
H	-2.9451390	1.5584314	-1.7634327

2b_sy_c_5_ts2.log

E = -1188.200729

H = -1187.836733

G = -1187.907087

NImag=1

C	-2.5234070	-0.3679316	0.6874543
C	-1.9852320	0.6857744	-0.2554366
C	-2.8043986	-1.6884239	0.2890433
O	-3.2896278	-2.5522495	1.0745717
C	-0.6772110	0.8297433	0.4627856
C	0.5592309	0.0223603	0.2991003
C	1.1941986	-0.1668376	-0.9384479
C	2.4007842	-0.8488374	-1.0188554
C	2.9884965	-1.3497110	0.1496004
C	2.3787490	-1.1606443	1.3955111
C	1.1786079	-0.4655737	1.4606310
C	-2.6506394	-2.0871061	-1.1744975
C	-1.9871797	0.2823060	-1.7311274
C	-1.7044415	-1.2023467	-1.9765747
S	0.0486639	2.9595667	0.0708886
C	1.5223577	2.9770949	1.1130246
C	0.8272422	3.0741128	-1.5542916
C	4.2386563	-2.0565374	0.0686766
N	5.2454832	-2.6253500	0.0036920
C	-2.9670940	0.0556885	2.0665748
H	-2.5344034	1.6330617	-0.1463418
H	-0.8252477	1.1140014	1.5042342
H	0.7527905	0.2268999	-1.8473448
H	2.8896493	-0.9908083	-1.9769145
H	2.8448847	-1.5473717	2.2955153
H	0.7059182	-0.3011555	2.4250996
H	-2.3282527	-3.1333989	-1.2096469
H	-3.6602648	-2.0577656	-1.6098605

H	-2.9904310	0.5036973	-2.1163888
H	-1.2917296	0.9138573	-2.2976811
H	-0.6774766	-1.4569306	-1.7049430
H	-1.8035848	-1.4135279	-3.0474902
H	1.9955249	3.9589722	1.0437999
H	1.2088894	2.7958096	2.1434132
H	2.2189943	2.1994334	0.7880513
H	1.2347229	4.0814195	-1.6694720
H	0.0632121	2.9010835	-2.3142342
H	1.6293223	2.3383862	-1.6433884
H	-3.9928404	-0.2831101	2.2601170
H	-2.3516073	-0.3584240	2.8779571
H	-2.9501007	1.1475040	2.1692564

2b_sy_c_6.log

E = -1188.218403

H = -1187.852994

G = -1187.924305

NImag=0

C	-5.3162285	0.2361304	-2.6372278
C	-4.1951746	0.8740521	-1.8435041
C	-5.3959958	-1.1247785	-2.8915534
O	-6.3246749	-1.6943751	-3.5705796
C	-4.7953399	1.8912219	-0.8227561
C	-5.6496231	1.3202962	0.2886172
C	-5.1053605	0.7105270	1.4272431
C	-5.9305673	0.1829462	2.4135404
C	-7.3189800	0.2631861	2.2629412
C	-7.8795953	0.8819264	1.1403749
C	-7.0410590	1.4131246	0.1681760
C	-4.2787975	-2.0431009	-2.3834567
C	-3.2542947	-0.1329249	-1.1761315
C	-2.9725824	-1.3043447	-2.1093518
S	-3.4546721	2.8999521	-0.0353067
C	-2.6963262	3.7215773	-1.4496569
C	-4.4126838	4.2585158	0.6641099
C	-8.1783756	-0.2845206	3.2788564
N	-8.8699759	-0.7250329	4.0966363
C	-6.2422832	1.1765876	-3.3662475
H	-3.5967782	1.4989969	-2.5310015
H	-5.3818803	2.6335131	-1.3760226
H	-4.0303365	0.6425530	1.5648871
H	-5.5038634	-0.2871117	3.2931184
H	-8.9573603	0.9511252	1.0370184
H	-7.4745096	1.9115836	-0.6931573
H	-4.6130851	-2.5590526	-1.4711614
H	-4.1409826	-2.8181919	-3.1459987
H	-2.3218375	0.3613299	-0.8707249
H	-3.7175173	-0.5397604	-0.2700146
H	-2.2285862	-1.9735728	-1.6621588
H	-2.5494148	-0.9337433	-3.0531111
H	-2.1346295	4.5691572	-1.0515133
H	-2.0123977	3.0208616	-1.9288513
H	-3.4736319	4.0579609	-2.1391459
H	-3.7012609	4.9971162	1.0379342
H	-5.0028139	3.8600436	1.4909506
H	-5.0538311	4.6858563	-0.1097223
H	-6.6925435	0.6543487	-4.2166188
H	-7.0757493	1.5787403	-2.7689753
H	-5.6958002	2.0528802	-3.7510543

2b_sy_c_6_ts1.log

E = -1188.199549
H = -1187.836904
G = -1187.906976

NImag=1

C	-0.4000855	-2.1956087	0.5689600
C	-1.2799632	-1.4765787	-0.2618940
C	0.9592676	-2.4234452	0.1935587
O	1.7929766	-2.9929653	0.9324426
C	-1.4081230	0.4520310	0.5056537
C	-0.0611703	0.9710330	0.4043255
C	0.4116538	1.7799203	-0.6577414
C	1.7561402	2.0785581	-0.7897667
C	2.6822908	1.5687797	0.1367852
C	2.2374042	0.7795580	1.2068460
C	0.8886057	0.4903765	1.3367649
C	1.3793554	-2.0033765	-1.2110521
C	-0.9477583	-1.2509280	-1.7312423
C	0.2205320	-2.1208654	-2.1991983
S	-2.6422807	1.3871551	-0.3384163
C	-4.0786402	0.2984350	-0.3423280
C	-3.2119155	2.6362320	0.8442940
C	4.0762273	1.8686699	-0.0039646
N	5.2048948	2.1116536	-0.1193353
C	-0.8515737	-2.6386743	1.9343695
H	-2.3345915	-1.6403707	-0.0462444
H	-1.7469557	0.1954283	1.5106410
H	-0.2776779	2.1822604	-1.3946535
H	2.0996385	2.7007727	-1.6102337
H	2.9517351	0.3938715	1.9278476
H	0.5510972	-0.1110009	2.1745126
H	1.7358046	-0.9619961	-1.1752549
H	2.2288586	-2.6275506	-1.5057662
H	-1.8417040	-1.4423477	-2.3362090
H	-0.6689614	-0.2044950	-1.9097745
H	0.5322852	-1.8139110	-3.2035898
H	-0.0943602	-3.1697313	-2.2619257
H	-4.9412999	0.9163865	-0.5983658
H	-3.9315634	-0.4626552	-1.1092875
H	-4.2034337	-0.1499106	0.6456762
H	-4.0531224	3.1697116	0.3963783
H	-2.3794333	3.3208524	1.0153697
H	-3.5066064	2.1400270	1.7712273
H	-0.5229132	-3.6605446	2.1547562
H	-0.4477462	-2.0068876	2.7406470
H	-1.9441540	-2.6067601	2.0136090

2b_sy_c_8.log

E = -1188.218087
H = -1187.852563
G = -1187.921414

NImag=0

C	-3.7688688	-0.2285509	-1.9878883
C	-5.2079356	-0.5644461	-1.6591759
C	-3.3885825	0.1766280	-3.2590651
O	-2.2014115	0.5286589	-3.5912851
C	-6.0579806	0.6262074	-1.0834736
C	-6.2673874	0.6752774	0.4072449
C	-5.2462597	0.3478709	1.3089553
C	-5.4715718	0.3867094	2.6794754

C	-6.7359543	0.7501929	3.1576708
C	-7.7709899	1.0713266	2.2726731
C	-7.5282107	1.0315043	0.9050605
C	-4.4031427	0.1562027	-4.4116453
C	-5.9394941	-1.1426686	-2.8808606
C	-5.8581236	-0.1849087	-4.0667035
S	-5.3708204	2.2223687	-1.7607801
C	-6.6211641	3.4041022	-1.2059321
C	-3.9828598	2.7422709	-0.7402231
C	-6.9757993	0.7863415	4.5761658
N	-7.1691709	0.8165610	5.7175676
C	-2.7070786	-0.4266894	-0.9367103
H	-5.2242776	-1.3228957	-0.8642866
H	-7.0488242	0.6388911	-1.5557831
H	-4.2689318	0.0543227	0.9421303
H	-4.6789363	0.1332363	3.3755402
H	-8.7498525	1.3430012	2.6532969
H	-8.3310151	1.2735027	0.2138661
H	-4.3466643	1.1238387	-4.9260855
H	-4.0105479	-0.5833037	-5.1238033
H	-5.4612485	-2.0943911	-3.1423017
H	-6.9865664	-1.3585781	-2.6338832
H	-6.4199609	0.7296294	-3.8335721
H	-6.3596246	-0.6220713	-4.9376112
H	-6.3309571	4.3767463	-1.6076572
H	-7.5818488	3.1042320	-1.6288675
H	-6.6643284	3.4388572	-0.1158364
H	-3.9003373	3.8226208	-0.8814623
H	-3.0936068	2.2403626	-1.1178014
H	-4.1669805	2.5158710	0.3119551
H	-2.5747310	0.4082418	-0.2271939
H	-2.9144265	-1.3162609	-0.3242928
H	-1.7367277	-0.5649120	-1.4253208

2b_sy_c_8_ts1.log

E = -1188.191256

H = -1187.828299

G = -1187.898462

NImag=1

C	1.5338367	-1.5013308	0.1944000
C	1.2225561	-0.8969922	-1.0410180
C	2.8619125	-1.5164404	0.7045790
O	3.1540983	-1.9995351	1.8237954
C	0.1746505	0.8948853	-0.8898394
C	-1.1980320	0.5343601	-0.5440656
C	-1.7280230	0.5028802	0.7626225
C	-3.0138205	0.0479508	1.0076368
C	-3.8123266	-0.4058464	-0.0527216
C	-3.3056730	-0.3949932	-1.3609604
C	-2.0235205	0.0727531	-1.5947783
C	4.0059064	-0.9982381	-0.1632585
C	2.3494184	-0.5587083	-1.9948971
C	3.5763436	-0.0294252	-1.2612854
S	1.0402876	2.1306290	0.0182942
C	-0.1290794	3.3741926	0.6360169
C	1.6400361	1.4403508	1.5887308
C	-5.1410212	-0.8799385	0.1994727
N	-6.2166801	-1.2635909	0.4025917
C	0.4515996	-2.1002648	1.0547299
H	0.3261893	-1.2725231	-1.5390212
H	0.2867435	1.1806286	-1.9344435

H	-1.1318593	0.8140099	1.6131051
H	-3.4019575	0.0329593	2.0211777
H	-3.9208237	-0.7451946	-2.1839715
H	-1.6413075	0.0891465	-2.6120500
H	4.7505568	-0.5455808	0.5003624
H	4.4825597	-1.8811874	-0.6134311
H	2.6164251	-1.4883432	-2.5189123
H	2.0145088	0.1470682	-2.7611602
H	3.3471517	0.9505650	-0.8235299
H	4.3980451	0.1365910	-1.9660269
H	0.4735794	4.1907013	1.0394400
H	-0.7062153	3.7248141	-0.2211958
H	-0.7821143	2.9660567	1.4060911
H	1.7396043	2.2942891	2.2625388
H	2.6198165	0.9961993	1.4168682
H	0.9507171	0.7027701	1.9972697
H	0.2317339	-1.4914898	1.9444769
H	-0.4833235	-2.2077864	0.4928737
H	0.7459825	-3.0883102	1.4285086

2b_sy_c_9.log

E = -1188.216787
H = -1187.851429
G = -1187.921593

NImag=0

C	-3.8637413	0.4148310	-2.8339298
C	-4.4578217	0.1300843	-1.4699595
C	-4.1658277	-0.3182329	-3.9741921
O	-3.6553067	-0.0980959	-5.1294544
C	-5.3421301	1.2795870	-0.8901924
C	-5.9261756	1.0303134	0.4784443
C	-5.1445742	0.5368233	1.5325073
C	-5.7098904	0.2985802	2.7789308
C	-7.0730223	0.5513678	2.9753876
C	-7.8690198	1.0362587	1.9321220
C	-7.2884700	1.2721934	0.6914595
C	-5.0972901	-1.5265743	-3.8581074
C	-5.3898358	-1.1086486	-1.4331732
C	-5.0196931	-2.1559697	-2.4724843
S	-4.4762118	2.9193250	-0.9596410
C	-5.6993496	4.0529661	-0.2777526
C	-3.2673884	2.8942928	0.3779238
C	-7.6627841	0.3040599	4.2643642
N	-8.1371552	0.1057580	5.3020637
C	-2.6773097	1.3515415	-2.9272803
H	-3.6382143	-0.0322516	-0.7483391
H	-6.1529898	1.4619708	-1.6067013
H	-4.0895689	0.3260073	1.3852771
H	-5.1051715	-0.0846042	3.5941125
H	-8.9256131	1.2224242	2.0932497
H	-7.9016032	1.6448838	-0.1245174
H	-6.1363173	-1.2383700	-4.0761561
H	-4.7942339	-2.2335213	-4.6381014
H	-5.3903520	-1.5350554	-0.4246076
H	-6.4225345	-0.7895061	-1.6376456
H	-5.6957852	-3.0147846	-2.3853688
H	-4.0011721	-2.5251041	-2.2922752
H	-5.2380841	5.0427591	-0.2776323
H	-6.5643707	4.0487935	-0.9436651
H	-5.9751898	3.7567213	0.7354935
H	-2.6838522	3.8123511	0.2813071

H	-2.6189675	2.0276656	0.2399471
H	-3.7758904	2.8601095	1.3425199
H	-1.9345059	0.9339595	-3.6192964
H	-2.8985573	2.3623665	-3.3014806
H	-2.1841288	1.4771242	-1.9522560

2b_sy_c_9_ts1.log

E = -1188.188341

H = -1187.825521

G = -1187.897608

NImag=1

C	-2.7646317	-0.2716715	-0.7494535
C	-1.4152775	-0.6372232	-0.8966762
C	-3.5858573	-0.9509452	0.2068640
O	-4.7465493	-0.5921046	0.4959389
C	-0.1888127	0.3904075	0.5188550
C	1.2314821	0.1494072	0.3218936
C	1.9830228	0.7296487	-0.7267240
C	3.3117101	0.3933255	-0.9319176
C	3.9341420	-0.5515567	-0.1022761
C	3.2062394	-1.1557160	0.9358557
C	1.8831678	-0.8047241	1.1401566
C	-2.9903675	-2.1793940	0.8794126
C	-0.9660214	-2.0627112	-0.5880090
C	-2.1143209	-2.9502870	-0.1044707
S	-0.8286096	2.0262993	0.5798614
C	0.2952177	3.0223665	1.5918187
C	-0.5745830	2.8364991	-1.0210620
C	5.3062272	-0.9023185	-0.3182179
N	6.4174797	-1.1863358	-0.4929625
C	-3.3480229	0.9317656	-1.4442117
H	-0.8822015	-0.1727201	-1.7275422
H	-0.6094034	-0.1071619	1.3931549
H	1.5219773	1.4351899	-1.4082162
H	3.8706588	0.8505743	-1.7424772
H	3.6864611	-1.8853766	1.5804455
H	1.3306028	-1.2637505	1.9555915
H	-2.3864195	-1.8568773	1.7410715
H	-3.8130126	-2.7891449	1.2647398
H	-0.5200009	-2.4827130	-1.4970798
H	-0.1728129	-2.0716617	0.1663012
H	-1.7130540	-3.8594250	0.3555934
H	-2.7311135	-3.2628888	-0.9558374
H	-0.0459007	4.0592698	1.5443517
H	0.2284773	2.6500235	2.6152104
H	1.3137095	2.9310516	1.2090974
H	-1.3177726	3.6337023	-1.0879385
H	-0.7380784	2.1086785	-1.8151745
H	0.4315957	3.2540051	-1.0744689
H	-4.3711344	0.7216417	-1.7745656
H	-3.4166345	1.8203013	-0.7976764
H	-2.7603736	1.2051693	-2.3266829

2b_sy_c_prod_1.log

E = -710.334261

H = -710.052948

G = -710.111105

NImag=0

C	-0.6981484	0.7235338	3.0334934
C	-1.8933110	-0.1177628	2.6222166

C	-1.4358362	1.0036597	1.7309932
C	-0.8801158	0.8013586	0.3580057
C	0.4333173	1.1578356	0.0325011
C	0.9228639	0.9701550	-1.2555934
C	0.0835296	0.4277821	-2.2355162
C	-1.2422231	0.0876100	-1.9327931
C	-1.7134863	0.2794429	-0.6411325
H	-2.0451422	1.9045386	1.7994098
C	-0.8528084	1.7573570	4.1294152
H	-2.7989237	0.0919437	3.1868922
C	-1.7194560	-1.5783547	2.2489307
C	-0.3276219	-1.9399050	1.7209506
C	0.7759914	-1.3838627	2.6166719
C	0.6580045	0.0779651	2.9912101
O	1.6412405	0.6977951	3.3672433
C	0.5838954	0.2243708	-3.5682679
N	0.9868202	0.0602115	-4.6420046
H	1.0827066	1.5839022	0.7915960
H	1.9438746	1.2413561	-1.5038693
H	-1.8857890	-0.3252442	-2.7029451
H	-2.7370863	0.0093609	-0.3964817
H	-1.8775482	2.1397198	4.1381289
H	-0.6402069	1.3204006	5.1106232
H	-0.1704328	2.5976381	3.9747905
H	-1.9172613	-2.1734159	3.1491636
H	-2.4804626	-1.8601695	1.5113048
H	-0.1921675	-1.5806758	0.6976045
H	-0.2347006	-3.0295562	1.6800074
H	1.7719739	-1.5499200	2.1964067
H	0.7479105	-1.9048702	3.5865444

2b_sy_c_prod_2.log

E = -710.334347
H = -710.052942
G = -710.110835

NImag=0

C	-0.6492659	0.7058635	2.9491919
C	-1.8759323	-0.1212810	2.5734209
C	-1.4261620	0.9944739	1.6718854
C	-0.8830992	0.8008121	0.2917863
C	0.3850121	1.2831821	-0.0558904
C	0.8681222	1.1521654	-1.3520130
C	0.0687135	0.5313401	-2.3199426
C	-1.2075705	0.0554954	-1.9952022
C	-1.6741278	0.1963499	-0.6934771
H	-2.0169045	1.9062433	1.7557933
C	-0.7534097	1.7301469	4.0570026
H	-2.7510504	0.1173446	3.1718431
C	-1.7333836	-1.5924615	2.1929653
C	-0.4158650	-2.1992860	2.6719499
C	0.7605063	-1.3365596	2.2049167
C	0.6869415	0.0330883	2.8447799
O	1.6768614	0.5552078	3.3356715
C	0.5607994	0.3858785	-3.6633661
N	0.9569173	0.2683535	-4.7456466
H	1.0015270	1.7671571	0.6968793
H	1.8523026	1.5244310	-1.6171570
H	-1.8203942	-0.4175963	-2.7555843
H	-2.6659914	-0.1655211	-0.4378984
H	-1.7715576	2.1268914	4.1025647
H	-0.5136635	1.2825872	5.0269005

H	-0.0647016	2.5628168	3.8870925
H	-2.5745424	-2.1419027	2.6249045
H	-1.8011653	-1.7161277	1.1059670
H	-0.3049326	-3.2181325	2.2883722
H	-0.4088469	-2.2602342	3.7674605
H	0.7252113	-1.2320205	1.1120859
H	1.7280516	-1.7705053	2.4695441

2b_sy_tr_1.log

E = -1188.219901
H = -1187.854516
G = -1187.924348

NImag=0

C	-1.6405163	0.0119388	1.3563683
C	-2.0932261	0.3528902	-0.0405779
C	-2.3973603	-0.7239280	2.2516794
O	-1.9626647	-1.1940645	3.3641970
C	-1.1188401	-0.2721771	-1.0879586
C	-1.3678258	0.1713308	-2.5105124
C	-2.4040310	-0.3379363	-3.3047891
C	-2.6269560	0.1618450	-4.5813539
C	-1.8130454	1.1915423	-5.0688756
C	-0.7757673	1.7124092	-4.2883038
C	-0.5569495	1.1931227	-3.0177085
C	-3.8739039	-0.9646605	1.9294344
C	-3.5614655	-0.0063763	-0.3403779
C	-4.4196453	0.0396745	0.9189462
S	-1.1810127	-2.1284144	-0.9517241
C	-0.1657548	-2.6374785	-2.3589775
C	-0.0276727	-2.5515300	0.3742396
C	-2.0428559	1.7152388	-6.3890342
N	-2.2277117	2.1369690	-7.4516929
C	-0.2653467	0.4816839	1.7510979
H	-1.9551222	1.4349188	-0.2227074
H	-0.0869234	-0.0245070	-0.8167666
H	-3.0470260	-1.1350913	-2.9415615
H	-3.4255141	-0.2381332	-5.1971791
H	-0.1475662	2.5074449	-4.6758789
H	0.2515573	1.5884438	-2.4092376
H	-4.0110278	-1.9884401	1.5485466
H	-4.4182050	-0.9107126	2.8795383
H	-3.9563655	0.6581266	-1.1161515
H	-3.6351878	-1.0279949	-0.7363677
H	-5.4626240	-0.1827878	0.6653043
H	-4.3988461	1.0484048	1.3520854
H	0.0636974	-3.6942000	-2.2077473
H	-0.7407365	-2.5125925	-3.2758598
H	0.7498213	-2.0424119	-2.3820975
H	0.1025388	-3.6343931	0.3139942
H	-0.4821324	-2.2672652	1.3243472
H	0.9221668	-2.0420074	0.2041499
H	-0.1975540	0.5530135	2.8416269
H	0.5680788	-0.1664515	1.4331886
H	-0.0538779	1.4752564	1.3275971

2b_sy_tr_1_r.log

E = -1188.215150
H = -1187.849671
G = -1187.919531

NImag=0

C	0.9890214	-1.7610648	-0.7455756
C	1.0536581	-0.8915309	0.4990606
C	0.6499246	-3.1108686	-0.7204950
O	0.5719298	-3.8619515	-1.7568738
C	0.1439878	0.3588031	0.3337930
C	0.5258842	1.3225349	-0.7613329
C	1.8136701	1.8687837	-0.8281215
C	2.1456823	2.7647431	-1.8353496
C	1.1792633	3.1164610	-2.7866052
C	-0.1139818	2.5858992	-2.7260580
C	-0.4334381	1.6969568	-1.7063177
C	0.4202731	-3.8090886	0.6218691
C	0.6345099	-1.6390823	1.7759238
C	1.1031262	-3.0857227	1.7742947
S	0.1431205	1.3923210	1.9265315
C	-0.6309513	2.9432980	1.4124696
C	-1.2304920	0.7367519	2.9080688
C	1.5193990	4.0407302	-3.8358767
N	1.7923001	4.7851354	-4.6799830
C	1.5425270	-1.2160901	-2.0430568
H	2.0821536	-0.5111532	0.6398959
H	-0.9011003	0.0481907	0.2205063
H	2.5699049	1.5918708	-0.0982583
H	3.1430058	3.1880112	-1.8923003
H	-0.8545952	2.8688161	-3.4666905
H	-1.4348060	1.2795796	-1.6497345
H	-0.6578460	-3.8943052	0.8226935
H	0.7993357	-4.8308283	0.5087154
H	1.0180891	-1.1144648	2.6608818
H	-0.4626315	-1.6489683	1.8451004
H	0.8695293	-3.5573304	2.7356853
H	2.1934277	-3.1255465	1.6479252
H	-0.8166060	3.5062000	2.3294903
H	0.0647231	3.4911498	0.7775451
H	-1.5663165	2.7325466	0.8895961
H	-1.5208165	1.5346586	3.5943822
H	-0.8860213	-0.1271068	3.4718886
H	-2.0592777	0.4776571	2.2465543
H	1.8352396	-2.0604935	-2.6757882
H	0.8504738	-0.6016915	-2.6387762
H	2.4299850	-0.5904046	-1.8685445

2b_sy_tr_1_ts1.log

E = -1188.194723

H = -1187.832357

G = -1187.903549

NImag=1

C	2.3883200	-0.9649561	0.9024865
C	1.0271415	-1.0654945	0.5773397
C	3.3997188	-1.0942555	-0.0986651
O	4.6021709	-0.8192480	0.1073482
C	0.0822968	0.8482032	0.5933460
C	-1.3090369	0.5273081	0.3856100
C	-1.9632187	0.5592537	-0.8708975
C	-3.2657596	0.1130871	-1.0142614
C	-3.9684170	-0.3818979	0.0961910
C	-3.3435004	-0.4178201	1.3550039
C	-2.0432861	0.0304721	1.4928375
C	2.9853496	-1.6072691	-1.4719801
C	0.5980336	-1.6377783	-0.7664599
C	1.7178188	-2.4538482	-1.4107285

S	0.8574098	1.8297894	-0.6472793
C	0.0601490	3.4583369	-0.5947971
C	2.4337192	2.2576851	0.1169503
C	-5.3164041	-0.8382599	-0.0508053
N	-6.4096425	-1.2098047	-0.1695880
C	2.7981722	-0.5369528	2.2846999
H	0.3539042	-1.2751525	1.4098844
H	0.3558512	1.1920444	1.5908677
H	-1.4523887	0.9368880	-1.7533520
H	-3.7482706	0.1478939	-1.9860875
H	-3.8866803	-0.7935964	2.2167261
H	-1.5699443	0.0072156	2.4707739
H	2.8180199	-0.7379396	-2.1267432
H	3.8324873	-2.1611263	-1.8889634
H	-0.3067250	-2.2403993	-0.6353248
H	0.3294061	-0.8337496	-1.4641982
H	1.4161611	-2.7743320	-2.4136456
H	1.9101179	-3.3583927	-0.8210829
H	0.6038112	4.1175758	-1.2755965
H	-0.9689844	3.3359881	-0.9367131
H	0.0886039	3.8338565	0.4297023
H	2.8817403	3.0318724	-0.5089417
H	3.0703187	1.3731255	0.1305658
H	2.2481054	2.6333863	1.1249978
H	3.6826498	-1.0833227	2.6289522
H	3.0561267	0.5322974	2.3339154
H	1.9866287	-0.7085335	3.0006438

2b_sy_tr_2.log

E = -1188.217872

H = -1187.852571

G = -1187.923122

NImag=0

C	-1.5588219	0.1978423	1.3416261
C	-2.0879536	0.4026713	-0.0540521
C	-2.2661100	-0.4182614	2.3576216
O	-1.8114068	-0.6350487	3.5396821
C	-1.2191424	-0.3334642	-1.1347940
C	-1.4421607	0.1744947	-2.5415191
C	-2.4784016	-0.2777786	-3.3684605
C	-2.6651927	0.2707246	-4.6317462
C	-1.8126193	1.2895131	-5.0718455
C	-0.7739142	1.7538367	-4.2569006
C	-0.5930198	1.1886479	-3.0009036
C	-3.7070814	-0.8721871	2.1077277
C	-3.5991835	0.1691480	-0.1729007
C	-4.0751715	-1.0362488	0.6365963
S	-1.4006400	-2.1744193	-1.1409842
C	-0.1216241	-2.6314164	-2.3318169
C	-0.5859864	-2.7106734	0.3798616
C	-2.0020615	1.8617731	-6.3781379
N	-2.1539233	2.3226757	-7.4297156
C	-0.1518101	0.6672215	1.6034920
H	-1.8973786	1.4490027	-0.3535805
H	-0.1653017	-0.1849678	-0.8719003
H	-3.1506838	-1.0667556	-3.0415056
H	-3.4649889	-0.0848074	-5.2725947
H	-0.1153200	2.5408784	-4.6088506
H	0.2167171	1.5385269	-2.3663724
H	-3.8520908	-1.8141572	2.6497879
H	-4.3776731	-0.1386386	2.5795859

H	-4.1002643	1.0622625	0.2215895
H	-3.9055034	0.0826634	-1.2209526
H	-3.6313963	-1.9625146	0.2491562
H	-5.1590044	-1.1534033	0.5199551
H	0.0212579	-3.7101033	-2.2432999
H	-0.4771824	-2.3860485	-3.3328607
H	0.8002198	-2.0947838	-2.0965893
H	-0.4066044	-3.7816531	0.2603295
H	-1.2534354	-2.5198058	1.2190214
H	0.3550396	-2.1687664	0.4924679
H	-0.0360937	0.9538749	2.6540402
H	0.6239121	-0.0937845	1.4063048
H	0.1046997	1.5364301	0.9801372

2b_sy_tr_2_r.log

E = -1188.219526

H = -1187.854152

G = -1187.924078

NImag=0

C	1.3126682	-1.5615427	-1.0175497
C	1.2146221	-0.9669777	0.3742043
C	0.7310235	-2.7756013	-1.3561317
O	0.8121902	-3.3278519	-2.5111987
C	0.1606947	0.1762532	0.3651325
C	0.5111107	1.3138737	-0.5606461
C	1.7194984	2.0081912	-0.4234437
C	2.0421980	3.0380814	-1.2963116
C	1.1475953	3.3730786	-2.3215222
C	-0.0659093	2.6923766	-2.4658256
C	-0.3795048	1.6702949	-1.5763292
C	-0.0135254	-3.5961139	-0.2964076
C	0.9081923	-2.0390263	1.4247785
C	-0.3021567	-2.8760444	1.0198956
S	-0.0579153	0.9157286	2.0936405
C	-0.8730935	2.4992106	1.7858887
C	-1.4803685	0.0114825	2.7492736
C	1.4791931	4.4355776	-3.2337681
N	1.7458536	5.2912522	-3.9671596
C	2.1708018	-0.8633503	-2.0457720
H	2.1749466	-0.4974301	0.6381384
H	-0.8350930	-0.2064958	0.1210401
H	2.4210015	1.7448547	0.3642989
H	2.9775829	3.5778706	-1.1935105
H	-0.7511821	2.9635423	-3.2620875
H	-1.3187987	1.1347362	-1.6799007
H	-0.9413607	-3.9641712	-0.7499683
H	0.6042864	-4.4857608	-0.1047359
H	1.7864168	-2.6931553	1.4921134
H	0.7862203	-1.6047008	2.4256056
H	-1.1857128	-2.2348672	0.9035841
H	-0.5471614	-3.5975289	1.8081008
H	-1.2275916	2.8548130	2.7556039
H	-0.1399162	3.1970042	1.3815935
H	-1.7070936	2.3554833	1.0958508
H	-1.7947278	0.5406930	3.6510287
H	-1.1733565	-1.0011802	3.0066263
H	-2.2783953	0.0077672	2.0043107
H	2.5841449	-1.6064527	-2.7370060
H	1.6432139	-0.1209398	-2.6671936
H	3.0064565	-0.3288872	-1.5731196

2b_sy_tr_2_ts1.log

E = -1188.196708

H = -1187.834290

G = -1187.905447

NImag=1

C	2.3638586	-1.0904754	0.8771830
C	1.0496815	-1.1638014	0.3874609
C	3.4928605	-1.1967949	0.0115402
O	4.6711877	-1.0766993	0.4151185
C	0.0679032	0.7066033	0.5272779
C	-1.3376131	0.3983575	0.3408240
C	-2.0394710	0.5609388	-0.8779245
C	-3.3532555	0.1460646	-1.0118322
C	-4.0148571	-0.4584359	0.0695592
C	-3.3383298	-0.6381333	1.2866658
C	-2.0272378	-0.2139112	1.4155514
C	3.2664222	-1.5394691	-1.4579266
C	0.7971723	-1.6232474	-1.0277642
C	1.8883323	-1.1405305	-1.9776759
S	0.7006589	1.9560022	-0.5430879
C	0.0661450	3.5249920	0.1090734
C	2.4225152	2.1051600	-0.0302351
C	-5.3742068	-0.8856302	-0.0675997
N	-6.4759336	-1.2328194	-0.1787553
C	2.6087372	-0.7777379	2.3279690
H	0.2880434	-1.4778177	1.1046164
H	0.3576661	0.9247467	1.5566739
H	-1.5545230	1.0175948	-1.7367556
H	-3.8750395	0.2861021	-1.9534135
H	-3.8482029	-1.1021722	2.1252993
H	-1.5151906	-0.3427134	2.3655501
H	4.0660352	-1.0675456	-2.0381113
H	3.4005791	-2.6263579	-1.5589401
H	0.7816021	-2.7232479	-1.0214553
H	-0.1930649	-1.3011231	-1.3668141
H	1.8346319	-0.0478684	-2.0737954
H	1.7261575	-1.5458669	-2.9819791
H	0.5236374	4.3391753	-0.4576173
H	-1.0150134	3.5242401	-0.0415386
H	0.3123611	3.5944441	1.1706393
H	2.7941628	3.0377410	-0.4587466
H	2.9844357	1.2618010	-0.4288081
H	2.4720270	2.1312533	1.0602459
H	3.3945799	-1.4125989	2.7518412
H	2.9381687	0.2621944	2.4773641
H	1.6961367	-0.9203755	2.9176619

2b_sy_tr_2_ts2.log

E = -1188.213398

H = -1187.849670

G = -1187.919527

NImag=1

C	1.4411750	-1.6704830	-0.5011500
C	1.5393910	-0.2585330	-1.0426500
C	2.4042590	-2.1840470	0.3814400
O	2.3491430	-3.3501320	0.8767420
C	0.6485860	0.3869750	-0.0223080
C	-0.8045700	0.0661330	0.0018480
C	-1.5658890	0.0484610	-1.1754980
C	-2.9276290	-0.2141920	-1.1297500

C	-3.5373660	-0.4677780	0.1067680
C	-2.7914880	-0.4530500	1.2907830
C	-1.4304480	-0.1781920	1.2297900
C	3.6684700	-1.3786960	0.6956870
C	2.9657570	0.2870280	-1.0634290
C	3.6629000	0.0943430	0.2825760
S	0.5748240	2.5609810	-0.4257640
C	-0.8830310	3.0856690	0.5042320
C	1.8537080	3.1767620	0.6944300
C	-4.9480760	-0.7446850	0.1589590
N	-6.0840820	-0.9665960	0.2008810
C	0.3365220	-2.5823710	-0.9682090
H	1.0968590	-0.1879980	-2.0436770
H	1.0817960	0.4694220	0.9749020
H	-1.0956720	0.2462450	-2.1346920
H	-3.5197660	-0.2242730	-2.0387250
H	-3.2748870	-0.6519770	2.2415290
H	-0.8416700	-0.1614200	2.1427240
H	3.8740090	-1.4790560	1.7673560
H	4.4835690	-1.9064720	0.1801930
H	3.5159110	-0.2603680	-1.8389620
H	2.9750120	1.3434940	-1.3617760
H	3.1643280	0.6919610	1.0542890
H	4.6895280	0.4730740	0.2258330
H	-0.8859050	4.1770710	0.5445880
H	-1.7717950	2.7375040	-0.0247880
H	-0.8530770	2.6694590	1.5141950
H	1.7213590	4.2554680	0.8024890
H	2.8301160	2.9743110	0.2527370
H	1.7637610	2.6865220	1.6667770
H	0.7301220	-3.5964850	-1.1046510
H	-0.5083460	-2.6716590	-0.2660340
H	-0.0788490	-2.2460780	-1.9248930

2b_sy_tr_3.log

E = -1188.213041

H = -1187.847617

G = -1187.916449

NImag=0

C	-1.5641630	-0.1348334	1.2796164
C	-1.9628631	0.2399020	-0.1255324
C	-2.4306245	-0.7145519	2.1950410
O	-2.1295572	-1.0498972	3.3964809
C	-0.9489222	-0.2681348	-1.2022629
C	-1.2688526	0.2325343	-2.5927639
C	-2.1153870	-0.4520263	-3.4721825
C	-2.4332119	0.0871982	-4.7124800
C	-1.9056424	1.3321361	-5.0749020
C	-1.0623070	2.0317914	-4.2044947
C	-0.7469006	1.4747084	-2.9713779
C	-3.8890704	-0.9341750	1.7776607
C	-3.4211855	-0.0649868	-0.5115000
C	-4.3430017	0.0423781	0.6970499
S	-0.5891362	-2.0913411	-1.3042920
C	0.5884005	-2.3939087	0.0274423
C	-1.9836268	-3.0689688	-0.7010428
C	-2.2312659	1.8968021	-6.3571754
N	-2.4933905	2.3519887	-7.3894253
C	-0.2329743	0.3967186	1.7441812
H	-1.8215331	1.3334013	-0.2433170
H	0.0458006	0.0993688	-0.9232253

H	-2.5471833	-1.4120901	-3.1999966
H	-3.0874133	-0.4462824	-5.3938289
H	-0.6559236	2.9945505	-4.4961285
H	-0.0863385	2.0085566	-2.2936284
H	-4.0355774	-1.9689250	1.4305033
H	-4.4921450	-0.8250629	2.6858273
H	-3.7373851	0.6213723	-1.3046996
H	-3.5212121	-1.0744833	-0.9236696
H	-5.3780638	-0.1560813	0.3950388
H	-4.3141285	1.0659505	1.0947287
H	0.8905395	-3.4385234	-0.0719507
H	1.4501129	-1.7446364	-0.1336209
H	0.1089482	-2.2065177	0.9883501
H	-1.5914816	-4.0859656	-0.6201739
H	-2.7831089	-3.0472392	-1.4414893
H	-2.3056917	-2.6963379	0.2707814
H	-0.1506158	0.2669864	2.8273998
H	0.6524641	-0.0778984	1.2949729
H	-0.1371811	1.4725233	1.5192859

2b_sy_tr_3_r.log

E = -1188.210536
H = -1187.844775
G = -1187.913962

NImag=0

C	1.2541381	-1.4996381	-0.7144032
C	1.1271478	-0.6848989	0.5648996
C	0.8772437	-2.8351079	-0.8152944
O	0.9381293	-3.5285735	-1.8917448
C	0.1104363	0.4703601	0.3415367
C	0.3788829	1.4022609	-0.8196904
C	1.5894275	2.0964839	-0.9302665
C	1.8201857	2.9444087	-2.0050935
C	0.8290026	3.0969913	-2.9828984
C	-0.3877260	2.4134191	-2.8831534
C	-0.6064916	1.5754165	-1.7957305
C	0.4460529	-3.5853931	0.4459330
C	0.6613136	-1.5163827	1.7800019
C	1.0714621	-2.9793913	1.6946691
S	-0.1722926	1.6705533	1.7781329
C	-1.1890514	0.8344651	3.0152858
C	1.3963352	1.8491708	2.6519780
C	1.0652720	3.9689693	-4.1027499
N	1.2553043	4.6717623	-5.0034317
C	2.0055014	-0.9099476	-1.8864132
H	2.1003062	-0.2160924	0.7951651
H	-0.8922745	0.0401070	0.2334405
H	2.3758013	1.9520547	-0.1950607
H	2.7604033	3.4778483	-2.0966890
H	-1.1478621	2.5393512	-3.6470103
H	-1.5472870	1.0390731	-1.7109025
H	-0.6499428	-3.5833372	0.5417278
H	0.7496863	-4.6288260	0.3078325
H	1.0371713	-1.0731241	2.7083743
H	-0.4357952	-1.4946281	1.8343093
H	0.7474503	-3.5051424	2.6005197
H	2.1647394	-3.0660854	1.6412063
H	-1.5279194	1.6180678	3.6962672
H	-2.0474227	0.3997157	2.5000645
H	-0.6201776	0.0768423	3.5503722
H	1.1682970	2.4300121	3.5488711

H	2.0805404	2.4156568	2.0199244
H	1.8098774	0.8774269	2.9194214
H	2.4479393	-1.7285564	-2.4649333
H	1.4042155	-0.3186188	-2.5951042
H	2.8152529	-0.2483663	-1.5477227

2b_sy_tr_4.log

E = -1188.209724

H = -1187.844162

G = -1187.913236

NImag=0

C	-1.6485376	0.1376363	1.3377361
C	-2.1982663	0.2370954	-0.0696621
C	-2.2415706	-0.5980123	2.3464354
O	-1.6996520	-0.8596071	3.4818141
C	-1.0919407	-0.0894281	-1.1158940
C	-1.3449391	0.3261969	-2.5513066
C	-2.4316469	-0.1359306	-3.3078215
C	-2.6387943	0.3233650	-4.6026912
C	-1.7524920	1.2558415	-5.1539228
C	-0.6598348	1.7242782	-4.4178801
C	-0.4647094	1.2534725	-3.1249861
C	-3.6488268	-1.1503071	2.1272822
C	-3.5128353	-0.5288140	-0.2785057
C	-4.3831707	-0.4807580	0.9725734
S	-0.3521183	-1.8130374	-1.1338655
C	-0.6323464	-2.6278896	0.4588271
C	-1.3415609	-2.8759051	-2.2070958
C	-1.9670643	1.7355194	-6.4937682
N	-2.1392000	2.1214950	-7.5718693
C	-0.3131480	0.7794033	1.6035530
H	-2.3856850	1.3004814	-0.3209833
H	-0.1990195	0.4538350	-0.7968498
H	-3.1213073	-0.8666915	-2.9023433
H	-3.4804058	-0.0366536	-5.1848272
H	0.0242336	2.4451160	-4.8528856
H	0.3819971	1.6166887	-2.5496326
H	-3.5813410	-2.2353815	1.9473248
H	-4.1943497	-1.0290758	3.0707431
H	-4.0571619	-0.1156458	-1.1326323
H	-3.3111049	-1.5843350	-0.5049586
H	-5.3425554	-0.9737854	0.7772108
H	-4.6040132	0.5647705	1.2264374
H	-0.1304879	-3.5935794	0.3561692
H	-0.1654929	-2.0350477	1.2447427
H	-1.6978366	-2.7580367	0.6443234
H	-0.9094718	-3.8728746	-2.0929136
H	-1.2113028	-2.5429875	-3.2362845
H	-2.3903172	-2.8780030	-1.9114728
H	-0.2024154	0.9689503	2.6753071
H	0.5612529	0.1653208	1.3111427
H	-0.2032608	1.7362207	1.0712299

2b_sy_tr_4_ts1.log

E = -1188.190142

H = -1187.827116

G = -1187.897392

NImag=1

C	2.5698532	-0.6790460	0.8987127
C	1.1893531	-0.9239823	0.7804470

C	3.4828921	-1.0106500	-0.1473954
O	4.6911741	-0.6842453	-0.1338818
C	0.0813260	0.8783356	0.8131746
C	-1.2896123	0.5246170	0.5077134
C	-1.8773924	0.5738226	-0.7771477
C	-3.1576692	0.0947373	-1.0014054
C	-3.8949267	-0.4663263	0.0527507
C	-3.3317195	-0.5325829	1.3380210
C	-2.0578784	-0.0400451	1.5562698
C	2.9816907	-1.8748451	-1.3029478
C	0.6557716	-1.6564936	-0.4376667
C	1.7007731	-2.6357950	-0.9729193
S	0.9679802	2.1403433	-0.0283387
C	1.4412913	1.5771145	-1.6780245
C	-0.1639320	3.4906633	-0.4466873
C	-5.2158130	-0.9668932	-0.1804534
N	-6.2862109	-1.3732450	-0.3693235
C	3.0969403	0.0074919	2.1298063
H	0.6530920	-1.1205489	1.7102879
H	0.2700533	1.0633324	1.8690600
H	-1.3326285	0.9807833	-1.6212652
H	-3.5905227	0.1456304	-1.9956174
H	-3.9009463	-0.9624028	2.1564838
H	-1.6338235	-0.0832065	2.5558764
H	2.8109760	-1.2269017	-2.1758519
H	3.7989681	-2.5513913	-1.5740470
H	-0.2790951	-2.1675982	-0.1862106
H	0.4154147	-0.9455362	-1.2385297
H	1.3155357	-3.1456056	-1.8627167
H	1.9097077	-3.4054703	-0.2199232
H	1.9680536	2.4167895	-2.1369636
H	2.1299652	0.7437543	-1.5493260
H	0.5803164	1.2939038	-2.2814926
H	0.4289333	4.2595359	-0.9469818
H	-0.5615110	3.8768212	0.4932454
H	-0.9679217	3.1433817	-1.0954886
H	4.0871129	-0.3698575	2.4047435
H	3.2043494	1.0941439	1.9893751
H	2.4204873	-0.1423732	2.9793854

2b_sy_tr_prod_1.log

E = -710.338002

H = -710.056222

G = -710.114710

NImag=0

C	1.8239530	-0.1721755	1.1671979
C	0.9736663	-1.4344023	1.2199408
C	0.7962070	-0.5014398	0.0705756
C	-0.3816679	0.3971841	-0.1084146
C	-1.6074289	0.1656474	0.5254854
C	-2.6828023	1.0260337	0.3309392
C	-2.5334718	2.1345110	-0.5099800
C	-1.3143532	2.3803166	-1.1564791
C	-0.2518880	1.5112198	-0.9509923
H	1.2323098	-0.8289239	-0.8716230
C	1.5349887	0.9712077	2.1101343
H	0.2064628	-1.3874355	1.9888212
C	1.5951639	-2.8105790	0.9871663
C	3.1231502	-2.7855048	1.0311028
C	3.6753957	-1.6450726	0.1661468
C	3.2510740	-0.3170693	0.7537603

O	4.0510879	0.5884110	0.9387445
C	-3.6418819	3.0269402	-0.7153575
N	-4.5349435	3.7462402	-0.8808778
H	-1.7311482	-0.6967322	1.1728114
H	-3.6329398	0.8409629	0.8214589
H	-1.2082055	3.2421860	-1.8072208
H	0.6970080	1.6967790	-1.4473218
H	1.7363324	1.9361983	1.6341179
H	0.4890855	0.9550054	2.4273967
H	2.1652196	0.8961523	3.0015129
H	1.2177701	-3.5034666	1.7446485
H	1.2700668	-3.1932103	0.0121572
H	3.5269300	-3.7428967	0.6881513
H	3.4615555	-2.6428636	2.0651473
H	3.2903763	-1.7373911	-0.8581064
H	4.7668275	-1.6549326	0.1178561

2b_sy_tr_prod_2.log

E = -710.338504

H = -710.056883

G = -710.115660

NImag=0

C	1.8074537	-0.1593280	1.3324123
C	0.9728579	-1.4223126	1.3638949
C	0.8405314	-0.5161986	0.1850748
C	-0.3352165	0.3701414	-0.0571304
C	-1.5865374	0.1368095	0.5243198
C	-2.6574265	0.9884522	0.2746435
C	-2.4782093	2.0901424	-0.5693118
C	-1.2337506	2.3366666	-1.1652004
C	-0.1762078	1.4762951	-0.9051946
H	1.3281606	-0.8287588	-0.7350407
C	1.4587402	1.0084239	2.2257228
H	0.1638600	-1.3848584	2.0901108
C	1.6420079	-2.7750533	1.2139796
C	2.8239158	-2.7336778	0.2456101
C	3.8275643	-1.6496795	0.6399927
C	3.2581470	-0.2876521	0.9949191
O	4.0005488	0.6794051	1.0801213
C	-3.5810643	2.9749574	-0.8299330
N	-4.4694659	3.6883971	-1.0400079
H	-1.7334475	-0.7201139	1.1739389
H	-3.6269940	0.8023236	0.7251307
H	-1.1046024	3.1928429	-1.8192437
H	0.7921749	1.6626615	-1.3620185
H	1.6723598	1.9618289	1.7326333
H	0.3984986	0.9867348	2.4906989
H	2.0432395	0.9669899	3.1500691
H	1.9944974	-3.0992002	2.2013018
H	0.9047697	-3.5117024	0.8759818
H	2.4699003	-2.5702071	-0.7774102
H	3.3306000	-3.7033843	0.2436129
H	4.5985919	-1.5062133	-0.1225600
H	4.3493024	-1.9616319	1.5568823

2c.log

E = -347.858736

H = -347.694230

G = -347.734626

NImag=0

C	-0.0242654	0.8178314	-0.7870990
C	0.6247208	-0.3640732	-0.8185145
C	0.0667766	-1.5901415	-0.1437263
C	-0.9382326	-1.2471192	0.9527045
C	-1.9818612	-0.2605679	0.4326379
C	-1.3392020	0.9806932	-0.1470572
O	-1.9060339	2.0678163	-0.1245316
C	1.9273840	-0.5340698	-1.5361939
H	0.3934632	1.6991407	-1.2694235
H	-0.4104847	-2.2110749	-0.9169063
H	0.8955867	-2.1849269	0.2562490
H	-1.4260879	-2.1549996	1.3187197
H	-0.4060253	-0.7978506	1.8002179
H	-2.5568406	-0.7260570	-0.3815110
H	-2.6919207	0.0435743	1.2060567
H	2.2269248	0.3749620	-2.0624913
H	2.7136536	-0.8112821	-0.8243583
H	1.8513436	-1.3562552	-2.2577708

2c_sy_c_1.log

E = -1188.221464

H = -1187.856149

G = -1187.925399

NImag=0

C	-4.5060822	2.3976240	-2.5370028
C	-3.8178913	2.4265724	-1.1958208
C	-3.8937788	2.5867603	-3.7624736
O	-4.4547472	2.4030779	-4.8971117
C	-3.3643392	0.9646840	-0.8024740
C	-2.9266981	0.7438840	0.6260008
C	-3.8272225	0.6684038	1.6982045
C	-3.3694497	0.5020361	2.9979559
C	-1.9915797	0.4178882	3.2361758
C	-1.0786906	0.4886398	2.1791261
C	-1.5542494	0.6439317	0.8817520
C	-2.4522941	3.1066260	-3.7934899
C	-2.5376938	3.2805221	-1.2715025
C	-1.6722382	2.9479310	-2.4868686
S	-4.7007105	-0.2477516	-1.2761051
C	-4.2942846	-0.6911255	-2.9852923
C	-4.1361636	-1.7717480	-0.4802414
C	-1.5114063	0.2498745	4.5819744
N	-1.1249345	0.1147055	5.6653512
C	-4.7566044	3.0166719	-0.1374985
H	-5.5552493	2.0918893	-2.5441040
H	-2.5443942	0.6722418	-1.4647922
H	-4.8989182	0.7336668	1.5296494
H	-4.0694385	0.4391517	3.8244113
H	-0.0136833	0.4154724	2.3723058
H	-0.8499651	0.6918406	0.0554908
H	-1.9328035	2.6052631	-4.6181594
H	-2.5081180	4.1700505	-4.0679679
H	-2.8574665	4.3292279	-1.3350603
H	-1.9582417	3.1805340	-0.3441885
H	-1.2927757	1.9212471	-2.4082043
H	-0.7875088	3.5948316	-2.4928901
H	-4.8165917	-1.6290975	-3.1877944
H	-4.6416219	0.1043456	-3.6441429
H	-3.2131148	-0.8257123	-3.0670951
H	-4.7135901	-2.5834855	-0.9269965
H	-4.3477011	-1.7169672	0.5866575

H	-3.0686428	-1.9106738	-0.6651867
H	-5.6614868	2.4085578	-0.0127615
H	-4.2747280	3.1248278	0.8398024
H	-5.0732014	4.0092801	-0.4718328

2c_sy_c_1_r.log

E = -1188.215464
H = -1187.850298
G = -1187.919253

NImag=0

C	0.5259049	-0.5211218	2.1400438
C	1.2547840	-0.5387599	0.8154444
C	1.0297673	-0.1003713	3.3591824
O	0.4187120	-0.1808308	4.4805809
C	0.3678668	0.3197422	-0.1672574
C	0.4293633	1.8150743	0.0458154
C	1.4557619	2.6094169	-0.4818703
C	1.5055320	3.9715676	-0.2191763
C	0.5190030	4.5500100	0.5887113
C	-0.5191959	3.7739657	1.1145677
C	-0.5620669	2.4133864	0.8299889
C	2.4449110	0.4808226	3.3941780
C	2.7005295	-0.0122257	0.9492330
C	2.9026852	1.0325078	2.0482516
S	0.7166243	-0.0002200	-1.9927276
C	-0.2822279	-1.4600677	-2.3860543
C	-0.3366872	1.2303187	-2.8028167
C	0.5669506	5.9604881	0.8686479
N	0.6056045	7.0960609	1.0928496
C	1.3243419	-1.9833847	0.2875388
H	-0.4718826	-0.9656710	2.1354743
H	-0.6691159	-0.0192811	-0.0640668
H	2.2389160	2.1752292	-1.0987134
H	2.3023743	4.5833156	-0.6288405
H	-1.2845572	4.2333889	1.7312115
H	-1.3699983	1.8067909	1.2270838
H	2.4633314	1.2607096	4.1638165
H	3.1304702	-0.3104683	3.7322426
H	3.3328543	-0.8744439	1.1992518
H	3.0660822	0.3531604	-0.0196944
H	2.3414451	1.9468273	1.8318832
H	3.9622124	1.3135059	2.0849865
H	-0.4653026	-1.4161420	-3.4612891
H	0.2806531	-2.3587048	-2.1467085
H	-1.2228604	-1.4169432	-1.8330381
H	-0.4089211	0.9302778	-3.8498724
H	0.1371294	2.2076088	-2.7303109
H	-1.3212264	1.2303107	-2.3295312
H	0.3241698	-2.4024053	0.1319778
H	1.9026025	-2.0693294	-0.6437680
H	1.8302048	-2.5987860	1.0365203

2c_sy_c_1_ts1.log

E = -1188.197325
H = -1187.835277
G = -1187.905201

NImag=1

C	2.4172900	-0.5815380	1.1772323
C	1.2613775	-1.1236564	0.5807384
C	3.7227743	-0.6761157	0.6176193

O	4.7454813	-0.2176658	1.1708408
C	0.1542534	0.4565521	-0.4868127
C	-1.2686157	0.2708367	-0.3255491
C	-2.0083046	0.7458239	0.7858082
C	-3.3471364	0.4353325	0.9456818
C	-4.0030267	-0.3653569	-0.0035968
C	-3.2950063	-0.8378626	-1.1229725
C	-1.9595567	-0.5179405	-1.2798218
C	3.8914864	-1.4392508	-0.6925187
C	1.4490312	-2.0188382	-0.6251434
C	2.6056615	-1.5605122	-1.5070791
S	0.8332882	1.9301738	0.2323005
C	2.3127353	2.1723294	-0.7701717
C	-0.1436623	3.3121736	-0.4189660
C	-5.3869097	-0.6883299	0.1623418
N	-6.5094278	-0.9513554	0.2970714
C	0.1572998	-1.5450659	1.5179538
H	2.3342764	-0.1012084	2.1516382
H	0.5146908	0.3517898	-1.5091635
H	-1.5259558	1.3492918	1.5511551
H	-3.8931302	0.8058362	1.8078957
H	-3.8028147	-1.4460818	-1.8652706
H	-1.4219962	-0.8795076	-2.1521688
H	4.6866349	-0.9517555	-1.2663760
H	4.2620749	-2.4394270	-0.4256026
H	1.6577254	-3.0309532	-0.2430777
H	0.5132448	-2.0863907	-1.1916533
H	2.3621317	-0.5862037	-1.9490191
H	2.7483956	-2.2591011	-2.3380478
H	2.7344856	3.1389024	-0.4888624
H	3.0174033	1.3760430	-0.5404086
H	2.0275487	2.1609825	-1.8242171
H	0.3644471	4.2343457	-0.1272834
H	-1.1346780	3.2792387	0.0344581
H	-0.2100705	3.2256400	-1.5049101
H	-0.0841503	-0.7575690	2.2399173
H	-0.7550988	-1.8345736	0.9906574
H	0.5111485	-2.4165232	2.0830857

2c_sy_c_1_ts2.log

E = -1188.206877
H = -1187.843183
G = -1187.912240

NImag=1

C	-1.9278263	1.3246460	-0.9095594
C	-2.0235930	0.2869512	0.1854530
C	-1.5617436	2.6697419	-0.7405185
O	-1.5120292	3.5095678	-1.6820783
C	-0.8961115	-0.5346322	-0.3933876
C	0.5611791	-0.2281886	-0.2349173
C	1.2039829	-0.2881769	1.0096021
C	2.5727699	-0.0802858	1.1117585
C	3.3152195	0.1851901	-0.0455083
C	2.6937915	0.2319017	-1.2988339
C	1.3241265	0.0141361	-1.3841197
C	-1.3060779	3.1819181	0.6741200
C	-1.8175637	0.8827664	1.5874185
C	-0.8889058	2.0977495	1.6626886
S	-0.9021439	-2.6171496	0.4411183
C	-2.1488885	-3.4300459	-0.5887002
C	0.5682799	-3.2813344	-0.3795796

C	4.7341340	0.3999621	0.0541863
N	5.8765942	0.5724737	0.1345985
C	-3.3488436	-0.4764640	0.1480081
H	-2.2483626	1.0177618	-1.9040017
H	-1.1345404	-0.8925062	-1.3970184
H	0.6386957	-0.5092214	1.9103544
H	3.0668945	-0.1280815	2.0763468
H	3.2789249	0.4301566	-2.1906655
H	0.8350016	0.0401519	-2.3536777
H	-0.5497962	3.9718426	0.6170883
H	-2.2377956	3.6616749	1.0073121
H	-2.8098062	1.2043076	1.9302292
H	-1.4969443	0.0950528	2.2815143
H	0.1473620	1.8188391	1.4607398
H	-0.9094983	2.4918673	2.6852477
H	-1.9209464	-4.4978790	-0.6091670
H	-3.1301475	-3.2777569	-0.1410987
H	-2.1226441	-3.0211629	-1.6021949
H	0.5347595	-4.3703798	-0.3061621
H	1.4546022	-2.9076971	0.1342705
H	0.5783355	-2.9726299	-1.4284737
H	-3.5037800	-0.9574797	-0.8237311
H	-3.4025057	-1.2399106	0.9349997
H	-4.1682461	0.2303334	0.3112039

2c_sy_c_2.log

E = -1188.222327

H = -1187.857156

G = -1187.925864

NImag=0

C	-4.1816160	2.5443584	-1.8110642
C	-2.7037216	2.3165580	-1.5722753
C	-4.7795109	2.8781080	-3.0178448
O	-6.0330800	3.0544697	-3.1954512
C	-2.4138388	0.9243544	-0.9097912
C	-2.5329757	0.7587330	0.5853337
C	-3.6278538	1.2295341	1.3251857
C	-3.6805195	1.0570482	2.7017882
C	-2.6281298	0.4046386	3.3560923
C	-1.5272292	-0.0709774	2.6379242
C	-1.4897398	0.1105723	1.2597718
C	-3.8855429	3.0605865	-4.2470857
C	-1.9237220	2.3136240	-2.9085443
C	-2.4344181	3.3636703	-3.8874393
S	-3.4310948	-0.3348683	-1.8307530
C	-2.5161429	-1.8499455	-1.4664975
C	-4.9190078	-0.6541750	-0.8649700
C	-2.6803811	0.2240673	4.7828668
N	-2.7224469	0.0776531	5.9308548
C	-2.0886127	3.3871981	-0.6483928
H	-4.8415638	2.5143143	-0.9450076
H	-1.3971920	0.6169472	-1.1867259
H	-4.4493193	1.7356883	0.8320980
H	-4.5290313	1.4247635	3.2690661
H	-0.7140865	-0.5722145	3.1521027
H	-0.6323306	-0.2520178	0.6992084
H	-3.9352354	2.1453890	-4.8560891
H	-4.3229277	3.8628997	-4.8515633
H	-0.8572594	2.4542194	-2.6911553
H	-2.0186148	1.3339151	-3.3987917
H	-1.8033429	3.3733589	-4.7836007

H	-2.3652724	4.3628311	-3.4381067
H	-3.0836855	-2.6781932	-1.8953093
H	-1.5422575	-1.7768590	-1.9536641
H	-2.4079216	-1.9795146	-0.3875357
H	-5.4451469	-1.4534614	-1.3923420
H	-5.5210584	0.2540267	-0.8621624
H	-4.6550081	-0.9724647	0.1445658
H	-2.6931765	3.5353059	0.2511463
H	-1.0687358	3.1219686	-0.3387645
H	-2.0475492	4.3417898	-1.1823775

2c_sy_c_2_r.log

E = -1188.216956

H = -1187.851617

G = -1187.920097

NImag=0

C	0.9186404	-1.6983799	0.3520834
C	1.4501230	-0.6658337	-0.6190650
C	1.5919795	-2.2172778	1.4426454
O	1.1088194	-3.0406516	2.2970032
C	0.3487728	0.4438873	-0.7506737
C	-0.4042259	0.9184970	0.4701528
C	0.2146778	1.3177565	1.6641850
C	-0.5419880	1.7353547	2.7501675
C	-1.9393313	1.7590923	2.6516886
C	-2.5756832	1.3682925	1.4709629
C	-1.8022086	0.9528771	0.3920004
C	3.0464848	-1.7894042	1.6626994
C	2.8127412	-0.1040121	-0.1626126
C	3.7043489	-1.1991572	0.4186657
S	0.9836401	1.8842263	-1.7652604
C	-0.5448401	2.6417535	-2.3488906
C	1.5444850	3.1514817	-0.6123439
C	-2.7248989	2.1888770	3.7777998
N	-3.3569494	2.5362888	4.6839473
C	1.6118756	-1.2799875	-2.0268452
H	-0.1089478	-2.0288745	0.1857040
H	-0.3989824	0.0505402	-1.4506188
H	1.2934209	1.3059139	1.7628163
H	-0.0571541	2.0390147	3.6719550
H	-3.6581890	1.3855979	1.4013402
H	-2.2949297	0.6375005	-0.5237642
H	3.0700978	-1.0552944	2.4824517
H	3.5946631	-2.6693716	2.0182577
H	3.3113132	0.3861467	-1.0109206
H	2.6871329	0.6538785	0.6166173
H	4.6889285	-0.7825331	0.6597860
H	3.8657818	-1.9885821	-0.3260167
H	-0.2636100	3.5257958	-2.9242987
H	-1.0465554	1.9197652	-2.9954471
H	-1.1717540	2.9183487	-1.4990114
H	1.8406159	4.0025753	-1.2299068
H	2.4107858	2.7725111	-0.0696546
H	0.7364311	3.4316012	0.0648680
H	0.6844470	-1.7755100	-2.3335264
H	1.8746060	-0.5365763	-2.7914224
H	2.4045721	-2.0332504	-2.0110658

2c_sy_c_2_ts1.log

E = -1188.190157

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H =      -1187.827726
G =      -1187.898392
NImag=1
C      1.6284838      -1.4360164      0.6338362
C      1.3942420      -1.1663351      -0.7263833
C      2.8183266      -1.0598589      1.3201679
O      2.9783649      -1.1808892      2.5530827
C      0.1540009      0.6194420      -0.9599218
C      -1.2042221      0.3409238      -0.5241201
C      -1.5674884      0.2129043      0.8356431
C      -2.8517769      -0.1610321      1.2047761
C      -3.8134470      -0.4307040      0.2217261
C      -3.4735640      -0.3248549      -1.1378889
C      -2.1928654      0.0562692      -1.4956030
C      3.9479630      -0.4836407      0.4772328
C      2.5814035      -0.7448421      -1.6003682
C      3.9271332      -1.0472620      -0.9407576
S      1.0273861      2.0030859      -0.3152553
C      -0.0895463      3.4288377      -0.3752598
C      1.2080627      1.8640410      1.4838194
C      -5.1402386      -0.8149963      0.6025078
N      -6.2146842      -1.1261364      0.9099980
C      0.3906451      -2.0553523      -1.4237621
H      0.8415648      -1.9067122      1.2222572
H      0.2692274      0.7035734      -2.0417176
H      -0.8371331      0.3810101      1.6178120
H      -3.1116441      -0.2556133      2.2546098
H      -4.2187701      -0.5321357      -1.8994694
H      -1.9368698      0.1438576      -2.5479405
H      3.8305558      0.6117609      0.4456342
H      4.8918465      -0.6893900      0.9908527
H      2.5014798      -1.2600247      -2.5645883
H      2.5485248      0.3263788      -1.8254695
H      4.7362544      -0.6187748      -1.5415313
H      4.0892272      -2.1313351      -0.9002990
H      0.4168044      4.2679303      0.1081253
H      -0.2766592      3.6536087      -1.4264106
H      -1.0180588      3.1821851      0.1439872
H      2.0526680      2.4998597      1.7563015
H      1.4204675      0.8273214      1.7421756
H      0.2991641      2.2136675      1.9747679
H      -0.4724290      -2.2723433      -0.7873383
H      0.0397990      -1.6305589      -2.3690726
H      0.8911937      -3.0062599      -1.6497093

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2c_sy_c_2_ts2.log
E =      -1188.206186
H =      -1187.842817
G =      -1187.912587
NImag=1
C      1.7687542      -0.5529476      -1.4892296
C      1.9818232      0.4202628      -0.3486291
C      1.4948208      -1.9166976      -1.3220321
O      1.1555450      -2.7050176      -2.2493610
C      0.5437401      0.8948944      -0.4009434
C      -0.6072781      0.0399722      0.0587286
C      -0.8724247      -0.2265386      1.4086768
C      -1.9625165      -1.0058708      1.7810346
C      -2.8078099      -1.5220310      0.7945847
C      -2.5766330      -1.2429311      -0.5589008
C      -1.4880814      -0.4582655      -0.9122971

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C	1.6770485	-2.4817357	0.0839385
C	2.4251658	-0.2442309	0.9808132
C	2.7680579	-1.7288943	0.8435485
S	0.2243325	2.7124315	0.7840223
C	0.7828843	3.9799877	-0.3804598
C	-1.5580555	2.9235311	0.5511858
C	-3.9344077	-2.3319463	1.1736693
N	-4.8420139	-2.9836342	1.4788710
C	2.9592979	1.5283572	-0.7393079
H	1.7097162	-0.1306711	-2.4911327
H	0.3204010	1.3952645	-1.3460702
H	-0.2517991	0.1913464	2.1941994
H	-2.1608234	-1.2068916	2.8285978
H	-3.2443994	-1.6357044	-1.3184407
H	-1.3011225	-0.2417321	-1.9598677
H	0.7235149	-2.4186312	0.6294890
H	1.9205941	-3.5444158	-0.0164311
H	3.2974457	0.2970088	1.3627601
H	1.6519716	-0.1359514	1.7439855
H	2.9170181	-2.1582166	1.8407210
H	3.7159520	-1.8407070	0.3023454
H	0.2938081	4.9182611	-0.1107372
H	1.8615247	4.0955833	-0.2862453
H	0.5146363	3.6955203	-1.4012411
H	-1.8112442	3.9580415	0.7918771
H	-2.0810414	2.2507990	1.2313861
H	-1.8236142	2.6991147	-0.4855296
H	2.6407653	2.0424463	-1.6531118
H	3.0788115	2.2671666	0.0617817
H	3.9412531	1.0795041	-0.9233821

2c_sy_c_3.log

E = -1188.219690

H = -1187.854687

G = -1187.923455

NImag=0

C	-4.2746217	2.7084256	-1.7846520
C	-2.8099555	2.6435603	-1.4246013
C	-4.7849662	2.5699153	-3.0658637
O	-6.0265747	2.5616019	-3.3679746
C	-2.3894870	1.2037375	-0.9189949
C	-2.4664341	0.9010767	0.5562990
C	-3.6027715	1.1956323	1.3250616
C	-3.6363736	0.9017570	2.6810094
C	-2.5219266	0.3030502	3.2833905
C	-1.3805579	0.0018489	2.5346695
C	-1.3631507	0.3022033	1.1766678
C	-3.8183846	2.4609553	-4.2556946
C	-1.9453729	3.0029965	-2.6528388
C	-2.3334717	2.2625836	-3.9288882
S	-3.3538987	-0.0618006	-1.8966099
C	-2.3581724	-1.5409216	-1.6021265
C	-4.8306397	-0.5116518	-0.9686626
C	-2.5533995	-0.0036520	4.6888997
N	-2.5794118	-0.2510622	5.8199813
C	-2.4536248	3.6557420	-0.3222102
H	-4.9910270	2.8133751	-0.9685324
H	-1.3660703	0.9825598	-1.2489135
H	-4.4683375	1.6621348	0.8654603
H	-4.5156012	1.1328999	3.2730374
H	-0.5218167	-0.4602454	3.0099473

H	-0.4776374	0.0718078	0.5907049
H	-4.1847806	1.6529676	-4.9004376
H	-3.9481566	3.3880478	-4.8315312
H	-2.0753869	4.0786985	-2.8262715
H	-0.8851746	2.8411258	-2.4176279
H	-2.0953446	1.1962013	-3.8385059
H	-1.7160020	2.6277251	-4.7576563
H	-2.8714033	-2.3738441	-2.0865681
H	-1.3838350	-1.3861668	-2.0693619
H	-2.2552563	-1.7269627	-0.5309025
H	-5.2965487	-1.3157960	-1.5432426
H	-5.4859098	0.3586612	-0.9420652
H	-4.5681664	-0.8618297	0.0303641
H	-3.1157308	3.5775085	0.5435944
H	-1.4199690	3.5284088	0.0252670
H	-2.5562496	4.6668245	-0.7279201

2c_sy_c_3_r.log

E = -1188.213699

H = -1187.848434

G = -1187.917754

NImag=0

C	0.2228929	-2.1499699	0.2965529
C	1.2222182	-1.1761780	-0.2937531
C	0.3087430	-2.7907955	1.5219154
O	-0.4880484	-3.7001533	1.9393007
C	0.3723823	0.0929377	-0.6696016
C	-0.1501581	0.9988364	0.4190563
C	0.6781032	1.7987018	1.2186317
C	0.1371124	2.6382510	2.1846962
C	-1.2503377	2.6813096	2.3618697
C	-2.0940226	1.8900683	1.5755300
C	-1.5371005	1.0632367	0.6072748
C	1.4580085	-2.4097452	2.4564676
C	2.3964051	-0.9174734	0.6772889
C	2.0374235	-1.0317052	2.1588566
S	1.0785695	1.0931257	-2.1016098
C	-0.1543953	2.3922463	-2.3039125
C	2.4942727	2.0648436	-1.5567790
C	-1.8131077	3.5478400	3.3634697
N	-2.2655071	4.2463501	4.1687791
C	1.8058360	-1.7550542	-1.5995369
H	-0.5842727	-2.4571015	-0.3727105
H	-0.4931396	-0.3061589	-1.2140530
H	1.7566880	1.7614365	1.1164367
H	0.7841169	3.2520045	2.8024434
H	-3.1687047	1.9274240	1.7190495
H	-2.1906074	0.4547857	-0.0113966
H	1.0808406	-2.4649006	3.4839085
H	2.2411915	-3.1772287	2.3672422
H	3.1548730	-1.6835728	0.4669348
H	2.8773786	0.0429280	0.4604623
H	1.3044162	-0.2712671	2.4453577
H	2.9357008	-0.8495683	2.7611318
H	0.1584738	2.9912290	-3.1615427
H	-1.1113380	1.9116558	-2.5167921
H	-0.2116191	3.0047583	-1.4024017
H	2.8169953	2.6265988	-2.4368259
H	3.2891170	1.3845832	-1.2497661
H	2.2115094	2.7489102	-0.7567730
H	1.0299195	-1.8878827	-2.3630831

H	2.6067865	-1.1321767	-2.0225434
H	2.2356256	-2.7363806	-1.3813237

2c_sy_c_3_ts1.log

E = -1188.194357
H = -1187.831674
G = -1187.901557

NImag=1

C	2.6064796	-0.2572632	1.0652222
C	1.4304808	-0.9558327	0.7184772
C	3.8634994	-0.4292342	0.4204042
O	4.8959853	0.1955118	0.7477212
C	0.2026776	0.2642643	-0.5899101
C	-1.2280053	0.1200422	-0.3939899
C	-1.9890388	0.8527260	0.5465081
C	-3.3318120	0.5832321	0.7542072
C	-3.9652276	-0.4396410	0.0322110
C	-3.2331271	-1.1820681	-0.9097332
C	-1.8956128	-0.8984921	-1.1183674
C	3.9816204	-1.5014487	-0.6568309
C	1.5835200	-2.1237152	-0.2375921
C	2.6500400	-1.8778303	-1.3005820
S	0.9879360	1.8428889	-0.5450871
C	-0.0635091	2.9866283	-1.4728024
C	0.8337512	2.5586435	1.1174617
C	-5.3523990	-0.7194469	0.2495595
N	-6.4767107	-0.9464117	0.4255716
C	0.4074869	-1.1858887	1.8051481
H	2.5845795	0.4452248	1.8970794
H	0.5495455	-0.1782490	-1.5219965
H	-1.5278902	1.6340153	1.1395824
H	-3.8957606	1.1585521	1.4819173
H	-3.7220158	-1.9677215	-1.4774450
H	-1.3402562	-1.4688920	-1.8580709
H	4.7057602	-1.1575209	-1.4021907
H	4.4233607	-2.3825898	-0.1693674
H	1.8736376	-2.9935973	0.3726387
H	0.6158711	-2.3696966	-0.6892833
H	2.3313302	-1.0674432	-1.9679353
H	2.7688623	-2.7692646	-1.9253535
H	0.3740431	3.9832632	-1.3806316
H	-0.0520109	2.6665327	-2.5158297
H	-1.0789844	2.9723660	-1.0725123
H	1.7300743	3.1572613	1.2867395
H	0.7799570	1.7565419	1.8509655
H	-0.0551536	3.1886107	1.1629232
H	0.1861870	-0.2743255	2.3692542
H	-0.5289660	-1.5897596	1.4108097
H	0.8208105	-1.9190234	2.5097243

2c_sy_c_3_ts2.log

E = -1188.204986
H = -1187.841498
G = -1187.911301

NImag=1

C	2.2944822	-0.8880720	-0.9852007
C	2.0907581	0.2931243	-0.0624451
C	2.4302373	-2.2308725	-0.5956964
O	2.6572880	-3.1769627	-1.4003240
C	0.7499186	0.6406316	-0.6682233

C	-0.5721037	0.0196647	-0.3741980
C	-1.1179517	-0.0489255	0.9164240
C	-2.3968708	-0.5504368	1.1204815
C	-3.1485473	-0.9883164	0.0233148
C	-2.6276621	-0.9155440	-1.2739620
C	-1.3510626	-0.4033186	-1.4619092
C	2.3943310	-2.5624852	0.8923298
C	2.1267103	-0.1115830	1.4213311
C	1.6432950	-1.5315896	1.7269570
S	0.3089850	2.8364481	-0.3276253
C	-1.3875401	2.9864755	-0.9250513
C	0.0496567	3.1284489	1.4346619
C	-4.4729429	-1.5101547	0.2304109
N	-5.5394607	-1.9299176	0.3970282
C	3.1105217	1.4101081	-0.3116255
H	2.4653028	-0.6604104	-2.0364901
H	0.8597370	0.8596418	-1.7305632
H	-0.5490780	0.2937235	1.7732263
H	-2.8141145	-0.6007343	2.1206711
H	-3.2190890	-1.2514538	-2.1191637
H	-0.9452554	-0.3331344	-2.4672804
H	1.9538377	-3.5584542	1.0074995
H	3.4386111	-2.6376057	1.2284752
H	3.1787999	-0.0491889	1.7293445
H	1.5903985	0.6309141	2.0251411
H	0.5740653	-1.6391952	1.5301603
H	1.7852679	-1.7307184	2.7953286
H	-1.7028892	4.0269167	-0.8194460
H	-1.3963858	2.7092963	-1.9812445
H	-2.0508301	2.3305036	-0.3555004
H	-0.2387335	4.1739100	1.5671599
H	0.9928116	2.9439317	1.9522222
H	-0.7356820	2.4764011	1.8217954
H	3.0542037	1.7780043	-1.3421969
H	2.9662632	2.2592543	0.3693273
H	4.1163688	1.0129354	-0.1445915

2c_sy_c_4.log

E = -1188.221039

H = -1187.855967

G = -1187.924680

NImag=0

C	-4.2089913	2.5265541	-1.7460491
C	-2.7576652	2.1579059	-1.5202897
C	-4.7635687	2.9847477	-2.9315214
O	-5.9960621	3.2750775	-3.1090552
C	-2.6180319	0.7168538	-0.8899545
C	-2.5695735	0.6279050	0.6204786
C	-3.6645031	0.9819460	1.4203856
C	-3.5817204	0.9023700	2.8045386
C	-2.3912715	0.4640698	3.3977408
C	-1.2911227	0.1037956	2.6123412
C	-1.3909212	0.1840525	1.2279433
C	-3.8425778	3.1648904	-4.1422648
C	-1.9652430	2.1487731	-2.8488344
C	-2.3687360	3.2959505	-3.7690161
S	-4.0487836	-0.3489386	-1.3856846
C	-3.8997363	-0.6215508	-3.1616602
C	-3.4586027	-1.9601469	-0.8073100
C	-2.3000636	0.3803299	4.8314613
N	-2.2262526	0.3127932	5.9852267

C	-2.0639507	3.1500521	-0.5626890
H	-4.8684698	2.4910005	-0.8776354
H	-1.7289935	0.2161561	-1.2918588
H	-4.5895372	1.3292088	0.9690774
H	-4.4289010	1.1783660	3.4234418
H	-0.3748760	-0.2388158	3.0817944
H	-0.5426405	-0.0991495	0.6112531
H	-3.9825292	2.3075535	-4.8185241
H	-4.1935087	4.0486695	-4.6868032
H	-0.8934363	2.1869083	-2.6151606
H	-2.1320936	1.2110896	-3.3895189
H	-1.7390924	3.2888759	-4.6663510
H	-2.1984609	4.2587501	-3.2707639
H	-4.6055053	-1.4213611	-3.3978085
H	-4.1905763	0.2962912	-3.6709884
H	-2.8810057	-0.9245232	-3.4100579
H	-4.1460293	-2.7100314	-1.2036325
H	-3.4979658	-1.9661641	0.2825918
H	-2.4425584	-2.1388059	-1.1651704
H	-2.6521331	3.3088390	0.3460708
H	-1.0621258	2.8077814	-0.2706374
H	-1.9619834	4.1159305	-1.0665057

2c_sy_c_4_r.log

E = -1188.215831

H = -1187.850391

G = -1187.919912

NImag=0

C	0.6136375	-1.8148424	0.2844052
C	1.3893576	-0.7530305	-0.4693949
C	1.0533037	-2.5037644	1.4016656
O	0.3827209	-3.3863406	2.0423992
C	0.3606941	0.4061888	-0.7153445
C	-0.1604668	1.1035428	0.5218469
C	0.5796643	2.0654743	1.2214481
C	0.0660193	2.6639679	2.3654663
C	-1.2060437	2.2978197	2.8187565
C	-1.9661186	1.3505052	2.1240975
C	-1.4402906	0.7676730	0.9774887
C	2.4593195	-2.2070743	1.9355562
C	2.6103857	-0.2910690	0.3439777
C	3.3612116	-1.4814909	0.9395312
S	1.0116488	1.7116286	-1.9059874
C	0.4982208	1.0969165	-3.5304561
C	-0.2113298	3.0390059	-1.7619042
C	-1.7423487	2.9113622	4.0044175
N	-2.1745242	3.4056287	4.9584496
C	1.8605472	-1.2891958	-1.8359635
H	-0.3708723	-2.0712071	-0.1117709
H	-0.4899349	-0.0142576	-1.2648753
H	1.5654637	2.3693381	0.8780363
H	0.6429150	3.4090217	2.9028286
H	-2.9558658	1.0800489	2.4766289
H	-2.0290493	0.0372572	0.4309133
H	2.3549434	-1.6064804	2.8512973
H	2.8985325	-3.1635912	2.2414337
H	3.2729632	0.3195987	-0.2837998
H	2.2895390	0.3304994	1.1854566
H	4.2748114	-1.1303124	1.4327006
H	3.6757260	-2.1716073	0.1470551
H	0.5584868	1.9503535	-4.2085885

H	1.1841754	0.3190061	-3.8562817
H	-0.5264093	0.7253176	-3.4666311
H	-0.0621311	3.6838119	-2.6301390
H	-0.0225323	3.6004160	-0.8485003
H	-1.2153138	2.6088956	-1.7644419
H	1.0058936	-1.5716747	-2.4613612
H	2.4856101	-0.5719359	-2.3859851
H	2.4644884	-2.1864418	-1.6816570

2c_sy_c_4_ts1.log

E = -1188.191200

H = -1187.829008

G = -1187.898661

NImag=1

C	1.9448247	-0.8464048	1.0556812
C	1.2973155	-1.1696943	-0.1514877
C	3.3485483	-0.6204050	1.1742067
O	3.9041579	-0.2451962	2.2277782
C	0.0312015	0.5686427	-0.7575451
C	-1.3533354	0.3140472	-0.4253121
C	-1.8762367	0.4494101	0.8843769
C	-3.1833183	0.0977799	1.1776781
C	-4.0204660	-0.4043482	0.1694605
C	-3.5261262	-0.5440681	-1.1402193
C	-2.2222688	-0.1871184	-1.4261619
C	4.2293616	-0.9551816	-0.0309318
C	2.1664732	-1.2717909	-1.4003586
C	3.5339963	-1.8608446	-1.0448490
S	0.7484976	1.8802653	0.1856511
C	2.2844232	2.2126753	-0.6886172
C	-0.1718701	3.3684867	-0.2846303
C	-5.3719807	-0.7652892	0.4707460
N	-6.4683334	-1.0587903	0.7137920
C	0.1642031	-2.1621502	-0.0904260
H	1.3659576	-0.8275488	1.9787765
H	0.2405915	0.6997929	-1.8200171
H	-1.2488792	0.8197187	1.6916135
H	-3.5621335	0.2063247	2.1892972
H	-4.1738183	-0.9258340	-1.9234907
H	-1.8477318	-0.2967574	-2.4404176
H	4.5353721	-0.0173760	-0.5169020
H	5.1434509	-1.4120826	0.3620072
H	1.6539789	-1.8809672	-2.1526999
H	2.3293573	-0.2856286	-1.8478265
H	4.1430601	-1.9625565	-1.9494861
H	3.4072998	-2.8650656	-0.6215298
H	2.6606814	3.1672984	-0.3164512
H	2.9935325	1.4234153	-0.4515488
H	2.0858962	2.2647732	-1.7613073
H	0.3035409	4.2233491	0.2018150
H	-1.1939155	3.2546905	0.0809960
H	-0.1587002	3.4755274	-1.3708173
H	-0.4737702	-2.0074229	0.7850603
H	-0.4551363	-2.1496572	-0.9910669
H	0.6130549	-3.1616458	-0.0071441

2c_sy_c_5.log

E = -1188.218014

H = -1187.852742

G = -1187.921647

NImag=0

C	-4.1932359	2.1676978	-2.7785333
C	-3.6318155	2.2058537	-1.3732456
C	-3.6662752	2.7896123	-3.8980537
O	-4.1578845	2.7334005	-5.0781756
C	-3.3491996	0.7431652	-0.8685192
C	-2.8650201	0.6072344	0.5558850
C	-1.5091920	0.3296160	0.7643258
C	-0.9892178	0.2367855	2.0503996
C	-1.8418936	0.4084542	3.1453683
C	-3.2045604	0.6712330	2.9563245
C	-3.7053667	0.7727475	1.6655577
C	-2.4032524	3.6388623	-3.7237791
C	-2.2491372	2.8988053	-1.3466517
C	-2.1930701	4.1001529	-2.2848659
S	-4.8468072	-0.3378641	-1.1649105
C	-4.4145841	-1.1428730	-2.7262702
C	-4.6081244	-1.7584740	-0.0720750
C	-1.3154091	0.3043320	4.4803679
N	-0.8910496	0.2203470	5.5546474
C	-4.6010794	2.9450530	-0.4332367
H	-5.1651009	1.6849804	-2.9074402
H	-2.6034769	0.3032917	-1.5380856
H	-0.8528321	0.1870621	-0.0892310
H	0.0636798	0.0268128	2.2062558
H	-3.8596888	0.7935127	3.8122734
H	-4.7652042	0.9738689	1.5331463
H	-1.5324111	3.0582508	-4.0622673
H	-2.4936613	4.4928125	-4.4044075
H	-2.0081884	3.1893189	-0.3168488
H	-1.4760661	2.1860826	-1.6674823
H	-1.2279788	4.6079262	-2.1746774
H	-2.9689084	4.8273379	-2.0120079
H	-5.2234644	-1.8378993	-2.9596432
H	-4.3372172	-0.3684692	-3.4877819
H	-3.4677295	-1.6713155	-2.5991902
H	-5.2591201	-2.5439399	-0.4620787
H	-4.9201398	-1.4917743	0.9363124
H	-3.5635477	-2.0752705	-0.0956347
H	-5.5804883	2.4515820	-0.3977475
H	-4.2192380	3.0375546	0.5884748
H	-4.7636432	3.9538333	-0.8229981

2c_sy_c_5_ts1.log

E = -1188.192721

H = -1187.830563

G = -1187.900655

NImag=1

C	2.6445787	-0.4595541	1.0504322
C	1.3309710	-0.9499769	0.9144561
C	3.6357905	-0.6603767	0.0503513
O	4.7523386	-0.0974905	0.0502863
C	0.2617126	0.4764620	-0.3528368
C	-1.1655048	0.2687905	-0.2840837
C	-1.7807467	-0.5915721	-1.2286180
C	-3.1232931	-0.9145339	-1.1487048
C	-3.9161344	-0.3722095	-0.1232206
C	-3.3368548	0.4990791	0.8148354
C	-1.9918905	0.8101349	0.7345292
C	3.2578826	-1.5877315	-1.0937011
C	1.1055491	-2.2021107	0.0717572

C	2.3789287	-2.7318481	-0.5940627
S	0.8265417	2.0543020	0.2485594
C	2.3822439	2.3069099	-0.6340981
C	-0.1642011	3.2925111	-0.6307999
C	-5.3073907	-0.6950438	-0.0417588
N	-6.4360812	-0.9580365	0.0240412
C	0.4369466	-0.8553389	2.1262662
H	2.8708641	0.2429297	1.8529329
H	0.7189794	0.2676186	-1.3202370
H	-1.1840303	-0.9952382	-2.0416288
H	-3.5708357	-1.5749168	-1.8852050
H	-3.9477471	0.9245069	1.6050495
H	-1.5720014	1.4726324	1.4880641
H	2.7145977	-0.9949469	-1.8458308
H	4.1762405	-1.9519745	-1.5634068
H	0.6921504	-2.9708184	0.7374595
H	0.3343408	-2.0207548	-0.6835173
H	2.1158046	-3.4072153	-1.4145315
H	2.9543043	-3.3184675	0.1323326
H	2.5998657	3.3748422	-0.5662584
H	3.1710357	1.7343407	-0.1497667
H	2.2504474	2.0057481	-1.6758891
H	0.2379037	4.2749920	-0.3736744
H	-1.1963077	3.2134023	-0.2880993
H	-0.0950908	3.1058198	-1.7042155
H	0.4559138	0.1426791	2.5771960
H	-0.5970471	-1.1233941	1.8959287
H	0.8041925	-1.5675504	2.8760971

2c_sy_c_6.log

E = -1188.211850

H = -1187.846201

G = -1187.914346

NImag=0

C	-4.2921941	2.3665606	-1.7144399
C	-2.8060354	2.2809427	-1.4634580
C	-4.9068628	2.5768966	-2.9336872
O	-6.1662513	2.4717540	-3.1517508
C	-2.3608508	0.9054948	-0.8465517
C	-2.3929198	0.7282334	0.6627437
C	-3.4954232	1.0942020	1.4461034
C	-3.4798052	0.9061663	2.8227067
C	-2.3502514	0.3440990	3.4281044
C	-1.2402028	-0.0280031	2.6624989
C	-1.2720777	0.1659507	1.2869602
C	-4.0358093	2.9823793	-4.1251233
C	-2.0007994	2.4662857	-2.7748411
C	-2.6516765	3.4771492	-3.7131805
S	-3.1642726	-0.6633760	-1.4746170
C	-4.9382266	-0.6368152	-1.1290210
C	-3.2101442	-0.6372681	-3.2769514
C	-2.3310997	0.1491248	4.8538714
N	-2.3156494	-0.0082732	6.0010275
C	-2.3288861	3.3734706	-0.4779296
H	-4.9493395	2.1486190	-0.8736596
H	-1.3265864	0.7130118	-1.1618616
H	-4.3723531	1.5408824	0.9904026
H	-4.3342824	1.1939560	3.4259331
H	-0.3673525	-0.4604596	3.1401983
H	-0.4116186	-0.1200448	0.6883555
H	-3.9418471	2.1245522	-4.8086156

H	-4.5838619	3.7547890	-4.6773991
H	-0.9785331	2.7697059	-2.5149096
H	-1.9112589	1.5177841	-3.3133155
H	-2.0145798	3.6291615	-4.5921355
H	-2.7416326	4.4503462	-3.2137313
H	-5.2793891	-1.6500096	-1.3560892
H	-5.0868428	-0.4380658	-0.0672276
H	-5.4308645	0.1087506	-1.7528862
H	-3.7145210	-1.5646675	-3.5607140
H	-2.1863712	-0.6488484	-3.6523591
H	-3.7694739	0.2315463	-3.6234362
H	-2.9757441	3.4412010	0.4005529
H	-1.2984711	3.2015425	-0.1387275
H	-2.3622381	4.3402732	-0.9903394

2c_sy_c_6_ts1.log

E = -1188.181433

H = -1187.818969

G = -1187.887990

NImag=1

C	2.0418390	-0.5440043	1.1961041
C	1.2427514	-1.1883509	0.2361165
C	3.4239966	-0.2676410	1.0238101
O	4.0699455	0.5055141	1.7690800
C	-0.0037446	0.3108731	-0.7795274
C	-1.4259858	0.2051685	-0.4917799
C	-2.0567255	0.9060304	0.5608542
C	-3.4003961	0.7197531	0.8488355
C	-4.1593215	-0.1865303	0.0951380
C	-3.5546549	-0.8979068	-0.9573554
C	-2.2173002	-0.6986540	-1.2416054
C	4.1637687	-1.0024388	-0.0901181
C	1.9676071	-1.7598718	-0.9832239
C	3.3832671	-2.2062383	-0.6123428
S	0.5769637	2.0002028	-0.6654478
C	1.3201492	2.4024601	0.9523998
C	2.0667827	1.9630866	-1.6766623
C	-5.5458002	-0.3848479	0.3928169
N	-6.6695702	-0.5467710	0.6325569
C	0.0966828	-2.0267412	0.7456452
H	1.5744675	-0.1777283	2.1086384
H	0.2539154	-0.0072207	-1.7890693
H	-1.4935614	1.6030430	1.1757777
H	-3.8655028	1.2699406	1.6608427
H	-4.1436789	-1.5930676	-1.5475666
H	-1.7575351	-1.2459174	-2.0604856
H	4.3548266	-0.2961051	-0.9113289
H	5.1427536	-1.2901819	0.3078306
H	1.3829558	-2.5877069	-1.3999205
H	2.0610603	-1.0078847	-1.7733144
H	3.8788324	-2.6356325	-1.4897332
H	3.3427679	-2.9875985	0.1565889
H	1.3657499	3.4938272	0.9523992
H	0.6494643	2.0654470	1.7428305
H	2.3124985	1.9690917	1.0743524
H	2.5335700	2.9468663	-1.5995990
H	1.7694385	1.7679962	-2.7079353
H	2.7373887	1.1875949	-1.3053893
H	-0.4493662	-1.5258298	1.5514709
H	-0.6065409	-2.3051939	-0.0421152
H	0.5237994	-2.9543541	1.1508398

2c_sy_c_7.log

E = -1188.213307
H = -1187.848227
G = -1187.917057

NImag=0

C	-4.4225073	2.1941863	-2.6257400
C	-3.8876978	2.2344407	-1.2158320
C	-3.7482540	2.5887949	-3.7674016
O	-4.2040999	2.4929440	-4.9600126
C	-3.2756788	0.8390016	-0.7946227
C	-2.7930223	0.7024793	0.6352860
C	-3.6658015	0.4911529	1.7102176
C	-3.1807838	0.3870805	3.0076721
C	-1.8045100	0.5016566	3.2373278
C	-0.9180065	0.7125418	2.1755635
C	-1.4190114	0.8049339	0.8826757
C	-2.3723173	3.2491727	-3.6293186
C	-2.7223630	3.2466430	-1.1371157
C	-1.7053051	3.0820305	-2.2640191
S	-4.2234272	-0.7152344	-1.1782190
C	-6.0074766	-0.4676153	-1.0604429
C	-4.0142153	-0.9780761	-2.9523003
C	-1.2960943	0.3966001	4.5790236
N	-0.8864561	0.3119495	5.6590295
C	-4.9685041	2.6863073	-0.2226626
H	-5.4211820	1.7834498	-2.7710686
H	-2.4179876	0.6606242	-1.4514816
H	-4.7373916	0.4131225	1.5498149
H	-3.8591479	0.2204926	3.8377340
H	0.1473791	0.7950230	2.3631318
H	-0.7350089	0.9612633	0.0526490
H	-1.7316570	2.8589524	-4.4285656
H	-2.5151743	4.3178523	-3.8460549
H	-3.1738773	4.2451353	-1.2116230
H	-2.2339727	3.1948140	-0.1562626
H	-1.2247417	2.0970882	-2.2030987
H	-0.9008869	3.8163232	-2.1404942
H	-6.4416284	-1.4141743	-1.3918216
H	-6.2692860	-0.2990028	-0.0160070
H	-6.3361978	0.3503776	-1.6981050
H	-4.4481483	-1.9582621	-3.1628295
H	-2.9408520	-0.9988614	-3.1502195
H	-4.5005462	-0.1829503	-3.5150300
H	-5.8130846	1.9926679	-0.1712247
H	-4.5690752	2.8162942	0.7889662
H	-5.3584006	3.6529808	-0.5559183

2c_sy_c_7_ts1.log

E = -1188.190960
H = -1187.828359
G = -1187.897350

NImag=1

C	2.7098233	-0.2350597	0.8817092
C	1.3598487	-0.6082678	1.0190090
C	3.6674131	-0.9567432	0.1134406
O	4.8512311	-0.5816541	-0.0307705
C	0.1892029	0.4705744	-0.4721085
C	-1.2429029	0.2446021	-0.3710851
C	-2.0927244	1.0644567	0.4083898

C	-3.4435599	0.7872519	0.5380037
C	-3.9919048	-0.3361144	-0.0995979
C	-3.1683064	-1.1712902	-0.8742275
C	-1.8226920	-0.8796943	-1.0069836
C	3.2567082	-2.2971550	-0.4857388
C	0.9883541	-2.0030373	0.5570041
C	1.7508332	-2.4518156	-0.6856764
S	0.5914035	2.2017814	-0.6673505
C	1.1801214	2.9205296	0.8883059
C	2.1394190	2.1268213	-1.5896968
C	-5.3865214	-0.6291720	0.0374535
N	-6.5169606	-0.8669502	0.1478535
C	0.6154348	-0.1651217	2.2554375
H	3.0759266	0.6596897	1.3805743
H	0.6596112	-0.0262815	-1.3176224
H	-1.6907334	1.9263565	0.9362472
H	-4.0787624	1.4314336	1.1380583
H	-3.5943672	-2.0342695	-1.3764854
H	-1.1960800	-1.5180244	-1.6246474
H	3.8035928	-2.4335211	-1.4240103
H	3.6216889	-3.0678988	0.2085171
H	1.2357991	-2.6754661	1.3935167
H	-0.0936565	-2.0832037	0.4142232
H	1.4355470	-1.8598195	-1.5530178
H	1.5052041	-3.4939654	-0.9160437
H	1.4438856	3.9531623	0.6482239
H	0.3530152	2.9148418	1.5993350
H	2.0431570	2.3822364	1.2734495
H	2.5273039	3.1447441	-1.6597705
H	1.9082545	1.7443039	-2.5850084
H	2.8377953	1.4706274	-1.0675532
H	0.8748889	0.8530549	2.5529534
H	-0.4689283	-0.2398402	2.1332857
H	0.9023997	-0.8320162	3.0795647

2c_sy_c_8.log

E = -1188.219059

H = -1187.853690

G = -1187.922248

NImag=0

C	-4.1318753	2.2280761	-2.9715328
C	-4.0323360	2.2929832	-1.4622330
C	-3.2032671	2.7384458	-3.8651745
O	-3.3040588	2.7076853	-5.1398600
C	-3.4852704	0.9101754	-0.9270601
C	-2.9732125	0.7642808	0.4866991
C	-3.7182921	1.0847974	1.6316004
C	-3.1631791	0.9585131	2.8986045
C	-1.8453028	0.5059040	3.0342803
C	-1.0866162	0.1758212	1.9073690
C	-1.6573978	0.3057672	0.6467625
C	-1.9605577	3.4502162	-3.3157750
C	-3.0156021	3.3711328	-1.0422333
C	-1.7070133	3.2609544	-1.8201196
S	-4.6787773	-0.4333204	-1.4008039
C	-3.5925331	-1.8706853	-1.4517526
C	-5.6514358	-0.8321296	0.0652635
C	-1.2678103	0.3758382	4.3458229
N	-0.8029286	0.2703587	5.4012301
C	-5.4050841	2.6423803	-0.8698777
H	-5.0292116	1.7695055	-3.3898126

H	-2.6605241	0.6486826	-1.5964034
H	-4.7427739	1.4271563	1.5525409
H	-3.7458689	1.2073739	3.7792047
H	-0.0667717	-0.1768651	2.0187004
H	-1.0690049	0.0508033	-0.2305372
H	-1.0994863	3.1159564	-3.9061465
H	-2.0865946	4.5199110	-3.5377071
H	-3.4735996	4.3470132	-1.2526776
H	-2.8385027	3.3289683	0.0393612
H	-1.2438507	2.2821809	-1.6371601
H	-0.9932412	4.0092261	-1.4570168
H	-4.2244526	-2.7479574	-1.6017821
H	-2.9186013	-1.7455526	-2.3007914
H	-3.0385981	-1.9505267	-0.5141089
H	-6.3123661	-1.6491091	-0.2327236
H	-6.2468389	0.0404765	0.3373927
H	-5.0001655	-1.1442779	0.8826427
H	-6.1695353	1.9028437	-1.1410600
H	-5.3913500	2.7478444	0.2187744
H	-5.7304117	3.5988520	-1.2902994

2c_sy_c_8_ts1.log

E = -1188.191867

H = -1187.829211

G = -1187.898887

NImag=1

C	3.0405062	-0.1736112	0.5271691
C	1.7670989	-0.3961576	1.0634185
C	3.7269600	-1.1108203	-0.3049437
O	4.8576498	-0.8993608	-0.7865217
C	0.3493201	0.5913583	-0.3399572
C	-1.0608146	0.2385995	-0.2560620
C	-1.9230119	0.6657036	0.7826052
C	-3.2271980	0.2054459	0.8738184
C	-3.7149142	-0.7187577	-0.0620675
C	-2.8757480	-1.1768551	-1.0906009
C	-1.5795953	-0.7005563	-1.1817464
C	3.0833542	-2.4742697	-0.5325551
C	1.1741751	-1.7828927	0.9441782
C	1.5665072	-2.4776194	-0.3556668
S	0.8859556	2.2652079	-0.3962421
C	0.1417948	3.0082512	-1.8753622
C	0.0036577	3.2401006	0.8419040
C	-5.0608288	-1.1985067	0.0358176
N	-6.1513329	-1.5868697	0.1142187
C	1.3861558	0.3418268	2.3221899
H	3.5572626	0.7601122	0.7443083
H	0.8550682	0.1412546	-1.1941135
H	-1.5655580	1.3433383	1.5486001
H	-3.8698100	0.5480606	1.6789568
H	-3.2505835	-1.8913604	-1.8169782
H	-0.9424628	-1.0472452	-1.9905889
H	3.3753393	-2.8257707	-1.5270236
H	3.5439291	-3.1590893	0.1943129
H	1.5581881	-2.3641252	1.7976899
H	0.0857722	-1.7398448	1.0626524
H	1.0990073	-1.9637298	-1.2035491
H	1.1866688	-3.5047851	-0.3620494
H	0.3999898	4.0699229	-1.8907750
H	0.5728615	2.5045837	-2.7419573
H	-0.9409302	2.8692968	-1.8431395

H	0.4461917	4.2377751	0.8033198
H	0.1647705	2.8059070	1.8280439
H	-1.0574281	3.2901221	0.5948261
H	1.8088487	1.3514009	2.3412916
H	0.3019954	0.3942205	2.4592634
H	1.8049457	-0.2005999	3.1808110

2c_sy_c_prod_1.log

E = -710.335667
H = -710.054467
G = -710.112280

NImag=0

C	-0.9740416	-0.5445733	3.7220209
C	-2.0089369	-1.2173839	2.8384078
C	-1.4481066	0.1126167	2.4287630
C	-0.5888233	0.3396290	1.2275889
C	0.7309222	0.7911796	1.3392055
C	1.5060075	1.0080888	0.2053194
C	0.9500274	0.7786918	-1.0587670
C	-0.3770301	0.3466907	-1.1892134
C	-1.1362220	0.1342367	-0.0463486
H	-2.1203202	0.9484103	2.6196412
H	-1.3145461	-0.0520741	4.6291999
C	-3.4367308	-1.2385524	3.3392167
C	-1.5968482	-2.4881423	2.1074230
C	-0.0945442	-2.6591472	1.8606546
C	0.7219699	-2.4050544	3.1261881
C	0.3920644	-1.1276653	3.8658855
O	1.1886872	-0.6356235	4.6513397
C	1.7458899	0.9960593	-2.2366099
N	2.3868113	1.1711894	-3.1856843
H	1.1598183	0.9721742	2.3204791
H	2.5313677	1.3526522	0.2929929
H	-0.7982464	0.1786064	-2.1750716
H	-2.1636069	-0.2076522	-0.1378091
H	-4.1338653	-1.3640763	2.5026194
H	-3.5882060	-2.0707835	4.0353320
H	-3.6876343	-0.3073126	3.8561084
H	-1.9467261	-3.3329007	2.7157985
H	-2.1397510	-2.5417777	1.1550669
H	0.2492084	-2.0016618	1.0581757
H	0.0907103	-3.6824684	1.5198842
H	1.7986153	-2.4265657	2.9352214
H	0.5101866	-3.1994100	3.8585711

2c_sy_c_prod_2.log

E = -710.334844
H = -710.053541
G = -710.111145

NImag=0

C	-0.9664839	-0.5604659	3.6818417
C	-2.0147799	-1.2277268	2.7977082
C	-1.4400802	0.0968245	2.3890743
C	-0.5564369	0.3152067	1.2025606
C	0.7367731	0.8317440	1.3455470
C	1.5319152	1.0833408	0.2334933
C	1.0247473	0.8175032	-1.0440470
C	-0.2710989	0.3116247	-1.2080779
C	-1.0511817	0.0670376	-0.0847545
H	-2.1003419	0.9434002	2.5751274

H	-1.3042448	-0.0773058	4.5945854
C	-3.4327757	-1.2271558	3.3281756
C	-1.6053102	-2.5054765	2.0569019
C	-0.4513466	-3.2441989	2.7328833
C	0.7508977	-2.3100628	2.9004106
C	0.3931742	-1.1564720	3.8098236
O	1.1610879	-0.7602424	4.6748897
C	1.8410244	1.0708157	-2.2007475
N	2.4985501	1.2748099	-3.1324545
H	1.1271949	1.0414121	2.3376686
H	2.5346927	1.4821300	0.3479441
H	-0.6550911	0.1145048	-2.2036329
H	-2.0581895	-0.3230068	-0.2051202
H	-4.1498498	-1.3183953	2.5046556
H	-3.5865003	-2.0728353	4.0078314
H	-3.6510450	-0.3033269	3.8728639
H	-2.4814391	-3.1594434	2.0024851
H	-1.3188427	-2.2776985	1.0237647
H	-0.1627596	-4.1165799	2.1386842
H	-0.7685799	-3.6106988	3.7175011
H	1.0418896	-1.9112945	1.9184876
H	1.6200304	-2.8160681	3.3284256

2c_sy_tr_1.log

E = -1188.223312

H = -1187.858030

G = -1187.926841

NImag=0

C	-1.1386594	1.8516688	-6.2900687
C	-0.2030682	1.6179405	-5.1295002
C	-2.4834487	2.1609969	-6.2069831
O	-3.1925344	2.6155148	-7.1718026
C	0.9027288	2.7222889	-5.2292439
C	1.9891799	2.7050025	-4.1791498
C	1.7581444	3.0339340	-2.8361552
C	2.7857666	2.9624440	-1.9041012
C	4.0599002	2.5517119	-2.3140764
C	4.3094844	2.2255934	-3.6512536
C	3.2733748	2.3115663	-4.5735831
C	-3.1865461	1.9361073	-4.8674521
C	-0.9579985	1.6777035	-3.7847521
C	-2.3616776	1.0872237	-3.9034632
S	0.0778235	4.3976838	-5.2742619
C	1.5078481	5.5008835	-5.1468646
C	-0.3414824	4.7096152	-7.0086466
C	5.1260408	2.4736131	-1.3509736
N	5.9840475	2.4112006	-0.5756611
C	0.5317243	0.2699088	-5.2539862
H	-0.6593308	1.9653212	-7.2644524
H	1.3708007	2.6428603	-6.2175563
H	0.7793071	3.3632016	-2.5017505
H	2.6057057	3.2223092	-0.8663194
H	5.3020818	1.9160880	-3.9610396
H	3.4620790	2.0660410	-5.6147219
H	-3.4040086	2.9149224	-4.4141694
H	-4.1556432	1.4698858	-5.0812541
H	-0.3767047	1.1648579	-3.0095309
H	-1.0806702	2.7187128	-3.4575028
H	-2.8329010	1.0529203	-2.9146969
H	-2.3063997	0.0536762	-4.2691962
H	1.1454979	6.5057347	-5.3708339

H	1.8926539	5.4683698	-4.1280287
H	2.2707912	5.1965558	-5.8671375
H	-0.3977321	5.7963985	-7.1090417
H	-1.3066982	4.2441325	-7.2161652
H	0.4463532	4.3057921	-7.6477779
H	1.2740598	0.1241108	-4.4601494
H	-0.1994194	-0.5422985	-5.1924485
H	1.0392293	0.1933060	-6.2226479

2c_sy_tr_1_r.log

E = -1188.218497
H = -1187.853165
G = -1187.921982

NImag=0

C	0.9754389	-1.4866600	-0.8246636
C	1.1771483	-0.8534785	0.5384365
C	0.6721427	-2.8155881	-1.0796909
O	0.5088255	-3.3260607	-2.2406429
C	0.2337845	0.3965304	0.5683758
C	0.5122071	1.4465433	-0.4845331
C	1.6345273	2.2839582	-0.4351872
C	1.8623851	3.2212446	-1.4349818
C	0.9587652	3.3237370	-2.4990846
C	-0.1740687	2.5048021	-2.5560730
C	-0.3921593	1.5776290	-1.5437925
C	0.5220549	-3.7708961	0.1072334
C	0.7409695	-1.8238794	1.6548807
C	1.1871195	-3.2570774	1.3793153
S	0.2351059	1.2847417	2.2334296
C	-0.7586670	2.7545212	1.8781306
C	-0.9861593	0.3905526	3.2259274
C	1.1925132	4.2891063	-3.5403291
N	1.3800393	5.0659202	-4.3784928
C	2.6495166	-0.4565157	0.7556468
H	1.1475422	-0.8456072	-1.6895048
H	-0.8006251	0.0510518	0.4684727
H	2.3383674	2.2231706	0.3900381
H	2.7310464	3.8696933	-1.3936459
H	-0.8738056	2.5980636	-3.3798555
H	-1.2717475	0.9416037	-1.5790212
H	-0.5503325	-3.9388365	0.2853339
H	0.9425060	-4.7360535	-0.1967352
H	1.1472681	-1.4856429	2.6181014
H	-0.3550964	-1.8245914	1.7349347
H	0.9320997	-3.8908490	2.2362764
H	2.2781117	-3.2964848	1.2689437
H	-1.0102846	3.1957296	2.8443534
H	-0.1574771	3.4534626	1.2978234
H	-1.6609535	2.4610325	1.3370039
H	-1.2880572	1.0790778	4.0178320
H	-0.5185141	-0.4888426	3.6624436
H	-1.8402327	0.1231317	2.6008812
H	2.8023491	0.1627054	1.6503408
H	3.2436381	-1.3670044	0.8777544
H	3.0508253	0.0763013	-0.1103840

2c_sy_tr_1_ts1.log

E = -1188.193159
H = -1187.830829
G = -1187.900369

NImag=1

C	2.6578216	-0.7384592	0.9189161
C	1.3085412	-1.1229872	0.8385784
C	3.5505185	-0.7377682	-0.1898390
O	4.6781873	-0.1972272	-0.1644255
C	0.1448561	0.7459886	0.7597877
C	-1.2272019	0.4790096	0.4076926
C	-1.6992539	0.3577331	-0.9251992
C	-3.0079699	-0.0013183	-1.1985371
C	-3.9061470	-0.2496264	-0.1491229
C	-3.4697884	-0.1201591	1.1823796
C	-2.1638114	0.2412549	1.4488211
C	3.1088647	-1.4758533	-1.4488322
C	0.8502484	-1.7996413	-0.4474359
C	2.0112981	-2.4964490	-1.1587670
S	1.0776814	1.6877857	-0.4211329
C	0.1188447	3.2002750	-0.7117691
C	2.4093310	2.4169092	0.5604029
C	-5.2593699	-0.6160145	-0.4320188
N	-6.3578925	-0.9141636	-0.6601854
C	0.6440241	-1.6038848	2.1040434
H	3.0314635	-0.3281574	1.8565219
H	0.3143714	1.1249117	1.7672316
H	-1.0374896	0.5456736	-1.7673787
H	-3.3429418	-0.0883992	-2.2275379
H	-4.1654388	-0.2944838	1.9975304
H	-1.8406685	0.3518858	2.4801889
H	2.7441022	-0.7341011	-2.1743667
H	3.9978683	-1.9403477	-1.8875967
H	0.0399189	-2.5019080	-0.2217940
H	0.4354021	-1.0645509	-1.1467961
H	1.6551742	-2.9545887	-2.0874756
H	2.4101956	-3.3000925	-0.5275234
H	0.7146706	3.8433640	-1.3630161
H	-0.8118930	2.9289983	-1.2107437
H	-0.0801903	3.6840405	0.2462185
H	2.7714651	3.2744503	-0.0107562
H	3.2052693	1.6834317	0.6764361
H	2.0058764	2.7369714	1.5231647
H	-0.4461660	-1.6032353	2.0289042
H	0.9602834	-2.6420395	2.2758982
H	0.9487409	-1.0102910	2.9710381

2c_sy_tr_1_ts2.log

E = -1188.209239

H = -1187.845795

G = -1187.915302

NImag=1

C	-1.4886532	-1.5810999	0.2087178
C	-1.5875648	-0.1697932	0.7461466
C	-2.4927488	-2.2509035	-0.5128283
O	-2.3692195	-3.4157495	-0.9829932
C	-0.5032653	0.3389871	-0.1634799
C	0.9300801	-0.0706513	-0.0515820
C	1.6685982	0.0773423	1.1311957
C	3.0132034	-0.2713511	1.1719401
C	3.6314952	-0.7690017	0.0191472
C	2.9131533	-0.9067457	-1.1750685
C	1.5719589	-0.5499113	-1.2019077
C	-3.8463390	-1.5592640	-0.6698975
C	-2.9317753	0.4940387	0.3798620

C	-4.0846337	-0.5031631	0.4067736
S	-0.2199510	2.5574660	0.1488426
C	1.1646456	2.8424137	-0.9795678
C	-1.5380758	3.2807692	-0.8567877
C	5.0230737	-1.1317209	0.0584269
N	6.1433745	-1.4238844	0.0891274
C	-1.3368673	-0.0782501	2.2521534
H	-0.5962226	-2.1470620	0.4659712
H	-0.8338641	0.4438348	-1.1977112
H	1.2104035	0.4929194	2.0218400
H	3.5843212	-0.1522395	2.0865946
H	3.4033744	-1.2853830	-2.0657683
H	1.0064879	-0.6513630	-2.1238796
H	-3.8972426	-1.0920575	-1.6638990
H	-4.6110582	-2.3426479	-0.6472708
H	-3.1116391	1.3342059	1.0621944
H	-2.8813347	0.9061036	-0.6355514
H	-5.0329388	0.0178217	0.2363773
H	-4.1512443	-0.9831217	1.3918541
H	1.2505734	3.9175562	-1.1507032
H	2.0767859	2.4740557	-0.5076210
H	0.9890206	2.3211183	-1.9244737
H	-1.2586050	4.3103612	-1.0909633
H	-2.4589493	3.2781365	-0.2739476
H	-1.6668278	2.7073881	-1.7780928
H	-1.1292192	0.9490684	2.5764878
H	-2.2383900	-0.4215870	2.7711612
H	-0.5135883	-0.7241447	2.5667397

2c_sy_tr_2.log

E = -1188.222035

H = -1187.856691

G = -1187.925091

NImag=0

C	-1.1651012	1.7514989	-6.3525524
C	-0.1229524	1.4383450	-5.3135524
C	-2.4420562	2.2175129	-6.0942817
O	-3.2416613	2.6735313	-6.9838432
C	0.8892169	2.6492755	-5.2773387
C	1.9239012	2.6543557	-4.1786900
C	1.6118328	2.9597251	-2.8465373
C	2.5903675	2.9185743	-1.8624503
C	3.8986517	2.5584526	-2.2090178
C	4.2287066	2.2530513	-3.5335074
C	3.2399319	2.3114341	-4.5090269
C	-2.9761452	2.1698449	-4.6580173
C	-0.7892953	1.1076029	-3.9680456
C	-1.9074317	2.0685678	-3.5662906
S	-0.0269486	4.2786373	-5.3114896
C	1.3384390	5.4474700	-5.0845834
C	-0.3644480	4.6147347	-7.0591109
C	4.9148026	2.5083744	-1.1915416
N	5.7324724	2.4679913	-0.3723742
C	0.7379215	0.2324605	-5.7310497
H	-0.8144970	1.7984614	-7.3857885
H	1.4077392	2.6561432	-6.2431847
H	0.6021289	3.2445627	-2.5627223
H	2.3466911	3.1606757	-0.8334210
H	5.2464134	1.9814878	-3.7933770
H	3.4913315	2.0842286	-5.5412087
H	-3.6003486	3.0580898	-4.5077705

H	-3.6524574	1.3049426	-4.5979900
H	-1.2255808	0.1066305	-4.0846966
H	-0.0386514	1.0233960	-3.1740608
H	-1.5011617	3.0644754	-3.3556558
H	-2.3579511	1.7251097	-2.6278544
H	0.9363725	6.4383565	-5.3035511
H	1.6733708	5.4096028	-4.0485230
H	2.1518758	5.2009993	-5.7712550
H	-0.4190399	5.7023813	-7.1495466
H	-1.3197483	4.1522673	-7.3131022
H	0.4524966	4.2203522	-7.6668613
H	1.5156896	0.0073277	-4.9910775
H	0.0965959	-0.6484657	-5.8310486
H	1.2232269	0.4110346	-6.6975033

2c_sy_tr_2_r.log

E = -1188.219126

H = -1187.853986

G = -1187.922576

NImag=0

C	1.0572847	-1.7584130	-0.4603702
C	1.2528550	-0.9606569	0.8099553
C	0.3053128	-2.9168997	-0.5846552
O	0.1585755	-3.5902607	-1.6610291
C	0.3011177	0.2879252	0.6935589
C	0.6077126	1.2120801	-0.4633083
C	1.7046265	2.0835846	-0.4642621
C	1.9650760	2.8944718	-1.5617724
C	1.1211562	2.8316833	-2.6769628
C	0.0153695	1.9750920	-2.6887930
C	-0.2368765	1.1779809	-1.5783799
C	-0.3804977	-3.4936130	0.6602261
C	0.8718566	-1.8203218	2.0270016
C	-0.4639916	-2.5362680	1.8489319
S	0.2460547	1.3195446	2.2782637
C	-0.5427252	2.8638665	1.7602015
C	-1.1643884	0.6124137	3.1654236
C	1.3881120	3.6652722	-3.8189630
N	1.6029145	4.3365720	-4.7379071
C	2.7188215	-0.5313426	0.9601931
H	1.5405883	-1.3720322	-1.3586759
H	-0.7316757	-0.0591845	0.5977218
H	2.3644757	2.1495789	0.3969532
H	2.8132871	3.5706958	-1.5576363
H	-0.6379038	1.9396233	-3.5542284
H	-1.0972673	0.5154099	-1.5780261
H	-1.3780944	-3.8334103	0.3596939
H	0.1790691	-4.3957240	0.9467962
H	1.6565207	-2.5801362	2.1356283
H	0.9086890	-1.2303390	2.9526668
H	-1.2741133	-1.8147860	1.6841376
H	-0.7206813	-3.0812767	2.7648051
H	-0.8712693	3.3600412	2.6756997
H	0.1927555	3.4830796	1.2487031
H	-1.3931074	2.6397403	1.1126008
H	-1.3945116	1.3062497	3.9763518
H	-0.8837158	-0.3539137	3.5805735
H	-2.0101227	0.5225026	2.4807526
H	2.8770095	0.1502713	1.8068666
H	3.3262942	-1.4248468	1.1331346
H	3.0961438	-0.0504500	0.0537270

2c_sy_tr_2_ts1.log

E = -1188.196459

H = -1187.834061

G = -1187.904147

NImag=1

C	2.7186593	-0.8072860	0.8217754
C	1.3575021	-1.0885986	1.0341801
C	3.4035135	-1.0553190	-0.3990333
O	4.5856511	-0.6999034	-0.6056493
C	0.2453334	0.7780155	0.7452710
C	-1.1341398	0.5197970	0.3937059
C	-1.6038765	0.3826016	-0.9376388
C	-2.9110958	0.0186397	-1.2090428
C	-3.8104838	-0.2195425	-0.1575632
C	-3.3788955	-0.0639409	1.1713252
C	-2.0734423	0.3062772	1.4351701
C	2.6826465	-1.8608715	-1.4744606
C	0.6755631	-2.0021298	0.0401853
C	1.1593934	-1.7772891	-1.3886902
S	1.1507584	1.7186126	-0.4642075
C	0.2632461	3.2964598	-0.5724304
C	2.6181438	2.2998564	0.4188955
C	-5.1615831	-0.5971185	-0.4377203
N	-6.2578228	-0.9044166	-0.6640192
C	0.8953642	-1.2617981	2.4604521
H	3.2775299	-0.2998667	1.6069652
H	0.3966232	1.2172518	1.7318796
H	-0.9402122	0.5605742	-1.7798760
H	-3.2441423	-0.0820296	-2.2374338
H	-4.0769337	-0.2226745	1.9876302
H	-1.7585049	0.4450029	2.4653237
H	3.0477897	-1.5297746	-2.4517457
H	3.0050106	-2.9049774	-1.3507405
H	0.9165865	-3.0311101	0.3502091
H	-0.4127337	-1.9046287	0.1128582
H	0.8342367	-0.7893185	-1.7327421
H	0.7000873	-2.5095000	-2.0613126
H	0.8248236	3.9482555	-1.2451868
H	-0.7269216	3.0997134	-0.9856291
H	0.1886630	3.7299579	0.4269138
H	2.8991165	3.2436360	-0.0532093
H	3.4148895	1.5683960	0.2995369
H	2.3673056	2.4542946	1.4703786
H	-0.1935532	-1.2190034	2.5494741
H	1.2166412	-2.2529079	2.8065699
H	1.3411821	-0.5133436	3.1218614

2c_sy_tr_2_ts1_rot1.log

E = -1188.197381

H = -1187.835245

G = -1187.904938

NImag=1

C	0.2607323	-1.8158340	-0.8657203
C	1.3819531	-0.9606843	-0.8878214
C	0.1445644	-2.9796737	-0.0575453
O	-0.8473325	-3.7423991	-0.0770222
C	0.9209551	0.7381618	0.3309574
C	-0.5304260	0.8104304	0.2635271
C	-1.2368424	1.5328804	-0.7229926

C	-2.6155885	1.4422181	-0.8304425
C	-3.3332969	0.6168831	0.0493421
C	-2.6532775	-0.1147943	1.0339582
C	-1.2748509	-0.0159733	1.1332190
C	1.3356319	-3.3767060	0.8083979
C	2.6265639	-1.4614431	-0.1772079
C	2.2940423	-2.2262372	1.1005354
S	1.6964615	2.2624108	-0.1517038
C	1.3275721	3.4366088	1.1812016
C	3.4447693	1.9937186	0.1908808
C	-4.7595666	0.5245622	-0.0573162
N	-5.9139671	0.4503563	-0.1436827
C	1.6285497	-0.2229786	-2.1853852
H	-0.5862846	-1.5893698	-1.5138570
H	1.3089400	0.4409086	1.3065903
H	-0.7066432	2.1700964	-1.4258387
H	-3.1421897	2.0055096	-1.5944222
H	-3.2082317	-0.7538961	1.7138413
H	-0.7525616	-0.5819798	1.8996438
H	0.9499384	-3.8247606	1.7299913
H	1.8639104	-4.1745090	0.2664593
H	3.1479620	-2.1330374	-0.8780222
H	3.3134279	-0.6370836	0.0300487
H	1.8335067	-1.5436534	1.8256332
H	3.2124791	-2.6044807	1.5619532
H	1.8717721	4.3618599	0.9784463
H	0.2524559	3.6226197	1.1625377
H	1.6312078	2.9997941	2.1348011
H	3.9146897	2.9790876	0.2054776
H	3.8760174	1.3966363	-0.6116686
H	3.5540331	1.5000595	1.1589379
H	2.4634832	0.4818433	-2.1202041
H	1.8811408	-0.9516454	-2.9661949
H	0.7318630	0.3141917	-2.5142954

2c_sy_tr_2_ts2.log

E = -1188.212485

H = -1187.848748

G = -1187.917664

NImag=1

C	-1.4290446	-1.7127128	0.5314322
C	-1.5738915	-0.2864595	1.0130178
C	-2.3133761	-2.3591245	-0.3445303
O	-2.1712665	-3.5493886	-0.7454672
C	-0.6043775	0.2678077	-0.0036729
C	0.8588643	-0.0541738	0.0315374
C	1.6747921	0.2625029	1.1266455
C	3.0367948	-0.0116435	1.0972249
C	3.5957881	-0.6025320	-0.0416314
C	2.7997802	-0.9064886	-1.1526875
C	1.4413834	-0.6230257	-1.1093276
C	-3.5835602	-1.6288046	-0.7875231
C	-3.0003644	0.2347279	0.7991074
C	-3.5781953	-0.1148638	-0.5710684
S	-0.5270561	2.4819910	0.1201094
C	0.9364629	2.8692795	-0.8708856
C	-1.7854364	2.9320841	-1.0993006
C	5.0052255	-0.8881016	-0.0764519
N	6.1401022	-1.1176565	-0.1047688
C	-1.1741091	-0.1163255	2.4772648
H	-0.5589987	-2.2674354	0.8772893

H	-0.9956959	0.2577873	-1.0203234
H	1.2609730	0.7538155	2.0007824
H	3.6659163	0.2380673	1.9450674
H	3.2437857	-1.3554307	-2.0348701
H	0.8164118	-0.8546053	-1.9671853
H	-3.7588471	-1.8737409	-1.8405948
H	-4.4096793	-2.0838654	-0.2229598
H	-3.6258814	-0.2327169	1.5706621
H	-3.0372676	1.3162065	0.9873166
H	-3.0064051	0.3701293	-1.3704665
H	-4.5972572	0.2801624	-0.6476530
H	0.9019415	3.9312918	-1.1232786
H	1.8253205	2.6638193	-0.2731886
H	0.9407222	2.2631539	-1.7806002
H	-1.6470652	3.9850981	-1.3536553
H	-2.7723551	2.7949147	-0.6569646
H	-1.6761222	2.3115185	-1.9920780
H	-1.0632436	0.9395473	2.7538576
H	-1.9604039	-0.5509616	3.1027969
H	-0.2449295	-0.6413491	2.7109347

2c_sy_tr_3.log

E = -1188.219683

H = -1187.854931

G = -1187.924555

NImag=0

C	-1.3599904	2.6487584	-5.2505666
C	-0.2489905	1.8786158	-5.9290679
C	-2.2151880	2.1691296	-4.2754010
O	-3.1210946	2.8480729	-3.6771168
C	1.1331728	2.6111174	-5.8414879
C	1.8624339	2.6513436	-4.5224922
C	1.2300721	2.9926362	-3.3167954
C	1.9411924	2.9932606	-2.1243139
C	3.3011986	2.6572399	-2.1301522
C	3.9477096	2.3165465	-3.3219661
C	3.2219532	2.3150429	-4.5083983
C	-2.0818529	0.6993462	-3.8640722
C	-0.0478631	0.4855629	-5.2885309
C	-1.3793510	-0.1591059	-4.9125872
S	0.9534876	4.3307741	-6.5600024
C	0.8311863	5.4837488	-5.1794962
C	2.6374718	4.6700756	-7.1051846
C	4.0406061	2.6610636	-0.8957486
N	4.6357367	2.6646543	0.0977709
C	-0.5574094	1.6842181	-7.4303007
H	-1.5269764	3.6752394	-5.5881901
H	1.8055198	2.1623538	-6.5834163
H	0.1748121	3.2453235	-3.3175742
H	1.4505202	3.2528875	-1.1921127
H	5.0002789	2.0539129	-3.3166789
H	3.7171248	2.0402550	-5.4356821
H	-1.5303924	0.6518829	-2.9125034
H	-3.0918464	0.3273179	-3.6580410
H	0.5229893	-0.1471230	-5.9803166
H	0.5429856	0.5696865	-4.3693249
H	-1.2024406	-1.1714063	-4.5311742
H	-2.0193427	-0.2598125	-5.7984526
H	0.7667680	6.4762010	-5.6314658
H	-0.0845076	5.2651297	-4.6291486
H	1.7129896	5.4057464	-4.5420865

H	2.6596013	5.7048616	-7.4524883
H	2.8611732	3.9936536	-7.9315528
H	3.3335665	4.5273320	-6.2758755
H	0.2896889	1.2422924	-7.9710774
H	-1.4187252	1.0183334	-7.5382200
H	-0.8232683	2.6299310	-7.9147078

2c_sy_tr_3_r.log

E = -1188.217718
H = -1187.852375
G = -1187.921956

NImag=0

C	-1.4374711	-1.2152127	-0.2229172
C	-1.8942649	0.1646311	-0.6548730
C	-1.5979315	-2.3977099	-0.9288692
O	-1.1725757	-3.5450083	-0.5570431
C	-0.6110997	1.0568018	-0.6326739
C	0.2322318	1.1122718	0.6182751
C	-0.2610706	1.5136047	1.8680679
C	0.5614601	1.5144862	2.9881117
C	1.8961521	1.1122796	2.8648614
C	2.4090259	0.7140494	1.6263569
C	1.5740415	0.7201022	0.5156271
C	-2.3525696	-2.3524220	-2.2600638
C	-2.4176716	0.1415336	-2.1106233
C	-3.2303088	-1.1148570	-2.4093809
S	-0.9583047	2.7844455	-1.3088173
C	-1.1464966	3.9287500	0.0728055
C	0.6821017	3.2644333	-1.8844000
C	2.7499061	1.1121584	4.0234890
N	3.4374381	1.1134089	4.9553318
C	-3.0085682	0.7034849	0.2613847
H	-0.9509137	-1.2811482	0.7510083
H	0.0248268	0.6841837	-1.4427809
H	-1.2876282	1.8396634	1.9849673
H	0.1742286	1.8259272	3.9523571
H	3.4444677	0.4026791	1.5382760
H	1.9678338	0.4043169	-0.4463588
H	-1.6190480	-2.3936274	-3.0787589
H	-2.9471281	-3.2705209	-2.3277866
H	-3.0228410	1.0364283	-2.3005410
H	-1.5702466	0.1696073	-2.8116153
H	-3.6456437	-1.0501152	-3.4215962
H	-4.0826995	-1.1810182	-1.7209854
H	-1.2639341	4.9157954	-0.3803310
H	-2.0502315	3.6701550	0.6253757
H	-0.2627774	3.9023349	0.7115114
H	0.6142722	4.3007819	-2.2208355
H	0.9423336	2.6158228	-2.7222405
H	1.4034219	3.1692757	-1.0700216
H	-3.2319611	1.7664411	0.0927762
H	-3.9281904	0.1453186	0.0593517
H	-2.7736971	0.5565191	1.3180299

2c_sy_tr_3_ts1.log

E = -1188.194255
H = -1187.831773
G = -1187.901401

NImag=1

C	-1.1715070	-1.6896985	0.9264466
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C	-1.6413814	-1.3838028	-0.3667261
C	0.1259216	-2.2084567	1.2040779
O	0.5641133	-2.4086489	2.3576642
C	-1.2509204	0.6629861	-0.8225181
C	0.1614954	0.8678329	-0.5457119
C	0.6783882	0.8848586	0.7671163
C	2.0466106	0.9293913	0.9980430
C	2.9363987	0.9445642	-0.0838133
C	2.4472111	0.9318014	-1.4009299
C	1.0808694	0.8969237	-1.6187394
C	0.9818384	-2.5972790	0.0048595
C	-0.8819612	-1.9856067	-1.5567930
C	0.1032175	-3.0813480	-1.1468562
S	-2.4521185	1.7379081	-0.1025256
C	-2.5787289	1.4784144	1.6836794
C	-1.7484031	3.4074368	-0.0877012
C	4.3506663	0.9811987	0.1533940
N	5.4942993	1.0108513	0.3434654
C	-3.1451545	-1.3481349	-0.5629031
H	-1.8040742	-1.4802113	1.7875148
H	-1.5045864	0.6640450	-1.8836831
H	0.0109675	0.8373070	1.6189215
H	2.4303000	0.9349015	2.0134801
H	3.1391489	0.9551397	-2.2369175
H	0.7029348	0.8945712	-2.6375757
H	1.5690089	-1.7218213	-0.3110988
H	1.6885096	-3.3666608	0.3308966
H	-1.6164253	-2.3821417	-2.2680453
H	-0.3202897	-1.2169407	-2.0964743
H	0.7144414	-3.3647076	-2.0107354
H	-0.4434643	-3.9775546	-0.8279566
H	-3.4651568	2.0333824	1.9986885
H	-2.7210310	0.4174795	1.8810107
H	-1.6967718	1.8628537	2.1958375
H	-2.4680022	4.0658557	0.4046323
H	-1.6079594	3.7108839	-1.1263223
H	-0.7978587	3.4009444	0.4493216
H	-3.4285539	-0.8338819	-1.4866342
H	-3.5072068	-2.3821614	-0.6349434
H	-3.6648722	-0.8819958	0.2804071

2c_sy_tr_3_ts2.log

E = -1188.209102

H = -1187.845682

G = -1187.916115

NImag=1

C	-1.7076400	-1.4635428	0.3404124
C	-1.7030080	0.0042434	0.7101128
C	-2.7165954	-2.1183007	-0.3846497
O	-2.6687888	-3.3313134	-0.7337076
C	-0.5597230	0.3381608	-0.2084016
C	0.8432958	-0.1391214	-0.0813383
C	1.5286189	-0.2255482	1.1408263
C	2.8504328	-0.6479097	1.1827225
C	3.5092542	-0.9783520	-0.0078986
C	2.8498567	-0.8823150	-1.2385190
C	1.5265031	-0.4627298	-1.2648884
C	-3.9857045	-1.3319693	-0.7108215
C	-2.9721193	0.7401439	0.2166725
C	-4.2010976	-0.1607225	0.2442656
S	-0.3020140	2.5804762	-0.1397633

C	1.2849130	2.9120987	0.6535954
C	0.1624165	2.8315282	-1.8657919
C	4.8797891	-1.4131668	0.0342732
N	5.9835328	-1.7624770	0.0681840
C	-1.5075524	0.2589660	2.2074768
H	-0.8724652	-2.0631413	0.6963615
H	-0.8821782	0.3671417	-1.2491922
H	1.0465297	0.0593913	2.0672520
H	3.3757807	-0.7132134	2.1296691
H	3.3681984	-1.1376358	-2.1567492
H	1.0056153	-0.3985905	-2.2161695
H	-3.9212063	-0.9601771	-1.7436827
H	-4.8202596	-2.0402057	-0.6793239
H	-3.1230734	1.6358405	0.8299287
H	-2.8330564	1.0823061	-0.8180650
H	-5.0900480	0.4134883	-0.0385153
H	-4.3699394	-0.5377570	1.2616264
H	1.5039628	3.9769598	0.5458112
H	1.1945633	2.6640408	1.7128959
H	2.0731278	2.3151278	0.1886863
H	0.4755791	3.8686529	-2.0014751
H	-0.7160485	2.6305574	-2.4818022
H	0.9776343	2.1546283	-2.1355707
H	-1.1623766	1.2810833	2.4126314
H	-2.4733800	0.1260080	2.7071526
H	-0.8119906	-0.4500029	2.6608230

2c_sy_tr_4.log

E = -1188.215193

H = -1187.849446

G = -1187.917227

NImag=0

C	-1.0828181	1.9762565	-6.3060038
C	-0.1220773	1.7298038	-5.1680496
C	-2.4445603	2.1780297	-6.2019487
O	-3.2243274	2.5076086	-7.1651496
C	1.0743986	2.7381369	-5.2875762
C	2.1327599	2.6631134	-4.2059797
C	3.3360572	2.0094768	-4.4968512
C	4.3296284	1.8812530	-3.5342382
C	4.1214426	2.4266015	-2.2623785
C	2.9304915	3.0958594	-1.9581894
C	1.9436666	3.2086593	-2.9299767
C	-3.0937417	1.9917163	-4.8271165
C	-0.8207780	1.8082109	-3.7950049
C	-2.2239313	1.2055149	-3.8489471
S	0.7071198	4.5511582	-5.5395131
C	0.1919405	4.7224720	-7.2627685
C	-0.8197655	5.0497821	-4.7152727
C	5.1446546	2.3052319	-1.2581386
N	5.9682982	2.2069391	-0.4499145
C	0.5346730	0.3365323	-5.3111683
H	-0.6348575	2.0459376	-7.2988530
H	1.5607208	2.5306064	-6.2493835
H	3.4937658	1.5927446	-5.4877190
H	5.2591693	1.3709548	-3.7639319
H	2.7816768	3.5214720	-0.9715102
H	1.0251845	3.7299133	-2.6753683
H	-3.3290338	2.9825829	-4.4083265
H	-4.0555894	1.4913126	-4.9889875
H	-0.2069227	1.2980077	-3.0429969

H	-0.9238088	2.8462540	-3.4631930
H	-2.6651529	1.2131785	-2.8456244
H	-2.1703784	0.1556324	-4.1639010
H	0.2138925	5.7941106	-7.4734787
H	0.9253793	4.2084104	-7.8862789
H	-0.8053888	4.3032454	-7.3931387
H	-0.9905318	6.0751994	-5.0530385
H	-0.6634983	5.0462955	-3.6365943
H	-1.6365617	4.3969548	-5.0211712
H	1.2844289	0.1393760	-4.5359763
H	-0.2432620	-0.4288568	-5.2347264
H	1.0109367	0.2319115	-6.2927157

2c_sy_tr_4_r.log

E = -1188.211473
H = -1187.845816
G = -1187.913923

NImag=0

C	1.0381197	-1.3445429	-0.7513091
C	1.1911768	-0.7463756	0.6355276
C	0.7325783	-2.6632627	-1.0535420
O	0.5816468	-3.1338200	-2.2329268
C	0.2008294	0.4685210	0.6587455
C	0.4827578	1.5726012	-0.3413471
C	-0.3397882	1.6787859	-1.4687406
C	-0.1132165	2.6592348	-2.4269273
C	0.9455068	3.5566135	-2.2485968
C	1.7691227	3.4746207	-1.1203925
C	1.5337735	2.4830701	-0.1753486
C	0.5822435	-3.6597692	0.0987405
C	0.7479322	-1.7625217	1.7065198
C	1.2271639	-3.1770613	1.3930459
S	-0.2035690	1.3851767	2.2679271
C	-1.3273511	0.3056952	3.1822159
C	1.1958558	1.4424976	3.4070971
C	1.1863047	4.5791357	-3.2319105
N	1.3802131	5.4023953	-4.0230304
C	2.6495223	-0.3145680	0.8711917
H	1.2225686	-0.6762762	-1.5926119
H	-0.7972844	0.0650127	0.4544648
H	-1.1621914	0.9817755	-1.5998015
H	-0.7495161	2.7340012	-3.3024672
H	2.5839596	4.1785503	-0.9882717
H	2.1869069	2.4296234	0.6904411
H	-0.4891949	-3.8483166	0.2614561
H	1.0188544	-4.6082456	-0.2339452
H	1.1109907	-1.4495547	2.6931559
H	-0.3494209	-1.7905570	1.7493157
H	0.9752413	-3.8427807	2.2264206
H	2.3198550	-3.1927765	1.2926021
H	-1.7698063	0.9268031	3.9636845
H	-2.1053447	-0.0289982	2.4938545
H	-0.7898162	-0.5355623	3.6168657
H	0.8019320	1.9214148	4.3071609
H	1.9773843	2.0686814	2.9769968
H	1.5590790	0.4415618	3.6354732
H	2.7952129	0.2798671	1.7790915
H	3.2690640	-1.2124144	0.9580925
H	3.0299592	0.2575184	0.0200936

2c_sy_tr_4_ts1.log

E = -1188.186984
H = -1187.824695
G = -1187.894064

NImag=1

C	2.6296902	-0.5166932	0.9088032
C	1.2701509	-0.8663672	0.9822706
C	3.4898141	-0.9011180	-0.1562247
O	4.6462979	-0.4502811	-0.3095607
C	0.0749041	0.9462989	0.6756573
C	-1.3028639	0.6157613	0.3613712
C	-2.2414377	0.3953569	1.3991223
C	-3.5374377	-0.0045467	1.1285815
C	-3.9516799	-0.1883280	-0.2022760
C	-3.0466076	0.0380748	-1.2504641
C	-1.7473625	0.4261765	-0.9695251
C	2.9810102	-1.9464658	-1.1419879
C	0.7216031	-1.7707306	-0.1134554
C	1.7969123	-2.7433253	-0.6008866
S	0.7493536	2.1570846	-0.4423083
C	1.9260364	3.0377490	0.5998084
C	1.8971651	1.4148494	-1.6457943
C	-5.2937755	-0.5958091	-0.4881096
N	-6.3821596	-0.9259414	-0.7189226
C	0.6953238	-1.1026666	2.3590816
H	3.0677440	0.0822202	1.7064468
H	0.2490174	1.3174940	1.6840257
H	-1.9409408	0.5639668	2.4292039
H	-4.2424845	-0.1604861	1.9393210
H	-3.3653935	-0.0987240	-2.2791333
H	-1.0627377	0.5749226	-1.8019246
H	2.6881189	-1.4239884	-2.0652207
H	3.8279552	-2.5907915	-1.3996473
H	-0.1630104	-2.3023172	0.2553034
H	0.3943817	-1.1782026	-0.9751293
H	1.3846147	-3.3959712	-1.3777949
H	2.1251682	-3.3854601	0.2259525
H	2.4720251	3.7329025	-0.0410293
H	1.3594457	3.5858834	1.3535031
H	2.6028632	2.3164753	1.0608951
H	2.0040954	2.1698690	-2.4276019
H	1.4258555	0.5237875	-2.0628263
H	2.8613983	1.1881163	-1.1937614
H	-0.3965733	-1.0775498	2.3731393
H	1.0021215	-2.1093527	2.6749814
H	1.0866099	-0.3878813	3.0891178

2c_sy_tr_5.log

E = -1188.218650
H = -1187.853628
G = -1187.922762

NImag=0

C	-1.4201185	2.5655740	-5.3740472
C	-0.2810150	1.9051232	-6.1052017
C	-2.0365962	2.1016761	-4.2265593
O	-2.9942718	2.6866492	-3.6110927
C	1.0830880	2.6738176	-5.9454950
C	1.7608958	2.6730284	-4.6013917
C	1.1446066	3.1468548	-3.4321567
C	1.7990044	3.0702245	-2.2098046
C	3.0827657	2.5137962	-2.1465485

C	3.7137989	2.0402540	-3.3013258
C	3.0494088	2.1301536	-4.5194203
C	-1.6012282	0.7512271	-3.6446389
C	-0.0615918	0.4500292	-5.6264821
C	-0.2525308	0.2151169	-4.1284038
S	0.9065482	4.4027533	-6.6333020
C	0.5348367	5.5447894	-5.2891721
C	2.6322327	4.8314454	-6.9319601
C	3.7607797	2.4314158	-0.8798525
N	4.3068803	2.3654722	0.1393136
C	-0.5773856	1.8380087	-7.6180424
H	-1.7963427	3.5009328	-5.7981347
H	1.7892776	2.2627878	-6.6787099
H	0.1374880	3.5445097	-3.4711716
H	1.3187129	3.4312805	-1.3063214
H	4.7085392	1.6112706	-3.2438113
H	3.5347857	1.7621035	-5.4190132
H	-1.6074786	0.8481995	-2.5523660
H	-2.3984872	0.0347376	-3.8908266
H	-0.7978497	-0.1660998	-6.1588385
H	0.9293190	0.1007393	-5.9490750
H	0.5588671	0.6752493	-3.5585152
H	-0.1876794	-0.8622075	-3.9333301
H	0.4989852	6.5326006	-5.7550924
H	-0.4439062	5.2909797	-4.8815139
H	1.3158746	5.5082770	-4.5290753
H	2.6529847	5.8744152	-7.2536412
H	3.0025880	4.1869238	-7.7305375
H	3.2108306	4.6984455	-6.0152721
H	0.2636419	1.4083474	-8.1780503
H	-1.4562425	1.2071558	-7.7785874
H	-0.8056164	2.8214421	-8.0415327

2c_sy_tr_5_r.log

E = -1188.218691

H = -1187.853694

G = -1187.922493

NImag=0

C	-2.9388519	-0.1076130	-1.4140488
C	-1.7050504	-0.5553178	-0.6623371
C	-4.1769183	0.1885144	-0.8651308
O	-5.2175897	0.5238166	-1.5288477
C	-0.7103245	0.6602004	-0.6085064
C	-0.5651518	1.5699233	-1.8050984
C	-0.3300757	1.1018625	-3.1058578
C	-0.1997782	1.9886180	-4.1662263
C	-0.3005049	3.3656464	-3.9314238
C	-0.5325487	3.8530147	-2.6420072
C	-0.6617061	2.9511763	-1.5917319
C	-4.3553079	0.0793058	0.6518428
C	-2.0684248	-0.9281123	0.7908960
C	-3.0459692	0.0511558	1.4342916
S	0.9779144	0.1252618	0.0257662
C	2.0059013	-0.2049156	-1.4181619
C	1.6949937	1.6816526	0.5858546
C	-0.1628534	4.2870366	-5.0279281
N	-0.0502340	5.0291675	-5.9098714
C	-1.0795516	-1.7986723	-1.3190420
H	-2.8440793	-0.0271793	-2.4974648
H	-1.0236164	1.2871563	0.2333726
H	-0.2486916	0.0402861	-3.3068782

H	-0.0219502	1.6205900	-5.1711600
H	-0.6123822	4.9207649	-2.4672137
H	-0.8492129	3.3263892	-0.5892696
H	-4.9881420	0.9151059	0.9714144
H	-4.9293879	-0.8375228	0.8507776
H	-2.5341400	-1.9222181	0.7683273
H	-1.1580420	-1.0267371	1.3977436
H	-2.6136519	1.0602224	1.4631922
H	-3.2238970	-0.2365749	2.4767660
H	2.9775914	-0.5194061	-1.0308791
H	1.5539018	-1.0182751	-1.9872475
H	2.1058691	0.6972909	-2.0230570
H	2.7062358	1.4605304	0.9331610
H	1.0879761	2.0473603	1.4158417
H	1.7192187	2.4005349	-0.2354477
H	-0.2088518	-2.1754078	-0.7640873
H	-1.8269038	-2.5977240	-1.3235001
H	-0.7808056	-1.6284508	-2.3567472

2c_sy_tr_5_ts1.log

E = -1188.194165

H = -1187.831598

G = -1187.901154

NImag=1

C	-1.6609014	-1.5534397	0.6923286
C	-1.8286660	-1.0861464	-0.6208707
C	-0.6758780	-2.5016310	1.1010902
O	-0.5498688	-2.8885054	2.2823333
C	-1.0331876	0.9281584	-0.8328420
C	0.3802142	0.8960907	-0.4977358
C	0.8441654	0.6442076	0.8115140
C	2.1980247	0.4804745	1.0712915
C	3.1259381	0.5662120	0.0247395
C	2.6889609	0.8318024	-1.2852589
C	1.3380274	0.9961004	-1.5328968
C	0.1674989	-3.1689925	0.0240875
C	-1.0007206	-1.7539504	-1.7078887
C	0.3375164	-2.3175551	-1.2291136
S	-2.0771433	2.1015685	-0.0269420
C	-2.5101591	1.5872646	1.6529422
C	-1.0569769	3.5403885	0.3875348
C	4.5239545	0.3938595	0.2930426
N	5.6551769	0.2544955	0.5081138
C	-3.2296391	-0.7284004	-1.0759350
H	-2.3474800	-1.2245119	1.4695738
H	-1.2289605	1.0892711	-1.8932609
H	0.1430105	0.5448177	1.6318284
H	2.5402501	0.2761178	2.0811195
H	3.4117740	0.9107911	-2.0913338
H	1.0000033	1.1970585	-2.5459533
H	1.1349570	-3.4374574	0.4603114
H	-0.3428682	-4.1108794	-0.2253686
H	-1.6175316	-2.5826637	-2.0903640
H	-0.8558793	-1.0675293	-2.5501461
H	1.0350296	-1.5051299	-1.0121343
H	0.7865163	-2.9124641	-2.0322207
H	-3.0394021	2.4412544	2.0825115
H	-3.1845671	0.7349013	1.6003230
H	-1.6257789	1.3590118	2.2461811
H	-1.7040162	4.2730030	0.8745010
H	-0.6687950	3.9435758	-0.5490780

H	-0.2417441	3.2433603	1.0499846
H	-3.2273955	-0.1222858	-1.9871908
H	-3.7666515	-1.6607310	-1.2951239
H	-3.7993958	-0.2073479	-0.3006584

2c_sy_tr_prod_1.log

E = -710.339129
H = -710.057779
G = -710.116305

NImag=0

C	0.6586037	-1.9309460	0.7731920
C	0.6158423	-1.7602452	-0.7310123
C	0.7446415	-0.5453023	0.1470149
C	-0.3750511	0.4340905	0.2859702
C	-1.2825344	0.4068597	1.3497881
C	-2.3092876	1.3420171	1.4336628
C	-2.4317250	2.3198786	0.4406362
C	-1.5281111	2.3659903	-0.6300801
C	-0.5095077	1.4259415	-0.6974709
H	1.7245609	-0.0741375	0.1632746
H	-0.2724604	-2.1684181	1.2813195
C	-0.7026800	-2.0231965	-1.4224343
C	1.8388952	-2.2012691	-1.5189923
C	3.1525607	-2.0599328	-0.7493286
C	3.0914010	-2.7804453	0.5983666
C	1.8654443	-2.4903676	1.4406866
O	1.8417938	-2.7762832	2.6283616
C	-3.4918967	3.2878184	0.5196757
N	-4.3461702	4.0679665	0.5825271
H	-1.1881126	-0.3458414	2.1260998
H	-3.0102823	1.3187352	2.2617589
H	-1.6309211	3.1283504	-1.3955054
H	0.1927911	1.4541685	-1.5263408
H	-0.7925264	-3.0869370	-1.6671807
H	-1.5541427	-1.7444237	-0.7949253
H	-0.7661440	-1.4530094	-2.3568314
H	1.6974943	-3.2555033	-1.7942302
H	1.8850178	-1.6296150	-2.4541145
H	3.4000120	-1.0033998	-0.6025048
H	3.9670635	-2.4846943	-1.3434358
H	3.9797993	-2.5930192	1.2080792
H	3.0502321	-3.8661299	0.4245737

2c_sy_tr_prod_2.log

E = -710.337435
H = -710.055899
G = -710.114187

NImag=0

C	0.5871785	-1.9905241	0.7114159
C	0.6749412	-1.6991220	-0.7815204
C	0.7441769	-0.5662526	0.2034292
C	-0.3594600	0.4315993	0.3351057
C	-0.3886064	1.5071754	-0.5653622
C	-1.3874617	2.4682350	-0.4981660
C	-2.3781746	2.3572962	0.4872720
C	-2.3620075	1.2944604	1.3970161
C	-1.3531557	0.3398819	1.3149866
H	1.7364255	-0.1324518	0.3179777
H	-0.3881564	-2.2613151	1.1068589
C	-0.5963501	-1.8861718	-1.5803222

C	1.9699609	-2.0676440	-1.5155774
C	2.8363351	-3.0717689	-0.7541021
C	3.0554332	-2.6267706	0.6982403
C	1.7297597	-2.6186350	1.4223311
O	1.5800612	-3.1437949	2.5159521
C	-3.4186206	3.3466082	0.5645421
N	-4.2566915	4.1442238	0.6259532
H	0.3812540	1.5856059	-1.3283699
H	-1.4083096	3.2967359	-1.1987298
H	-3.1302340	1.2212199	2.1599526
H	-1.3400221	-0.4793320	2.0270127
H	-0.6807270	-2.9257653	-1.9142522
H	-1.4859591	-1.6421747	-0.9923698
H	-0.5869054	-1.2439599	-2.4689528
H	1.7077165	-2.4846754	-2.4934247
H	2.5531234	-1.1578049	-1.7031023
H	3.8017130	-3.1890272	-1.2556504
H	2.3494813	-4.0553555	-0.7551740
H	3.4809845	-1.6140153	0.7142429
H	3.7354969	-3.2907810	1.2368870

3_1.log

E = -347.841829
H = -347.676461
G = -347.717170

NImag=0

C	-0.8611824	-0.5364645	1.0241927
C	-1.8465304	0.3331989	1.3096339
C	-1.9084994	1.5449569	2.1855551
C	-0.7838952	1.7647804	3.1881489
C	0.6085180	1.7603819	2.5579621
C	1.2061245	0.3643173	2.4192309
C	0.5538479	-0.6121831	1.4636883
O	1.2269091	-1.5417248	1.0294969
H	-1.0977502	-1.3408201	0.3301162
H	-2.7856891	0.1377087	0.7906100
H	-2.8731909	1.5188387	2.7072185
H	-1.9737393	2.4120491	1.5103441
H	-0.8297070	0.9952892	3.9702053
H	-0.9638538	2.7251602	3.6826035
H	1.2923056	2.3408037	3.1857696
H	0.5799664	2.2617884	1.5814056
H	1.1926547	-0.1305540	3.4009858
H	2.2568106	0.4183731	2.1178324

3_2.log

E = -347.842288
H = -347.676827
G = -347.716448

NImag=0

C	-0.8859987	-0.5686308	0.9764523
C	-1.8430167	0.3363761	1.2368327
C	-1.7197607	1.5805239	2.0772209
C	-0.7994250	1.4116043	3.2961449
C	0.6940746	1.5311281	2.9769210
C	1.1002473	0.9295894	1.6189880
C	0.5390578	-0.4524327	1.3763174
O	1.2424747	-1.4524383	1.4443431
H	-1.1352564	-1.4813547	0.4393876
H	-2.8398437	0.1210229	0.8544494

H	-2.7245020	1.8528530	2.4127742
H	-1.3721414	2.4187955	1.4550014
H	-1.0061960	0.4324680	3.7448789
H	-1.0594391	2.1624937	4.0490652
H	1.2748440	1.0526580	3.7725605
H	0.9833265	2.5874877	2.9597043
H	2.1892139	0.8694021	1.5485438
H	0.7389430	1.5842548	0.8175135

3_3.log

E = -347.841624
H = -347.676131
G = -347.715929

NImag=0

C	-0.7625753	-0.2865153	0.7451928
C	-1.7787848	0.4222117	1.2637790
C	-1.8243120	1.0360340	2.6360005
C	-0.7720040	2.1350279	2.8759405
C	0.6478711	1.7474576	2.4420934
C	0.9687203	0.2533879	2.6067330
C	0.5249275	-0.5815152	1.4214460
O	1.2413239	-1.4734694	0.9834496
H	-0.8625835	-0.7325833	-0.2419051
H	-2.6676076	0.5354874	0.6447577
H	-1.6794035	0.2425177	3.3785182
H	-2.8199427	1.4490469	2.8150812
H	-0.7811507	2.3612863	3.9480461
H	-1.0720333	3.0505231	2.3552124
H	1.3682980	2.3286268	3.0255529
H	0.8086578	2.0247521	1.3940898
H	0.4924288	-0.1458657	3.5127450
H	2.0441691	0.0889896	2.7124691

3_sy_c_1.log

E = -1188.219004
H = -1187.852904
G = -1187.921972

NImag=0

C	-0.5770320	4.0771109	-2.0059103
C	-0.3968130	2.6229852	-2.3712272
C	-1.6644591	4.8899690	-2.2905595
O	-1.8656134	6.0276838	-1.7404084
C	-1.3911002	1.7006457	-1.6096579
C	-1.0949857	0.2265291	-1.7181204
C	0.1673393	-0.2838021	-1.3859985
C	0.4338369	-1.6404758	-1.5124295
C	-0.5701138	-2.4955991	-1.9858889
C	-1.8335467	-2.0001212	-2.3246904
C	-2.0885863	-0.6403608	-2.1829082
C	-2.7527944	4.4305118	-3.2715045
C	-0.4216842	2.2620498	-3.8701306
S	-1.3639007	2.2163695	0.1841307
C	-2.7192733	3.4039966	0.3385501
C	-2.1536410	0.8085046	1.0006760
C	-0.2988838	-3.9020388	-2.1232804
N	-0.0809617	-5.0340850	-2.2334891
C	-2.2977087	3.8637257	-4.6207243
C	-1.7597580	2.4329210	-4.5882239
H	0.1301326	4.4729776	-1.2763348
H	0.6023001	2.3362137	-2.0185888

H	-2.4254785	1.8911533	-1.9127213
H	0.9507590	0.3749110	-1.0201829
H	1.4081802	-2.0393066	-1.2505508
H	-2.6028584	-2.6730021	-2.6887752
H	-3.0689637	-0.2475378	-2.4379421
H	-3.3979421	3.6910411	-2.7699105
H	-3.3776351	5.3123570	-3.4450019
H	-0.0901476	1.2223491	-3.9921380
H	0.3304994	2.8923561	-4.3604224
H	-2.9508516	3.4649135	1.4045740
H	-2.3840299	4.3697356	-0.0426011
H	-3.5815229	3.0315694	-0.2191372
H	-2.3444014	1.1162452	2.0307525
H	-1.4649773	-0.0364137	0.9909507
H	-3.0887736	0.5623635	0.4925843
H	-3.1553403	3.8856727	-5.3044310
H	-1.5369646	4.5281725	-5.0544564
H	-1.6335166	2.0809894	-5.6193946
H	-2.5173880	1.7757199	-4.1368773

3_sy_c_10.log

E = -1188.213830
H = -1187.847606
G = -1187.917055

NImag=0

C	-0.7253236	3.9621861	-2.0456355
C	-0.6499240	2.5125428	-2.4590005
C	-1.7483199	4.8435842	-2.3511982
O	-1.8898664	6.0115722	-1.8495925
C	-1.4962960	1.5910069	-1.5357163
C	-1.1786580	0.1219372	-1.6556562
C	-2.1953768	-0.7783787	-1.9889596
C	-1.9219873	-2.1338381	-2.1357912
C	-0.6152633	-2.5912716	-1.9350180
C	0.4129357	-1.7027127	-1.5944832
C	0.1264797	-0.3504441	-1.4617278
C	-2.7910762	4.3886601	-3.3782460
C	-1.0381146	2.1460623	-3.9262140
S	-1.2565416	2.1408404	0.2287900
C	-2.5694159	3.3577812	0.4935210
C	-1.9761560	0.7609033	1.1506605
C	-0.3240950	-3.9931159	-2.0787963
N	-0.0904456	-5.1215390	-2.1938545
C	-2.2232153	4.2328525	-4.7991095
C	-0.9816731	3.3279138	-4.8952265
H	0.0382073	4.3060779	-1.3469332
H	0.3933923	2.2011180	-2.3214316
H	-2.5652199	1.7567277	-1.7108635
H	-3.2079681	-0.4141671	-2.1373916
H	-2.7090991	-2.8327042	-2.3989892
H	1.4208816	-2.0724164	-1.4388571
H	0.9278659	0.3346813	-1.1974549
H	-3.2365825	3.4341281	-3.0663500
H	-3.5975494	5.1285465	-3.3859314
H	-2.0509439	1.7194826	-3.9519257
H	-0.3699238	1.3483448	-4.2697087
H	-2.6972919	3.4422057	1.5753083
H	-2.2520657	4.3059573	0.0592625
H	-3.4874637	2.9959021	0.0247970
H	-2.0599743	1.0888767	2.1885575
H	-1.2998901	-0.0919583	1.0888921

H	-2.9592182	0.5150512	0.7429781
H	-3.0135767	3.8189667	-5.4386831
H	-1.9821359	5.2237895	-5.2041494
H	-0.0742998	3.9076484	-4.6964925
H	-0.8954108	2.9532986	-5.9217792

3_sy_c_10_ts1.log

E = -1188.184416

H = -1187.821274

G = -1187.891969

NImag=1

C	-2.3473443	-0.1840781	-1.2156853
C	-1.1014068	-0.6370856	-0.7706540
C	-3.6026859	-0.3984413	-0.5569376
O	-4.6879631	-0.0125144	-1.0328149
C	-0.0149346	0.7658879	0.5043201
C	1.3584254	0.3774531	0.3105431
C	1.9816211	-0.4639358	1.2675996
C	3.2588369	-0.9539636	1.0753469
C	3.9751342	-0.6145026	-0.0875264
C	3.3824706	0.2192514	-1.0486984
C	2.0992532	0.7017705	-0.8540968
C	-3.5895521	-1.0949733	0.7942300
C	-0.9040733	-1.8738893	0.1048662
S	-0.5032620	2.3053390	-0.2002430
C	-2.0684768	2.6017034	0.6411101
C	0.5076359	3.5790359	0.5997683
C	5.3011966	-1.1118040	-0.2870076
N	6.3772208	-1.5164789	-0.4486177
C	-3.2777531	-2.5988613	0.7067375
C	-2.0028896	-2.9293487	-0.0835231
H	-2.3826353	0.4379835	-2.1086075
H	-0.3059325	-0.4987002	-1.5038951
H	-0.4152289	0.6567270	1.5119775
H	1.4390668	-0.7235481	2.1724002
H	3.7171525	-1.5942812	1.8228604
H	3.9323928	0.4822947	-1.9471820
H	1.6646317	1.3376087	-1.6220045
H	-2.8390641	-0.6081792	1.4319252
H	-4.5681923	-0.9461020	1.2587192
H	-0.8525213	-1.6092021	1.1675477
H	0.0701552	-2.3044068	-0.1467417
H	-2.3820728	3.6168124	0.3916681
H	-2.7937169	1.8828415	0.2626270
H	-1.9184636	2.4918821	1.7171392
H	0.1357122	4.5538618	0.2757836
H	1.5372218	3.4442171	0.2634163
H	0.4336920	3.4665523	1.6829146
H	-3.1740658	-2.9741481	1.7316478
H	-4.1332280	-3.1214212	0.2635851
H	-2.2306631	-3.0228608	-1.1506002
H	-1.6252435	-3.9042706	0.2437791

3_sy_c_11.log

E = -1188.203218

H = -1187.837240

G = -1187.906152

NImag=0

C	-0.8186777	3.1130205	-2.1064749
C	-1.9406101	2.3378277	-2.7666757

C	-0.4372101	4.4295260	-2.3215229
O	0.4499908	5.0396196	-1.6253363
C	-2.4282431	1.1453326	-1.9191426
C	-1.5398230	-0.0878393	-1.8915649
C	-0.2095110	-0.0516455	-2.3217786
C	0.5710848	-1.2028075	-2.2954422
C	0.0195706	-2.4003071	-1.8293804
C	-1.3129729	-2.4548879	-1.4037397
C	-2.0825783	-1.3001883	-1.4426718
C	-1.0441701	5.2651182	-3.4649688
C	-3.1232745	3.2164668	-3.2286374
S	-2.8708727	1.4551329	-0.1239272
C	-1.3503634	1.6360156	0.8338802
C	-3.5612512	3.1142019	-0.0027830
C	0.8263222	-3.5913935	-1.7958198
N	1.4749004	-4.5503786	-1.7681685
C	-1.4786883	4.4896988	-4.7122701
C	-2.8687336	3.8584939	-4.5949125
H	-0.2447661	2.5917364	-1.3444693
H	-1.6066891	1.8049064	-3.6809406
H	-3.4099580	0.8265938	-2.2900071
H	0.2249959	0.8739300	-2.6837658
H	1.6016989	-1.1742041	-2.6332066
H	-1.7380038	-3.3911361	-1.0578576
H	-3.1230136	-1.3491675	-1.1311952
H	-1.8831005	5.8632311	-3.0777264
H	-0.2605128	5.9821153	-3.7315597
H	-3.3021728	4.0068597	-2.4939215
H	-4.0426503	2.6192876	-3.2853548
H	-1.6419306	1.4943532	1.8768391
H	-0.6583032	0.8455867	0.5364114
H	-0.9197497	2.6230059	0.6743134
H	-3.7927024	3.2585438	1.0553189
H	-4.4800313	3.1439099	-0.5896002
H	-2.8260895	3.8402532	-0.3511032
H	-1.4658175	5.1529511	-5.5852944
H	-0.7346507	3.7070794	-4.9110983
H	-2.9943465	3.1065081	-5.3842401
H	-3.6343954	4.6261493	-4.7644050

3_sy_c_11_ts1.log

E = -1188.174490

H = -1187.811035

G = -1187.881602

NImag=1

C	1.7522951	-0.3617256	1.2414418
C	0.9766751	-0.9457564	0.2371878
C	3.1459939	-0.0473138	1.1810811
O	3.6656777	0.7645808	1.9779158
C	-0.1787477	0.4811510	-0.8846833
C	-1.5639670	0.2522750	-0.5398914
C	-2.3097657	1.0690322	0.3421315
C	-3.6043450	0.7378777	0.7086852
C	-4.1966494	-0.4357523	0.2189856
C	-3.4700594	-1.2730251	-0.6467221
C	-2.1824538	-0.9320658	-1.0150529
C	4.0596395	-0.7725729	0.1959133
C	1.5893924	-1.6696892	-0.9471747
S	0.3448104	2.1805666	-0.8195529
C	0.9586749	2.6176507	0.8423650
C	1.9074235	2.0923172	-1.7117834

C	-5.5322316	-0.7793850	0.6007724
N	-6.6158099	-1.0581049	0.9094576
C	3.8429298	-2.2933432	0.1837451
C	2.5664843	-2.7805900	-0.5425665
H	1.2317543	0.0417195	2.1082716
H	0.0239944	-1.3610773	0.5662379
H	0.1200716	0.1116802	-1.8639257
H	-1.8849421	1.9837367	0.7466393
H	-4.1622948	1.3860416	1.3773674
H	-3.9266461	-2.1810785	-1.0283582
H	-1.6309110	-1.5790086	-1.6923413
H	3.9449043	-0.3577781	-0.8136905
H	5.0826903	-0.5485062	0.5118643
H	2.1044203	-0.9577797	-1.6003780
H	0.7833405	-2.1061152	-1.5467087
H	1.0129939	3.7082148	0.8322422
H	0.2275948	2.2923520	1.5831311
H	1.9351477	2.1778586	1.0431263
H	2.3787557	3.0740048	-1.6398096
H	1.6867978	1.8562669	-2.7538529
H	2.5352264	1.3250991	-1.2555716
H	4.7171241	-2.7593519	-0.2834194
H	3.8346096	-2.6375030	1.2240277
H	2.0388873	-3.5104226	0.0820043
H	2.8497141	-3.3090650	-1.4598860

3_sy_c_12.log

E = -1188.215197

H = -1187.848968

G = -1187.917715

NImag=0

C	-1.0658392	4.1565383	-1.8313624
C	-0.7021259	2.7308812	-2.1819568
C	-1.6076552	5.1580394	-2.6282603
O	-1.7055947	6.3810054	-2.2634251
C	-1.6856500	1.6553957	-1.6321742
C	-1.2356397	0.2221508	-1.7503211
C	0.0734453	-0.1717810	-1.4401109
C	0.4586832	-1.5014211	-1.5625631
C	-0.4711026	-2.4493180	-2.0051435
C	-1.7792516	-2.0722038	-2.3293627
C	-2.1503762	-0.7397552	-2.1980063
C	-2.1390904	4.8673066	-4.0433835
C	-0.4827449	2.4572556	-3.6834375
S	-2.1405037	2.1139999	0.1089238
C	-2.9381851	0.6253681	0.7418271
C	-0.5920869	2.0690108	1.0287126
C	-0.0741042	-3.8263172	-2.1339531
N	0.2455028	-4.9346670	-2.2366157
C	-2.7670412	3.4922942	-4.2766789
C	-1.7526224	2.3726367	-4.5360411
H	-0.7117512	4.5001238	-0.8573016
H	0.2635069	2.5244803	-1.6996750
H	-2.6612622	1.7673812	-2.1179145
H	0.8095993	0.5554499	-1.1124334
H	1.4721233	-1.8055130	-1.3227622
H	-2.4902320	-2.8139927	-2.6776297
H	-3.1643770	-0.4388616	-2.4475317
H	-2.8845921	5.6470583	-4.2306514
H	-1.3303317	5.0390169	-4.7700101
H	0.0840225	1.5262042	-3.8070271

H	0.1584046	3.2631186	-4.0574672
H	-3.2295142	0.8440983	1.7712862
H	-3.8292996	0.4415122	0.1380739
H	-2.2536591	-0.2239151	0.7059283
H	-0.8471564	2.2902744	2.0673284
H	0.0628424	2.8480801	0.6362925
H	-0.1329418	1.0821207	0.9518205
H	-3.3898744	3.2480672	-3.4064193
H	-3.4514776	3.5430119	-5.1320073
H	-1.4470066	2.4012025	-5.5893485
H	-2.2393404	1.3989624	-4.3885178

3_sy_c_13.log

E = -1188.214574

H = -1187.848557

G = -1187.918247

NImag=0

C	-1.9907163	3.9443501	-2.0045264
C	-1.4860950	2.5736669	-2.3882272
C	-1.6046706	5.1053815	-2.6627039
O	-2.1054964	6.2640636	-2.4839100
C	-1.9003083	1.5474247	-1.3232616
C	-1.3930759	0.1436437	-1.5422779
C	-0.0492347	-0.1015264	-1.8539994
C	0.4020522	-1.4004511	-2.0473494
C	-0.5010991	-2.4652469	-1.9345043
C	-1.8463710	-2.2351399	-1.6277827
C	-2.2818806	-0.9293643	-1.4298512
C	-0.5361927	4.9752637	-3.7556343
C	-1.9453886	2.1003516	-3.7869946
S	-1.2371937	2.1672923	0.3220651
C	-2.6083202	3.0573006	1.1003585
C	-1.2892992	0.6832981	1.3582562
C	-0.0380858	-3.8126382	-2.1383313
N	0.3349629	-4.8966508	-2.3017889
C	-1.0879966	4.2548963	-4.9985328
C	-1.1047623	2.7241217	-4.9077376
H	-2.9054614	3.9905644	-1.4132638
H	-0.3846134	2.5716934	-2.4079380
H	-2.9886139	1.5336827	-1.1893294
H	0.6562906	0.7195548	-1.9460511
H	1.4425330	-1.5933008	-2.2866349
H	-2.5369528	-3.0678115	-1.5454346
H	-3.3239472	-0.7408076	-1.1879542
H	-0.2226581	5.9895681	-4.0209719
H	0.3517521	4.4372632	-3.3938130
H	-3.0068992	2.3521370	-3.9115968
H	-1.8573641	1.0102806	-3.8837294
H	-2.4314659	3.0115009	2.1770255
H	-2.5864159	4.0881193	0.7547565
H	-3.5505477	2.5687256	0.8446442
H	-1.0402810	1.0103737	2.3697932
H	-0.5352292	-0.0198399	1.0048394
H	-2.2875645	0.2413301	1.3291199
H	-2.1023924	4.6265194	-5.2018623
H	-0.4790526	4.5242495	-5.8705068
H	-0.0683321	2.3767358	-4.7824849
H	-1.4507124	2.3212244	-5.8674738

3_sy_c_14.log


```

E =      -1188.211194
H =      -1187.845078
G =      -1187.915061
NImag=0
C        -0.6293099      3.2362313      -2.5567811
C        -1.6202145      2.2633899      -3.1610793
C        -0.7956460      4.5771279      -2.2343264
O         0.1247493      5.3146201      -1.7375277
C        -2.1788352      1.2153775      -2.1455738
C        -1.4051250      -0.0634276     -1.9594014
C        -0.0049204      -0.0943893     -2.0077219
C         0.6822171      -1.2889484     -1.8353108
C        -0.0361580      -2.4705621     -1.6143692
C        -1.4340876      -2.4605060     -1.5710309
C        -2.1073266      -1.2568341     -1.7458097
C        -2.1462475      5.2583168      -2.4851619
C        -2.8280902      2.8682490      -3.9163029
S        -2.4169694      2.1256527      -0.5409652
C        -3.5701457      1.0390044      0.3281337
C        -0.9403855      1.8334109      0.4518805
C         0.6725567      -3.7105743     -1.4375619
N         1.2424502      -4.7084807     -1.2942618
C        -2.5039597      5.4054134      -3.9714228
C        -2.4626303      4.0864750      -4.7654010
H         0.3765736      2.8503387      -2.3922928
H        -1.0809521      1.6536060      -3.9010012
H        -3.2132516      0.9513533      -2.4002708
H         0.5576260      0.8165219      -2.1799713
H         1.7662715      -1.3107256     -1.8725271
H        -1.9819523      -3.3828777     -1.4096324
H        -3.1938695      -1.2449376     -1.7265971
H        -2.9494038      4.7151290      -1.9731057
H        -2.0939894      6.2505974      -2.0267266
H        -3.6270727      3.1359189      -3.2112401
H        -3.2436135      2.0757407      -4.5496344
H        -3.7406746      1.4801723      1.3123196
H        -4.5047554      1.0201467      -0.2349209
H        -3.1513970      0.0360155      0.4304472
H        -1.1324193      2.2996171      1.4209426
H        -0.1049716      2.3237658      -0.0467149
H        -0.7736458      0.7610993      0.5688125
H        -3.5127553      5.8325323      -4.0383915
H        -1.8281093      6.1329518      -4.4377869
H        -1.4624185      3.9298952      -5.1861470
H        -3.1473413      4.1624922      -5.6174656

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3_sy_c_14_ts1.log

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E =      -1188.180926
H =      -1187.817199
G =      -1187.887748
NImag=1
C         1.3440908      -1.4172580      0.4924527
C         1.1520951      -0.9112985     -0.8015964
C         2.5081500      -1.2520383      1.3068229
O         2.6215826      -1.7778072      2.4331904
C        -0.0537170      0.8410665     -0.9490072
C        -1.3869563      0.4142937     -0.5754532
C        -1.9029070      0.4563934      0.7386639
C        -3.1455912      -0.0818100      1.0404338
C        -3.9094338      -0.6945721      0.0381642
C        -3.4116032      -0.7631060     -1.2745460

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C	-2.1758336	-0.2170614	-1.5682472
C	3.6572971	-0.4035690	0.7796450
C	2.2905262	-0.5118537	-1.7393049
S	0.7452173	2.1994978	-0.1824593
C	-0.4358241	3.5706632	-0.0573904
C	1.0039708	1.8384751	1.5802808
C	-5.1916612	-1.2509898	0.3513242
N	-6.2304330	-1.7018964	0.6036766
C	4.4111070	-1.0341158	-0.4033210
C	3.5176229	-1.4236342	-1.5935049
H	0.5357067	-1.9926667	0.9405409
H	0.3289319	-1.3916614	-1.3293813
H	0.1059508	0.9637159	-2.0192783
H	-1.3395543	0.9143928	1.5428499
H	-3.5261961	-0.0333936	2.0559019
H	-4.0007328	-1.2380725	-2.0528363
H	-1.7991410	-0.2675653	-2.5864342
H	3.2736332	0.5774200	0.4705986
H	4.3494266	-0.2331255	1.6088916
H	2.6047867	0.5271866	-1.5848877
H	1.9068597	-0.5611285	-2.7631848
H	0.0535519	4.3709161	0.5030401
H	-0.6556917	3.8996941	-1.0740742
H	-1.3418334	3.2368905	0.4513383
H	1.9657894	2.2718112	1.8578965
H	1.0218579	0.7560815	1.7133683
H	0.2043860	2.2897279	2.1690700
H	5.1582419	-0.3050493	-0.7379674
H	4.9645215	-1.9127683	-0.0530814
H	3.1778034	-2.4596884	-1.4920650
H	4.1110331	-1.3775255	-2.5131445

3_sy_c_15.log

E = -1188.211851

H = -1187.846176

G = -1187.916058

NImag=0

C	-0.8386794	3.2463886	-2.2594261
C	-2.0522400	2.4355499	-2.6623090
C	-0.2416204	4.2258524	-3.0353628
O	0.7763692	4.9209991	-2.6943424
C	-2.3498124	1.2846528	-1.6828936
C	-1.4692391	0.0617188	-1.7244789
C	-0.0846448	0.1343078	-1.9294304
C	0.6828167	-1.0231606	-1.9706821
C	0.0657322	-2.2679059	-1.7981135
C	-1.3154540	-2.3591158	-1.5968801
C	-2.0721250	-1.1938650	-1.5657660
C	-0.8473728	4.5252366	-4.4125049
C	-3.3384456	3.2712141	-2.8595913
S	-2.4749469	1.9954984	0.0570446
C	-3.6893194	0.8913337	0.8061095
C	-0.9999407	1.4556279	0.9459666
C	0.8601991	-3.4673035	-1.8349193
N	1.4995340	-4.4324431	-1.8642071
C	-2.2639047	5.1135648	-4.3514603
C	-3.3687338	4.0722891	-4.1635530
H	-0.3693557	3.0482212	-1.2974100
H	-1.8830715	1.9047086	-3.6177661
H	-3.3830356	0.9542532	-1.8308254
H	0.3930306	1.0989425	-2.0624889

H	1.7539576	-0.9664246	-2.1338281
H	-1.7869414	-3.3285372	-1.4751142
H	-3.1479783	-1.2605539	-1.4292906
H	-0.1707473	5.2316439	-4.9027650
H	-0.8725514	3.6130669	-5.0283721
H	-3.4589789	3.9509183	-2.0043778
H	-4.2100264	2.6016594	-2.8704964
H	-3.7824644	1.1835971	1.8539577
H	-4.6393333	1.0439343	0.2915489
H	-3.3555687	-0.1450320	0.7276451
H	-1.1434061	1.7749366	1.9806862
H	-0.1282855	1.9541150	0.5223935
H	-0.9049550	0.3699716	0.8864156
H	-2.3118758	5.8603604	-3.5463960
H	-2.4692782	5.6496000	-5.2864480
H	-3.3210506	3.3639929	-5.0035367
H	-4.3429560	4.5711857	-4.2352317

3_sy_c_15_ts1.log

E = -1188.144571

H = -1187.782372

G = -1187.853562

NImag=1

C	2.7818513	0.3742425	-0.3884581
C	1.6010843	-0.3117336	-0.5431567
C	3.6255695	-0.0434520	0.7269764
O	4.6488611	0.5369292	1.0948202
C	-0.3432768	1.1223782	-0.9183967
C	-1.4770764	0.4024567	-0.4437288
C	-1.9896267	0.4697557	0.8816859
C	-3.0544223	-0.3148951	1.2861767
C	-3.6634333	-1.2103286	0.3907820
C	-3.1804139	-1.2944742	-0.9301720
C	-2.1220962	-0.5072498	-1.3324312
C	3.3369938	-1.4825156	1.1789886
C	1.4183455	-1.3385169	-1.6028225
S	0.3049550	2.5612786	-0.2218918
C	-1.0372080	3.7543228	0.0416029
C	0.7835282	2.2599092	1.5136845
C	-4.7602873	-2.0203960	0.8133219
N	-5.6526513	-2.6804203	1.1566687
C	3.2808714	-2.4495921	-0.0456901
C	1.9596521	-2.5964772	-0.8435624
H	3.3095094	0.7785389	-1.2521892
H	1.1055728	-0.6168246	0.3806724
H	-0.1197786	1.1015913	-1.9797444
H	-1.5475415	1.1395041	1.6108033
H	-3.4224028	-0.2411699	2.3053069
H	-3.6506617	-1.9758773	-1.6330357
H	-1.7705840	-0.5719765	-2.3584887
H	4.1443701	-1.7866573	1.8515101
H	2.3986110	-1.5365959	1.7460776
H	2.0240151	-1.1172944	-2.4878228
H	0.3822695	-1.5252498	-1.9011998
H	-0.6188080	4.6071109	0.5814922
H	-1.3846893	4.0666412	-0.9441872
H	-1.8481143	3.2975472	0.6114072
H	1.6995795	2.8228267	1.6982357
H	0.9656740	1.1958446	1.6553099
H	-0.0110832	2.6084102	2.1742809
H	4.0884151	-2.1719685	-0.7366900

H	3.5252630	-3.4527803	0.3215440
H	1.1734847	-2.9211469	-0.1499287
H	2.0975313	-3.4047223	-1.5711775

3_sy_c_16.log

E = -1188.211006
H = -1187.845011
G = -1187.914012

NImag=0

C	-2.2199701	3.7760619	-1.9604022
C	-1.5456154	2.4665494	-2.2966036
C	-1.8382148	4.9935685	-2.4956168
O	-2.4375830	6.1106419	-2.3232000
C	-2.0274279	1.3555357	-1.3525144
C	-1.4754903	-0.0322863	-1.6096809
C	-2.3372358	-1.1315696	-1.5520625
C	-1.8599688	-2.4192944	-1.7675867
C	-0.4998115	-2.6059151	-2.0372605
C	0.3760303	-1.5149566	-2.0954196
C	-0.1164295	-0.2336099	-1.8826216
C	-0.6250606	5.0005051	-3.4357863
C	-1.7620286	2.0271176	-3.7679999
S	-1.6320115	1.6500534	0.4557299
C	-0.0796879	2.5632865	0.4594195
C	-2.7804049	2.8822041	1.1066124
C	0.0057518	-3.9348296	-2.2598872
N	0.4129030	-5.0041959	-2.4380403
C	-0.9299541	4.2978036	-4.7694443
C	-0.8288529	2.7684853	-4.7326592
H	-3.1683760	3.7291236	-1.4262525
H	-0.4541068	2.5456349	-2.1660594
H	-3.1241182	1.3127001	-1.3413735
H	-3.3918012	-0.9782434	-1.3404916
H	-2.5300348	-3.2716150	-1.7291348
H	1.4277819	-1.6729880	-2.3096147
H	0.5652810	0.6100812	-1.9439749
H	-0.3670302	6.0485594	-3.6168570
H	0.2490981	4.5204964	-2.9703962
H	-2.8127886	2.2032791	-4.0320763
H	-1.5716241	0.9548399	-3.8979713
H	0.1332274	2.7912089	1.5061201
H	0.7004191	1.9126287	0.0611032
H	-0.1944245	3.4762936	-0.1278873
H	-2.6752854	2.8388881	2.1929440
H	-3.7898721	2.5803571	0.8213764
H	-2.5352983	3.8683796	0.7171699
H	-1.9329850	4.5965556	-5.1057272
H	-0.2279137	4.6532882	-5.5341831
H	0.2058419	2.4995721	-4.4720348
H	-1.0011279	2.3824044	-5.7448547

3_sy_c_16_ts1.log

E = -1188.145192
H = -1187.783566
G = -1187.855855

NImag=1

C	2.4992763	-0.7751942	-0.9513184
C	1.4320731	-0.7736633	-0.0840674
C	3.7929218	-1.1430327	-0.3913862
O	4.8661582	-1.0872310	-0.9975091

C	0.0711653	1.2554017	-0.4380294
C	-1.2708441	0.7724919	-0.4154446
C	-1.7901615	0.1672104	-1.5950889
C	-3.0402039	-0.4156899	-1.6224916
C	-3.8471975	-0.4179454	-0.4679507
C	-3.3640735	0.1869292	0.7068942
C	-2.1114616	0.7691122	0.7323079
C	3.6687759	-1.9653159	0.8984878
C	0.4287914	-1.8723446	-0.0719006
S	0.5907725	2.3293664	0.8174653
C	2.3803895	2.3959976	0.6116739
C	0.1798131	4.0214321	0.2940242
C	-5.1426528	-1.0162239	-0.4922376
N	-6.1969332	-1.5043472	-0.5124281
C	2.6550129	-3.1364218	0.7061484
C	1.1419889	-2.8696695	0.9043194
H	2.3569682	-1.0129124	-2.0055159
H	1.6502978	-0.4472900	0.9351514
H	0.5381167	1.4513748	-1.3994463
H	-1.1752927	0.1569556	-2.4912518
H	-3.4074219	-0.8745251	-2.5358575
H	-3.9831247	0.1963095	1.5991233
H	-1.7716046	1.2210463	1.6599615
H	4.6584922	-2.3682745	1.1322561
H	3.3615113	-1.3356679	1.7437327
H	0.2978862	-2.3146122	-1.0656181
H	-0.5487385	-1.6164167	0.3477429
H	2.7338436	3.2582222	1.1799951
H	2.8145254	1.4818928	1.0167032
H	2.6197165	2.5065994	-0.4481511
H	0.5739369	4.7202034	1.0357926
H	-0.9092968	4.0862730	0.2575775
H	0.6127803	4.2038250	-0.6917128
H	2.8178337	-3.5689020	-0.2903872
H	2.9204729	-3.9194745	1.4254583
H	0.9920586	-2.4896028	1.9228503
H	0.6222911	-3.8330171	0.8443304

3_sy_c_17.log

E = -1188.204376

H = -1187.838577

G = -1187.908324

NImag=0

C	-0.8627918	3.1722717	-1.9779128
C	-2.0432687	2.4133697	-2.5405001
C	-0.1125875	4.0856279	-2.6984561
O	0.8940543	4.7371761	-2.2494999
C	-2.4776085	1.1952297	-1.7053519
C	-1.6076490	-0.0463802	-1.7900294
C	-2.1698949	-1.2852452	-1.4530773
C	-1.4158209	-2.4493795	-1.5174359
C	-0.0811851	-2.3738969	-1.9331209
C	0.4898065	-1.1465332	-2.2861103
C	-0.2747244	0.0128324	-2.2093439
C	-0.5088714	4.3587888	-4.1567484
C	-3.2584416	3.2937276	-2.9252268
S	-2.8014294	1.4229222	0.1290363
C	-1.2214155	1.5402361	1.0006291
C	-3.4747314	3.0790764	0.3505815
C	0.7092288	-3.5743293	-2.0038073
N	1.3447221	-4.5408537	-2.0595030

C	-1.8953746	4.9953613	-4.3334620
C	-3.0659554	4.0111812	-4.2639288
H	-0.5433964	2.9712498	-0.9606202
H	-1.7556216	1.9152147	-3.4871559
H	-3.4879455	0.9026360	-2.0142877
H	-3.2115946	-1.3437166	-1.1474864
H	-1.8536585	-3.4075414	-1.2585035
H	1.5228922	-1.1025146	-2.6146931
H	0.1655265	0.9698857	-2.4718577
H	0.2570829	5.0263199	-4.5629864
H	-0.4730731	3.4266786	-4.7425392
H	-3.4450731	4.0388959	-2.1444202
H	-4.1603207	2.6707878	-3.0062443
H	-1.4145281	1.1935628	2.0171496
H	-0.5050561	0.8742503	0.5152029
H	-0.8650220	2.5693986	1.0039664
H	-3.6318280	3.1965896	1.4253173
H	-4.4320823	3.1238348	-0.1706019
H	-2.7686384	3.8191871	-0.0272182
H	-2.0284700	5.7841730	-3.5793953
H	-1.9357279	5.4905356	-5.3117246
H	-2.9303962	3.2536955	-5.0498216
H	-3.9923308	4.5465938	-4.5055121

3_sy_c_18.log

E = -1188.218447

H = -1187.852400

G = -1187.920656

NImag=0

C	-2.2920003	3.8536615	-1.9980849
C	-1.6704507	2.5316482	-2.3871481
C	-1.8926945	5.0690956	-2.5350076
O	-2.4513995	6.1972019	-2.3260128
C	-2.1670398	1.4190773	-1.4513812
C	-1.5490513	0.0562677	-1.6240095
C	-0.1802613	-0.1063384	-1.8750948
C	0.3654834	-1.3765535	-2.0156497
C	-0.4662128	-2.4975123	-1.9115592
C	-1.8374053	-2.3524487	-1.6731232
C	-2.3673519	-1.0758606	-1.5305330
C	-0.7120915	5.0535264	-3.5153333
C	-1.9288221	2.1151644	-3.8544218
S	-1.9773503	2.0419252	0.3038765
C	-2.0929194	0.5431028	1.3025744
C	-0.2210525	2.4008918	0.4723852
C	0.0953980	-3.8140515	-2.0609347
N	0.5478351	-4.8733166	-2.1803228
C	-1.0743466	4.3752116	-4.8476371
C	-1.0032059	2.8440018	-4.8343884
H	-3.2295199	3.8303286	-1.4410465
H	-0.5758071	2.5800175	-2.2723649
H	-3.2589849	1.3373047	-1.5256179
H	0.4692894	0.7576798	-1.9767742
H	1.4252297	-1.5021993	-2.2109804
H	-2.4742929	-3.2279893	-1.6029899
H	-3.4310752	-0.9552475	-1.3452388
H	-0.4327146	6.0965966	-3.6926094
H	0.1627028	4.5461097	-3.0819879
H	-2.9819298	2.3145136	-4.0925380
H	-1.7637528	1.0381860	-3.9897560
H	-1.9868676	0.8593552	2.3425299

H	-3.0848318	0.1135427	1.1496781
H	-1.3091066	-0.1664238	1.0323263
H	-0.0637774	2.6587009	1.5220092
H	0.0074265	3.2607504	-0.1587528
H	0.3747454	1.5269842	0.2038087
H	-2.0809789	4.6984710	-5.1485573
H	-0.3891635	4.7283361	-5.6283624
H	0.0315820	2.5503705	-4.6027400
H	-1.2085334	2.4748177	-5.8466299

3_sy_c_18_ts1.log

E = -1188.144341
H = -1187.782008
G = -1187.853174

NImag=1

C	2.8297947	0.3244824	-0.6175459
C	1.6266743	-0.3317289	-0.5119725
C	3.8216018	0.0182624	0.4089625
O	4.9084929	0.5871382	0.5301978
C	-0.3239167	1.1279069	-0.8621032
C	-1.4937609	0.4119330	-0.4676969
C	-2.0494534	0.4058628	0.8404365
C	-3.1570106	-0.3615758	1.1542963
C	-3.7654156	-1.1689470	0.1790267
C	-3.2356650	-1.1855941	-1.1262160
C	-2.1354396	-0.4140912	-1.4364401
C	3.5630605	-1.3273991	1.1003050
C	1.2773336	-1.4818445	-1.3854131
S	0.2836337	2.5685647	-0.1323477
C	-1.0952150	3.6849289	0.2459738
C	0.8726395	2.2665738	1.5574791
C	-4.9070297	-1.9616137	0.5064376
N	-5.8357947	-2.6068704	0.7720743
C	3.3139243	-2.4511030	0.0450481
C	1.8910575	-2.6474023	-0.5376585
H	3.2344985	0.5875128	-1.5947449
H	1.2540565	-0.4856052	0.5029367
H	-0.0696084	1.1381133	-1.9169615
H	-1.6066447	1.0012677	1.6297942
H	-3.5572005	-0.3440121	2.1637071
H	-3.7021991	-1.8016145	-1.8892535
H	-1.7458754	-0.4269824	-2.4507955
H	4.4480526	-1.5703753	1.6954758
H	2.7103498	-1.2601719	1.7884076
H	1.7607967	-1.4067648	-2.3649961
H	0.2067646	-1.6669154	-1.5131788
H	-0.6792346	4.5613019	0.7481913
H	-1.5444401	3.9733428	-0.7054127
H	-1.8274791	3.1892326	0.8848106
H	1.3192399	3.2064059	1.8896706
H	1.6398438	1.4944205	1.5183078
H	0.0580805	1.9852004	2.2227541
H	4.0238337	-2.3072107	-0.7808022
H	3.5822833	-3.4038977	0.5151764
H	1.2026690	-2.8424846	0.2944288
H	1.9062015	-3.5507943	-1.1583516

3_sy_c_19.log

E = -1188.210132
H = -1187.844082

G = -1187.914059
NImag=0

C	-0.8061927	3.2202075	-2.3229862
C	-1.9337462	2.3591345	-2.8640615
C	-0.5305871	4.5616394	-2.5681505
O	0.3881072	5.2163104	-1.9656014
C	-2.2957256	1.2272397	-1.8771367
C	-1.4078712	0.0070104	-1.8334838
C	-0.0495595	0.0513031	-2.1738005
C	0.7304452	-1.0979734	-2.1219981
C	0.1510357	-2.3084010	-1.7254941
C	-1.2090535	-2.3768801	-1.4054585
C	-1.9778274	-1.2214840	-1.4697534
C	-1.3044155	5.3652085	-3.6277793
C	-3.2074570	3.1638921	-3.1918402
S	-2.4984024	2.0224693	-0.1869833
C	-3.6772061	0.9112259	0.6147845
C	-1.0307835	1.6084446	0.7783501
C	0.9566645	-3.4992191	-1.6647135
N	1.6042646	-4.4579058	-1.6138554
C	-1.8264554	4.5703541	-4.8262667
C	-3.1520235	3.8573615	-4.5558301
H	-0.1053406	2.7486514	-1.6386116
H	-1.6604278	1.8053848	-3.7828607
H	-3.3188517	0.8849882	-2.0697711
H	0.4063900	0.9813951	-2.4934252
H	1.7814210	-1.0601424	-2.3885938
H	-1.6568487	-3.3237569	-1.1230590
H	-3.0409799	-1.2815954	-1.2549281
H	-2.1310974	5.9061742	-3.1429549
H	-0.5996432	6.1311109	-3.9678942
H	-3.3626328	3.9097769	-2.4015500
H	-4.0821587	2.5012852	-3.1802533
H	-3.8884392	1.3365476	1.5979851
H	-4.5884257	0.8967097	0.0144363
H	-3.2550366	-0.0894350	0.7190310
H	-1.2644580	1.8837186	1.8094325
H	-0.1943452	2.2026893	0.4139364
H	-0.8260447	0.5386582	0.7052129
H	-1.9541174	5.2366064	-5.6876501
H	-1.0645777	3.8348740	-5.1163258
H	-3.3329318	3.1172410	-5.3454695
H	-3.9739642	4.5824805	-4.6091285

3_sy_c_1_r.log
E = -1188.209494
H = -1187.843697
G = -1187.912810
NImag=0

C	0.2129446	-0.6899499	1.9860076
C	1.1517724	-0.5347797	0.8150608
C	0.1212789	0.0347817	3.1690787
O	-0.8153673	-0.1294718	4.0248534
C	0.5504955	0.5038658	-0.1990803
C	0.3226208	1.9197293	0.2776449
C	1.2891067	2.9279269	0.1918544
C	1.0408236	4.1962512	0.7032734
C	-0.1918488	4.4608253	1.3098429
C	-1.1798468	3.4714081	1.3816706
C	-0.9206354	2.2138761	0.8515259
C	1.1672017	1.0945930	3.5435452

C	2.6607699	-0.4145036	1.0975297
S	1.5327152	0.5729519	-1.7750482
C	1.4885461	-1.1440605	-2.3210352
C	0.3367626	1.3129080	-2.9055030
C	-0.4529655	5.7691747	1.8482611
N	-0.6630949	6.8227893	2.2808629
C	2.6393554	0.6916817	3.4260689
C	3.1893117	0.6990796	2.0022647
H	-0.6149450	-1.3780648	1.8084367
H	1.0659554	-1.4775785	0.2604589
H	-0.4125419	0.0915462	-0.5216297
H	2.2569578	2.7360755	-0.2627859
H	1.7949291	4.9733571	0.6380234
H	-2.1387016	3.6914063	1.8392119
H	-1.6861096	1.4456856	0.8946639
H	0.9994641	2.0032975	2.9445410
H	0.9474360	1.3616076	4.5820798
H	3.2052050	-0.3640428	0.1419302
H	2.9490398	-1.3736004	1.5478313
H	1.7783255	-1.1437790	-3.3737098
H	2.2173499	-1.7087092	-1.7384915
H	0.4799429	-1.5437104	-2.1958242
H	0.7634433	1.2605873	-3.9087469
H	0.2025823	2.3554461	-2.6129183
H	-0.6048369	0.7630319	-2.8489153
H	3.2360180	1.3947807	4.0205679
H	2.7870733	-0.3008728	3.8752459
H	4.2800438	0.5860316	2.0437132
H	3.0033882	1.6833547	1.5599683

3_sy_c_1_ts1.log

E = -1188.185890
H = -1187.822808
G = -1187.893969

NImag=1

C	2.2988625	-0.2531909	1.3862858
C	1.0653775	-0.7407119	0.9479633
C	3.6157789	-0.4406590	0.8441709
O	4.6082840	0.0716564	1.3988132
C	0.0352670	0.5727013	-0.5124507
C	-1.3608422	0.3039853	-0.2765318
C	-2.0664107	0.7892044	0.8534400
C	-3.3820665	0.4283294	1.0907753
C	-4.0450128	-0.4396064	0.2090150
C	-3.3651976	-0.9395102	-0.9170061
C	-2.0541932	-0.5718227	-1.1509949
C	3.8566998	-1.1705885	-0.4709028
C	0.8105620	-2.0493219	0.2363297
S	0.6130374	2.1490107	0.0314277
C	2.1905730	2.2840117	-0.8272257
C	-0.3321274	3.3788622	-0.9052858
C	-5.4044985	-0.8115552	0.4536200
N	-6.5075289	-1.1144352	0.6515754
C	3.1549434	-2.5106849	-0.6928686
C	1.6606185	-2.3946086	-0.9799410
H	2.2767272	0.4531301	2.2153996
H	0.2521179	-0.5017457	1.6361066
H	0.4051744	0.3547347	-1.5136906
H	-1.5780326	1.4566845	1.5597749
H	-3.9035029	0.8137407	1.9616582
H	-3.8764885	-1.6080408	-1.6029044

H	-1.5378890	-0.9571332	-2.0264468
H	3.5593968	-0.4807851	-1.2768484
H	4.9404946	-1.2974893	-0.5465435
H	-0.2479783	-2.0917194	-0.0391144
H	0.9544922	-2.8330919	0.9960564
H	2.5075614	3.3254138	-0.7477782
H	2.9081786	1.6387335	-0.3240711
H	2.0532574	1.9965433	-1.8718002
H	0.0787026	4.3643570	-0.6736831
H	-1.3699834	3.3220653	-0.5721393
H	-0.2537462	3.1574345	-1.9713006
H	3.6377973	-2.9969444	-1.5480398
H	3.3176250	-3.1674111	0.1725500
H	1.2971338	-3.3494847	-1.3775072
H	1.5031864	-1.6470421	-1.7692109

3_sy_c_1_ts2.log

E = -1188.198829

H = -1187.834525

G = -1187.904511

NImag=1

C	-1.7225602	1.4354368	-1.2126577
C	-2.1055540	0.5118777	-0.0775198
C	-0.7268643	2.4270990	-1.2936697
O	-0.4339619	2.9908678	-2.3871355
C	-1.1157646	-0.5360498	-0.4874682
C	0.3601559	-0.4692043	-0.2391576
C	0.9039086	-0.5973927	1.0444623
C	2.2789388	-0.5495704	1.2406673
C	3.1224150	-0.3813347	0.1366796
C	2.5970909	-0.2822388	-1.1580004
C	1.2211524	-0.3406047	-1.3367638
C	0.0386466	2.9054709	-0.0612733
C	-2.2099458	1.0047620	1.3695928
S	-1.6151948	-2.4531651	0.5091707
C	-3.2414671	-2.6772527	-0.2403857
C	-0.6238788	-3.5236864	-0.5550313
C	4.5466575	-0.3253754	0.3315372
N	5.6933923	-0.2807439	0.4879197
C	-0.7870942	3.1577878	1.2032823
C	-1.1299260	1.8957772	1.9901883
H	-2.1993955	1.2004066	-2.1625033
H	-3.0954880	0.1077776	-0.3157158
H	-1.3480124	-0.9410850	-1.4735263
H	0.2531400	-0.7425468	1.9013436
H	2.6978239	-0.6443285	2.2370232
H	3.2610751	-0.1655447	-2.0080625
H	0.8040850	-0.2638215	-2.3366737
H	0.8381695	2.1845298	0.1691262
H	0.5342496	3.8306832	-0.3707660
H	-2.3574414	0.1271196	2.0154342
H	-3.1511292	1.5685605	1.4085835
H	-3.5092201	-3.7347243	-0.1938346
H	-3.9612946	-2.0953268	0.3376102
H	-3.2251409	-2.3368688	-1.2797727
H	-0.9806530	-4.5507833	-0.4573529
H	0.4124549	-3.4636089	-0.2170946
H	-0.7019467	-3.1919856	-1.5942757
H	-0.2065179	3.8162997	1.8601920
H	-1.7049444	3.7042140	0.9452842
H	-1.5004294	2.1850251	2.9814075

H -0.2036409 1.3409679 2.1655394

3_sy_c_2.log

E = -1188.214634

H = -1187.848539

G = -1187.917953

NImag=0

C	-0.6533842	4.0449356	-1.9139054
C	-0.5487186	2.6023072	-2.3447924
C	-1.3195705	5.1082971	-2.5054754
O	-1.3026255	6.3018727	-2.0415022
C	-1.5114694	1.6284176	-1.5977137
C	-1.1339828	0.1745719	-1.7292222
C	0.1408185	-0.2790410	-1.3638578
C	0.4822496	-1.6167568	-1.5142257
C	-0.4581756	-2.5098638	-2.0431090
C	-1.7348805	-2.0718944	-2.4118548
C	-2.0654270	-0.7316246	-2.2466210
C	-2.1420821	4.9265795	-3.7940250
C	-0.6886055	2.3463854	-3.8573640
S	-1.5453813	2.0970095	0.2028998
C	-2.9148709	3.2733036	0.2950191
C	-2.3562695	0.6709214	0.9596736
C	-0.1075419	-3.8959208	-2.2055736
N	0.1742527	-5.0115984	-2.3361030
C	-2.9336344	3.6222258	-3.9157366
C	-2.1131826	2.4282154	-4.4182020
H	-0.0954847	4.2992320	-1.0103383
H	0.4608625	2.2648166	-2.0723201
H	-2.5496949	1.7683372	-1.9139018
H	0.8753546	0.4070515	-0.9505935
H	1.4666949	-1.9711121	-1.2272986
H	-2.4559410	-2.7741411	-2.8169398
H	-3.0564929	-0.3837530	-2.5241687
H	-2.8311918	5.7769292	-3.8141590
H	-1.4810316	5.0457379	-4.6658034
H	-0.2750668	1.3590545	-4.0998403
H	-0.0518485	3.0827402	-4.3602843
H	-3.1241363	3.4268327	1.3561435
H	-2.5862839	4.1984767	-0.1769942
H	-3.7818665	2.8482060	-0.2151606
H	-2.6044390	0.9621964	1.9823886
H	-1.6541092	-0.1628855	0.9739979
H	-3.2592765	0.4187442	0.3994386
H	-3.3752445	3.3972503	-2.9356632
H	-3.7789506	3.7696132	-4.5985784
H	-2.0369310	2.4813137	-5.5113416
H	-2.6554408	1.4990166	-4.1978916

3_sy_c_20.log

E = -1188.208113

H = -1187.842180

G = -1187.912387

NImag=0

C	-1.4409045	4.0010079	-1.9512001
C	-1.3057113	2.5667419	-2.4107920
C	-1.7816181	5.1422926	-2.6676641
O	-1.8693033	6.3060993	-2.1415898
C	-1.8134667	1.5524288	-1.3455077
C	-1.3409462	0.1385955	-1.5850654

C	0.0241080	-0.1552904	-1.7000402
C	0.4471068	-1.4600636	-1.9205480
C	-0.5056693	-2.4796740	-2.0361012
C	-1.8723442	-2.2002645	-1.9280896
C	-2.2800019	-0.8911480	-1.6986133
C	-2.0204306	5.0959531	-4.1882698
C	-2.1117478	2.2314170	-3.6812755
S	-1.2955819	2.0520459	0.3825932
C	-2.7454818	2.9539482	0.9768506
C	-1.5098174	0.5375848	1.3433262
C	-0.0730179	-3.8326269	-2.2667207
N	0.2749545	-4.9214831	-2.4520070
C	-1.0483532	4.1911929	-4.9524217
C	-1.4802652	2.7228164	-4.9837087
H	-1.1030191	4.2202863	-0.9375942
H	-0.2535317	2.2954607	-2.6059189
H	-2.9086265	1.5799474	-1.2981319
H	0.7685847	0.6305505	-1.6058905
H	1.5038017	-1.6913624	-2.0029794
H	-2.6009550	-2.9987902	-2.0198118
H	-3.3386977	-0.6649666	-1.6093524
H	-3.0588091	4.8098108	-4.4094213
H	-1.9080293	6.1317529	-4.5225442
H	-3.1153441	2.6592749	-3.5611734
H	-2.2457203	1.1460021	-3.7631630
H	-2.5575291	3.2048401	2.0226917
H	-2.8499520	3.8574850	0.3779182
H	-3.6234552	2.3122408	0.8804436
H	-1.4480537	0.8355885	2.3922872
H	-0.6957269	-0.1473893	1.1063591
H	-2.4822651	0.0918935	1.1253985
H	-0.9341024	4.5471348	-5.9832262
H	-0.0585480	4.2758798	-4.4855904
H	-0.6176766	2.0909153	-5.2304803
H	-2.2146526	2.5773713	-5.7861756

3_sy_c_2_r.log

E = -1188.206945

H = -1187.840954

G = -1187.909878

NImag=0

C	0.3701233	-0.2259329	-2.0428564
C	-0.6938297	-0.3394687	-0.9802516
C	0.2893792	0.1816873	-3.3657646
O	1.2728471	0.1181553	-4.1862804
C	-0.3673993	0.6215447	0.2232063
C	-0.3132121	2.1072125	-0.0486796
C	-1.3891208	2.9787563	0.1528632
C	-1.2924865	4.3212423	-0.1933266
C	-0.1013123	4.8032115	-0.7468113
C	0.9961277	3.9532806	-0.9258506
C	0.8866935	2.6164860	-0.5638762
C	-1.0134659	0.7390124	-3.9674764
C	-2.1524815	-0.3409059	-1.4647382
S	-1.5176915	0.3114155	1.6387202
C	-1.2701723	-1.4444240	1.9649812
C	-0.5985946	1.0320768	3.0146531
C	0.0026185	6.1897357	-1.1162773
N	0.0858669	7.3060029	-1.4137421
C	-1.8320446	1.6661245	-3.0660355
C	-2.7452628	0.9322943	-2.0801778

H	1.3531790	-0.5837061	-1.7307985
H	-0.5575643	-1.3306456	-0.5260118
H	0.6091805	0.3070159	0.6109388
H	-2.3282814	2.6258896	0.5689600
H	-2.1326717	4.9899424	-0.0394879
H	1.9230658	4.3388367	-1.3372269
H	1.7383722	1.9563634	-0.6885546
H	-0.6994332	1.2830540	-4.8637959
H	-1.6418337	-0.0938703	-4.3180882
H	-2.8101987	-0.6626187	-0.6438331
H	-2.2050154	-1.1459388	-2.2074287
H	-1.6725759	-1.6310688	2.9628728
H	-1.8355206	-2.0155015	1.2283027
H	-0.2047399	-1.6802721	1.9245578
H	-1.1230132	0.7587728	3.9321587
H	-0.6050339	2.1159852	2.8920840
H	0.4204809	0.6405561	3.0129649
H	-1.1409405	2.3251634	-2.5261248
H	-2.4558353	2.3216704	-3.6863261
H	-3.6609238	0.6312451	-2.6054519
H	-3.0678300	1.6240028	-1.2950224

3_sy_c_2_ts1.log

E = -1188.186643

H = -1187.823337

G = -1187.892858

NImag=1

C	-2.3761409	-0.2718737	-1.3598664
C	-1.1044172	-0.6925122	-0.9583391
C	-3.6495158	-0.7383938	-0.8919246
O	-4.7164629	-0.3060184	-1.3714097
C	-0.0994766	0.6132888	0.4915507
C	1.2961492	0.3156493	0.2772988
C	2.0039336	0.7246887	-0.8802016
C	3.3140852	0.3315172	-1.0999152
C	3.9665787	-0.4925351	-0.1708267
C	3.2845207	-0.9139736	0.9859602
C	1.9801583	-0.5136774	1.2020559
C	-3.7389018	-1.7843051	0.2158309
C	-0.8377480	-2.0137935	-0.2674801
S	-0.6544536	2.1760068	-0.1137815
C	-2.2425672	2.3415218	0.7183145
C	0.2886154	3.4348569	0.7843108
C	5.3205002	-0.8966510	-0.3961373
N	6.4186747	-1.2255129	-0.5784342
C	-2.7635707	-1.5507138	1.3766997
C	-1.3901398	-2.1836867	1.1552345
H	-2.4352921	0.5183528	-2.1074477
H	-0.3085177	-0.3980457	-1.6442862
H	-0.4794842	0.4414084	1.4978652
H	1.5233056	1.3589445	-1.6214640
H	3.8384195	0.6584969	-1.9926811
H	3.7899575	-1.5461071	1.7096292
H	1.4638245	-0.8352396	2.1023679
H	-4.7742351	-1.7613525	0.5667684
H	-3.5721337	-2.7796386	-0.2206414
H	0.2420528	-2.1947754	-0.2535011
H	-1.2687002	-2.7906093	-0.9131873
H	-2.6174244	3.3433407	0.5013839
H	-2.9143309	1.5892315	0.3050964
H	-2.0962152	2.2023706	1.7916249

H	-0.1290619	4.4116780	0.5290434
H	1.3247014	3.3748790	0.4460292
H	0.2173152	3.2414408	1.8562068
H	-2.6534156	-0.4700853	1.5350087
H	-3.1931903	-1.9545423	2.2998237
H	-1.4500227	-3.2588627	1.3632970
H	-0.6810417	-1.7666139	1.8788065

3_sy_c_2_ts2.log

E = -1188.191007
H = -1187.826573
G = -1187.896588

NImag=1

C	-1.9773889	1.2613649	-0.9707461
C	-2.0882741	0.2600132	0.1553776
C	-1.5579040	2.6085108	-0.9709587
O	-1.6227828	3.3195115	-2.0119212
C	-1.0341942	-0.6154778	-0.4426210
C	0.4447607	-0.4464555	-0.2976754
C	1.1019399	-0.6972185	0.9127665
C	2.4788529	-0.5464922	1.0166520
C	3.2121875	-0.1561218	-0.1098921
C	2.5764373	0.0600708	-1.3389747
C	1.1994529	-0.0997316	-1.4263069
C	-1.0661296	3.3112154	0.2959714
C	-2.0189209	0.7463984	1.6067141
S	-1.2889438	-2.6990489	0.4214060
C	-2.9239765	-3.0329145	-0.2671696
C	-0.2607884	-3.5556802	-0.7920880
C	4.6378229	0.0076799	-0.0065896
N	5.7854416	0.1396609	0.0768257
C	-0.1183169	2.5045378	1.1827005
C	-0.8176107	1.5453106	2.1480462
H	-2.4057979	0.9304087	-1.9144407
H	-3.0458474	-0.2696493	0.0702680
H	-1.3174460	-0.9840920	-1.4293524
H	0.5383704	-1.0157486	1.7839608
H	2.9850264	-0.7331517	1.9580207
H	3.1566234	0.3471099	-2.2096269
H	0.6961761	0.0685539	-2.3738663
H	-0.5710110	4.2233412	-0.0499585
H	-1.9428657	3.6314562	0.8783412
H	-2.1717367	-0.1238437	2.2588262
H	-2.9184225	1.3631108	1.7234427
H	-3.0627677	-4.1134517	-0.3434995
H	-3.6687332	-2.6197148	0.4148705
H	-3.0183796	-2.5718240	-1.2543878
H	-0.5036164	-4.6200231	-0.7786154
H	0.7834701	-3.4163138	-0.5058005
H	-0.4354490	-3.1407907	-1.7890042
H	0.5870585	1.9621654	0.5422867
H	0.4872215	3.1965403	1.7800628
H	-1.1997939	2.1326068	2.9926762
H	-0.0708221	0.8709429	2.5755826

3_sy_c_3.log

E = -1188.213514
H = -1187.847375
G = -1187.915601

NImag=0

C	-0.8171097	4.0719919	-1.8001545
C	-0.4709424	2.6321469	-2.0920654
C	-1.8988917	4.7955890	-2.2758740
O	-2.2693900	5.9216194	-1.7915599
C	-1.5314115	1.6210653	-1.5711679
C	-1.1934301	0.1559204	-1.7620083
C	-2.1563760	-0.7059799	-2.2974944
C	-1.8743162	-2.0528901	-2.4930715
C	-0.6119654	-2.5432486	-2.1409626
C	0.3622347	-1.6942234	-1.6016241
C	0.0671314	-0.3491632	-1.4183139
C	-2.7588109	4.2546260	-3.4281720
C	-0.1737019	2.3000633	-3.5731567
S	-1.9783979	1.7888131	0.2250731
C	-0.4657884	2.2560274	1.0828805
C	-2.9914317	3.2768851	0.3792084
C	-0.3101697	-3.9363570	-2.3380097
N	-0.0673462	-5.0576289	-2.4960846
C	-2.0177829	3.7433606	-4.6685543
C	-1.3624740	2.3677415	-4.5325259
H	-0.2900075	4.5286964	-0.9624963
H	0.4579435	2.4119065	-1.5499179
H	-2.5038819	1.8185745	-2.0354123
H	-3.1351012	-0.3181721	-2.5672596
H	-2.6202670	-2.7196129	-2.9126873
H	1.3386359	-2.0860187	-1.3366673
H	0.8333621	0.3081402	-1.0173488
H	-3.4224803	3.4602018	-3.0508790
H	-3.4122908	5.0837390	-3.7177745
H	0.2717843	1.2999715	-3.6431318
H	0.5939487	3.0104636	-3.9033003
H	-0.7417500	2.3877155	2.1315426
H	0.2423771	1.4305199	0.9945266
H	-0.0644877	3.1796753	0.6670331
H	-3.3433659	3.2873216	1.4135624
H	-3.8408946	3.1530643	-0.2964357
H	-2.4202009	4.1684191	0.1242489
H	-2.7351761	3.6913887	-5.4970599
H	-1.2564854	4.4801053	-4.9617556
H	-1.0102789	2.0495571	-5.5214323
H	-2.1280131	1.6344847	-4.2383174

3_sy_c_3_r.log

E = -1188.203491

H = -1187.837489

G = -1187.905974

NImag=0

C	2.3226873	-0.7158489	0.2581882
C	0.9932924	-0.4686705	0.9335445
C	2.8598193	-1.7929363	-0.4394685
O	3.9433322	-1.7029166	-1.1168167
C	0.0292846	0.2357664	-0.0928028
C	-0.8474553	-0.6739920	-0.9134293
C	-0.3341384	-1.1643526	-2.1196018
C	-1.0510869	-2.0881942	-2.8705692
C	-2.3087719	-2.5067908	-2.4215679
C	-2.8480643	-2.0027892	-1.2317561
C	-2.1119141	-1.0934323	-0.4838250
C	2.2191076	-3.1851058	-0.4598121
C	0.3298525	-1.6086531	1.7286609
S	-1.0136591	1.6198358	0.6099397

C	-1.3802398	1.2568733	2.3402062
C	0.2430926	2.8974300	0.8107584
C	-3.0628930	-3.4554929	-3.1969764
N	-3.6703052	-4.2192183	-3.8207692
C	1.5336498	-3.6898159	0.8066384
C	0.2056480	-3.0062317	1.1144604
H	2.8926733	0.2065584	0.1203078
H	1.1950172	0.3068453	1.6851388
H	0.6541960	0.8240860	-0.7718131
H	0.6381432	-0.8269300	-2.4668475
H	-0.6478535	-2.4762880	-3.8001486
H	-3.8274070	-2.3277522	-0.8968836
H	-2.5347638	-0.7357713	0.4515629
H	1.4984023	-3.2240161	-1.2915720
H	3.0317282	-3.8679452	-0.7293197
H	-0.6711642	-1.2857948	2.0413862
H	0.9120862	-1.7131191	2.6540179
H	-1.8023353	2.1793959	2.7454027
H	-2.1285402	0.4656203	2.3850338
H	-0.4718845	0.9849518	2.8791958
H	-0.2272526	3.7298961	1.3371924
H	0.5518723	3.2126320	-0.1869645
H	1.0881807	2.5062169	1.3802856
H	1.3466111	-4.7639756	0.6837208
H	2.2122715	-3.5872924	1.6655865
H	-0.3496614	-3.6155859	1.8388882
H	-0.3993645	-2.9933789	0.2000916

3_sy_c_3_ts1.log

E = -1188.180471

H = -1187.817205

G = -1187.887217

NImag=1

C	2.6767689	-0.0751726	0.9874888
C	1.3082383	-0.2822924	1.1595895
C	3.6408697	-0.7945592	0.2001658
O	4.8367940	-0.4430079	0.1931134
C	0.1415649	0.6941111	-0.4658206
C	-1.2723903	0.4096053	-0.3617727
C	-1.8479639	-0.6540456	-1.1022243
C	-3.1751099	-1.0067533	-0.9487324
C	-3.9922701	-0.2976338	-0.0489566
C	-3.4513402	0.7679040	0.6872228
C	-2.1171290	1.1072844	0.5365296
C	3.2472899	-1.9500293	-0.7078915
C	0.5935364	-1.6146449	1.1483038
S	0.5109063	2.4309189	-0.4943799
C	1.1021874	2.9877079	1.1294573
C	2.0564278	2.4656172	-1.4218000
C	-5.3672670	-0.6579852	0.1118276
N	-6.4830299	-0.9507395	0.2418883
C	2.3273751	-3.0219223	-0.1214167
C	0.8711012	-2.5828115	0.0044119
H	3.1045912	0.8186682	1.4367758
H	0.8538804	0.3945572	1.8841439
H	0.6666415	0.2243562	-1.2954946
H	-1.2351293	-1.1918533	-1.8192112
H	-3.5957102	-1.8204586	-1.5317400
H	-4.0790345	1.3173305	1.3821987
H	-1.7214406	1.9179618	1.1431194
H	2.7637827	-1.5161946	-1.5967862

H	4.1857785	-2.4001024	-1.0440098
H	-0.4836077	-1.4338116	1.2179559
H	0.8770199	-2.1034233	2.0933033
H	1.2847492	4.0595559	1.0238948
H	0.3035617	2.8242135	1.8543104
H	2.0134753	2.4699289	1.4204434
H	2.4465771	3.4839224	-1.3758983
H	1.8265012	2.1960890	-2.4535666
H	2.7541898	1.7550010	-0.9745443
H	2.3714534	-3.8944274	-0.7828673
H	2.7078270	-3.3500733	0.8555461
H	0.2382778	-3.4651555	0.1576605
H	0.5594388	-2.1369759	-0.9479999

3_sy_c_3_ts2.log

E = -1188.194080

H = -1187.829485

G = -1187.898993

NImag=1

C	-1.2971809	1.8641373	-1.0797521
C	-1.8316405	0.8905648	-0.0508650
C	-0.1094451	2.6170149	-1.1129453
O	0.2539258	3.2426598	-2.1522361
C	-1.1139179	-0.2974498	-0.6375418
C	0.3261683	-0.6060428	-0.3688512
C	1.2535614	-0.4910115	-1.4109288
C	2.5997140	-0.7581761	-1.1944139
C	3.0178850	-1.1699741	0.0767762
C	2.0967638	-1.3250683	1.1202235
C	0.7563261	-1.0454482	0.8880453
C	0.7978861	2.7604138	0.1076172
C	-1.7599494	1.2292309	1.4460989
S	-2.0902492	-2.2273755	-0.1231505
C	-3.1576526	-1.9363438	1.3047940
C	-3.3271788	-2.1439018	-1.4350125
C	4.4093265	-1.4520606	0.3102760
N	5.5294207	-1.6792142	0.4979987
C	0.1025307	3.0319642	1.4428184
C	-0.4878750	1.7861949	2.0939269
H	-1.8377671	1.8504486	-2.0251116
H	-2.8975796	0.7462039	-0.2652637
H	-1.3794648	-0.4399474	-1.6842038
H	0.9189937	-0.1689822	-2.3927335
H	3.3213304	-0.6526179	-1.9976806
H	2.4307178	-1.6617448	2.0959754
H	0.0393945	-1.1710151	1.6961192
H	1.4204130	1.8578345	0.2064254
H	1.4777093	3.5834028	-0.1329534
H	-2.0718211	0.3490117	2.0190849
H	-2.5477531	1.9795602	1.5953100
H	-3.8466303	-2.7805611	1.3831167
H	-2.5329202	-1.8950155	2.1983678
H	-3.7172117	-1.0070114	1.1798153
H	-4.0780713	-2.9175460	-1.2637910
H	-2.8211318	-2.3300949	-2.3839669
H	-3.7946891	-1.1555842	-1.4426743
H	0.8425217	3.4550927	2.1326840
H	-0.6753725	3.7966518	1.3098944
H	-0.7546568	2.0206329	3.1320770
H	0.2971539	1.0260156	2.1495736

3_sy_c_4.log

E = -1188.209052
H = -1187.843014
G = -1187.912496

NImag=0

C	-1.0097032	4.0770740	-1.7179749
C	-0.6539097	2.6406589	-2.0266521
C	-1.5405517	5.0645717	-2.5352850
O	-1.6639936	6.2894773	-2.1759604
C	-1.6678454	1.5686195	-1.5337651
C	-1.2519115	0.1282791	-1.7631713
C	-2.1774849	-0.7752174	-2.2980576
C	-1.8284828	-2.1009307	-2.5242255
C	-0.5350175	-2.5293469	-2.2039038
C	0.4011853	-1.6400981	-1.6638577
C	0.0382014	-0.3162800	-1.4473495
C	-2.0289789	4.7678593	-3.9641547
C	-0.3709822	2.3653311	-3.5208604
S	-2.1226942	1.6421870	0.2675793
C	-0.6274132	2.1180597	1.1528002
C	-3.1798845	3.0890757	0.4799164
C	-0.1609369	-3.8997078	-2.4337902
N	0.1404177	-5.0026025	-2.6181642
C	-2.6365094	3.3874026	-4.2150634
C	-1.6033701	2.2750555	-4.4272351
H	-0.6948646	4.4381217	-0.7386559
H	0.2864264	2.4247802	-1.4997772
H	-2.6486253	1.7327067	-1.9935022
H	-3.1796408	-0.4346563	-2.5444485
H	-2.5455455	-2.7988227	-2.9435444
H	1.4010321	-1.9844291	-1.4212543
H	0.7746613	0.3693643	-1.0389043
H	-2.7759712	5.5405226	-4.1740218
H	-1.2010692	4.9458093	-4.6675207
H	0.2070328	1.4395650	-3.6259559
H	0.2778559	3.1776476	-3.8661243
H	-0.9145088	2.2042796	2.2031713
H	0.1024151	1.3145878	1.0406472
H	-0.2424789	3.0653884	0.7776377
H	-3.5562179	3.0370005	1.5040485
H	-4.0074703	2.9893595	-0.2254761
H	-2.6189812	4.0027466	0.2963159
H	-3.2962086	3.1434761	-3.3719418
H	-3.2844349	3.4285712	-5.0989664
H	-1.2515311	2.3072231	-5.4659644
H	-2.0911099	1.2989901	-4.3035873

3_sy_c_4_r.log

E = -1188.199929
H = -1187.833648
G = -1187.902294

NImag=0

C	-2.5133803	-0.4581821	0.5799957
C	-1.4151274	-0.4068479	-0.4603115
C	-3.2653475	-1.5113526	1.0813145
O	-4.2766671	-1.3480689	1.8519193
C	-0.1415227	0.2120853	0.2092274
C	0.7675932	-0.6911999	1.0047827
C	0.5789617	-0.7648655	2.3899045
C	1.3592850	-1.6118688	3.1681511

C	2.3552313	-2.3784755	2.5532518
C	2.5747743	-2.2953277	1.1726606
C	1.7792434	-1.4512716	0.4087512
C	-2.9417270	-2.9771540	0.7511823
C	-1.2389779	-1.6695083	-1.3287725
S	0.9227881	1.2874155	-0.8931604
C	0.8282969	0.6815764	-2.5904965
C	-0.1078951	2.7610881	-1.0260597
C	3.1741134	-3.2526227	3.3504197
N	3.8334853	-3.9563976	3.9917210
C	-1.4594381	-3.3371395	0.6492551
C	-0.8424196	-3.0202129	-0.7109332
H	-2.8362824	0.5295988	0.9167432
H	-1.7191275	0.3647850	-1.1852221
H	-0.5088624	0.9924723	0.8850875
H	-0.1885467	-0.1568564	2.8595798
H	1.2065082	-1.6751531	4.2403441
H	3.3564235	-2.8872709	0.7083467
H	1.9474110	-1.4083138	-0.6650497
H	-3.4100261	-3.5563886	1.5533381
H	-3.4595234	-3.2643391	-0.1769862
H	-0.5387697	-1.4596593	-2.1435355
H	-2.2167852	-1.7946279	-1.8105054
H	1.3683879	1.4181827	-3.1898868
H	1.3376463	-0.2804990	-2.6516583
H	-0.2105392	0.6138504	-2.9154769
H	0.3705321	3.4231378	-1.7502179
H	-0.1304917	3.2359287	-0.0443344
H	-1.1118778	2.4873308	-1.3557010
H	-0.9125927	-2.8123758	1.4421722
H	-1.3286920	-4.4093389	0.8420190
H	-1.1630476	-3.7904026	-1.4251371
H	0.2447853	-3.1119298	-0.6439853

3_sy_c_4_ts1.log

E = -1188.177862

H = -1187.814698

G = -1187.885701

NImag=1

C	-2.5761395	-0.0583090	-1.1257210
C	-1.2147171	-0.3549037	-1.0489152
C	-3.6983556	-0.8473497	-0.6940842
O	-4.8648522	-0.4958492	-0.9550869
C	-0.0807516	0.6419933	0.5891825
C	1.3264539	0.3598842	0.3892961
C	1.9884989	-0.6203525	1.1708148
C	3.3017033	-0.9752882	0.9279381
C	4.0189302	-0.3480403	-0.1076662
C	3.3954704	0.6387209	-0.8844195
C	2.0741034	0.9796677	-0.6411894
C	-3.5029127	-2.1402578	0.0870081
C	-0.6945851	-1.7567140	-0.8017768
S	-0.4616215	2.3798986	0.6417258
C	-0.9862522	2.9828761	-0.9896927
C	-2.0591998	2.3469331	1.4777619
C	5.3804550	-0.7089859	-0.3617674
N	6.4843090	-1.0027153	-0.5673167
C	-2.3843239	-2.0732935	1.1293798
C	-1.0045247	-2.3991185	0.5602572
H	-2.8781920	0.8587420	-1.6244355
H	-0.5822805	0.2333467	-1.7145316

H	-0.5285914	0.2035734	1.4798823
H	1.4581546	-1.0874382	1.9948821
H	3.7891583	-1.7238898	1.5450014
H	3.9467194	1.1267085	-1.6823198
H	1.6137747	1.7280034	-1.2795354
H	-4.4659716	-2.3572403	0.5574111
H	-3.3062135	-2.9545335	-0.6254694
H	0.3884374	-1.7702701	-0.9612045
H	-1.1264295	-2.3829446	-1.5941258
H	-1.1901728	4.0471994	-0.8507524
H	-0.1595626	2.8629973	-1.6898033
H	-1.8757635	2.4647186	-1.3371986
H	-2.4691718	3.3578550	1.4482626
H	-1.8861357	2.0408154	2.5104142
H	-2.7116675	1.6406008	0.9599765
H	-2.3800030	-1.0711593	1.5782019
H	-2.6003958	-2.7733737	1.9436387
H	-0.9149828	-3.4856281	0.4399585
H	-0.2443347	-2.1083322	1.2905708

3_sy_c_4_ts2.log

E = -1188.187454

H = -1187.822719

G = -1187.891773

NImag=1

C	-1.6107874	1.6801944	-0.9090400
C	-1.8941309	0.5865141	0.0955995
C	-0.9255590	2.9051128	-0.7791644
O	-0.8688964	3.7316471	-1.7336875
C	-1.0355919	-0.4059473	-0.6372223
C	0.4458233	-0.5416478	-0.4784223
C	1.2863035	-0.1447064	-1.5260733
C	2.6667707	-0.2431601	-1.4036288
C	3.2122671	-0.7675089	-0.2254691
C	2.3841073	-1.2072766	0.8143424
C	1.0068135	-1.0983221	0.6760286
C	-0.2682773	3.3508522	0.5293193
C	-1.7049638	0.9143431	1.5836079
S	-1.7114359	-2.5346986	-0.2025623
C	-2.5884830	-2.4711804	1.3758351
C	-3.1208331	-2.5194207	-1.3307946
C	4.6404199	-0.8735630	-0.0873779
N	5.7900000	-0.9593664	0.0246627
C	0.5130109	2.2817663	1.2913493
C	-0.3541404	1.3729969	2.1637684
H	-2.1004124	1.5480565	-1.8718376
H	-2.9396140	0.2663250	-0.0057818
H	-1.3639365	-0.5407013	-1.6664280
H	0.8533320	0.2659503	-2.4331999
H	3.3179175	0.0812482	-2.2084073
H	2.8174872	-1.6313283	1.7139591
H	0.3658111	-1.4479658	1.4808342
H	0.3969150	4.1741815	0.2528507
H	-1.0448038	3.7808285	1.1793848
H	-2.0466700	0.0588354	2.1757510
H	-2.4381652	1.7099026	1.7661568
H	-3.1081039	-3.4214104	1.5181434
H	-1.8528743	-2.3381234	2.1713019
H	-3.3060823	-1.6483829	1.3757954
H	-3.7464493	-3.3920640	-1.1318766
H	-2.7340073	-2.5745913	-2.3498625

H	-3.6996895	-1.6018022	-1.1970762
H	1.0935041	1.6901548	0.5744155
H	1.2464713	2.7723141	1.9423642
H	-0.5951345	1.9160751	3.0866945
H	0.2397275	0.5106309	2.4783488

3_sy_c_5.log

E = -1188.212430

H = -1187.846127

G = -1187.914097

NImag=0

C	-0.4401880	3.3276993	-2.5274680
C	-1.2159756	2.3003968	-3.3185016
C	-0.8235714	4.5322876	-1.9480683
O	-0.1278160	5.0924101	-1.0275090
C	-2.0202551	1.2960289	-2.4135732
C	-1.3489093	-0.0229054	-2.1317859
C	0.0242449	-0.1021037	-1.8595936
C	0.6275268	-1.3293589	-1.6168525
C	-0.1481760	-2.4948536	-1.6524008
C	-1.5179747	-2.4357032	-1.9291294
C	-2.1078347	-1.1994047	-2.1656882
C	-2.1119238	5.2853064	-2.3035273
C	-2.1188836	2.7946321	-4.4585071
S	-2.5254753	2.1666675	-0.8482080
C	-3.6217709	0.9404737	-0.1019859
C	-1.1590386	2.1226729	0.3279808
C	0.4727916	-3.7698124	-1.4082939
N	0.9717507	-4.7961475	-1.2112847
C	-2.7166424	5.1604130	-3.7001596
C	-3.2294308	3.7719625	-4.0809763
H	0.5021741	2.9517876	-2.1255347
H	-0.4732076	1.6585352	-3.8075128
H	-3.0076476	1.0906178	-2.8473762
H	0.6303548	0.7986808	-1.8386158
H	1.6899340	-1.3897718	-1.4055915
H	-2.1078370	-3.3455880	-1.9622020
H	-3.1701339	-1.1476015	-2.3883083
H	-2.8740046	5.0113207	-1.5585284
H	-1.8809590	6.3393779	-2.1135448
H	-2.5609627	1.9140615	-4.9429185
H	-1.4750471	3.2750011	-5.2062810
H	-4.0115164	1.3829789	0.8168162
H	-4.4424875	0.7525446	-0.7967704
H	-3.0750692	0.0220275	0.1193610
H	-1.6123860	2.3009943	1.3066626
H	-0.4767374	2.9349201	0.0680364
H	-0.6754541	1.1442682	0.3150292
H	-3.5511834	5.8699382	-3.7603638
H	-1.9816531	5.4832607	-4.4509930
H	-3.9017626	3.8672239	-4.9419487
H	-3.8438615	3.3658610	-3.2624829

3_sy_c_5_r.log

E = -1188.202315

H = -1187.836149

G = -1187.906217

NImag=0

C	-0.1923234	0.9644775	-1.9907904
C	0.9416909	0.9405923	-0.9917963

C	-0.6831233	-0.0358499	-2.8226097
O	-1.7686878	0.0699727	-3.4904348
C	0.3669652	0.4497045	0.3778152
C	-0.0961013	-0.9754453	0.5369993
C	0.7743118	-2.0664138	0.6421046
C	0.2823175	-3.3632803	0.7269315
C	-1.1003778	-3.5767977	0.6981698
C	-1.9873535	-2.4991360	0.6011579
C	-1.4780055	-1.2080046	0.5344286
C	0.0765934	-1.3544833	-3.0131418
C	2.3085892	0.3852886	-1.4375589
S	1.3992155	1.0845922	1.8109770
C	0.2089225	0.9773059	3.1619153
C	2.6022111	-0.1381379	2.3710934
C	-1.6152541	-4.9183637	0.7757486
N	-2.0297020	-5.9978231	0.8397776
C	1.5734508	-1.2392145	-3.3133520
C	2.4413641	-0.9979691	-2.0816421
H	-0.8433025	1.8357874	-1.8980755
H	1.1606329	1.9962035	-0.7769776
H	-0.5042671	1.0930940	0.5485412
H	1.8474629	-1.9205907	0.6409294
H	0.9622511	-4.2049520	0.8057589
H	-3.0580619	-2.6729607	0.5833039
H	-2.1621645	-0.3671649	0.4647778
H	-0.0615575	-1.9906147	-2.1244780
H	-0.4257763	-1.8623310	-3.8424193
H	3.0080054	0.4401210	-0.5901913
H	2.6817862	1.1134849	-2.1699088
H	0.7323321	1.2549653	4.0788213
H	-0.5920189	1.6895319	2.9584358
H	-0.1759649	-0.0425435	3.2291616
H	3.1402960	0.3456594	3.1897136
H	3.2965847	-0.3575930	1.5596251
H	2.0962883	-1.0356966	2.7279381
H	1.9075333	-2.1750730	-3.7783817
H	1.7407047	-0.4443643	-4.0540593
H	3.4960664	-1.1101423	-2.3637636
H	2.2366365	-1.7958800	-1.3626860

3_sy_c_5_ts1.log

E = -1188.183749

H = -1187.820370

G = -1187.891186

NImag=1

C	2.6500960	0.1297860	1.1500611
C	1.4125300	-0.4969083	0.9894948
C	3.8698646	-0.0433624	0.4124289
O	4.8944277	0.5997954	0.7124728
C	0.2105878	0.4872633	-0.5750365
C	-1.1839952	0.1312675	-0.4731388
C	-2.0961215	0.7246840	0.4329546
C	-3.4015596	0.2732452	0.5418887
C	-3.8458571	-0.8000931	-0.2449290
C	-2.9572653	-1.4153593	-1.1453996
C	-1.6598324	-0.9539657	-1.2548011
C	3.9455083	-0.9575739	-0.8029916
C	1.1621154	-1.9225949	0.5501454
S	0.7842776	2.1358075	-0.4450106
C	-0.3507473	3.1997003	-1.3689490
C	0.4944474	2.7663502	1.2343340

C	-5.1934688	-1.2669727	-0.1307621
N	-6.2865242	-1.6466520	-0.0388775
C	3.3912193	-2.3757585	-0.6455875
C	1.8679172	-2.4580485	-0.6904099
H	2.6957119	0.9563052	1.8582997
H	0.6758853	-0.1978354	1.7372342
H	0.7378148	0.0584507	-1.4247445
H	-1.7831236	1.5423044	1.0726140
H	-4.0830543	0.7460716	1.2424692
H	-3.2971546	-2.2449374	-1.7577561
H	-0.9818315	-1.4303623	-1.9584592
H	3.4126023	-0.4570360	-1.6258631
H	5.0019719	-0.9964187	-1.0832425
H	0.0820854	-2.0638297	0.4384688
H	1.4572693	-2.5419147	1.4111868
H	-0.0383470	4.2338166	-1.2062706
H	-0.2541631	2.9387063	-2.4238447
H	-1.3745938	3.0468887	-1.0227428
H	1.2577099	3.5246539	1.4177720
H	0.6048356	1.9497623	1.9466032
H	-0.4987965	3.2108247	1.3009189
H	3.7949800	-2.9836722	-1.4629416
H	3.7625650	-2.8205537	0.2878501
H	1.5679891	-3.5058573	-0.8102429
H	1.5104189	-1.9312244	-1.5849970

3_sy_c_6.log

E = -1188.212155

H = -1187.846400

G = -1187.916524

NImag=0

C	-0.7409501	3.2236751	-2.1953016
C	-2.0161925	2.4434814	-2.4261520
C	-0.1530971	4.0450102	-3.1447627
O	0.9001422	4.7464776	-2.9672014
C	-2.2606737	1.3494080	-1.3583288
C	-1.4579414	0.0848512	-1.5688383
C	-2.1441348	-1.0949522	-1.8777324
C	-1.4528134	-2.2766487	-2.1159687
C	-0.0556977	-2.2773824	-2.0332601
C	0.6441653	-1.1082928	-1.7136990
C	-0.0596167	0.0676598	-1.4810043
C	-0.8258946	4.1508858	-4.5203513
C	-3.2795730	3.3093186	-2.6498791
S	-1.8969951	1.9156923	0.3713332
C	-3.0904952	3.2341993	0.6635212
C	-2.6583346	0.5745373	1.3072167
C	0.6700593	-3.4968764	-2.2710351
N	1.2534496	-4.4787902	-2.4625565
C	-2.2122026	4.8123186	-4.4841061
C	-3.3548515	3.8809508	-4.0687312
H	-0.2541428	3.1752016	-1.2220653
H	-1.9276718	1.8349892	-3.3448259
H	-3.3246289	1.0914516	-1.3271728
H	-3.2288838	-1.0872177	-1.9339100
H	-1.9853048	-3.1902006	-2.3587221
H	1.7269478	-1.1235279	-1.6471952
H	0.4864456	0.9718446	-1.2328227
H	-0.1515297	4.7387074	-5.1503610
H	-0.9218282	3.1561431	-4.9815395
H	-3.3039494	4.1331142	-1.9273861

H	-4.1806546	2.7015594	-2.4876754
H	-3.1521016	3.3603796	1.7467033
H	-2.7013355	4.1443707	0.2067302
H	-4.0610200	2.9547277	0.2490417
H	-2.6414171	0.8686740	2.3581965
H	-2.0512679	-0.3209188	1.1650703
H	-3.6818350	0.4180428	0.9599477
H	-2.1785112	5.6822884	-3.8129051
H	-2.4475472	5.1996216	-5.4832492
H	-3.3926260	3.0421174	-4.7791106
H	-4.3046904	4.4193084	-4.1742113

3_sy_c_6_ts1.log

E = -1188.149506

H = -1187.787452

G = -1187.859207

NImag=1

C	-1.8520451	-0.3433011	-0.9093928
C	-1.5390815	-0.1133239	0.4055291
C	-1.7461555	-1.7322318	-1.3586438
O	-1.8625423	-2.1062332	-2.5257796
C	0.1857622	1.6534136	0.6870860
C	1.2480150	0.7458130	0.4323779
C	1.9060535	0.1284490	1.5371658
C	2.8650060	-0.8449722	1.3598569
C	3.2239281	-1.2611391	0.0601695
C	2.5888978	-0.6723908	-1.0460106
C	1.6257468	0.3050809	-0.8678030
C	-1.8495480	-2.7354739	-0.1999801
C	-2.5775027	0.1336511	1.4448130
S	-0.3652026	2.6942886	-0.5777642
C	-1.9968973	3.2150188	-0.0184966
C	0.5220570	4.2672353	-0.3914547
C	4.2215050	-2.2635660	-0.1287915
N	5.0337996	-3.0805505	-0.2813155
C	-3.0531473	-2.3927756	0.7343315
C	-2.8734343	-1.3461415	1.8643127
H	-2.6040606	0.2580538	-1.4224268
H	-0.7351164	-0.7314494	0.8035717
H	0.0285059	2.0398513	1.6910499
H	1.6366611	0.4363132	2.5440362
H	3.3505973	-1.2945240	2.2210826
H	2.8573930	-0.9884856	-2.0499565
H	1.1595661	0.7385857	-1.7473809
H	-1.9955661	-3.7274695	-0.6370532
H	-0.9171974	-2.7662533	0.3786714
H	-3.4723143	0.6066710	1.0270541
H	-2.2395517	0.6946716	2.3219991
H	-2.2816817	4.0891577	-0.6071052
H	-2.6952761	2.3989509	-0.2024168
H	-1.9493836	3.4632662	1.0440155
H	0.1315930	4.9740499	-1.1273609
H	1.5761237	4.0633619	-0.5889648
H	0.3839468	4.6394527	0.6257090
H	-3.9015974	-2.0957004	0.1027287
H	-3.3528795	-3.3232476	1.2295006
H	-2.0503340	-1.6751299	2.5110414
H	-3.7838412	-1.3553062	2.4748439

3_sy_c_7.log


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E =      -1188.209216
H =      -1187.843144
G =      -1187.912247
NImag=0
C        -0.4459504      3.3497370      -2.3958017
C        -1.2014964      2.3367639      -3.2274114
C        -0.5400410      4.7372821      -2.3658727
O         0.2832558      5.4815038      -1.7278247
C        -1.9915983      1.2703021      -2.3979478
C        -1.2680750      -0.0177647      -2.0984276
C         0.1026929      -0.0379966      -1.8061425
C         0.7503380      -1.2360133      -1.5351554
C         0.0222053      -2.4322967      -1.5608029
C        -1.3437718      -2.4325124      -1.8602269
C        -1.9779762      -1.2244488      -2.1279488
C        -1.6644902      5.4994512      -3.0917580
C        -2.1196533      2.9156722      -4.3157266
S        -2.6125656      2.0840954      -0.8471629
C        -3.9036525      0.9297191      -0.3301124
C        -1.3966215      1.7551381       0.4431785
C         0.6899905      -3.6766103      -1.2842024
N         1.2267998      -4.6781141      -1.0607001
C        -3.0682727      4.9079871      -2.9475992
C        -3.3529669      3.6925916      -3.8492677
H         0.4113640      2.9570801      -1.8473393
H        -0.4668382      1.7257758      -3.7728496
H        -2.9363774      1.0196516      -2.8963142
H         0.6732132      0.8850939      -1.7899505
H         1.8110732      -1.2501625      -1.3080210
H        -1.8960966      -3.3657783      -1.8891870
H        -3.0363637      -1.2202606      -2.3742257
H        -1.6517623      6.5033836      -2.6561601
H        -1.4082987      5.6215906      -4.1539106
H        -2.4593921      2.0855795      -4.9483074
H        -1.5075719      3.5595674      -4.9568511
H        -4.3219344      1.3202937       0.5996372
H        -4.6731282      0.9182168      -1.1043875
H        -3.4897639      -0.0676786      -0.1704814
H        -1.8195361      2.1647859       1.3634819
H        -0.4793017      2.2816086       0.1827543
H        -1.2342385      0.6804835       0.5416689
H        -3.2128893      4.6409104      -1.8952744
H        -3.8105494      5.6847872      -3.1668842
H        -3.8741017      4.0305832      -4.7530878
H        -4.0571570      3.0139018      -3.3462973

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3_sy_c_7_ts1.log

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E =      -1188.182986
H =      -1187.819372
G =      -1187.889490
NImag=1
C         2.6507861       0.0763725       1.1107689
C         1.3579395      -0.4353010       0.9988490
C         3.8790962      -0.4970123       0.6341785
O         4.9793926       0.0270920       0.8922363
C         0.1434208       0.5004851      -0.6007632
C        -1.2464657       0.1986351      -0.3363833
C        -1.9618166       0.7236130       0.7665581
C        -3.2641646       0.3308763       1.0343050
C        -3.8961084      -0.6170464       0.2164069
C        -3.2020800      -1.1672648      -0.8760324

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C	-1.9078698	-0.7617745	-1.1429010
C	3.8754665	-1.7786233	-0.1914639
C	1.0427894	-1.8768580	0.6570215
S	0.7668895	2.1346794	-0.6107723
C	-0.4042389	3.1699944	-1.5248801
C	0.5892827	2.8981036	1.0252075
C	-5.2405697	-1.0234138	0.4940022
N	-6.3304935	-1.3530948	0.7179739
C	2.7744189	-1.8324272	-1.2564282
C	1.4490552	-2.3869011	-0.7346046
H	2.7835132	1.0199510	1.6383349
H	0.6337084	0.0006658	1.6877359
H	0.5571425	0.0316305	-1.4912445
H	-1.4911693	1.4311383	1.4398439
H	-3.7942810	0.7476690	1.8852379
H	-3.6899533	-1.8986811	-1.5130084
H	-1.3855385	-1.1789384	-1.9994585
H	4.8659778	-1.8443443	-0.6498144
H	3.7819681	-2.6366840	0.4898581
H	-0.0304847	-2.0446447	0.7957946
H	1.5473654	-2.4848306	1.4202044
H	-0.0645733	4.2057451	-1.4492694
H	-0.3865882	2.8417986	-2.5651497
H	-1.4030091	3.0572773	-1.0978276
H	1.2843161	3.7399517	1.0435651
H	0.8645731	2.1776579	1.7942241
H	-0.4318715	3.2533570	1.1648464
H	2.6274060	-0.8226023	-1.6608679
H	3.1081180	-2.4533096	-2.0947976
H	1.5145611	-3.4801978	-0.6793633
H	0.6564416	-2.1626586	-1.4565468

3_sy_c_8.log

E = -1188.218091

H = -1187.851820

G = -1187.920458

NImag=0

C	-0.8766609	4.1551341	-1.9057207
C	-0.5535559	2.7194683	-2.2540154
C	-1.9088944	4.9406488	-2.4005518
O	-2.1444508	6.1404524	-2.0287760
C	-1.5856944	1.6981544	-1.6994919
C	-1.2057913	0.2423767	-1.7793698
C	0.0818607	-0.2042547	-1.4523442
C	0.4031240	-1.5537175	-1.5330911
C	-0.5699566	-2.4684616	-1.9528590
C	-1.8573224	-2.0387589	-2.2936457
C	-2.1647159	-0.6867058	-2.2021611
C	-2.8547885	4.3794849	-3.4759310
C	-0.3114630	2.4106365	-3.7487072
S	-2.0320707	2.2301048	0.0233230
C	-2.8353263	0.7657699	0.7107339
C	-0.4828360	2.1963070	0.9413029
C	-0.2394808	-3.8662151	-2.0419329
N	0.0260742	-4.9911898	-2.1128323
C	-2.1822308	3.8821695	-4.7616816
C	-1.5280272	2.5021768	-4.6706711
H	-0.2394755	4.6208551	-1.1538149
H	0.3968050	2.4922444	-1.7550778
H	-2.5520377	1.8371642	-2.1950642
H	0.8503778	0.4981883	-1.1452433

H	1.3999663	-1.8990292	-1.2798844
H	-2.6019406	-2.7554522	-2.6238025
H	-3.1630428	-0.3460562	-2.4635880
H	-3.4744144	3.5713787	-3.0583065
H	-3.5384503	5.1978831	-3.7215795
H	0.1184054	1.4046556	-3.8429667
H	0.4553138	3.1144645	-4.0949241
H	-3.1251334	1.0231798	1.7316336
H	-3.7285290	0.5648419	0.1155141
H	-2.1578277	-0.0899132	0.7052033
H	-0.7407306	2.4112575	1.9807136
H	0.1626136	2.9831434	0.5504089
H	-0.0159915	1.2133289	0.8626397
H	-2.9396633	3.8416212	-5.5543730
H	-1.4333017	4.6198109	-5.0838885
H	-1.2076533	2.1999784	-5.6752940
H	-2.2875831	1.7670741	-4.3659829

3_sy_c_9.log

E = -1188.210105

H = -1187.844119

G = -1187.913570

NImag=0

C	-0.7191121	3.2443336	-2.2056684
C	-1.8700887	2.3482519	-2.6309404
C	-0.4320694	4.5427436	-2.6133618
O	0.5202102	5.2439549	-2.1260394
C	-2.1927553	1.2737079	-1.5562340
C	-1.4262138	-0.0260536	-1.6817353
C	-0.0581995	-0.0486031	-1.9826686
C	0.6168873	-1.2568801	-2.1028790
C	-0.0826967	-2.4566163	-1.9251675
C	-1.4507350	-2.4513247	-1.6334311
C	-2.1121940	-1.2348146	-1.5132209
C	-1.2386256	5.2340487	-3.7278720
C	-3.1474570	3.1216980	-3.0210904
S	-1.8825938	1.9283446	0.1581902
C	-3.1023204	3.2459768	0.3326038
C	-2.6852561	0.6526129	1.1543024
C	0.6119173	-3.7106466	-2.0512531
N	1.1705293	-4.7200491	-2.1519573
C	-1.7835032	4.3174604	-4.8265077
C	-3.1062118	3.6399142	-4.4610659
H	-0.0011029	2.8316604	-1.4992748
H	-1.6163420	1.7256707	-3.5100173
H	-3.2634377	1.0433204	-1.5523342
H	0.4844594	0.8787595	-2.1356478
H	1.6761512	-1.2746581	-2.3363112
H	-1.9852781	-3.3867051	-1.5059001
H	-3.1757338	-1.2237338	-1.2918419
H	-2.0568536	5.8188065	-3.2810908
H	-0.5467600	5.9631503	-4.1619600
H	-3.2848132	3.9646387	-2.3353052
H	-4.0271271	2.4750697	-2.9114796
H	-3.1987937	3.4389918	1.4032019
H	-2.7128272	4.1271910	-0.1762410
H	-4.0562376	2.9226261	-0.0891406
H	-2.7314727	1.0372727	2.1751701
H	-2.0630378	-0.2427135	1.1304863
H	-3.6878266	0.4503471	0.7714858
H	-1.9239492	4.8886407	-5.7517660

H	-1.0270422	3.5535339	-5.0492674
H	-3.2913766	2.8088070	-5.1532813
H	-3.9302106	4.3521647	-4.5951883

3_sy_c_9_ts1.log

E = -1188.182786
H = -1187.819260
G = -1187.890041

NImag=1

C	-1.7500988	-0.5377462	-1.1630208
C	-1.0260066	-0.9143263	-0.0219400
C	-3.1623001	-0.3245123	-1.2745282
O	-3.6783976	0.1612191	-2.3025273
C	0.1450664	0.7005467	0.7903823
C	1.4976768	0.3363157	0.4416435
C	2.0781639	0.5995978	-0.8227226
C	3.3359233	0.1202969	-1.1491082
C	4.0575701	-0.6510284	-0.2249074
C	3.4954104	-0.9380866	1.0314288
C	2.2414532	-0.4524466	1.3532580
C	-4.1038595	-0.8312169	-0.1798500
C	-1.6835583	-1.3465646	1.2719755
S	-0.5150257	2.1052211	-0.0391207
C	-2.0703362	2.3304666	0.8351195
C	0.4046578	3.5330528	0.5877295
C	5.3589332	-1.1430458	-0.5607511
N	6.4142036	-1.5425587	-0.8323613
C	-3.8403196	-2.3013937	0.1844428
C	-2.6295326	-2.5447592	1.1134352
H	-1.1899630	-0.3620400	-2.0808029
H	-0.0795243	-1.4143947	-0.2253732
H	-0.0862271	0.7313679	1.8549611
H	1.5415572	1.1859268	-1.5645126
H	3.7659642	0.3386425	-2.1218076
H	4.0510356	-1.5357609	1.7475081
H	1.8161494	-0.6731338	2.3285591
H	-4.0510458	-0.1991713	0.7153252
H	-5.1151846	-0.7256783	-0.5822437
H	-2.2353637	-0.5092358	1.7118600
H	-0.8991679	-1.6073691	1.9905757
H	-2.5115114	3.2639450	0.4820264
H	-2.7182137	1.4926436	0.5816754
H	-1.8757021	2.3698077	1.9089467
H	-0.0612286	4.4351605	0.1844117
H	1.4293863	3.4491502	0.2207066
H	0.3819184	3.5302439	1.6788433
H	-4.7395819	-2.7067636	0.6604200
H	-3.7132980	-2.8595130	-0.7501410
H	-2.0570923	-3.4088971	0.7573802
H	-2.9864282	-2.8040918	2.1167708

3_sy_c_prod_1.log

E = -710.326302
H = -710.044255
G = -710.101515

NImag=0

C	-1.2910136	-0.1900856	-3.9122146
C	-1.2842830	1.2964330	-3.6196355
C	-1.9266683	0.3296545	-2.6525238
C	-1.4210469	0.0877660	-1.2638743

C	-1.3431570	-1.2132169	-0.7497896
C	-0.9684545	-1.4379625	0.5679389
C	-0.6631614	-0.3448470	1.3907892
C	-0.7410389	0.9624790	0.8977746
C	-1.1237027	1.1675889	-0.4236441
H	-3.0149233	0.3203077	-2.6938058
H	-1.9567300	-0.5196841	-4.7070907
H	-1.9704373	1.8950715	-4.2134918
C	0.0461006	1.9727965	-3.3439907
C	0.9218684	2.0773976	-4.6038834
C	1.7114000	0.8049991	-4.9259698
C	0.8623117	-0.4504738	-5.2161685
C	0.0603630	-0.8368459	-3.9925375
O	0.5176921	-1.5696639	-3.1337067
C	-0.2715481	-0.5689330	2.7558497
N	0.0435950	-0.7496115	3.8561471
H	-1.5688461	-2.0549805	-1.3957955
H	-0.9073088	-2.4469131	0.9629097
H	-0.5084779	1.8023047	1.5444052
H	-1.1957843	2.1811024	-0.8076272
H	0.6016079	1.4299014	-2.5675777
H	-0.1469771	2.9736000	-2.9418108
H	0.2943325	2.3518691	-5.4627767
H	1.6426880	2.8914683	-4.4690932
H	2.3886563	0.5827418	-4.0911964
H	2.3398637	0.9877206	-5.8039043
H	1.5222813	-1.2827050	-5.4773244
H	0.1873986	-0.2495792	-6.0556814

3_sy_c_prod_2.log

E = -710.325325

H = -710.043566

G = -710.101287

NImag=0

C	-1.2224686	-0.1488308	-3.9363757
C	-1.1975354	1.3246657	-3.6297027
C	-1.8845304	0.3701489	-2.6810969
C	-1.3964404	0.1217979	-1.2877351
C	-1.2518366	-1.1807216	-0.7933698
C	-0.8765622	-1.4040588	0.5263503
C	-0.6428993	-0.3100570	1.3686750
C	-0.7897517	0.9996625	0.8948673
C	-1.1668907	1.2040243	-0.4267891
H	-2.9713036	0.3738563	-2.7428280
H	-1.8989453	-0.4934396	-4.7172143
H	-1.8461250	1.9585810	-4.2301679
C	0.1518125	1.9201806	-3.2878889
C	1.0072379	2.1443144	-4.5410124
C	1.0476335	0.9183980	-5.4625056
C	1.2597969	-0.4003866	-4.7192743
C	0.0635192	-0.9410174	-3.9448303
O	0.1309021	-2.0347972	-3.4126998
C	-0.2537738	-0.5337227	2.7346813
N	0.0591494	-0.7135562	3.8356715
H	-1.4236931	-2.0228441	-1.4547884
H	-0.7640184	-2.4143722	0.9064388
H	-0.6126759	1.8404912	1.5577099
H	-1.2885956	2.2176664	-0.7976558
H	0.6826221	1.2431635	-2.6049515
H	0.0291302	2.8639592	-2.7447438
H	0.6227925	3.0028979	-5.1043857

H	2.0262615	2.4015772	-4.2274093
H	1.8554312	1.0440982	-6.1907755
H	0.1190483	0.8549999	-6.0416688
H	2.0915073	-0.3219900	-4.0059438
H	1.5379011	-1.1958892	-5.4203809

3_sy_c_prod_3.log

E = -710.321169

H = -710.038860

G = -710.095727

NImag=0

C	-1.4599368	-0.1659089	-4.0611243
C	-1.4587977	1.3121984	-3.7763723
C	-2.0400639	0.3399499	-2.7653476
C	-1.4579459	0.1442531	-1.4015304
C	-1.0250478	-1.1095643	-0.9531055
C	-0.5295908	-1.2708088	0.3360490
C	-0.4699032	-0.1653333	1.1933134
C	-0.9141945	1.0932344	0.7669938
C	-1.4068048	1.2366419	-0.5237118
H	-3.1285711	0.3236087	-2.7461915
H	-2.1941452	-0.5114487	-4.7891048
H	-2.2047074	1.8863934	-4.3196018
C	-0.1817491	2.1060553	-3.5159474
C	1.0677020	1.3265689	-3.0829590
C	1.7933495	0.5930137	-4.2164768
C	0.8677249	-0.2688018	-5.1012430
C	-0.1801066	-0.9443637	-4.2495642
O	-0.0286126	-2.0647637	-3.7959290
C	0.0460882	-0.3241414	2.5259361
N	0.4616969	-0.4519923	3.5999066
H	-1.0619501	-1.9585400	-1.6273849
H	-0.1898716	-2.2424168	0.6801778
H	-0.8707792	1.9419180	1.4419951
H	-1.7548757	2.2093937	-0.8594220
H	-0.4082304	2.8648185	-2.7569954
H	0.0580415	2.6595054	-4.4335197
H	1.7709101	2.0317711	-2.6268690
H	0.8172240	0.6087876	-2.2932793
H	2.5615322	-0.0525758	-3.7775672
H	2.3077981	1.3147978	-4.8599085
H	1.4490066	-1.0281124	-5.6306490
H	0.3603107	0.3660619	-5.8348675

3_sy_c_prod_4.log

E = -710.327045

H = -710.044354

G = -710.101123

NImag=0

C	-1.4266238	-0.1589608	-3.9894509
C	-1.4500641	1.3437960	-3.7086828
C	-2.0125703	0.3978430	-2.6971114
C	-1.4316224	0.1544163	-1.3402233
C	-1.1610332	-1.1485192	-0.9028063
C	-0.6870973	-1.3843863	0.3810922
C	-0.4816851	-0.3002145	1.2445837
C	-0.7553888	1.0078877	0.8276099
C	-1.2303800	1.2248892	-0.4610448
H	-3.0994642	0.3379699	-2.6876539
H	-2.1603560	-0.5281291	-4.6987314

H	-2.2030551	1.8498965	-4.3064848
C	-0.1754380	2.1652682	-3.5427763
C	0.8837597	1.8289614	-4.6041373
C	1.7977600	0.6644242	-4.1917360
C	1.0915550	-0.4357841	-3.3739993
C	-0.1524539	-0.9269472	-4.0765499
O	-0.1080995	-1.9246289	-4.7848404
C	0.0123643	-0.5346120	2.5747693
N	0.4099159	-0.7238581	3.6463273
H	-1.3176831	-1.9856492	-1.5782841
H	-0.4747041	-2.3940558	0.7172309
H	-0.5972014	1.8389429	1.5072500
H	-1.4487282	2.2371023	-0.7897491
H	0.2549464	2.0491085	-2.5421161
H	-0.4629704	3.2174140	-3.6289919
H	0.3722463	1.5902556	-5.5449556
H	1.5066455	2.7068277	-4.8034944
H	2.6164510	1.0461280	-3.5721721
H	2.2519012	0.2166143	-5.0821620
H	0.8469202	-0.0455708	-2.3835427
H	1.7608533	-1.2903296	-3.2450665

3_sy_c_prod_5.log

E = -710.325137

H = -710.042577

G = -710.099745

NImag=0

C	-1.4001697	0.0734630	-3.9161775
C	-1.0726549	1.4957517	-3.5806118
C	-1.8511831	0.6261548	-2.5876191
C	-1.3603357	0.2636274	-1.2278664
C	-0.1248651	-0.3387193	-0.9385541
C	0.2496727	-0.6138889	0.3711774
C	-0.6144630	-0.2951133	1.4246956
C	-1.8547029	0.2990869	1.1622512
C	-2.2116025	0.5693887	-0.1511063
H	-2.9124373	0.8570609	-2.5701382
H	-2.2020645	-0.0670171	-4.6414091
H	-1.6826795	2.2425678	-4.0827903
C	0.3558158	1.9397998	-3.3394451
C	1.2428604	1.8116961	-4.5848282
C	1.7212941	0.3852845	-4.8677403
C	0.6312402	-0.6230997	-5.2838085
C	-0.3255805	-0.9491858	-4.1608619
O	-0.2619646	-1.9949104	-3.5388310
C	-0.2293448	-0.5857879	2.7781182
N	0.0812543	-0.8199847	3.8696841
H	0.5558516	-0.6178399	-1.7323384
H	1.2070966	-1.0809743	0.5784375
H	-2.5270679	0.5422132	1.9785877
H	-3.1755429	1.0281902	-0.3521779
H	0.8177948	1.3697245	-2.5258026
H	0.3320902	2.9831927	-3.0065966
H	0.7105744	2.2036321	-5.4623209
H	2.1296361	2.4408360	-4.4478191
H	2.2500115	-0.0008497	-3.9857211
H	2.4527319	0.4149179	-5.6821758
H	1.1001164	-1.5566996	-5.6066766
H	0.0593179	-0.2041176	-6.1214351

3_sy_tr_1.log

E = -1188.207326
H = -1187.841468
G = -1187.911046

NImag=0

C	3.9482456	-2.2203021	-6.3807997
C	3.2674630	-3.4655119	-6.8871588
C	4.7810738	-2.0131112	-5.2942672
O	5.3468973	-0.8879792	-5.0477173
C	3.7283751	-3.8025421	-8.3412400
C	2.9290869	-4.8911861	-9.0199189
C	3.1407145	-6.2556153	-8.7834060
C	2.3458335	-7.2126327	-9.4006169
C	1.3170323	-6.8019764	-10.2571976
C	1.0893681	-5.4436497	-10.5012129
C	1.9024102	-4.4987816	-9.8860326
C	5.1278842	-3.1444949	-4.3101791
C	3.2006726	-4.6516627	-5.9132377
S	5.5410131	-4.1904169	-8.4690889
C	5.6984379	-4.5132994	-10.2405332
C	6.3529188	-2.5739149	-8.4184079
C	0.4885916	-7.7885341	-10.8976680
N	-0.1780025	-8.5825959	-11.4137543
C	5.6211859	-4.4263046	-4.9859655
C	4.4975237	-5.3480970	-5.4800268
H	3.8315220	-1.3542413	-7.0365346
H	2.2097393	-3.2217367	-7.0912308
H	3.6366624	-2.8824058	-8.9299820
H	3.9335965	-6.5888525	-8.1189196
H	2.5155643	-8.2688528	-9.2208731
H	0.2928386	-5.1358136	-11.1703415
H	1.7378275	-3.4427630	-10.0802789
H	5.9173594	-2.7390024	-3.6708265
H	4.2748761	-3.3701313	-3.6548736
H	2.5246302	-5.4117715	-6.3222855
H	2.7009663	-4.2657580	-5.0172710
H	6.7669909	-4.5072288	-10.4648430
H	5.2807561	-5.4961709	-10.4573227
H	5.1799153	-3.7305619	-10.7990131
H	7.3684253	-2.7390936	-8.7857703
H	6.3585348	-2.2212746	-7.3883038
H	5.8118486	-1.8818209	-9.0671725
H	6.2798484	-4.1403627	-5.8171023
H	6.2523352	-4.9948444	-4.2924489
H	4.2207450	-6.0293348	-4.6656786
H	4.8823925	-5.9917701	-6.2801986

3_sy_tr_10.log

E = -1188.209132
H = -1187.843143
G = -1187.912577

NImag=0

C	5.0963773	-4.1485697	-6.7253709
C	3.8308726	-3.3606893	-6.9811805
C	5.8325019	-4.0427516	-5.5578492
O	6.8877834	-4.7111407	-5.2767396
C	3.3318984	-3.3769142	-8.4336202
C	2.7457288	-4.6465644	-9.0210232
C	3.0317103	-5.9193973	-8.5155137
C	2.4663749	-7.0511762	-9.0941508
C	1.6135052	-6.9121155	-10.1934264

C	1.3117310	-5.6455639	-10.7077769
C	1.8756359	-4.5246282	-10.1140848
C	5.3291565	-3.0708379	-4.4807913
C	2.6295781	-3.7219807	-6.0679276
S	4.5543341	-2.7391692	-9.6957996
C	5.4405957	-1.4286043	-8.8361206
C	5.8478785	-3.9763535	-9.9295256
C	1.0350955	-8.0822383	-10.7997398
N	0.5697290	-9.0229541	-11.2891402
C	3.9867048	-3.4892538	-3.8586190
C	2.7489714	-3.1001997	-4.6736089
H	5.4180786	-4.8904979	-7.4504408
H	4.0156373	-2.2921746	-6.7793660
H	2.5674033	-2.5962871	-8.5320669
H	3.6897373	-6.0342545	-7.6623302
H	2.6861708	-8.0368189	-8.6976379
H	0.6397438	-5.5452901	-11.5535154
H	1.6286294	-3.5393572	-10.5016924
H	6.1013334	-3.0369439	-3.7062201
H	5.2288914	-2.0523513	-4.8873594
H	2.5490924	-4.8126512	-5.9882802
H	1.6927043	-3.3599198	-6.5157911
H	6.1869349	-1.0509941	-9.5383033
H	4.7239729	-0.6405587	-8.5987576
H	5.9119357	-1.8365008	-7.9397764
H	6.3605093	-3.6975458	-10.8522382
H	5.3700342	-4.9502316	-10.0566492
H	6.5287354	-3.9754650	-9.0803718
H	3.9945196	-4.5753110	-3.6887533
H	3.8896328	-3.0212761	-2.8709737
H	2.7389717	-2.0058450	-4.7828331
H	1.8517682	-3.3619229	-4.0993340

3_sy_tr_11.log

E = -1188.209338

H = -1187.843750

G = -1187.913773

NImag=0

C	5.1915715	-3.7593618	-6.4104886
C	4.4022295	-2.7744053	-7.2306058
C	4.8420471	-4.4642687	-5.2678585
O	5.6642886	-5.1897206	-4.6036520
C	4.1086165	-3.2142154	-8.7044275
C	3.3548740	-4.4990895	-8.9295934
C	3.9222237	-5.7477152	-8.6369260
C	3.1932632	-6.9153459	-8.8304319
C	1.8860047	-6.8351861	-9.3233604
C	1.3151835	-5.5971021	-9.6437383
C	2.0600276	-4.4394340	-9.4559186
C	3.4143741	-4.4220227	-4.6885279
C	3.1371748	-2.1819467	-6.5783599
S	5.7236211	-3.4136159	-9.5944928
C	5.1679747	-3.4484853	-11.3097226
C	6.4511180	-1.7663335	-9.5162247
C	1.1246466	-8.0406056	-9.5178391
N	0.5110131	-9.0103840	-9.6739862
C	2.2611702	-4.4489724	-5.6955822
C	1.9300565	-3.0863778	-6.3110168
H	6.2346493	-3.8805905	-6.7151909
H	5.0308964	-1.8818597	-7.3689399
H	3.6099058	-2.3929334	-9.2342185

H	4.9317440	-5.8121920	-8.2448283
H	3.6292904	-7.8813486	-8.5984681
H	0.3069717	-5.5484060	-10.0414923
H	1.6272974	-3.4755496	-9.7087620
H	3.3509938	-5.3005990	-4.0388069
H	3.3144102	-3.5462300	-4.0293657
H	2.8041907	-1.3317521	-7.1875089
H	3.4761283	-1.7595458	-5.6247990
H	6.0603099	-3.4156666	-11.9375597
H	4.6373634	-4.3882864	-11.4710004
H	4.5209853	-2.5901738	-11.5022564
H	7.2171621	-1.7286571	-10.2937696
H	6.9172636	-1.6422526	-8.5388705
H	5.6805422	-1.0130049	-9.6929975
H	2.5056488	-5.1675535	-6.4866473
H	1.3590300	-4.8327213	-5.2032314
H	1.2718846	-2.5371615	-5.6251041
H	1.3513531	-3.2322272	-7.2295296

3_sy_tr_12.log

E = -1188.205200

H = -1187.838671

G = -1187.906442

NImag=0

C	5.1526154	-3.3441607	-6.5662963
C	3.9931482	-2.6218097	-7.1998930
C	5.2586496	-4.5214674	-5.8351758
O	6.3888013	-5.0698396	-5.5782737
C	3.6624427	-2.9893546	-8.6862176
C	3.0771651	-4.3489681	-8.9771165
C	3.7458099	-5.5385291	-8.6583810
C	3.1383479	-6.7685604	-8.8830177
C	1.8524399	-6.8130771	-9.4331086
C	1.1755801	-5.6341186	-9.7673199
C	1.7958714	-4.4123325	-9.5412464
C	4.0525196	-5.2842278	-5.2710722
C	2.6596828	-2.5387242	-6.4254389
S	5.0322387	-2.6962413	-9.9089187
C	5.8375677	-1.1890184	-9.3339365
C	6.3354387	-3.9235276	-9.6668915
C	1.2204504	-8.0855481	-9.6616826
N	0.7111678	-9.1092714	-9.8456121
C	2.8316709	-4.5039373	-4.7896530
C	2.0224954	-3.8212791	-5.8893518
H	6.1267214	-2.9483117	-6.8576981
H	4.2953749	-1.5694021	-7.2833994
H	2.9536596	-2.2370813	-9.0546321
H	4.7320032	-5.5104201	-8.2092382
H	3.6524704	-7.6894906	-8.6280557
H	0.1803093	-5.6794053	-10.1965734
H	1.2731885	-3.4932349	-9.7907887
H	3.7292738	-6.0241765	-6.0183510
H	4.4562290	-5.8628196	-4.4330410
H	1.9291157	-2.0176353	-7.0594593
H	2.8446193	-1.8812830	-5.5656088
H	6.5809889	-0.9346245	-10.0920697
H	5.0798078	-0.4048844	-9.2844772
H	6.3124263	-1.3483869	-8.3657329
H	7.2063095	-3.5227209	-10.1915963
H	6.0175648	-4.8477417	-10.1489830
H	6.5418942	-4.0636100	-8.6062594

H	2.1747596	-5.2070101	-4.2622094
H	3.1404279	-3.7525583	-4.0486161
H	1.0412172	-3.5442867	-5.4836906
H	1.8272355	-4.5404232	-6.6950160

3_sy_tr_13.log

E = -1188.209593

H = -1187.843241

G = -1187.911592

NImag=0

C	5.0418271	-3.0925408	-6.4410075
C	3.8416604	-2.4988529	-7.1330126
C	5.2339260	-4.2442785	-5.6876864
O	6.3993035	-4.7182438	-5.4433775
C	3.6751181	-2.9494562	-8.6239468
C	3.1564584	-4.3298773	-8.9147202
C	3.7803779	-5.4951546	-8.4454467
C	3.2127444	-6.7414246	-8.6794327
C	2.0106867	-6.8305367	-9.3918855
C	1.3808844	-5.6796623	-9.8779012
C	1.9625895	-4.4403636	-9.6402922
C	4.0887555	-5.0606149	-5.0743553
C	2.4665689	-2.5287139	-6.4400275
S	5.2640002	-2.5627625	-9.5058454
C	6.3417831	-4.0076485	-9.4470500
C	4.7392863	-2.6347816	-11.2286579
C	1.4184550	-8.1200549	-9.6309297
N	0.9407983	-9.1572897	-9.8239254
C	2.7820700	-4.3703916	-4.6910144
C	1.9504574	-3.8457608	-5.8594800
H	5.9847522	-2.6378933	-6.7579656
H	4.0538888	-1.4254777	-7.2462514
H	3.0125886	-2.2264720	-9.1177171
H	4.7001561	-5.4330900	-7.8760193
H	3.6917125	-7.6415285	-8.3079732
H	0.4517861	-5.7585369	-10.4324942
H	1.4755725	-3.5427536	-10.0113723
H	3.8646496	-5.8977901	-5.7523877
H	4.5233205	-5.5163803	-4.1774946
H	1.7233604	-2.1332727	-7.1464641
H	2.5192482	-1.8075350	-5.6137965
H	7.2476973	-3.7143932	-9.9827401
H	6.5727846	-4.2186526	-8.4014677
H	5.8642121	-4.8545232	-9.9410862
H	5.6312876	-2.4999552	-11.8435991
H	4.0405853	-1.8145505	-11.4002501
H	4.2726958	-3.6008994	-11.4325501
H	2.1776179	-5.0964479	-4.1329703
H	2.9898955	-3.5431050	-3.9972773
H	0.9277116	-3.6602065	-5.5080625
H	1.8719256	-4.6224263	-6.6309658

3_sy_tr_14.log

E = -1188.210222

H = -1187.843869

G = -1187.912825

NImag=0

C	5.1344731	-3.3637195	-6.5265513
C	3.8941382	-2.7395796	-7.1239741
C	5.2535573	-4.3261631	-5.5363562

O	6.3679754	-4.7401075	-5.0582556
C	3.6321596	-3.0667574	-8.6255066
C	3.0798725	-4.4211711	-8.9812097
C	3.6140088	-5.6086288	-8.4590460
C	3.0543087	-6.8367804	-8.7870848
C	1.9514938	-6.8842802	-9.6491932
C	1.4075618	-5.7104907	-10.1805960
C	1.9766691	-4.4881056	-9.8419163
C	3.9876851	-4.9521366	-4.9351475
C	2.5569064	-2.9197624	-6.3726997
S	5.1813472	-2.6660792	-9.5736874
C	6.1271058	-4.1912862	-9.7398254
C	4.5502153	-2.5019235	-11.2542037
C	1.3698621	-8.1550923	-9.9912815
N	0.9011269	-9.1775903	-10.2670575
C	3.1313476	-3.9792168	-4.1107378
C	2.7101412	-2.7033718	-4.8646609
H	6.0758612	-2.9151093	-6.8536217
H	4.0612633	-1.6496674	-7.1377218
H	2.9540562	-2.3033696	-9.0286509
H	4.4677672	-5.5654447	-7.7910382
H	3.4649470	-7.7550728	-8.3801955
H	0.5516354	-5.7573460	-10.8455748
H	1.5543864	-3.5719093	-10.2460425
H	3.3672785	-5.3929639	-5.7245515
H	4.3144903	-5.7755605	-4.2924506
H	2.1272223	-3.9101351	-6.5631922
H	1.8465923	-2.1943359	-6.7882224
H	7.0102885	-3.9309027	-10.3274972
H	6.4208061	-4.5145952	-8.7407773
H	5.5326318	-4.9486611	-10.2527604
H	5.4104266	-2.3441979	-11.9073710
H	3.8964482	-1.6287887	-11.2815449
H	4.0121909	-3.4084557	-11.5391323
H	2.2315737	-4.5150616	-3.7822620
H	3.6739832	-3.6997549	-3.1990079
H	3.4469566	-1.9077876	-4.7014300
H	1.7655385	-2.3387374	-4.4459641

3_sy_tr_15.log

E = -1188.205831

H = -1187.839602

G = -1187.908595

NImag=0

C	5.2045844	-3.5878333	-6.6749629
C	4.0303069	-2.8079648	-7.2154731
C	5.2162575	-4.6344073	-5.7666982
O	6.2764367	-5.1937269	-5.3133104
C	3.6080739	-3.0688693	-8.6941705
C	2.9993438	-4.4129804	-9.0236452
C	3.6384851	-5.6219168	-8.7139405
C	3.0265584	-6.8356156	-9.0051405
C	1.7659363	-6.8450444	-9.6128578
C	1.1149341	-5.6473794	-9.9296848
C	1.7383588	-4.4417310	-9.6333413
C	3.8842434	-5.1687308	-5.2265595
C	2.7088391	-2.8319006	-6.4001461
S	4.9012464	-2.7134006	-9.9809139
C	5.8091895	-1.2992009	-9.3290353
C	6.1482905	-4.0156161	-9.9143635
C	1.1324681	-8.1013810	-9.9148499

N	0.6225724	-9.1123858	-10.1579911
C	3.1714412	-4.1884101	-4.2828354
C	2.9454554	-2.7908798	-4.8881592
H	6.1876133	-3.2118920	-6.9612301
H	4.3248571	-1.7480317	-7.2151796
H	2.8755605	-2.2984908	-8.9679208
H	4.6075919	-5.6125110	-8.2277571
H	3.5187530	-7.7714182	-8.7614580
H	0.1368581	-5.6651577	-10.3989112
H	1.2366812	-3.5078874	-9.8713979
H	3.2095608	-5.4242502	-6.0520664
H	4.1001470	-6.0983331	-4.6905269
H	2.1083438	-3.7148461	-6.6506970
H	2.1161371	-1.9636855	-6.7118724
H	6.5279771	-1.0167722	-10.1006787
H	5.0942444	-0.4883608	-9.1774838
H	6.3186059	-1.5616451	-8.4016881
H	6.9935264	-3.6379001	-10.4948361
H	5.7365340	-4.8978964	-10.4046113
H	6.4343473	-4.2174755	-8.8826512
H	2.2007581	-4.6212448	-4.0084152
H	3.7440719	-4.0946374	-3.3515872
H	3.8085679	-2.1464307	-4.6846736
H	2.0861416	-2.3233584	-4.3943785

3_sy_tr_16.log

E = -1188.203612

H = -1187.837532

G = -1187.906745

NImag=0

C	4.1552523	-2.3787260	-6.4815679
C	3.5786061	-3.7121058	-6.9184990
C	4.4602894	-1.9657583	-5.1968600
O	4.9557154	-0.8232549	-4.8888298
C	3.8819239	-3.9253658	-8.4335855
C	2.9680527	-4.9378818	-9.0929657
C	3.2141959	-6.3154700	-9.1252012
C	2.2942636	-7.1855769	-9.6999379
C	1.1119369	-6.6747602	-10.2445647
C	0.8517070	-5.2995154	-10.2228454
C	1.7830817	-4.4430723	-9.6514651
C	4.2054187	-2.9384611	-4.0391147
C	3.9704612	-4.9583862	-6.0705100
S	5.6446245	-4.4043423	-8.7446601
C	5.6678664	-4.5207186	-10.5482249
C	6.5788358	-2.8698245	-8.5516745
C	0.1570978	-7.5712895	-10.8399585
N	-0.6118409	-8.2924248	-11.3193638
C	5.1964321	-4.1103751	-4.0007300
C	5.3153298	-4.8527156	-5.3417261
H	4.3274456	-1.6516021	-7.2755155
H	2.4744424	-3.6900247	-6.9326330
H	3.7714633	-2.9674949	-8.9542665
H	4.1280964	-6.7353640	-8.7130303
H	2.4909260	-8.2519956	-9.7270229
H	-0.0650259	-4.9108594	-10.6536497
H	1.5901529	-3.3739927	-9.6356649
H	4.2734513	-2.3689646	-3.1070544
H	3.1843081	-3.3364555	-4.1000868
H	3.9651960	-5.8472625	-6.7099057
H	3.1853517	-5.1422296	-5.3293766

H	6.7179622	-4.5454427	-10.8454566
H	5.1777852	-5.4474000	-10.8455962
H	5.1633330	-3.6508112	-10.9741134
H	7.5649183	-3.0676480	-8.9783807
H	6.6546464	-2.6440011	-7.4895967
H	6.0717671	-2.0676329	-9.0908257
H	6.1861663	-3.7478212	-3.6963520
H	4.8703072	-4.8180642	-3.2274939
H	5.7146464	-5.8578102	-5.1641064
H	6.0479100	-4.3399977	-5.9752872

3_sy_tr_17.log

E = -1188.213285

H = -1187.847221

G = -1187.916866

NImag=0

C	5.0860647	-3.9816959	-6.5027751
C	3.8278099	-3.2649209	-6.9421919
C	5.6629733	-3.8140779	-5.2522669
O	6.6869807	-4.4412991	-4.8165892
C	3.5403646	-3.3821477	-8.4518424
C	2.9536285	-4.6593111	-9.0004031
C	3.3058850	-5.9269111	-8.5164375
C	2.7353587	-7.0727079	-9.0562650
C	1.8044771	-6.9561099	-10.0954773
C	1.4344076	-5.6999619	-10.5860954
C	2.0092043	-4.5623364	-10.0313842
C	4.9943361	-2.8302864	-4.2826481
C	2.5402508	-3.6379870	-6.1704218
S	5.1029425	-2.8852270	-9.3558752
C	5.8939904	-4.4008142	-9.9342129
C	4.4430629	-2.3021199	-10.9327107
C	1.2145952	-8.1419995	-10.6583559
N	0.7407033	-9.0961106	-11.1123562
C	3.6025159	-3.2907883	-3.8184692
C	2.4633056	-2.9739994	-4.7926139
H	5.5052349	-4.7646350	-7.1287702
H	3.9572236	-2.1800897	-6.7877598
H	2.8732367	-2.5617526	-8.7390130
H	4.0201698	-6.0246715	-7.7071179
H	3.0064283	-8.0522699	-8.6767980
H	0.7028478	-5.6185409	-11.3830429
H	1.7112608	-3.5828813	-10.3960284
H	5.6619258	-2.7388997	-3.4205399
H	4.9039320	-1.8314514	-4.7356116
H	2.4851348	-4.7292039	-6.0685982
H	1.6560262	-3.3221525	-6.7432563
H	6.7065028	-4.0784491	-10.5895022
H	6.3006467	-4.9371919	-9.0782054
H	5.1751006	-5.0089245	-10.4863322
H	5.2987697	-2.0122701	-11.5457781
H	3.8162820	-1.4312199	-10.7347057
H	3.8760834	-3.0963314	-11.4220366
H	3.6309755	-4.3709350	-3.6163247
H	3.3649496	-2.8028456	-2.8649871
H	2.4284783	-1.8843496	-4.9372626
H	1.5113338	-3.2544223	-4.3254370

3_sy_tr_18.log

E = -1188.209489

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H =      -1187.843649
G =      -1187.913495
NImag=0
C      5.0833420      -3.8935056      -6.5053377
C      3.9213212      -3.0785531      -7.0319336
C      5.2922387      -4.3976476      -5.2308365
O      6.2707179      -5.1632429      -4.9153314
C      3.6806648      -3.2817683      -8.5466923
C      3.0693488      -4.5778989      -9.0136276
C      3.5070386      -5.8283885      -8.5524951
C      2.8969641      -6.9951132      -8.9950674
C      1.8413116      -6.9175902      -9.9121558
C      1.3919694      -5.6795635     -10.3823500
C      2.0089611      -4.5196488      -9.9275582
C      4.3462999      -4.0441486      -4.0687030
C      2.5757944      -3.3463942      -6.3266837
S      5.2557495      -2.8691846      -9.4718616
C      5.9725379      -4.4240063     -10.0412688
C      4.5956518      -2.2592873     -11.0355606
C      1.2088985      -8.1255083     -10.3732560
N      0.6995694      -9.0970242     -10.7445812
C      3.6955997      -2.6593799      -4.1267293
C      2.4380470      -2.6012325      -4.9965531
H      5.8608455      -4.1662796      -7.2196275
H      4.1032459      -1.9904012      -6.9476373
H      3.0389316      -2.4619911      -8.8892007
H      4.3232044      -5.8841298      -7.8402385
H      3.2328411      -7.9618999      -8.6348955
H      0.5699589      -5.6291382     -11.0886119
H      1.6568039      -3.5544704     -10.2816441
H      3.5731015      -4.8220488      -3.9769819
H      4.9646984      -4.1247111      -3.1685999
H      2.4776202      -4.4271611      -6.1679403
H      1.7444545      -3.0481876      -6.9798226
H      6.8405356      -4.1462284     -10.6431477
H      6.2924854      -5.0058537      -9.1769018
H      5.2449504      -4.9706020     -10.6431508
H      5.4468073      -2.0788255     -11.6950577
H      4.0744750      -1.3223090     -10.8340207
H      3.9230511      -3.0022609     -11.4692693
H      3.4358825      -2.3287534      -3.1140287
H      4.4360370      -1.9412568      -4.5030469
H      2.1844675      -1.5518682      -5.1929263
H      1.5920758      -3.0313367      -4.4455667

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3_sy_tr_19.log
E =      -1188.206143
H =      -1187.840071
G =      -1187.909306
NImag=0
C      5.1728354      -3.3302769      -6.4554133
C      4.0539584      -2.6004982      -7.1538097
C      5.1981918      -3.9948071      -5.2375372
O      6.2738615      -4.4293922      -4.6913978
C      3.7725593      -3.0285950      -8.6279640
C      3.1780439      -4.3748967      -8.9330062
C      3.7223711      -5.5696397      -8.4412965
C      3.1158771      -6.7885168      -8.7214366
C      1.9558007      -6.8183621      -9.5034581
C      1.4048630      -5.6364025     -10.0131185
C      2.0230877      -4.4261431      -9.7271060

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C	3.9114495	-4.2780173	-4.4389111
C	2.7259240	-2.4628655	-6.3878753
S	5.3286988	-2.7098373	-9.6070155
C	6.2500293	-4.2540821	-9.7308597
C	4.6862647	-2.5958782	-11.2868898
C	1.3254091	-8.0794582	-9.7914060
N	0.8176309	-9.0941334	-10.0235822
C	2.7277845	-4.8010127	-5.2561492
C	1.9365816	-3.7204270	-6.0097502
H	6.1618912	-3.1748472	-6.8955101
H	4.3764804	-1.5540255	-7.2912509
H	3.1253502	-2.2582218	-9.0668259
H	4.6146623	-5.5437911	-7.8259322
H	3.5333247	-7.7122076	-8.3341745
H	0.5070108	-5.6703152	-10.6211005
H	1.5966220	-3.5047896	-10.1145806
H	4.1992399	-5.0301180	-3.6978203
H	3.6162464	-3.3831021	-3.8719335
H	2.0654356	-1.8066542	-6.9699482
H	2.9647157	-1.9132529	-5.4697695
H	7.1321896	-4.0222889	-10.3322132
H	6.5527191	-4.5565713	-8.7282241
H	5.6425592	-5.0176595	-10.2186312
H	5.5458359	-2.5025221	-11.9535360
H	4.0675334	-1.6992070	-11.3472114
H	4.1100771	-3.4924682	-11.5251717
H	3.1071437	-5.5488556	-5.9608154
H	2.0365172	-5.3348968	-4.5924932
H	1.1088273	-3.3806187	-5.3742061
H	1.4693960	-4.1611449	-6.8981684

3_sy_tr_1_r.log

E = -1188.209881

H = -1187.843934

G = -1187.913529

NImag=0

C	1.5102034	-1.5974549	0.0028485
C	1.1201292	-0.6892164	1.1523921
C	1.2492877	-2.9457545	-0.2075006
O	1.8007155	-3.6373111	-1.1336963
C	0.0794586	0.3659441	0.6859599
C	0.4501128	1.0540201	-0.6068335
C	1.7031487	1.6606874	-0.7642583
C	2.0241899	2.3156659	-1.9453022
C	1.0832894	2.3609881	-2.9825384
C	-0.1701706	1.7565983	-2.8400680
C	-0.4799716	1.1110545	-1.6478021
C	0.2448927	-3.7213482	0.6606087
C	0.6927555	-1.4144627	2.4392164
S	-0.0607121	1.7497205	1.9659347
C	-0.9606215	3.0464070	1.0844283
C	-1.3787842	1.2380086	3.0917593
C	1.4116385	3.0386075	-4.2086950
N	1.6760522	3.5854251	-5.1947464
C	-0.9594513	-2.9271696	1.1649474
C	-0.6783702	-2.0997358	2.4220986
H	2.2114181	-1.1560397	-0.7053792
H	2.0182169	-0.1128013	1.4222828
H	-0.9317582	-0.0500163	0.6136516
H	2.4396527	1.6225123	0.0341918
H	2.9933174	2.7871571	-2.0696643

H	-0.8895810	1.7965745	-3.6512134
H	-1.4526683	0.6431816	-1.5259611
H	-0.0949302	-4.5485227	0.0290155
H	0.7745787	-4.1813488	1.5086673
H	0.7379882	-0.7233174	3.2921434
H	1.4654088	-2.1655032	2.6381112
H	-1.2361803	3.7907711	1.8342437
H	-0.2950191	3.4932836	0.3462157
H	-1.8491998	2.6205235	0.6136527
H	-1.6623209	2.1338392	3.6484290
H	-0.9902625	0.4905736	3.7813875
H	-2.2250613	0.8593203	2.5158726
H	-1.3056097	-2.2727278	0.3541093
H	-1.7895235	-3.6103377	1.3815367
H	-0.7281599	-2.7532767	3.3022272
H	-1.4830077	-1.3662894	2.5470447

3_sy_tr_1_ts1.log

E = -1188.184029

H = -1187.820732

G = -1187.889922

NImag=1

C	2.4463813	-0.8690312	1.3462401
C	1.0905507	-0.9909447	1.0029502
C	3.5952664	-1.2178129	0.5719435
O	4.7540166	-1.0786999	1.0217848
C	0.0950782	0.8741849	0.6998274
C	-1.2896703	0.5228505	0.4499583
C	-1.9077592	0.5424134	-0.8235514
C	-3.1958614	0.0695609	-1.0047242
C	-3.9198748	-0.4383253	0.0862356
C	-3.3367065	-0.4483363	1.3639340
C	-2.0504512	0.0302292	1.5386743
C	3.4511448	-1.7910184	-0.8369177
C	0.6023828	-1.8416728	-0.1507495
S	0.8381393	1.9376697	-0.4973855
C	0.0250016	3.5490253	-0.3109281
C	2.4212990	2.3192145	0.2731586
C	-5.2517679	-0.9283128	-0.1005170
N	-6.3311254	-1.3267987	-0.2520204
C	2.4799304	-1.0069545	-1.7261370
C	1.0125825	-1.4185074	-1.5656602
H	2.6758762	-0.4452130	2.3232100
H	0.4210690	-1.0368417	1.8623756
H	0.2994991	1.2589746	1.6996560
H	-1.3788750	0.9297773	-1.6906619
H	-3.6502160	0.0927773	-1.9903609
H	-3.9000651	-0.8256072	2.2119104
H	-1.6123223	0.0313856	2.5330441
H	4.4558262	-1.7828639	-1.2680444
H	3.1379264	-2.8424398	-0.7720378
H	-0.4898995	-1.9069752	-0.1091045
H	0.9720920	-2.8579827	0.0405601
H	0.5648713	4.2722233	-0.9268533
H	-1.0007202	3.4453510	-0.6695445
H	0.0426264	3.8348062	0.7425523
H	2.9016333	3.0804226	-0.3439085
H	3.0206725	1.4095297	0.2950364
H	2.2443904	2.6901212	1.2850605
H	2.6043956	0.0622579	-1.5132309
H	2.7652334	-1.1326214	-2.7762056

H	0.8031062	-2.2648006	-2.2306948
H	0.3684672	-0.5991975	-1.9054861

3_sy_tr_1_ts2.log

E = -1188.201534
H = -1187.836949
G = -1187.907174

NImag=1

C	1.3369521	-1.6314260	-0.6699958
C	1.4250417	-0.1729226	-1.0593030
C	2.2898131	-2.4667191	-0.0552928
O	2.1061137	-3.7116348	0.0669277
C	0.4855391	0.3350966	-0.0154777
C	-0.9388324	-0.0923140	-0.0013837
C	-1.6562967	-0.2797298	-1.1928106
C	-3.0039812	-0.6084212	-1.1572238
C	-3.6455472	-0.7528839	0.0806749
C	-2.9431524	-0.5683201	1.2778843
C	-1.5963743	-0.2339724	1.2276732
C	3.6156819	-1.9243692	0.4857405
C	2.8135669	0.4723423	-1.0549770
S	0.1338336	2.5126515	-0.5040537
C	-1.3176360	2.9301126	0.4891600
C	1.3780858	3.4423171	0.4210680
C	-5.0420139	-1.0943877	0.1206567
N	-6.1669974	-1.3684966	0.1529508
C	3.5209838	-0.5862746	1.2181124
C	3.5175387	0.6416159	0.2980848
H	0.4412894	-2.1447907	-1.0108442
H	0.9973728	-0.0266740	-2.0590023
H	0.9133111	0.4718168	0.9787109
H	-1.1630061	-0.1667067	-2.1538193
H	-3.5613320	-0.7528750	-2.0767971
H	-3.4500998	-0.6847498	2.2299939
H	-1.0428659	-0.0843906	2.1505330
H	3.9914727	-2.6971850	1.1627307
H	4.3380682	-1.8529980	-0.3402815
H	2.7439528	1.4596750	-1.5315731
H	3.4414767	-0.1335174	-1.7184416
H	-1.4600853	4.0120442	0.4404801
H	-2.1856844	2.4290946	0.0578398
H	-1.1701940	2.6139048	1.5245671
H	1.0625436	4.4877855	0.4531374
H	2.3271808	3.3685297	-0.1110226
H	1.4709036	3.0468721	1.4350529
H	2.6185490	-0.5977478	1.8419358
H	4.3648188	-0.4908819	1.9110185
H	4.5542744	0.9250852	0.0788922
H	3.0872860	1.4850627	0.8474220

3_sy_tr_2.log

E = -1188.208322
H = -1187.842319
G = -1187.913153

NImag=0

C	4.3056578	-2.4448437	-6.4409377
C	3.7371269	-3.7654376	-6.9124098
C	5.0041802	-2.1451871	-5.2824440
O	5.6289916	-1.0406769	-5.0956815
C	3.8904708	-3.8420716	-8.4611772

C	3.0457340	-4.9180462	-9.1091843
C	3.4517870	-6.2501837	-9.2549791
C	2.5951775	-7.1941886	-9.8096267
C	1.3147300	-6.8053447	-10.2168910
C	0.8932926	-5.4779163	-10.0781897
C	1.7637997	-4.5448255	-9.5304832
C	5.0329963	-3.1189708	-4.0908046
C	4.3387105	-5.0011643	-6.2250742
S	5.6659321	-4.0690457	-8.9519165
C	5.5314150	-4.0821312	-10.7544275
C	6.4357140	-2.4457375	-8.7449808
C	0.4242856	-7.7787728	-10.7910697
N	-0.2930779	-8.5616627	-11.2532732
C	3.7894850	-3.9972247	-3.9287757
C	3.8000343	-5.2458339	-4.8139495
H	4.2722989	-1.6391357	-7.1749342
H	2.6388457	-3.8299658	-6.7905744
H	3.6161781	-2.8731968	-8.8933115
H	4.4431956	-6.5724976	-8.9469934
H	2.9144695	-8.2243981	-9.9257801
H	-0.0996528	-5.1841553	-10.4019490
H	1.4465185	-3.5109634	-9.4264813
H	5.9374220	-3.7440575	-4.1393898
H	5.1537653	-2.4799881	-3.2095829
H	5.4295699	-4.8804644	-6.1837278
H	4.1425770	-5.9022135	-6.8166967
H	6.5452131	-3.9689259	-11.1432340
H	5.1202484	-5.0404316	-11.0703011
H	4.8967541	-3.2532684	-11.0754012
H	7.3855681	-2.5026496	-9.2821411
H	6.5943533	-2.2737998	-7.6816957
H	5.7876723	-1.6804683	-9.1760503
H	3.6852163	-4.3093497	-2.8827422
H	2.9049016	-3.3897144	-4.1593733
H	2.7842641	-5.6556283	-4.8798457
H	4.4209781	-6.0194621	-4.3448186

3_sy_tr_20.log

E = -1188.204846

H = -1187.838843

G = -1187.908400

NImag=0

C	5.1094942	-3.9863729	-6.7099906
C	3.9480899	-3.1069919	-7.1173271
C	5.3730829	-4.5759185	-5.4822744
O	6.3257604	-5.4104765	-5.2829364
C	3.5342314	-3.2352024	-8.6045140
C	2.9101470	-4.5339858	-9.0657082
C	3.4890218	-5.7854621	-8.8097542
C	2.8594457	-6.9506074	-9.2312008
C	1.6441462	-6.8684032	-9.9210427
C	1.0557634	-5.6280547	-10.1887885
C	1.6944671	-4.4711365	-9.7585822
C	4.5435942	-4.2340789	-4.2314497
C	2.6532965	-3.3583534	-6.3108364
S	4.8173834	-2.7322246	-9.8697416
C	5.9264197	-1.6160831	-8.9900800
C	5.8865282	-4.1372722	-10.2359517
C	0.9937662	-8.0740308	-10.3623597
N	0.4709040	-9.0441176	-10.7182055
C	3.9616321	-2.8195834	-4.1762477

C	2.6494547	-2.6645305	-4.9467784
H	5.8204087	-4.2568773	-7.4862605
H	4.1713644	-2.0300385	-7.0031706
H	2.8051120	-2.4397137	-8.7934297
H	4.4297620	-5.8496370	-8.2754208
H	3.3050491	-7.9193345	-9.0304848
H	0.1132257	-5.5744613	-10.7234478
H	1.2398241	-3.5047463	-9.9595654
H	3.7421889	-4.9783201	-4.1084926
H	5.2287884	-4.3856097	-3.3907454
H	2.5314499	-4.4413450	-6.1875364
H	1.7810865	-3.0071807	-6.8782568
H	6.7047328	-1.3349588	-9.7023637
H	5.3494566	-0.7334197	-8.7094225
H	6.3493606	-2.1133240	-8.1159955
H	6.6529188	-3.7444460	-10.9082153
H	5.2884373	-4.8790348	-10.7662618
H	6.3383340	-4.5531222	-9.3376038
H	3.7928415	-2.5267843	-3.1330977
H	4.7075586	-2.1193501	-4.5750842
H	2.4329492	-1.5974800	-5.0828600
H	1.8253218	-3.0796297	-4.3527149

3_sy_tr_21.log

E = -1188.202158

H = -1187.835887

G = -1187.904658

NImag=0

C	5.2354248	-3.5848827	-6.5905344
C	4.1627588	-2.7152577	-7.1929582
C	5.2183401	-4.3707454	-5.4470696
O	6.2630710	-4.9379565	-4.9652748
C	3.6693241	-3.0574900	-8.6338229
C	3.0751650	-4.4132984	-8.9329066
C	3.7615152	-5.6087149	-8.6772639
C	3.1726954	-6.8352879	-8.9643733
C	1.8849096	-6.8706318	-9.5092214
C	1.1866698	-5.6864736	-9.7753591
C	1.7906322	-4.4690010	-9.4907067
C	3.9265899	-4.6307353	-4.6473714
C	2.9368379	-2.4308177	-6.2994561
S	4.9166767	-2.7214915	-9.9902888
C	5.9090630	-1.3374578	-9.3992161
C	6.1482059	-4.0403028	-10.0023880
C	1.2724046	-8.1387811	-9.8048956
N	0.7785274	-9.1588268	-10.0433123
C	2.6494453	-4.8588414	-5.4592889
C	1.9783139	-3.5759238	-5.9650563
H	6.2248470	-3.4752685	-7.0381949
H	4.5915793	-1.7116463	-7.3230007
H	2.9238919	-2.2997050	-8.9065880
H	4.7503641	-5.5820753	-8.2348893
H	3.7031340	-7.7600364	-8.7627241
H	0.1892704	-5.7244589	-10.2004007
H	1.2541629	-3.5461646	-9.6935534
H	4.1416088	-5.5245286	-4.0530905
H	3.7734497	-3.8137048	-3.9261358
H	2.3582827	-1.6190887	-6.7588449
H	3.3417894	-2.0258374	-5.3644439
H	6.5886466	-1.0853976	-10.2157656
H	5.2385889	-0.4981279	-9.2071453

H	6.4666625	-1.6196755	-8.5050136
H	6.9450610	-3.6797698	-10.6575786
H	5.6933116	-4.9276878	-10.4420164
H	6.5265548	-4.2309408	-8.9987678
H	2.8913868	-5.5123707	-6.3040798
H	1.9249044	-5.4097503	-4.8469150
H	1.2983902	-3.1995277	-5.1897482
H	1.3473423	-3.8093190	-6.8307390

3_sy_tr_22.log

E = -1188.204892
H = -1187.838841
G = -1187.908924

NImag=0

C	4.5409386	-2.5149658	-6.4754625
C	4.1323076	-3.8899478	-6.9659133
C	4.2973862	-2.0017126	-5.2128844
O	4.5335500	-0.7910201	-4.8640844
C	4.1151788	-3.9414671	-8.5163540
C	3.1200542	-4.9305121	-9.0876353
C	3.3552961	-6.3106121	-9.1272151
C	2.3897349	-7.1758655	-9.6285675
C	1.1758968	-6.6574890	-10.0927840
C	0.9279457	-5.2803333	-10.0623974
C	1.9044032	-4.4268028	-9.5647293
C	3.7139769	-2.8664050	-4.0770134
C	4.8994415	-5.0687802	-6.3353750
S	5.7608342	-4.3482115	-9.2600684
C	5.4340002	-3.9935893	-10.9983283
C	6.8166697	-2.9509269	-8.8362259
C	0.1753145	-7.5497955	-10.6152354
N	-0.6302827	-8.2672694	-11.0363464
C	3.6705385	-4.3993527	-4.1860070
C	4.9462138	-4.9869634	-4.8011212
H	4.9282048	-1.8093959	-7.2087156
H	3.0714885	-4.0641261	-6.7315960
H	3.8830608	-2.9431613	-8.9026530
H	4.2942576	-6.7280326	-8.7751428
H	2.5730915	-8.2445839	-9.6617707
H	-0.0135968	-4.8874659	-10.4314769
H	1.7233682	-3.3559863	-9.5453911
H	4.3285250	-2.6073796	-3.2046557
H	2.7114919	-2.4751701	-3.8545734
H	5.9317047	-5.1076031	-6.7117034
H	4.4147245	-6.0094272	-6.6276811
H	6.3944697	-4.0276052	-11.5158015
H	4.7773624	-4.7739693	-11.3854841
H	4.9746353	-3.0071556	-11.0889874
H	7.7349401	-3.0796490	-9.4133991
H	7.0312142	-2.9997431	-7.7684604
H	6.3170402	-2.0172699	-9.0998058
H	3.5398383	-4.7974994	-3.1731089
H	2.7943507	-4.7369792	-4.7525423
H	5.1324195	-5.9926667	-4.4085510
H	5.7985099	-4.3702087	-4.4900515

3_sy_tr_23.log

E = -1188.211905
H = -1187.846008
G = -1187.916194

NImag=0

C	4.8299620	-4.3827193	-6.4033658
C	3.9035441	-3.4117861	-7.0881453
C	5.3145995	-4.0925619	-5.1308313
O	5.9572941	-4.8881221	-4.3711370
C	3.8251385	-3.5802142	-8.6196094
C	3.0657797	-4.7821302	-9.1366452
C	3.5795359	-6.0845924	-9.0948888
C	2.8208960	-7.1575277	-9.5492558
C	1.5351526	-6.9279575	-10.0509217
C	1.0111909	-5.6314514	-10.1079930
C	1.7834067	-4.5686867	-9.6568295
C	5.0444157	-2.6707827	-4.5969032
C	2.4794096	-3.3691008	-6.4919222
S	5.5472749	-3.6578963	-9.2758597
C	5.2521764	-3.2550354	-11.0118334
C	6.2483996	-2.1020049	-8.6981511
C	0.7460021	-8.0351347	-10.5221003
N	0.1100605	-8.9253033	-10.9019867
C	3.5437937	-2.3026687	-4.3905185
C	2.5219764	-3.2969374	-4.9598552
H	4.8687049	-5.4177876	-6.7383967
H	4.2981421	-2.3946938	-6.9541885
H	3.3931551	-2.6761567	-9.0638082
H	4.5777754	-6.2787736	-8.7152460
H	3.2208607	-8.1654567	-9.5174267
H	0.0162174	-5.4621569	-10.5059482
H	1.3849045	-3.5590901	-9.7037806
H	5.5785554	-2.5879557	-3.6465347
H	5.5032423	-1.9442648	-5.2807090
H	1.9154583	-4.2629034	-6.7884201
H	1.9422012	-2.4974031	-6.8947217
H	6.2271464	-3.1669006	-11.4945071
H	4.6958516	-4.0830117	-11.4553051
H	4.6921815	-2.3208990	-11.0863617
H	7.1652594	-1.9414371	-9.2689371
H	6.4820285	-2.2165874	-7.6389164
H	5.5368623	-1.2921176	-8.8722140
H	3.3496862	-2.2124126	-3.3161250
H	3.3467189	-1.3111407	-4.8189046
H	1.5244185	-3.0272589	-4.5933367
H	2.7400204	-4.2936782	-4.5596586

3_sy_tr_24.log

E = -1188.207351

H = -1187.841329

G = -1187.909305

NImag=0

C	5.2120002	-4.1428539	-6.5253467
C	4.6315242	-2.9341196	-7.2093164
C	4.5728965	-5.1690526	-5.8396116
O	5.1785094	-6.2104307	-5.4067003
C	4.0294682	-3.1731197	-8.6502545
C	3.2875205	-4.4606550	-8.9054282
C	3.9366828	-5.7020878	-8.8883829
C	3.2173711	-6.8759902	-9.0767402
C	1.8350919	-6.8086489	-9.2908772
C	1.1773781	-5.5747268	-9.3428508
C	1.9123481	-4.4096620	-9.1577347
C	3.0615900	-5.1385561	-5.5620218
C	3.6432915	-2.0655277	-6.4006989

S	5.2854202	-2.9917217	-10.0086588
C	5.5508341	-1.2089718	-10.0177011
C	6.8812259	-3.5560299	-9.3828285
C	1.0835779	-8.0220456	-9.4732159
N	0.4775448	-8.9980515	-9.6202674
C	2.4636565	-3.8537929	-4.9826066
C	2.3223793	-2.6980476	-5.9714810
H	6.2727982	-4.3171304	-6.7063796
H	5.4712724	-2.2468779	-7.3739661
H	3.3647090	-2.3383011	-8.9055335
H	5.0026988	-5.7642909	-8.7021448
H	3.7172532	-7.8386800	-9.0540489
H	0.1088919	-5.5325701	-9.5258921
H	1.4079205	-3.4482022	-9.1947074
H	2.5206180	-5.3946652	-6.4861613
H	2.8830256	-5.9608379	-4.8616286
H	3.4286791	-1.1616848	-6.9872871
H	4.1796932	-1.7379012	-5.5007221
H	6.3667368	-1.0094329	-10.7150772
H	4.6319461	-0.7420058	-10.3753272
H	5.8070431	-0.8613392	-9.0150726
H	7.5992883	-3.3136177	-10.1697243
H	6.8425785	-4.6363724	-9.2453191
H	7.1401251	-3.0407700	-8.4578278
H	1.4661053	-4.0912876	-4.5920615
H	3.0639710	-3.5242128	-4.1224020
H	1.7121962	-1.9115237	-5.5100732
H	1.7608384	-3.0427040	-6.8500199

3_sy_tr_25.log

E = -1188.209144

H = -1187.843037

G = -1187.912435

NImag=0

C	5.0927603	-3.8794145	-6.5827369
C	4.1815254	-2.9154716	-7.3119764
C	5.1113317	-4.1575317	-5.2240844
O	5.9099764	-4.9785371	-4.6536458
C	4.0325513	-3.2918463	-8.8139574
C	3.2589308	-4.5539501	-9.1123672
C	3.7732135	-5.8326424	-8.8567138
C	2.9972131	-6.9625681	-9.0860473
C	1.6947277	-6.8156752	-9.5768827
C	1.1734644	-5.5470567	-9.8542443
C	1.9636075	-4.4264100	-9.6275501
C	4.0912541	-3.4505188	-4.3245276
C	2.7338169	-2.7418767	-6.7507033
S	5.6927551	-3.4348485	-9.6173355
C	5.2297109	-3.2709219	-11.3521700
C	6.4124952	-1.8147838	-9.2977427
C	0.8870457	-7.9831580	-9.8118566
N	0.2361290	-8.9220119	-10.0018250
C	2.6554786	-3.9622385	-4.5171761
C	2.1892112	-3.9492810	-5.9832417
H	5.8342243	-4.4168914	-7.1743675
H	4.5988751	-1.8950185	-7.3470996
H	3.5622643	-2.4508697	-9.3358015
H	4.7786465	-5.9579649	-8.4692615
H	3.3940326	-7.9519367	-8.8843207
H	0.1670705	-5.4445872	-10.2464301
H	1.5677445	-3.4388958	-9.8467241

H	4.4005668	-3.6077720	-3.2866692
H	4.1139262	-2.3687443	-4.5081117
H	2.0643400	-2.4925641	-7.5828131
H	2.7178505	-1.8655272	-6.0938206
H	6.1529386	-3.2122084	-11.9313458
H	4.6749796	-4.1682439	-11.6323127
H	4.6227910	-2.3733333	-11.4868611
H	7.2755057	-1.7191626	-9.9596537
H	6.7395739	-1.7932152	-8.2571851
H	5.6744618	-1.0369030	-9.5042848
H	2.5716990	-4.9801477	-4.1163199
H	1.9815072	-3.3342874	-3.9200359
H	1.0932601	-3.9375707	-6.0116611
H	2.5035431	-4.8712128	-6.4836356

3_sy_tr_26.log

E = -1188.205010

H = -1187.838874

G = -1187.908474

NImag=0

C	5.2281777	-4.1758516	-6.5458615
C	4.6269271	-2.9828582	-7.2414556
C	4.7873247	-4.8801071	-5.4342531
O	5.4678323	-5.8133465	-4.8761963
C	4.0402927	-3.2140443	-8.6864994
C	3.2530350	-4.4712376	-8.9529371
C	3.8365478	-5.7418434	-8.8558745
C	3.0763505	-6.8852048	-9.0743549
C	1.7197474	-6.7580917	-9.3947278
C	1.1282899	-5.4955511	-9.5192725
C	1.9035465	-4.3621824	-9.3065267
C	3.4280015	-4.5966236	-4.7677681
C	3.5948496	-2.1857716	-6.4177136
S	5.3115557	-3.0740413	-10.0394191
C	5.6122691	-1.2976928	-10.0740288
C	6.8915229	-3.6573418	-9.3926102
C	0.9270927	-7.9386655	-9.6144394
N	0.2886147	-8.8884576	-9.7924542
C	2.2638233	-4.2818427	-5.7097086
C	2.2234733	-2.8271662	-6.1920080
H	6.1964778	-4.5043806	-6.9220498
H	5.4368868	-2.2560866	-7.4032322
H	3.4107854	-2.3529425	-8.9455503
H	4.8834783	-5.8481915	-8.5968120
H	3.5265925	-7.8691026	-8.9949710
H	0.0797428	-5.4079226	-9.7834105
H	1.4503226	-3.3797397	-9.4039708
H	3.2009895	-5.5027154	-4.1971011
H	3.5427246	-3.7898128	-4.0280630
H	3.4461669	-1.2107727	-6.8995199
H	4.0632471	-1.9849984	-5.4473454
H	6.4383196	-1.1276823	-10.7671046
H	4.7063069	-0.8177462	-10.4468222
H	5.8674402	-0.9402904	-9.0747261
H	7.6203822	-3.4520401	-10.1800801
H	6.8260333	-4.7329239	-9.2275322
H	7.1529091	-3.1220351	-8.4791524
H	2.3198695	-4.9637034	-6.5669928
H	1.3154635	-4.5054963	-5.2057806
H	1.7015647	-2.2164089	-5.4442533
H	1.6222224	-2.7594862	-7.1071204

3_sy_tr_28.log

E = -1188.215766

H = -1187.849715

G = -1187.918948

NImag=0

C	3.5612440	-4.6678750	-5.7671487
C	4.8085210	-4.7220035	-6.6239372
C	2.9248346	-3.5449764	-5.2539803
O	1.8121835	-3.5770682	-4.6240488
C	4.4610891	-4.1937381	-8.0392752
C	3.3439225	-4.9194600	-8.7453773
C	3.2407812	-6.3168207	-8.7250082
C	2.2076805	-6.9583096	-9.3959646
C	1.2615062	-6.1960544	-10.0925604
C	1.3462194	-4.7999779	-10.1182471
C	2.3884086	-4.1734008	-9.4453303
C	3.5498437	-2.1486207	-5.4162079
C	6.0719431	-4.0649968	-6.0348977
S	6.0046548	-4.1286885	-9.1157130
C	6.5161932	-5.8453191	-9.2964875
C	5.3843551	-3.7755750	-10.7701686
C	0.1869245	-6.8564825	-10.7849631
N	-0.6773669	-7.3878347	-11.3435010
C	5.0015533	-1.9846405	-4.9530384
C	6.0599394	-2.5420360	-5.9052860
H	3.0236868	-5.6091430	-5.6572786
H	5.0586897	-5.7837813	-6.7376038
H	4.2186958	-3.1270583	-7.9916004
H	3.9594142	-6.9146782	-8.1725433
H	2.1263838	-8.0399545	-9.3780410
H	0.6041409	-4.2184403	-10.6550648
H	2.4581580	-3.0890101	-9.4566250
H	3.4709950	-1.8214272	-6.4645241
H	2.9107935	-1.4763485	-4.8355114
H	6.9549126	-4.3587369	-6.6215566
H	6.2168533	-4.5047847	-5.0408519
H	7.4039556	-5.8378788	-9.9324992
H	6.7745517	-6.2298998	-8.3081471
H	5.7206253	-6.4319856	-9.7581472
H	6.2555748	-3.7184756	-11.4260603
H	4.8827827	-2.8063319	-10.7373159
H	4.7036310	-4.5635995	-11.0959639
H	5.2005245	-0.9140405	-4.8199179
H	5.1212632	-2.4496006	-3.9641128
H	7.0504882	-2.2287624	-5.5539052
H	5.9305486	-2.0721838	-6.8916882

3_sy_tr_28_ts1.log

E = -1188.184841

H = -1187.821003

G = -1187.890035

NImag=1

C	0.9325437	-1.4858629	-1.1322253
C	1.4914877	-0.2027690	-1.0951767
C	1.2328856	-2.6345855	-0.3289453
O	0.6567494	-3.7255665	-0.5169529
C	0.5276990	0.9418964	0.4440946
C	-0.8673626	0.5584073	0.3475812
C	-1.8255698	1.1794550	-0.4826585

C	-3.1044442	0.6633325	-0.6178040
C	-3.4643397	-0.5094115	0.0640690
C	-2.5253637	-1.1573572	0.8797735
C	-1.2529918	-0.6266831	1.0153011
C	2.2189671	-2.5564925	0.8312330
C	2.9492030	0.1224209	-0.8200733
S	1.0458238	2.6181603	0.3932015
C	1.0095368	3.2141994	-1.3156727
C	-0.2245998	3.6870996	1.1248974
C	-4.7862469	-1.0437315	-0.0780856
N	-5.8571409	-1.4746175	-0.1933603
C	3.5979849	-1.9605482	0.5363523
C	3.6113379	-0.4381477	0.4342408
H	0.0601317	-1.6221917	-1.7696354
H	1.0854667	0.4448411	-1.8739748
H	1.0457320	0.4986497	1.2924605
H	-1.5787601	2.0716630	-1.0462926
H	-3.8275641	1.1597628	-1.2572693
H	-2.7994532	-2.0677092	1.4040686
H	-0.5327285	-1.1280689	1.6558139
H	1.7447139	-1.9691632	1.6325466
H	2.3257633	-3.5795042	1.2031314
H	3.0824793	1.2103968	-0.8264986
H	3.5030479	-0.2458744	-1.6967859
H	1.2654316	4.2748066	-1.2679361
H	1.7756524	2.6825043	-1.8807668
H	0.0296176	3.0817666	-1.7712277
H	0.1689678	4.7058599	1.1149884
H	-0.3681291	3.3501308	2.1527643
H	-1.1564765	3.6291055	0.5622451
H	4.2713690	-2.2576610	1.3482818
H	4.0059094	-2.3994760	-0.3844771
H	4.6503094	-0.0882765	0.4395772
H	3.1397638	-0.0157853	1.3315848

3_sy_tr_2_ts1.log

E = -1188.183718

H = -1187.820554

G = -1187.891680

NImag=1

C	2.3986178	-0.6437668	1.3593407
C	1.0677415	-0.7969794	0.9470559
C	3.5669128	-0.7524516	0.5423150
O	4.7223555	-0.6629845	1.0074324
C	-0.0048552	1.0474222	0.6663976
C	-1.3625029	0.6203823	0.4154065
C	-1.9344195	0.4869590	-0.8736899
C	-3.1963959	-0.0537468	-1.0474537
C	-3.9401040	-0.4802221	0.0649150
C	-3.3992508	-0.3473850	1.3554454
C	-2.1389988	0.1961439	1.5227615
C	3.3967907	-0.9732247	-0.9542119
C	0.6520689	-1.5593525	-0.3074479
S	0.7618882	1.9802636	-0.6161698
C	-0.1318962	3.5565863	-0.7262455
C	2.2667156	2.5586708	0.1874844
C	-5.2463459	-1.0362513	-0.1142753
N	-6.3054910	-1.4882438	-0.2595521
C	2.8593664	-2.3658388	-1.3243289
C	1.5633753	-2.7605834	-0.5986078
H	2.5809203	-0.3868630	2.4014843

H	0.3720238	-0.9365894	1.7745430
H	0.1823818	1.5015131	1.6391245
H	-1.3853231	0.7995651	-1.7583913
H	-3.6149050	-0.1485449	-2.0446604
H	-3.9756250	-0.6679680	2.2178645
H	-1.7307382	0.3015317	2.5242530
H	2.7164717	-0.2101843	-1.3551381
H	4.3715387	-0.8175548	-1.4245248
H	0.6307512	-0.9097696	-1.1928097
H	-0.3768904	-1.9023558	-0.1653270
H	0.4203753	4.2062622	-1.4095457
H	-1.1250606	3.3497045	-1.1282719
H	-0.1978910	3.9943648	0.2716860
H	2.7546600	3.2471317	-0.5044207
H	2.9053344	1.6983414	0.3820210
H	2.0007212	3.0629644	1.1189043
H	2.6820634	-2.3707452	-2.4061813
H	3.6344162	-3.1157454	-1.1292454
H	1.7949142	-3.2658512	0.3450106
H	1.0184005	-3.4836337	-1.2151993

3_sy_tr_2_ts1_rot1.log

E = -1188.189309

H = -1187.825962

G = -1187.895467

NImag=1

C	0.7445694	-1.6837168	-1.1380193
C	1.3375045	-1.5395531	0.1203183
C	-0.6426502	-1.9208843	-1.4120971
O	-1.0704031	-2.1093678	-2.5695028
C	1.5687969	0.5577224	0.6423703
C	0.2306869	1.0621945	0.4918247
C	-0.3699793	1.2762733	-0.7740075
C	-1.7160941	1.5898385	-0.8830519
C	-2.5071219	1.7038251	0.2689009
C	-1.9269380	1.5236408	1.5394652
C	-0.5849658	1.2137848	1.6425850
C	-1.6264092	-1.9909899	-0.2518460
C	0.7079053	-2.0137861	1.4215729
S	2.7193871	1.0959510	-0.5790042
C	3.0242133	2.8478323	-0.2337355
C	4.2730594	0.3977984	0.0081931
C	-3.8978477	2.0240738	0.1548194
N	-5.0258351	2.2819634	0.0645560
C	-1.4327850	-3.2122634	0.6640036
C	-0.0186999	-3.3586953	1.2575162
H	1.3845940	-1.6186324	-2.0169266
H	2.4183623	-1.6658801	0.1170201
H	2.0047680	0.6028203	1.6412811
H	0.2180405	1.1931120	-1.6827425
H	-2.1632131	1.7398001	-1.8611704
H	-2.5360232	1.6320361	2.4315535
H	-0.1402980	1.0773489	2.6246108
H	-1.5432813	-1.0778318	0.3476049
H	-2.6331465	-2.0123729	-0.6796113
H	-0.0014878	-1.2780282	1.8183166
H	1.5047644	-2.1062503	2.1664501
H	3.8003418	3.1991096	-0.9173925
H	2.0904878	3.3808115	-0.4234602
H	3.3318447	2.9603133	0.8076556
H	5.0750426	0.9047096	-0.5311194

H	4.2897883	-0.6659816	-0.2268791
H	4.3595253	0.5680368	1.0832682
H	-2.1565396	-3.1186480	1.4821961
H	-1.6984170	-4.1237416	0.1159679
H	0.5917758	-4.0144906	0.6274345
H	-0.0937936	-3.8480165	2.2349004

3_sy_tr_3.log

E = -1188.216597
H = -1187.850598
G = -1187.919563

NImag=0

C	4.9645524	-4.2702737	-6.5089236
C	3.9632481	-3.3274661	-7.1340355
C	5.4064340	-4.1577511	-5.1983020
O	6.1957044	-4.9688870	-4.6078991
C	3.8422280	-3.5206602	-8.6623940
C	3.0993868	-4.7536563	-9.1314883
C	1.7916120	-4.5834913	-9.6030274
C	1.0300051	-5.6735915	-10.0049668
C	1.5903853	-6.9545178	-9.9507403
C	2.9030021	-7.1409868	-9.5042106
C	3.6503779	-6.0414116	-9.0978783
C	4.8686489	-2.9877897	-4.3639589
C	2.5422950	-3.3686279	-6.5273439
S	5.5314286	-3.5321211	-9.4054480
C	5.1305134	-3.2032954	-11.1345719
C	6.1722103	-1.9250016	-8.9033067
C	0.8123357	-8.0898671	-10.3704622
N	0.1851951	-9.0028206	-10.7085473
C	3.3650375	-3.1093092	-4.0661565
C	2.4474995	-2.6233162	-5.1927466
H	5.2569976	-5.1669027	-7.0503346
H	4.2955812	-2.2825284	-7.0167660
H	3.3579880	-2.6384231	-9.0946530
H	1.3641077	-3.5862520	-9.6529995
H	0.0153397	-5.5365721	-10.3636534
H	3.3329296	-8.1366289	-9.4774339
H	4.6697464	-6.2060591	-8.7644814
H	5.4345834	-2.9825866	-3.4274981
H	5.0546055	-2.0265670	-4.8668371
H	2.2365236	-4.4163403	-6.4068416
H	1.8264111	-2.8996800	-7.2177894
H	6.0743639	-3.0626904	-11.6643683
H	4.6141765	-4.0808187	-11.5284206
H	4.5040308	-2.3121957	-11.2066159
H	7.0596571	-1.7370892	-9.5108099
H	6.4480924	-1.9923886	-7.8500974
H	5.4139041	-1.1582833	-9.0752156
H	3.1321717	-4.1546683	-3.8187573
H	3.1283481	-2.5187185	-3.1724460
H	2.6667734	-1.5616608	-5.3782347
H	1.4080680	-2.6673044	-4.8452381

3_sy_tr_30.log

E = -1188.203749
H = -1187.837633
G = -1187.908469

NImag=0

C	5.0106853	-4.2487694	-6.6356290
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C	3.7838034	-3.4195227	-6.9319867
C	5.8022546	-4.0661907	-5.5155951
O	6.8753154	-4.7191797	-5.2626883
C	3.3041607	-3.4174845	-8.3885452
C	2.7178494	-4.6708997	-9.0111610
C	2.9623508	-5.9544423	-8.5108265
C	2.4057382	-7.0700622	-9.1276569
C	1.6024575	-6.9041339	-10.2602423
C	1.3406902	-5.6266360	-10.7689365
C	1.8960165	-4.5219297	-10.1374899
C	5.4408474	-3.0079901	-4.4472250
C	2.5620390	-3.7041543	-6.0255407
S	4.5644539	-2.7887649	-9.6196324
C	5.4709232	-1.5117486	-8.7314606
C	5.8284552	-4.0585269	-9.8355448
C	1.0331084	-8.0574165	-10.9059852
N	0.5753247	-8.9848484	-11.4268879
C	3.9714992	-2.5913256	-4.2064055
C	2.9511974	-3.6870019	-4.5396304
H	5.3157951	-5.0303021	-7.3251305
H	4.0196785	-2.3626826	-6.7434193
H	2.5506758	-2.6260672	-8.4905697
H	3.5764006	-6.0903596	-7.6285077
H	2.5936403	-8.0635640	-8.7345182
H	0.7062644	-5.5051050	-11.6404664
H	1.6798639	-3.5283671	-10.5223238
H	5.8319348	-3.4381016	-3.5182516
H	6.0543663	-2.1155581	-4.6394365
H	2.1059669	-4.6697475	-6.2740083
H	1.8037107	-2.9294334	-6.2108837
H	6.2322887	-1.1412013	-9.4212752
H	4.7702545	-0.7107191	-8.4897456
H	5.9250597	-1.9420007	-7.8367667
H	6.3992296	-3.7607981	-10.7174947
H	5.3261806	-5.0089113	-10.0290740
H	6.4606081	-4.1150325	-8.9513192
H	3.8744994	-2.3195346	-3.1492133
H	3.7189736	-1.6840929	-4.7691412
H	2.0414290	-3.5509220	-3.9440383
H	3.3683091	-4.6601715	-4.2532463

3_sy_tr_31.log

E = -1188.201950

H = -1187.835845

G = -1187.904686

NImag=0

C	4.1156681	-2.4333231	-6.3075316
C	3.8456562	-3.8194436	-6.8699483
C	4.8068176	-2.0833204	-5.1610379
O	5.1192589	-0.8772765	-4.8484346
C	3.5467864	-3.7032997	-8.3761698
C	2.7604367	-4.8290609	-9.0325550
C	2.5554162	-6.0638123	-8.4075327
C	1.8163594	-7.0609213	-9.0365262
C	1.2765867	-6.8248768	-10.3039073
C	1.4610439	-5.5911172	-10.9390592
C	2.1966331	-4.6045959	-10.2973530
C	5.2424463	-3.1443060	-4.1330215
C	4.9388414	-4.8503903	-6.5186317
S	4.9794125	-3.3962994	-9.5402726
C	6.1252152	-2.2265898	-8.7835233

C	5.9779378	-4.8991767	-9.5951391
C	0.5152937	-7.8560194	-10.9577511
N	-0.0966684	-8.6857568	-11.4849961
C	4.3919275	-4.4147923	-4.0573073
C	4.7379763	-5.4539098	-5.1262473
H	3.8142089	-1.5972793	-6.9399326
H	2.8921662	-4.2309946	-6.4890820
H	2.9822511	-2.7772525	-8.5408010
H	2.9513208	-6.2616718	-7.4183173
H	1.6580475	-8.0158340	-8.5465631
H	1.0255371	-5.4088287	-11.9157547
H	2.3217754	-3.6409724	-10.7844177
H	6.2978480	-3.4052499	-4.3078100
H	5.2176493	-2.6265155	-3.1679769
H	5.9149991	-4.3521749	-6.5618675
H	4.9750155	-5.6701871	-7.2431790
H	6.9473681	-2.1348133	-9.4983348
H	5.6113128	-1.2709408	-8.6795708
H	6.4739973	-2.5937365	-7.8201548
H	6.6103219	-4.8016940	-10.4797802
H	5.3050415	-5.7504280	-9.7182950
H	6.5826983	-4.9940947	-8.6947972
H	4.5037250	-4.8781914	-3.0698519
H	3.3344539	-4.1331665	-4.1459024
H	3.9404889	-6.2077543	-5.1699839
H	5.6562279	-5.9822316	-4.8404815

3_sy_tr_32.log

E = -1188.204204

H = -1187.838087

G = -1187.906718

NImag=0

C	4.3473970	-2.4072853	-6.3972320
C	4.0853850	-3.7909935	-6.9595962
C	4.3383276	-2.1096039	-5.0468661
O	4.5637527	-0.9578091	-4.5327169
C	3.7317514	-3.7003369	-8.4548396
C	2.8530490	-4.7966544	-9.0401452
C	2.6342603	-6.0127832	-8.3839703
C	1.8114446	-6.9822041	-8.9487088
C	1.2007498	-6.7366571	-10.1819394
C	1.3991613	-5.5206831	-10.8466469
C	2.2198244	-4.5617398	-10.2696232
C	4.0620919	-3.2563227	-4.0625639
C	5.1647220	-4.8439755	-6.6126148
S	5.1235608	-3.5179551	-9.6889340
C	6.3371045	-2.3699707	-9.0117399
C	6.0572098	-5.0630478	-9.7140217
C	0.3502313	-7.7386023	-10.7679715
N	-0.3338026	-8.5445209	-11.2407819
C	5.1384653	-4.3526396	-4.0592279
C	5.0160053	-5.3820447	-5.1866259
H	4.5669202	-1.5988887	-7.0924494
H	3.1459342	-4.1773819	-6.5274241
H	3.2185514	-2.7452963	-8.6235098
H	3.0834220	-6.2158600	-7.4186236
H	1.6411152	-7.9225876	-8.4352869
H	0.9092253	-5.3303888	-11.7956021
H	2.3581744	-3.6113810	-10.7788327
H	3.9965344	-2.8017552	-3.0693877
H	3.0868496	-3.7216513	-4.2736023

H	6.1601773	-4.3959230	-6.7278768
H	5.1187833	-5.7013848	-7.2944025
H	7.1737991	-2.3869368	-9.7145299
H	5.8868776	-1.3770711	-8.9954195
H	6.6530208	-2.6798521	-8.0166370
H	6.6523817	-5.0317559	-10.6288953
H	5.3462033	-5.8901040	-9.7681154
H	6.6978522	-5.1416267	-8.8375094
H	6.1314387	-3.8822417	-4.0942144
H	5.0871391	-4.8986548	-3.1089262
H	4.0342952	-5.8724844	-5.1041942
H	5.7678134	-6.1653438	-5.0316945

3_sy_tr_33.log

E = -1188.213534

H = -1187.847310

G = -1187.915842

NImag=0

C	3.4218956	-4.3785213	-5.8478114
C	4.7083455	-4.5397747	-6.6319960
C	3.0551954	-3.4015871	-4.9305455
O	1.9924979	-3.4616553	-4.2188569
C	4.4639447	-4.1870566	-8.1220104
C	3.3488522	-4.9437600	-8.7965362
C	3.1671244	-6.3184882	-8.5950749
C	2.1444025	-6.9980661	-9.2445984
C	1.2880204	-6.2957517	-10.1013517
C	1.4483552	-4.9209151	-10.3048610
C	2.4792757	-4.2564781	-9.6513295
C	3.9135899	-2.1453212	-4.6958176
C	5.9270201	-3.7999843	-6.0527113
S	6.0665436	-4.3632426	-9.0920277
C	6.4781439	-6.1146383	-9.0138032
C	5.5652945	-4.2081226	-10.8156857
C	0.2274627	-6.9957863	-10.7765240
N	-0.6249078	-7.5591274	-11.3217744
C	4.6361031	-1.5743496	-5.9170924
C	5.9539461	-2.2815082	-6.2530571
H	2.7206334	-5.2076965	-5.9415316
H	4.9655067	-5.6078231	-6.6059399
H	4.2882311	-3.1111059	-8.2261299
H	3.8156926	-6.8666167	-7.9183780
H	2.0029525	-8.0622085	-9.0877164
H	0.7739685	-4.3846463	-10.9641246
H	2.6096197	-3.1884938	-9.8033118
H	3.2178388	-1.3989928	-4.2991577
H	4.6369487	-2.3462344	-3.8910049
H	6.8556667	-4.2240606	-6.4600234
H	5.9472842	-4.0259061	-4.9810817
H	7.3800994	-6.2442127	-9.6157208
H	6.6899354	-6.3706117	-7.9742666
H	5.6619744	-6.7158324	-9.4170710
H	6.4742794	-4.2966453	-11.4144206
H	5.1304109	-3.2156150	-10.9483946
H	4.8516926	-4.9923611	-11.0735952
H	3.9510766	-1.6171774	-6.7735789
H	4.8486354	-0.5110287	-5.7539422
H	6.7505805	-1.8799364	-5.6147266
H	6.2445669	-2.0355600	-7.2832184

3_sy_tr_3_r.log

E = -1188.211486
H = -1187.845714
G = -1187.915408

NImag=0

C	-1.1307205	-1.0911551	0.3823396
C	-1.5255489	0.2244797	-0.2625034
C	-1.9737614	-1.8905274	1.1347664
O	-1.6591885	-3.0113869	1.6647655
C	-0.2035761	0.8566939	-0.7438573
C	0.7560090	1.1752597	0.3784625
C	2.0813795	0.7407201	0.2898627
C	2.9909695	1.0278684	1.3017997
C	2.5668294	1.7691770	2.4093250
C	1.2435039	2.2189027	2.5073504
C	0.3449266	1.9172174	1.4932935
C	-3.4246093	-1.4277869	1.3114985
C	-2.5750305	0.0942091	-1.3834847
S	-0.5304876	2.4318511	-1.7063287
C	1.0233300	3.3472179	-1.6142072
C	-0.4108134	1.8624185	-3.4185716
C	3.5004419	2.0759025	3.4602568
N	4.2517492	2.3237524	4.3060342
C	-4.2098735	-1.4186938	-0.0083049
C	-3.9930260	-0.1672815	-0.8622943
H	-0.1149995	-1.4482846	0.2115436
H	-1.9568960	0.9193464	0.4785200
H	0.2874725	0.2033137	-1.4749701
H	2.4021487	0.1681871	-0.5758329
H	4.0181795	0.6847380	1.2364131
H	0.9277845	2.7944880	3.3710424
H	-0.6796724	2.2686299	1.5772916
H	-3.8916891	-2.1167832	2.0217220
H	-3.4645688	-0.4206342	1.7536266
H	-2.2615995	-0.6966160	-2.0786264
H	-2.6515582	1.0252010	-1.9635028
H	0.9279763	4.1683202	-2.3279056
H	1.1357516	3.7448496	-0.6054546
H	1.8567165	2.6956198	-1.8830657
H	-0.5193519	2.7417201	-4.0562256
H	-1.2190394	1.1576026	-3.6106445
H	0.5627823	1.3908802	-3.5647524
H	-3.9550714	-2.3183751	-0.5858979
H	-5.2832863	-1.4823025	0.2098193
H	-4.2993569	0.7065171	-0.2688707
H	-4.6693177	-0.2052899	-1.7248373

3_sy_tr_3_ts1.log

E = -1188.149303
H = -1187.787588
G = -1187.859282

NImag=1

C	-1.6274688	-0.5095592	0.9063729
C	-1.3666532	-0.4045229	-0.4353827
C	-3.0282915	-0.7054158	1.2807668
O	-3.4641019	-0.6793942	2.4318230
C	0.2580299	1.4472703	-0.8780711
C	1.4009944	0.6955625	-0.4926822
C	2.1780651	0.0509617	-1.4996048
C	3.2356938	-0.7756115	-1.1848852
C	3.5829702	-1.0045485	0.1622056

C	2.8399139	-0.3735875	1.1760400
C	1.7813070	0.4565927	0.8599437
C	-3.8537617	-1.3173998	0.1408922
C	-0.7553902	-1.5138204	-1.2090924
S	-0.4243789	2.5676859	0.2485851
C	0.3018067	4.1893843	-0.1232856
C	-2.0955811	2.8578800	-0.3642364
C	4.6794107	-1.8552973	0.4923763
N	5.5722056	-2.5495348	0.7603201
C	-3.1155354	-2.5420144	-0.4869932
C	-2.0535710	-2.3055120	-1.5912346
H	-0.9013828	-0.9791224	1.5713519
H	-2.1104438	0.1243365	-1.0339576
H	0.0985726	1.7002623	-1.9235482
H	1.9232184	0.2178986	-2.5427228
H	3.8084820	-1.2510937	-1.9758141
H	3.1024356	-0.5412242	2.2166498
H	1.2319300	0.9255412	1.6707076
H	-4.8133527	-1.6373148	0.5573918
H	-4.0630087	-0.5678550	-0.6337449
H	-0.0845859	-2.1226576	-0.5921481
H	-0.2395280	-1.2144925	-2.1268947
H	-0.1613301	4.9330168	0.5295610
H	1.3696284	4.1158683	0.0896455
H	0.1329475	4.4281137	-1.1753020
H	-2.4548012	3.7776935	0.1010585
H	-2.7235428	2.0212778	-0.0580559
H	-2.0671199	2.9601148	-1.4509614
H	-2.6649316	-3.1248969	0.3276607
H	-3.8800257	-3.1860905	-0.9359621
H	-2.5336817	-1.7663700	-2.4176180
H	-1.7537840	-3.2849488	-1.9815605

3_sy_tr_3_ts2.log

E = -1188.189189

H = -1187.825576

G = -1187.896800

NImag=1

C	1.6572033	-0.8187644	1.1515143
C	1.5554669	0.2110049	0.0617235
C	2.3601135	-2.0333693	0.9233181
O	2.5249532	-2.9244425	1.7853603
C	0.2300658	0.6219578	0.5723614
C	-1.0124016	-0.0735327	0.1701781
C	-2.0540057	-0.1955368	1.1021726
C	-3.2559024	-0.7935279	0.7506461
C	-3.4269792	-1.2665792	-0.5567277
C	-2.4024365	-1.1378836	-1.5044826
C	-1.2049183	-0.5396892	-1.1398554
C	3.1493572	-2.1230262	-0.3855013
C	2.7488641	1.1388748	-0.1360773
S	-0.2231566	2.7306552	-0.4143885
C	-1.9582311	2.9529513	0.0379942
C	0.5429849	3.7758585	0.8461846
C	-4.6700393	-1.8821038	-0.9343399
N	-5.6720781	-2.3774175	-1.2387098
C	4.2336809	-1.0184804	-0.4407230
C	3.8081960	0.3730308	-0.9488236
H	1.5808445	-0.4926668	2.1862575
H	1.3907508	-0.3093727	-0.8877567
H	0.1986375	1.0867628	1.5578994

H	-1.9111514	0.1752758	2.1133001
H	-4.0572787	-0.8945448	1.4751811
H	-2.5532236	-1.4959910	-2.5175172
H	-0.4253280	-0.4209534	-1.8859093
H	3.6267430	-3.1067858	-0.4071293
H	2.4961581	-2.0530559	-1.2648694
H	3.1419834	1.4593687	0.8369185
H	2.4809994	2.0410952	-0.7025413
H	-2.2371387	3.9979288	-0.1151798
H	-2.5611237	2.3157935	-0.6124740
H	-2.1134744	2.6724599	1.0830678
H	0.1893404	4.8022791	0.7274030
H	1.6243124	3.7465004	0.7028733
H	0.2899625	3.4062244	1.8433600
H	4.6856647	-0.9255680	0.5565535
H	5.0326853	-1.3632250	-1.1076268
H	3.4175044	0.2523968	-1.9692825
H	4.7090402	0.9914590	-1.0345536

3_sy_tr_4.log

E = -1188.210041

H = -1187.844366

G = -1187.914807

NImag=0

C	4.4201655	-2.4482336	-6.5237012
C	4.0738462	-3.8534868	-6.9747410
C	4.2189749	-1.9656290	-5.2425546
O	4.4818780	-0.7771194	-4.8448833
C	4.0978211	-3.9351326	-8.5270198
C	3.1082402	-4.9281678	-9.1011711
C	3.3530552	-6.3043643	-9.1824838
C	2.3806063	-7.1655876	-9.6786684
C	1.1498969	-6.6474951	-10.0948271
C	0.8914361	-5.2735906	-10.0216578
C	1.8739035	-4.4245404	-9.5296722
C	3.6589253	-2.9322559	-4.1902411
C	4.8986481	-4.9815591	-6.3173295
S	5.7701156	-4.3588861	-9.1905788
C	5.5154837	-4.0694936	-10.9528665
C	6.7934099	-2.9344170	-8.7767023
C	0.1426709	-7.5350760	-10.6124070
N	-0.6682306	-8.2488844	-11.0295805
C	4.5794358	-4.1220759	-3.8803805
C	4.4785581	-5.2801827	-4.8756161
H	4.8200025	-1.7571190	-7.2636073
H	3.0203131	-4.0818492	-6.7359992
H	3.8829154	-2.9454505	-8.9437251
H	4.3046556	-6.7260288	-8.8717169
H	2.5731601	-8.2311011	-9.7451002
H	-0.0636823	-4.8801053	-10.3531862
H	1.6839911	-3.3563144	-9.4769540
H	3.4959465	-2.3425019	-3.2831216
H	2.6788866	-3.3207748	-4.5081999
H	5.9644625	-4.7103119	-6.3414672
H	4.7864090	-5.9171191	-6.8813265
H	6.4990158	-4.1028439	-11.4252352
H	4.8897348	-4.8734183	-11.3428389
H	5.0454989	-3.0942390	-11.0954380
H	7.7375655	-3.0780182	-9.3066313
H	6.9597572	-2.9369469	-7.6993782
H	6.2978542	-2.0178322	-9.1009535

H	5.6190351	-3.7700833	-3.8205201
H	4.3279462	-4.5190324	-2.8889770
H	3.4372004	-5.6332931	-4.8899725
H	5.0846909	-6.1174391	-4.5090687

3_sy_tr_4_ts1.log

E = -1188.147624
H = -1187.785619
G = -1187.857305

NImag=1

C	-2.7176401	-0.0433175	-0.6727787
C	-1.5360326	-0.1391507	0.0232805
C	-3.2355705	-1.2924413	-1.2248920
O	-4.2259406	-1.3788493	-1.9538238
C	0.2184778	1.4332499	-0.6071432
C	1.3287630	0.5697725	-0.3711732
C	2.0544063	0.4999966	0.8510297
C	3.0554370	-0.4329302	1.0440171
C	3.3868370	-1.3470742	0.0277248
C	2.6861910	-1.2984403	-1.1931655
C	1.6884451	-0.3650075	-1.3850886
C	-2.6797467	-2.5378507	-0.5186986
C	-1.4860253	-0.1182258	1.5122869
S	-0.0162195	2.8079344	0.4123496
C	0.7475130	4.2323213	-0.4183160
C	-1.7506564	3.2352918	0.1702720
C	4.4228922	-2.3075097	0.2300584
N	5.2655064	-3.0904231	0.3949140
C	-2.7900975	-2.3927026	1.0314727
C	-1.6781742	-1.6425317	1.8077945
H	-3.4754639	0.6903361	-0.3972693
H	-0.8254464	-0.8619786	-0.3776589
H	-0.1468187	1.5649118	-1.6221456
H	1.8290106	1.1891440	1.6597777
H	3.5926052	-0.4612029	1.9874420
H	2.9370912	-1.9974069	-1.9856259
H	1.1573875	-0.3377491	-2.3329328
H	-3.2730841	-3.3950247	-0.8497606
H	-1.6380884	-2.7281790	-0.8062508
H	-2.3047243	0.4721490	1.9382587
H	-0.5328885	0.2044650	1.9467144
H	0.5291249	5.1307963	0.1635914
H	1.8230842	4.0490231	-0.4404304
H	0.3465271	4.3100263	-1.4310192
H	-1.8941059	4.2448479	0.5600863
H	-2.3582916	2.5281015	0.7345291
H	-1.9865410	3.1938838	-0.8953843
H	-3.7612913	-1.9345852	1.2638402
H	-2.8219387	-3.4046108	1.4508533
H	-0.7193820	-2.1360685	1.6014470
H	-1.8779763	-1.7642779	2.8787112

3_sy_tr_4_ts2.log

E = -1188.174825
H = -1187.811496
G = -1187.884660

NImag=1

C	-1.7418764	-0.4760090	0.9902126
C	-1.4242710	-0.0510361	-0.3663394
C	-3.0114705	-0.9626392	1.3360597

O	-3.3553573	-1.2905978	2.5044591
C	-0.1371869	0.3712314	-0.8055493
C	1.1808746	-0.0845536	-0.3880915
C	1.4023620	-1.0730088	0.5896938
C	2.6943489	-1.4697504	0.9034621
C	3.7803813	-0.8643156	0.2584230
C	3.5811898	0.1158402	-0.7229239
C	2.2864811	0.4867185	-1.0481337
C	-4.0282180	-1.1577428	0.2092380
C	-1.2314853	-1.3240069	-1.5045931
S	-0.1444052	2.8088522	0.7013885
C	0.9121841	3.6871262	-0.4794303
C	-1.7587702	3.2307961	0.0017214
C	5.1201097	-1.2595741	0.6032763
N	6.1987731	-1.5774802	0.8797573
C	-3.5908074	-2.2108248	-0.8236814
C	-2.6493187	-1.7208861	-1.9232542
H	-0.9826541	-0.4220452	1.7635228
H	-2.2049387	0.5313096	-0.8644280
H	-0.1288529	1.0102151	-1.6877031
H	0.5688616	-1.5452669	1.0945040
H	2.8659889	-2.2376328	1.6500870
H	4.4308890	0.5675890	-1.2233434
H	2.1188040	1.2325138	-1.8199898
H	-4.9622508	-1.4725525	0.6824015
H	-4.2254199	-0.2056322	-0.3044925
H	-0.7099268	-2.1113081	-0.9584953
H	-0.6740968	-1.0746901	-2.4114122
H	0.7191787	4.7619631	-0.4352831
H	1.9520911	3.5007278	-0.2021226
H	0.7385760	3.3233690	-1.4963512
H	-1.9137100	4.3123104	0.0256268
H	-2.5240265	2.7442868	0.6110378
H	-1.8352116	2.8713541	-1.0290572
H	-3.1362955	-3.0640390	-0.3020746
H	-4.4852455	-2.5953741	-1.3270757
H	-3.1097321	-0.8794595	-2.4554696
H	-2.5176418	-2.5240756	-2.6600607

3_sy_tr_5.log

E = -1188.210591

H = -1187.844220

G = -1187.913495

NImag=0

C	4.1658275	-2.4156851	-6.2926997
C	3.3753429	-3.5815778	-6.8266319
C	5.3286760	-2.4144499	-5.5385969
O	6.0744770	-1.3798168	-5.4019608
C	3.6550586	-3.7121631	-8.3570055
C	2.9427803	-4.8444564	-9.0564125
C	3.3610281	-6.1800733	-8.9751501
C	2.6319155	-7.1883166	-9.5902965
C	1.4604260	-6.8628392	-10.2862106
C	1.0259489	-5.5365151	-10.3726093
C	1.7750099	-4.5364527	-9.7624130
C	5.8111002	-3.6903083	-4.8373844
C	3.5107190	-4.9168147	-6.0737631
S	5.5010791	-3.7953191	-8.6070730
C	5.6174333	-4.2397257	-10.3584749
C	6.0286759	-2.0671253	-8.7447616
C	0.7000080	-7.9042902	-10.9243814

N	0.0884557	-8.7428913	-11.4382420
C	4.7947011	-4.3717106	-3.9111091
C	3.4389142	-4.7233743	-4.5567592
H	3.9190926	-1.4604723	-6.7612096
H	2.3018399	-3.3292115	-6.8079819
H	3.3803829	-2.7682194	-8.8403161
H	4.2652039	-6.4478458	-8.4342538
H	2.9614405	-8.2202528	-9.5319952
H	0.1198021	-5.2939046	-10.9176832
H	1.4480153	-3.5030927	-9.8337060
H	6.1656676	-4.4098025	-5.5874225
H	6.6892556	-3.4048442	-4.2499253
H	4.4445584	-5.4304663	-6.3364663
H	2.6997670	-5.5773140	-6.3973365
H	6.6569223	-4.0784704	-10.6501890
H	5.3632747	-5.2916844	-10.4795582
H	4.9490310	-3.6031892	-10.9426984
H	6.9723013	-2.0858560	-9.2953339
H	6.1709220	-1.6667939	-7.7387518
H	5.2722627	-1.5091430	-9.3006405
H	5.2571632	-5.2903900	-3.5288990
H	4.6225680	-3.7297902	-3.0383594
H	2.7046369	-3.9371696	-4.3453093
H	3.0524149	-5.6363816	-4.0907286

3_sy_tr_5_r.log

E = -1188.209506

H = -1187.843425

G = -1187.913445

NImag=0

C	1.2796532	-1.5022821	-0.3111678
C	1.1556769	-0.6366084	0.9269611
C	0.7008954	-2.7386201	-0.5580372
O	0.8834136	-3.4340297	-1.6163461
C	0.1147203	0.4693360	0.6327345
C	0.4226233	1.2929074	-0.5952148
C	1.6597255	1.9336182	-0.7392710
C	1.9238185	2.7094049	-1.8605388
C	0.9417293	2.8417468	-2.8504228
C	-0.2971478	2.2045547	-2.7206432
C	-0.5496618	1.4379059	-1.5887957
C	-0.1939299	-3.3564253	0.5219843
C	0.8528461	-1.3452144	2.2703168
S	-0.0069670	1.7093337	2.0623516
C	-1.0037268	3.0410999	1.3543289
C	-1.2477177	1.0056264	3.1745202
C	1.2097844	3.6441321	-4.0144800
N	1.4243471	4.2911526	-4.9507239
C	0.5930638	-3.8271596	1.7546889
C	1.4828677	-2.7364877	2.3778403
H	1.9306749	-1.1071167	-1.0907744
H	2.1221737	-0.1297402	1.0636865
H	-0.8924596	0.0414200	0.5648294
H	2.4275026	1.8315034	0.0232729
H	2.8803544	3.2084218	-1.9744360
H	-1.0492491	2.3131811	-3.4950397
H	-1.5100921	0.9431644	-1.4762721
H	-0.9635303	-2.6406120	0.8365829
H	-0.7130319	-4.2084238	0.0724517
H	-0.2296397	-1.4374792	2.4218052
H	1.2277591	-0.7122531	3.0854086

H	-1.2773316	3.6971585	2.1830300
H	-0.3927825	3.5873604	0.6356376
H	-1.8942615	2.6214057	0.8814560
H	-1.6218540	1.8360424	3.7769974
H	-0.7691901	0.2703702	3.8181987
H	-2.0538995	0.5609455	2.5877824
H	-0.1231730	-4.1778457	2.5089542
H	1.2108783	-4.6926494	1.4847449
H	2.4630054	-2.7202589	1.8889030
H	1.6620986	-2.9804417	3.4308082

3_sy_tr_5_ts2.log

E = -1188.204024

H = -1187.839260

G = -1187.909002

NImag=1

C	1.3355360	-1.5678877	-0.4827076
C	1.3764428	-0.1245680	-0.9399962
C	2.1911091	-2.1892591	0.4386762
O	2.1100953	-3.4110813	0.7603227
C	0.3856906	0.3804535	0.0593368
C	-1.0370688	-0.0628573	-0.0118095
C	-1.7140961	-0.1365731	-1.2374866
C	-3.0557215	-0.4909119	-1.2801740
C	-3.7310493	-0.7749226	-0.0858644
C	-3.0693727	-0.7018828	1.1461167
C	-1.7289340	-0.3407631	1.1740789
C	3.3209698	-1.3664440	1.0565892
C	2.7285268	0.6210879	-0.9315591
S	0.1243628	2.5392415	-0.2464558
C	-1.2963042	2.8926967	0.8137841
C	1.4263710	3.2564427	0.7845036
C	-5.1204428	-1.1439161	-0.1258026
N	-6.2397661	-1.4402957	-0.1577223
C	4.4246616	-1.0067584	0.0475573
C	3.9155854	-0.3004962	-1.2227036
H	0.5568930	-2.1856623	-0.9240069
H	0.9628623	-0.0641861	-1.9524384
H	0.7771325	0.4431727	1.0776891
H	-1.1965430	0.0871607	-2.1656030
H	-3.5817474	-0.5471862	-2.2274019
H	-3.6026060	-0.9252922	2.0642163
H	-1.2063041	-0.2796345	2.1245780
H	2.9205464	-0.4456914	1.4986351
H	3.7493861	-1.9557878	1.8725307
H	2.8904500	1.1060192	0.0377013
H	2.6803671	1.4244729	-1.6762707
H	-1.3909468	3.9772501	0.9001099
H	-2.1897981	2.4843189	0.3391388
H	-1.1483253	2.4451997	1.7997039
H	1.1147431	4.2648130	1.0653558
H	2.3423575	3.3109336	0.1968756
H	1.5785180	2.6463430	1.6784210
H	5.1448859	-0.3521166	0.5540669
H	4.9708505	-1.9155950	-0.2326181
H	3.6153639	-1.0399567	-1.9737998
H	4.7367485	0.2756638	-1.6622695

3_sy_tr_6.log

E = -1188.212937

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H =      -1187.847121
G =      -1187.917412
NImag=0
C      5.0377034      -4.1532961      -6.5311761
C      4.1310785      -3.1584500      -7.2217499
C      5.0266973      -4.5756186      -5.2083037
O      5.7922482      -5.4917285      -4.7464124
C      3.9842234      -3.4497706      -8.7391153
C      3.1794877      -4.6716756      -9.1144765
C      3.6214819      -5.9745494      -8.8469845
C      2.8281352      -7.0682050      -9.1748329
C      1.5823896      -6.8595574      -9.7772126
C      1.1328606      -5.5653496     -10.0621273
C      1.9384425      -4.4817624      -9.7338341
C      4.0852969      -3.9356763      -4.1723494
C      2.7030696      -3.0822128      -6.6438521
S      5.6446145      -3.6024747      -9.5374596
C      5.2113218      -3.3301156     -11.2658866
C      6.4188369      -2.0298185      -9.1235983
C      0.7573926      -7.9888213     -10.1160267
N      0.0921912      -8.8967635     -10.3886992
C      3.7524580      -2.4573166      -4.3886591
C      2.6139902      -2.2188777      -5.3823262
H      5.7918177      -4.6483841      -7.1440725
H      4.5256038      -2.1261660      -7.1908455
H      3.5412449      -2.5695087      -9.2188252
H      4.5855698      -6.1443207      -8.3801550
H      3.1690543      -8.0767869      -8.9661339
H      0.1695054      -5.4148823     -10.5379326
H      1.5981421      -3.4746372      -9.9568833
H      3.1589326      -4.5262949      -4.1077008
H      4.5948106      -4.0646305      -3.2117480
H      2.3613342      -4.1034321      -6.4340185
H      2.0157060      -2.6678895      -7.3932598
H      6.1456381      -3.2673096     -11.8265017
H      4.6345781      -4.1932911     -11.6034359
H      4.6342877      -2.4080776     -11.3593470
H      7.2988718      -1.9359944      -9.7628244
H      6.7230561      -2.0736221      -8.0766283
H      5.7170241      -1.2132921      -9.3048255
H      3.4849889      -1.9929606      -3.4320517
H      4.6579613      -1.9430193      -4.7370451
H      2.6029792      -1.1596923      -5.6687312
H      1.6530733      -2.4218678      -4.8927513

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3_sy_tr_7.log
E =      -1188.212463
H =      -1187.846522
G =      -1187.915778
NImag=0
C      5.1478745      -3.3923951      -6.4346333
C      4.1496834      -2.6272671      -7.2650972
C      5.0437071      -4.5018112      -5.6011427
O      6.0670889      -5.1282779      -5.1546335
C      4.0182324      -3.1286751      -8.7467446
C      3.2830158      -4.4218876      -8.9748522
C      2.0362443      -4.3787331      -9.6100085
C      1.2902540      -5.5369885      -9.7859225
C      1.8082151      -6.7567925      -9.3331588
C      3.0661031      -6.8193810      -8.7220607
C      3.8005843      -5.6520305      -8.5490168

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C	3.7027213	-5.0813212	-5.1323361
C	2.7402667	-2.3545984	-6.7031883
S	5.7068556	-3.3392865	-9.4611759
C	5.3193112	-3.4107305	-11.2217145
C	6.3943513	-1.6776136	-9.3418031
C	1.0432250	-7.9624982	-9.5104711
N	0.4260028	-8.9320758	-9.6530048
C	2.5308552	-4.1378222	-4.8729149
C	1.9229057	-3.5103686	-6.1241873
H	6.1866428	-3.1273768	-6.6503592
H	4.5654316	-1.6187509	-7.3983374
H	3.5600464	-2.3381535	-9.3534959
H	1.6423073	-3.4274536	-9.9567261
H	0.3202845	-5.5032946	-10.2706819
H	3.4593907	-7.7728722	-8.3850364
H	4.7715324	-5.6991609	-8.0646126
H	3.3870698	-5.8474833	-5.8566274
H	3.9385613	-5.6200329	-4.2082176
H	2.1526856	-1.8624122	-7.4908248
H	2.8643421	-1.6115502	-5.9044696
H	6.2680386	-3.4046419	-11.7612982
H	4.7962090	-4.3503823	-11.4076776
H	4.7027692	-2.5546771	-11.5023344
H	7.2674478	-1.6524043	-9.9968163
H	6.7027523	-1.5083039	-8.3097223
H	5.6469713	-0.9481475	-9.6610976
H	1.7491651	-4.7115942	-4.3594106
H	2.8391926	-3.3429419	-4.1786398
H	0.9340850	-3.1057644	-5.8736636
H	1.7511770	-4.2956467	-6.8707832

3_sy_tr_8.log

E = -1188.212677

H = -1187.846858

G = -1187.916733

NImag=0

C	5.1718952	-3.7216369	-6.5217311
C	4.2516419	-2.8114214	-7.2947336
C	4.8386631	-4.7097626	-5.6077124
O	5.6795830	-5.4344243	-4.9711449
C	4.0477033	-3.2213110	-8.7929354
C	3.2875785	-4.5045789	-9.0139654
C	1.9600392	-4.4265485	-9.4515524
C	1.1929799	-5.5745837	-9.6056722
C	1.7684704	-6.8210612	-9.3312358
C	3.1006566	-6.9183655	-8.9135104
C	3.8545316	-5.7608517	-8.7569945
C	3.3563299	-4.9422439	-5.2884663
C	2.8492124	-2.5041907	-6.7065134
S	5.6938310	-3.4107506	-9.5999732
C	5.2263651	-3.3432447	-11.3410333
C	6.4312417	-1.7797597	-9.3900783
C	0.9840155	-8.0166528	-9.4907917
N	0.3518071	-8.9785715	-9.6190881
C	2.7123603	-3.7881052	-4.5043388
C	2.8567820	-2.4106824	-5.1787683
H	6.2400412	-3.5506849	-6.6745730
H	4.7418553	-1.8288643	-7.3535017
H	3.5598910	-2.4042498	-9.3394425
H	1.5219580	-3.4553448	-9.6642841
H	0.1624183	-5.5110694	-9.9388706

H	3.5377892	-7.8907403	-8.7120032
H	4.8839862	-5.8418261	-8.4238130
H	2.7879306	-5.1105917	-6.2118328
H	3.2903473	-5.8626156	-4.6996456
H	2.1162928	-3.2592894	-7.0121956
H	2.5094035	-1.5574731	-7.1428876
H	6.1484749	-3.3394959	-11.9250230
H	4.6511926	-4.2437609	-11.5643534
H	4.6384529	-2.4430750	-11.5299441
H	7.2594096	-1.7181878	-10.0992487
H	6.8130271	-1.7058994	-8.3714974
H	5.6852611	-1.0093201	-9.5958543
H	1.6453574	-4.0134455	-4.3793384
H	3.1417092	-3.7477372	-3.4953785
H	3.7854157	-1.9255765	-4.8573617
H	2.0371983	-1.7637049	-4.8461111

3_sy_tr_9.log

E = -1188.210529

H = -1187.844345

G = -1187.912761

NImag=0

C	4.0086743	-2.2787946	-6.2686540
C	3.1703519	-3.4110741	-6.8070046
C	5.2167943	-2.2569934	-5.5827608
O	5.9484289	-1.2025682	-5.5376891
C	3.5927814	-3.6930121	-8.2920294
C	2.8817065	-4.8255818	-8.9899322
C	3.1842432	-6.1749310	-8.7608633
C	2.4658620	-7.1795685	-9.3935881
C	1.4192587	-6.8346645	-10.2588274
C	1.0990857	-5.4941218	-10.4942062
C	1.8385271	-4.4994659	-9.8631385
C	5.8392782	-3.4652465	-4.8753044
C	2.9637649	-4.6490772	-5.9269891
S	5.4493397	-3.8555104	-8.4088377
C	5.6699862	-4.5066606	-10.0833822
C	6.0179155	-2.1625997	-8.7152682
C	0.6704085	-7.8721799	-10.9167596
N	0.0685585	-8.7076826	-11.4468359
C	4.9568443	-4.5837927	-4.3305196
C	4.1940050	-5.3786825	-5.3877414
H	3.7818626	-1.3232689	-6.7481125
H	2.1544423	-3.0180178	-6.9635929
H	3.4067823	-2.7717710	-8.8544248
H	3.9897355	-6.4565504	-8.0875306
H	2.7072101	-8.2229285	-9.2200287
H	0.2896108	-5.2369708	-11.1691550
H	1.6020963	-3.4558729	-10.0506345
H	6.5796480	-3.8994592	-5.5659314
H	6.4226256	-3.0387628	-4.0516762
H	2.3242767	-5.3585910	-6.4637974
H	2.3768718	-4.3123386	-5.0624948
H	6.7292567	-4.3888550	-10.3193895
H	5.4081279	-5.5638586	-10.0937283
H	5.0535444	-3.9406090	-10.7852557
H	7.0080619	-2.2551932	-9.1678432
H	6.0767597	-1.6364549	-7.7589121
H	5.3265653	-1.6765634	-9.4075599
H	5.6032185	-5.2716926	-3.7716830
H	4.2402608	-4.1727955	-3.6055794

H	3.8505808	-6.3221378	-4.9461371
H	4.8853471	-5.6561003	-6.1957015

3_sy_tr_prod_1.log

E = -710.333932
H = -710.051622
G = -710.108814

NImag=0

C	1.4046719	-0.8419815	0.0347981
C	1.3090618	0.5962713	0.4582470
C	0.2106107	-0.3845925	0.8257267
C	-1.1348960	-0.2981295	0.2023706
C	-1.3075860	0.0341555	-1.1504517
C	-2.5760389	0.1191692	-1.7069852
C	-3.6997481	-0.1314459	-0.9078089
C	-3.5478014	-0.4661878	0.4430836
C	-2.2712777	-0.5462578	0.9851701
H	0.2021269	-0.6980826	1.8671288
H	1.2814676	-1.0514188	-1.0262268
H	1.0650420	1.2991514	-0.3362021
C	2.2630012	1.1254891	1.5122294
C	3.7194459	1.1742882	1.0199362
C	4.4623295	-0.1638060	1.1021481
C	3.8873261	-1.3101359	0.2409525
C	2.4870130	-1.6434905	0.6981924
O	2.2703524	-2.4350854	1.5979507
C	-5.0150440	-0.0448391	-1.4794806
N	-6.0759137	0.0252932	-1.9405387
H	-0.4453566	0.2285170	-1.7822207
H	-2.7022760	0.3765280	-2.7536603
H	-4.4218288	-0.6599664	1.0565344
H	-2.1502798	-0.8056486	2.0329789
H	2.2066591	0.5008273	2.4143218
H	1.9349839	2.1278673	1.8068359
H	3.7416319	1.5479606	-0.0128192
H	4.2746339	1.8981273	1.6267663
H	4.4881063	-0.4947590	2.1483426
H	5.5014255	-0.0120793	0.7920684
H	4.5165733	-2.1976800	0.3520198
H	3.8727842	-1.0066588	-0.8116082

3_sy_tr_prod_3.log

E = -710.328888
H = -710.046475
G = -710.104027

NImag=0

C	1.2437419	-1.1280963	0.6394769
C	1.5440030	-0.1360600	-0.4363922
C	0.3923522	0.1126311	0.5261861
C	-1.0183271	0.0374073	0.0688806
C	-1.9515401	0.9539738	0.5746101
C	-3.2794298	0.9261715	0.1681808
C	-3.6917451	-0.0345134	-0.7629338
C	-2.7746078	-0.9596370	-1.2800667
C	-1.4515109	-0.9190160	-0.8632905
H	0.5649844	0.8704326	1.2864113
H	0.7768437	-2.0647847	0.3342819
H	1.2270770	-0.4353495	-1.4337092
C	2.7767612	0.7600744	-0.4401115
C	3.3798671	1.0965713	0.9287693

C	4.2614894	-0.0048975	1.5321439
C	3.6379418	-1.4176005	1.4899553
C	2.1677314	-1.3330710	1.8168155
O	1.7408403	-1.4259388	2.9528285
C	-5.0628550	-0.0741006	-1.1900286
N	-6.1688660	-0.1057833	-1.5346544
H	-1.6290639	1.6977668	1.2976544
H	-3.9939936	1.6396288	0.5657931
H	-3.1027673	-1.7019027	-2.0006103
H	-0.7537456	-1.6450068	-1.2717349
H	2.5038815	1.6904567	-0.9513588
H	3.5462321	0.2815775	-1.0604953
H	3.9884550	2.0010018	0.8281348
H	2.5832314	1.3582320	1.6374183
H	4.4784464	0.2520185	2.5743757
H	5.2196259	-0.0421820	1.0030275
H	4.1362432	-2.0701783	2.2114120
H	3.7502036	-1.8424256	0.4873301

3_sy_tr_prod_4.log

E = -710.335303

H = -710.052464

G = -710.109819

NImag=0

C	1.4848300	-0.8975165	-0.2878901
C	1.5089684	0.6162413	-0.3059230
C	0.4466573	-0.0853529	0.4832691
C	-0.9752488	-0.1022446	0.0496590
C	-1.9842862	-0.0797456	1.0226464
C	-3.3264758	-0.0862756	0.6646441
C	-3.6743369	-0.1177373	-0.6908928
C	-2.6798710	-0.1424499	-1.6780166
C	-1.3432778	-0.1342291	-1.3041623
H	0.5734863	-0.0795329	1.5616189
H	1.1345675	-1.3629994	-1.2051834
H	1.1656314	1.0091101	-1.2610110
C	2.5832942	1.4854760	0.3216826
C	3.0298636	1.1686162	1.7497140
C	3.8020711	-0.1396174	1.9190130
C	2.9583812	-1.4199516	1.8093909
C	2.5088815	-1.7327985	0.3993966
O	2.9868502	-2.6846018	-0.2027652
C	-5.0595905	-0.1246472	-1.0729564
N	-6.1766407	-0.1296816	-1.3811257
H	-1.7114320	-0.0557148	2.0737010
H	-4.1010731	-0.0676503	1.4244520
H	-2.9579314	-0.1675463	-2.7266412
H	-0.5847535	-0.1543542	-2.0814858
H	2.2058822	2.5145558	0.2999435
H	3.4622733	1.4647435	-0.3363710
H	3.6796538	1.9900781	2.0711637
H	2.1681897	1.1772843	2.4298571
H	4.2632830	-0.1459112	2.9119750
H	4.6229023	-0.1799199	1.1906708
H	2.0858320	-1.3371735	2.4679472
H	3.5493185	-2.2783532	2.1383795

3_sy_tr_prod_5.log

E = -710.331802

H = -710.050025

G = -710.107888
 NImag=0

C	1.4218967	-0.8627150	0.1004058
C	1.3459941	0.5613018	0.5530187
C	0.2273176	-0.4050804	0.8994711
C	-1.1104844	-0.2857306	0.2668823
C	-1.2680364	0.1062735	-1.0718406
C	-2.5301641	0.2171572	-1.6380537
C	-3.6628830	-0.0673090	-0.8631795
C	-3.5260607	-0.4605251	0.4734200
C	-2.2558001	-0.5657777	1.0255613
H	0.2022857	-0.7403526	1.9339433
H	1.2791105	-1.0761894	-0.9583528
H	1.1180204	1.3019684	-0.2118528
C	2.3291076	0.9868084	1.6232008
C	3.7447451	1.1793690	1.0550323
C	4.1770040	0.0649577	0.0911462
C	3.9152160	-1.3519659	0.6061329
C	2.4535638	-1.7397184	0.7693342
O	2.1373132	-2.7264237	1.4077577
C	-4.9717550	0.0448988	-1.4449436
N	-6.0273556	0.1357529	-1.9144462
H	-0.3984369	0.3280657	-1.6842167
H	-2.6448591	0.5204467	-2.6737203
H	-4.4070190	-0.6799549	1.0679615
H	-2.1465036	-0.8705543	2.0623779
H	2.3519768	0.2157844	2.4059084
H	1.9911165	1.9070643	2.1112245
H	3.8002593	2.1376986	0.5253303
H	4.4520261	1.2395921	1.8909568
H	5.2481069	0.1668049	-0.1119764
H	3.6691174	0.1926035	-0.8714906
H	4.4016038	-1.5255389	1.5737513
H	4.3439763	-2.0846119	-0.0906439

3_sy_tr_prod_6.log
 E = -710.325079
 H = -710.043126
 G = -710.102268
 NImag=0

C	1.4985200	-0.7473370	-0.0952595
C	1.3943332	0.7171928	0.2240294
C	0.3281112	-0.2482017	0.7093146
C	-1.0509762	-0.2209771	0.1621252
C	-1.3076757	0.0115727	-1.1985163
C	-2.6074413	0.0415790	-1.6839152
C	-3.6794094	-0.1637430	-0.8043479
C	-3.4437646	-0.3981927	0.5556634
C	-2.1370432	-0.4249326	1.0257905
H	0.3815348	-0.4864660	1.7701545
H	1.3054182	-1.0280109	-1.1313202
H	1.0744188	1.3178862	-0.6247011
C	2.2964695	1.4619902	1.2019297
C	3.4505870	0.6527028	1.8040937
C	4.3291558	0.0077159	0.7180766
C	3.9424598	-1.4502220	0.4126685
C	2.4626101	-1.7069712	0.5643303
O	2.0429903	-2.6775600	1.1678686
C	-5.0270232	-0.1340018	-1.3013240
N	-6.1140514	-0.1096796	-1.7024228
H	-0.4876972	0.1721179	-1.8932100

H	-2.7980475	0.2218739	-2.7370088
H	-4.2774384	-0.5576459	1.2318916
H	-1.9518568	-0.6076029	2.0804405
H	1.6851835	1.8981468	2.0009079
H	2.7401545	2.3027444	0.6564516
H	4.0482773	1.3342107	2.4177898
H	3.0717152	-0.1162295	2.4927060
H	5.3794830	0.0163059	1.0228989
H	4.2646397	0.6122208	-0.1940764
H	4.4553829	-2.1431711	1.0857766
H	4.2228800	-1.7146149	-0.6153056

3_sy_tr_prod_7.log

E = -710.333263
H = -710.050452
G = -710.107837

NImag=0

C	1.4517946	-0.7103400	-0.1822817
C	1.3721566	0.7734316	0.1233793
C	0.3179660	-0.1384169	0.6686756
C	-1.0725852	-0.1538622	0.1436540
C	-1.3659403	0.0831810	-1.2079734
C	-2.6768119	0.0697198	-1.6638767
C	-3.7201121	-0.1824863	-0.7630190
C	-3.4468739	-0.4211135	0.5890989
C	-2.1295455	-0.4056170	1.0296799
H	0.3854543	-0.3419267	1.7339201
H	1.1735317	-1.0100206	-1.1889930
H	1.0671393	1.3495611	-0.7473523
C	2.3793440	1.4903443	1.0197012
C	3.8252309	1.0195112	0.8050851
C	4.1934983	-0.2106638	1.6471076
C	3.0688506	-1.2600481	1.7637031
C	2.4974215	-1.5915161	0.4064079
O	2.9169532	-2.5428331	-0.2381979
C	-5.0786127	-0.1952186	-1.2314941
N	-6.1739892	-0.2050618	-1.6093546
H	-0.5696408	0.2806059	-1.9200145
H	-2.8973727	0.2531585	-2.7104122
H	-4.2590167	-0.6155381	1.2820514
H	-1.9140700	-0.5904417	2.0781267
H	2.1032065	1.3771739	2.0749422
H	2.3052165	2.5581152	0.7949668
H	3.9667603	0.7997287	-0.2608697
H	4.5211161	1.8283385	1.0498490
H	4.4478859	0.1071176	2.6640751
H	5.0853127	-0.6879236	1.2269500
H	2.2849650	-0.8815781	2.4251059
H	3.4640667	-2.1810813	2.1989591

4a.log

E = -305.169163
H = -305.087982
G = -305.121481

NImag=0

C	-0.1667507	-1.2305037	-0.3858679
C	1.2471598	-0.8945914	-0.0389624
O	1.2359204	0.5183600	0.1970488
C	-0.0194490	1.0036270	0.0211946
C	-0.9048190	-0.1195461	-0.3499969

O	-0.2756891	2.1770529	0.1665119
H	-0.4896581	-2.2375679	-0.6220131
H	1.5893856	-1.4034301	0.8674423
H	1.9429552	-1.1129223	-0.8549313
H	-1.9607571	0.0087202	-0.5451260

4a_c_sy_1.log

E = -1145.534118

H = -1145.252442

G = -1145.316808

NImag=0

C	2.5337255	1.2186910	-0.6212743
C	2.0048792	-0.1080715	-0.1704309
C	3.6061391	1.6156731	0.1603315
O	4.2703761	2.6656259	0.2450871
C	0.6133786	-0.1806761	0.5144383
C	-0.5773556	-0.2192445	-0.4265656
C	-1.7575712	-0.8445366	-0.0023671
C	-2.8682185	-0.9067158	-0.8327237
C	-2.7972751	-0.3351967	-2.1090206
C	-1.6260431	0.2891002	-2.5493222
C	-0.5214548	0.3442671	-1.7054206
O	3.9583639	0.5691196	1.0522145
C	3.1726169	-0.5753419	0.7320671
S	0.1704405	1.1042472	1.7800992
C	1.5421861	1.1741830	2.9440362
C	0.2464262	2.7287269	0.9958478
C	-3.9411827	-0.3970977	-2.9801998
N	-4.8618671	-0.4467864	-3.6808005
H	2.0422903	1.8975281	-1.3047573
H	1.8853780	-0.8492235	-0.9751626
H	0.5738392	-1.0840375	1.1381898
H	-1.8058861	-1.2952983	0.9855508
H	-3.7784528	-1.3967374	-0.5039470
H	-1.5814767	0.7242095	-3.5421575
H	0.3852686	0.8224557	-2.0582386
H	3.7978030	-1.2870948	0.1808613
H	2.8415368	-1.0499237	1.6619952
H	1.2820026	1.9532672	3.6641241
H	1.5908699	0.2084911	3.4508152
H	2.4780303	1.4046388	2.4340808
H	-0.2432364	3.4133573	1.6920242
H	-0.3243311	2.6813180	0.0661821
H	1.2815003	3.0080825	0.8084434

4a_c_sy_1_r.log

E = -1145.533225

H = -1145.251274

G = -1145.315769

NImag=0

C	-0.5640536	-2.1152317	-0.5819706
C	-1.1990515	-0.8806425	-1.1500312
C	-1.3029686	-2.5941170	0.4915638
O	-1.1289630	-3.4969961	1.3285829
C	-0.3262563	0.3628338	-0.8370096
C	0.1203329	0.6521578	0.5791193
C	1.3979667	1.1929443	0.7681595
C	1.8521715	1.5292139	2.0381685
C	1.0140685	1.3160011	3.1368271
C	-0.2651950	0.7722336	2.9660500

C	-0.7082838	0.4481867	1.6898988
O	-2.5092375	-1.8536256	0.5985695
C	-2.6098556	-0.9967542	-0.5338459
S	-0.9644000	2.0051331	-1.5182893
C	-2.1521361	1.5656442	-2.8038920
C	-2.0430547	2.7051981	-0.2530666
C	1.4718539	1.6570176	4.4577190
N	1.8401815	1.9333862	5.5203101
H	0.4353287	-2.4570096	-0.8182702
H	-1.2904118	-0.8918337	-2.2416378
H	0.5747676	0.2534222	-1.4509841
H	2.0490879	1.3482541	-0.0882676
H	2.8435894	1.9464156	2.1791690
H	-0.9040223	0.6072627	3.8273749
H	-1.6980836	0.0211331	1.5731086
H	-3.2780873	-1.4579857	-1.2720202
H	-3.0565778	-0.0514101	-0.2130672
H	-2.5452713	2.5098236	-3.1865845
H	-1.6123294	1.0447811	-3.5962501
H	-2.9563948	0.9508914	-2.3983863
H	-2.5525508	3.5453501	-0.7303541
H	-1.4117352	3.0720139	0.5570070
H	-2.7652068	1.9734952	0.1079556

4a_c_sy_1_ts1.log

E = -1145.510166

H = -1145.231096

G = -1145.295518

NImag=1

C	-1.0860362	-1.8891691	-0.1330989
C	-1.0927146	-0.9564439	-1.1615878
C	-2.4328380	-2.1309050	0.2894949
O	-2.8941186	-2.8032883	1.2019993
C	-0.4073835	1.0000063	-0.6211789
C	0.9805493	0.6961063	-0.3461410
C	1.8999813	0.6129062	-1.4185559
C	3.2037633	0.1969291	-1.2177449
C	3.6355496	-0.1532740	0.0734939
C	2.7383032	-0.0919951	1.1502964
C	1.4305331	0.3152983	0.9391137
O	-3.2979069	-1.4469100	-0.5456323
C	-2.5382629	-0.8123514	-1.5789017
S	-1.2162362	1.8846159	0.6812478
C	-2.2686880	3.0365964	-0.2211629
C	-2.4882574	0.8378358	1.4373242
C	4.9864112	-0.5768294	0.2883034
N	6.0813900	-0.9197895	0.4612785
H	-0.2297970	-2.3527871	0.3369653
H	-0.3243191	-0.8955772	-1.9262066
H	-0.6214646	1.4855009	-1.5718959
H	1.5748183	0.8933936	-2.4168595
H	3.8981548	0.1481869	-2.0509413
H	3.0682351	-0.3746092	2.1451933
H	0.7495885	0.3324481	1.7873199
H	-2.7095269	-1.3456260	-2.5218117
H	-2.8844259	0.2180140	-1.6921688
H	-2.9113616	3.5341308	0.5071223
H	-1.6189650	3.7634693	-0.7101063
H	-2.8642522	2.4879369	-0.9532337
H	-3.2096294	0.4992753	0.6931347
H	-2.9704812	1.4606730	2.1945279

H -1.9884515 -0.0034371 1.9204204

4a_c_sy_1_ts2.log

E = -1145.523943

H = -1145.243641

G = -1145.307250

NImag=1

C	-1.7620480	1.8325283	1.1138085
C	-2.2119651	0.5969103	0.3926087
C	-1.1796783	2.7195031	0.1890554
O	-0.5806355	3.7893241	0.3197575
C	-1.0796559	-0.2523099	0.8793084
C	0.3630323	-0.1129884	0.5309500
C	1.2884768	-0.4651820	1.5282884
C	2.6544018	-0.4373128	1.2871729
C	3.1141691	-0.0517844	0.0223533
C	2.2095107	0.2927732	-0.9885770
C	0.8442349	0.2507166	-0.7371151
O	-1.3635836	2.2254988	-1.1075743
C	-2.2313183	1.0888451	-1.0549260
S	-1.4067592	-2.4203025	0.3185927
C	-3.1361688	-2.4285038	-0.2066784
C	-0.5976900	-2.5875055	-1.2869405
C	4.5269238	-0.0169624	-0.2439130
N	5.6648643	0.0102364	-0.4585657
H	-1.7884009	1.9901282	2.1818501
H	-3.1716637	0.1715111	0.6919715
H	-1.2108076	-0.4787441	1.9366573
H	0.9276768	-0.7585081	2.5103018
H	3.3594065	-0.7065129	2.0664873
H	2.5753444	0.5803516	-1.9687166
H	0.1660316	0.5031105	-1.5403307
H	-3.2488147	1.4071714	-1.3087615
H	-1.8992078	0.3532188	-1.7927202
H	-3.3696078	-3.4178490	-0.6062633
H	-3.7568436	-2.2358885	0.6699048
H	-3.3080487	-1.6664891	-0.9700517
H	-0.9141367	-3.5341821	-1.7307726
H	0.4809473	-2.6069996	-1.1224550
H	-0.8689979	-1.7550173	-1.9396737

4a_c_sy_2.log

E = -1145.541329

H = -1145.259776

G = -1145.323806

NImag=0

C	2.7327793	1.0888515	-0.6519270
C	2.1636596	-0.2324739	-0.2175787
C	3.7423124	1.4955536	0.2134121
O	4.4171510	2.5353676	0.3173897
C	0.7748373	-0.1800982	0.4724674
C	-0.4306240	-0.1800918	-0.4294069
C	-0.4023031	0.4185637	-1.6958603
C	-1.5294199	0.4061109	-2.5077567
C	-2.6995810	-0.2125795	-2.0512671
C	-2.7421558	-0.8251403	-0.7944548
C	-1.6053530	-0.8071702	0.0050921
O	3.9901462	0.4752821	1.1588537
C	3.2735526	-0.6882269	0.7550236
S	0.8072812	1.3091413	1.5944150

C	0.0098313	2.6495312	0.6887447
C	-0.5121176	0.9211220	2.7645470
C	-3.8689708	-0.2277452	-2.8900884
N	-4.8103955	-0.2392807	-3.5643521
H	2.3525477	1.7226327	-1.4412688
H	2.0499944	-0.9817549	-1.0118354
H	0.6717986	-1.0028712	1.1903978
H	0.5016746	0.8956454	-2.0579602
H	-1.5067782	0.8685881	-3.4889253
H	-3.6495094	-1.3135225	-0.4552118
H	-1.6262618	-1.2972422	0.9747416
H	3.9608321	-1.3666903	0.2343924
H	2.8914513	-1.1919344	1.6491858
H	0.6389705	2.8925693	-0.1669443
H	-0.9941046	2.3502999	0.3819774
H	-0.0341221	3.4954610	1.3785497
H	-0.5862528	1.7684321	3.4490803
H	-0.2206714	0.0254166	3.3159833
H	-1.4583991	0.7725531	2.2414841

4a_c_sy_2_r.log

E = -1145.536344
H = -1145.254624
G = -1145.318996

NImag=0

C	-0.8015191	-2.1883137	-0.3884760
C	-1.4462273	-0.9909316	-1.0162708
C	-1.5048693	-2.5748037	0.7459777
O	-1.3022571	-3.4038173	1.6499763
C	-0.6032794	0.2951655	-0.7936710
C	-0.1013288	0.6450704	0.5829838
C	-0.9095532	0.5529214	1.7246531
C	-0.4136595	0.9160292	2.9696830
C	0.9029403	1.3821286	3.0799027
C	1.7240508	1.4772997	1.9528017
C	1.2144682	1.1058770	0.7133052
O	-2.7074064	-1.8247955	0.8311165
C	-2.8428047	-1.0679887	-0.3665023
S	-1.4872990	1.7511751	-1.5893696
C	-2.2469087	2.6954867	-0.2535292
C	-0.1235745	2.8523003	-2.0127218
C	1.4158310	1.7659007	4.3685239
N	1.8279608	2.0773590	5.4050120
H	0.2000407	-2.5340585	-0.6106726
H	-1.5665739	-1.0516669	-2.1059758
H	0.2608723	0.2111493	-1.4632346
H	-1.9272882	0.1849382	1.6532489
H	-1.0385062	0.8413501	3.8535490
H	2.7445705	1.8327477	2.0477292
H	1.8518370	1.1672109	-0.1647071
H	-3.5204461	-1.5970947	-1.0474285
H	-3.2954331	-0.1008436	-0.1206134
H	-3.0066184	2.0795292	0.2281355
H	-1.4843510	3.0154299	0.4583059
H	-2.7205615	3.5576797	-0.7282471
H	-0.5623185	3.7609064	-2.4298025
H	0.4871467	2.3513916	-2.7654358
H	0.4565322	3.0806781	-1.1163515

4a_c_sy_2_ts1.log

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E =      -1145.510667
H =      -1145.231318
G =      -1145.295834
NImag=1
C        -1.4584589      -1.8901492      0.1288860
C        -1.3615703      -1.2258360     -1.0863826
C        -2.7849683      -1.7124689      0.6443377
O        -3.2980215      -2.0391512      1.7056714
C        -0.4461942       0.7148291     -1.0030935
C         0.9091975       0.4321076     -0.5818370
C         1.3370041       0.4094187      0.7647500
C         2.6234730       0.0155238      1.1034303
C         3.5233881      -0.3817639      0.1055884
C         3.1180613      -0.3797041     -1.2405512
C         1.8373408       0.0224521     -1.5707720
O        -3.5407165      -1.0273635     -0.2904773
C        -2.7807814      -0.9172756     -1.4988669
S        -1.4710757       1.8551255     -0.1566157
C        -1.8253350       1.2240264      1.5144597
C        -0.4869669       3.3253983      0.2473215
C         4.8511021      -0.7883517      0.4567124
N         5.9267856      -1.1178748      0.7402655
H        -0.6733585      -2.3904972      0.6786324
H        -0.6246044      -1.4584002     -1.8482948
H        -0.5755003       0.9135485     -2.0655933
H         0.6697387       0.7078254      1.5655578
H         2.9342149       0.0121241      2.1434931
H         3.8140885      -0.6856311     -2.0153794
H         1.5330106       0.0304261     -2.6139089
H        -3.1328312      -1.6750833     -2.2104775
H        -2.9415599       0.0721834     -1.9310702
H        -1.5209009       0.1800779      1.5755291
H        -1.2762415       1.8214219      2.2441756
H        -2.8996731       1.3152106      1.6760571
H        -1.1270206       3.9953563      0.8259770
H        -0.2094809       3.7924406     -0.6988123
H         0.3983390       3.0439952      0.8195366

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4a_c_sy_2_ts2.log
E =      -1145.525706
H =      -1145.245502
G =      -1145.309361
NImag=1
C         2.2120375       1.5225239     -1.0504695
C         2.4141978       0.2962754     -0.2100368
C         1.5982948       2.5186638     -0.2669628
O         1.1195048       3.6215246     -0.5418438
C         1.2374440      -0.4315614     -0.7792982
C        -0.1956568      -0.1091322     -0.5522968
C        -0.7399447       0.2181685      0.6996808
C        -2.1054942       0.4354267      0.8409283
C        -2.9457571       0.3189951     -0.2714870
C        -2.4239591      -0.0166609     -1.5275113
C        -1.0600094      -0.2318535     -1.6542034
O         1.5589264       2.0982896      1.0659860
C         2.3320075       0.9010707      1.1918471
S         1.3966215      -2.5887690     -0.1249057
C         1.2669486      -2.5116034      1.6728505
C        -0.2262375      -3.2696259     -0.5263745
C        -4.3590312       0.5402479     -0.1210047
N        -5.4972731       0.7174982     -0.0003235

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H	2.3690921	1.5939610	-2.1167660
H	3.3367427	-0.2735983	-0.3539474
H	1.4284411	-0.7108646	-1.8146929
H	-0.1121403	0.3051978	1.5759413
H	-2.5205995	0.6885705	1.8107967
H	-3.0812865	-0.1069725	-2.3858701
H	-0.6487266	-0.4941786	-2.6249796
H	3.3454277	1.1654253	1.5157659
H	1.8775091	0.2632208	1.9524195
H	2.1980952	-2.0950586	2.0606348
H	0.4161777	-1.8932166	1.9681848
H	1.1377025	-3.5277259	2.0523760
H	-0.2647609	-4.3046855	-0.1799314
H	-0.3436795	-3.2429527	-1.6115619
H	-1.0117225	-2.6805485	-0.0460523

4a_c_sy_3.log

E = -1145.541560
H = -1145.259924
G = -1145.323898

NImag=0

C	2.6691217	1.0126870	-0.6660035
C	1.9619781	-0.1709614	-0.0763022
C	3.8148506	1.3232377	0.0522555
O	4.6630722	2.2296026	-0.0231366
C	0.5689908	0.0961335	0.5740605
C	-0.5944486	-0.0426702	-0.3787567
C	-1.6220808	-0.9415443	-0.0770682
C	-2.6956719	-1.1076185	-0.9449392
C	-2.7427510	-0.3549690	-2.1230593
C	-1.7238210	0.5536007	-2.4360302
C	-0.6540413	0.7037638	-1.5630069
O	3.9870540	0.3797646	1.0979860
C	3.0307073	-0.6638693	0.9304215
S	0.5092335	1.8135787	1.2514399
C	-1.0906316	1.7779171	2.0930388
C	1.6007220	1.7188224	2.6839090
C	-3.8525426	-0.5151861	-3.0251114
N	-4.7458251	-0.6439526	-3.7507403
H	2.3361195	1.5901313	-1.5174786
H	1.7533947	-0.9807038	-0.7881774
H	0.4081782	-0.5588948	1.4385223
H	-1.5804851	-1.5178324	0.8427146
H	-3.4911790	-1.8078190	-0.7128548
H	-1.7736331	1.1311433	-3.3531190
H	0.1352831	1.4075408	-1.8099247
H	3.5410530	-1.5449299	0.5252614
H	2.6142273	-0.9210417	1.9103074
H	-1.1380829	2.6744376	2.7144230
H	-1.8742955	1.8147266	1.3350747
H	-1.1747064	0.8777757	2.7053616
H	1.4739524	2.6530993	3.2344223
H	2.6291959	1.6249905	2.3320025
H	1.3107616	0.8648398	3.2999081

4a_c_sy_3_ts1.log

E = -1145.513676
H = -1145.234925
G = -1145.300727

NImag=1

C	1.5298982	-1.7171156	-0.6036361
C	1.1561280	-1.3487801	0.6792933
C	2.9590583	-1.6427119	-0.7130007
O	3.7156021	-1.8072095	-1.6588637
C	0.3625860	0.6955845	0.7648103
C	-1.0171980	0.4346467	0.4412312
C	-1.9132826	0.1268837	1.4965638
C	-3.2181343	-0.2544033	1.2489488
C	-3.6842103	-0.3449970	-0.0751889
C	-2.8158709	-0.0511127	-1.1373865
C	-1.5081862	0.3296554	-0.8839067
O	3.4883077	-1.3404663	0.5313220
C	2.4277118	-1.3178034	1.4925863
S	1.2754883	1.5708201	-0.4519531
C	0.6340858	3.2658913	-0.4437952
C	2.8641661	1.8417472	0.3510734
C	-5.0362722	-0.7321209	-0.3380204
N	-6.1330402	-1.0473325	-0.5501818
H	0.8892290	-1.9687344	-1.4374033
H	0.2308060	-1.6446816	1.1620733
H	0.5761932	1.0506922	1.7729201
H	-1.5617076	0.1968482	2.5223248
H	-3.8875476	-0.4804917	2.0733168
H	-3.1719844	-0.1224184	-2.1605085
H	-0.8639936	0.5487490	-1.7313231
H	2.4939353	-2.2204714	2.1123884
H	2.5455844	-0.4406210	2.1327335
H	1.2305013	3.8566449	-1.1425295
H	-0.4023453	3.2220670	-0.7833268
H	0.6950564	3.6680098	0.5689105
H	3.3859383	2.6024807	-0.2325976
H	3.4289047	0.9091521	0.3285552
H	2.6973532	2.1861140	1.3737550

4a_c_sy_4.log

E = -1145.540016

H = -1145.258397

G = -1145.323300

NImag=0

C	3.1130607	1.7000422	0.0736915
C	2.0021813	0.9538251	-0.6014505
C	3.9606525	0.7941414	0.7017889
O	4.9011474	0.9052249	1.5069687
C	0.7324368	0.7381132	0.2781099
C	-0.4872068	0.3056266	-0.4909519
C	-0.9717702	1.0700435	-1.5614045
C	-2.0863998	0.6527030	-2.2765426
C	-2.7162858	-0.5481546	-1.9246644
C	-2.2410659	-1.3238842	-0.8620230
C	-1.1303044	-0.8876402	-0.1481765
O	3.6087354	-0.5206042	0.2999963
C	2.6880458	-0.4091470	-0.7833413
S	0.3869341	2.3088327	1.2119335
C	-1.3187390	2.0893960	1.7642977
C	1.2291957	2.0110312	2.7831571
C	-3.8676376	-0.9898299	-2.6666067
N	-4.7941746	-1.3456779	-3.2632343
H	3.1304188	2.7649258	0.2687478
H	1.6822421	1.3591549	-1.5668541
H	0.9518857	0.0140215	1.0713866
H	-0.4852275	2.0020411	-1.8384087

H	-2.4676726	1.2448869	-3.1016048
H	-2.7380958	-2.2519413	-0.5998550
H	-0.7572237	-1.4796575	0.6826401
H	3.2390404	-0.4206186	-1.7326875
H	2.0038588	-1.2635091	-0.7521710
H	-1.5029140	2.8645521	2.5111850
H	-1.9834240	2.2328703	0.9120957
H	-1.4411430	1.0954858	2.1996036
H	0.9898956	2.8524800	3.4368180
H	2.2992180	1.9700898	2.5811033
H	0.8659356	1.0718766	3.2055531

4a_c_sy_4_ts1.log

E = -1145.513067
H = -1145.234213
G = -1145.299588

NImag=1

C	2.5944060	-0.8583739	-1.1979275
C	1.2886739	-1.0713779	-0.7823032
C	3.4807771	-1.4923633	-0.2627204
O	4.7005013	-1.4815951	-0.1656897
C	0.4481593	0.5072469	0.4665856
C	-0.9649981	0.2864315	0.3075590
C	-1.6934044	0.7006562	-0.8360943
C	-3.0248518	0.3609929	-1.0030966
C	-3.6804840	-0.4162531	-0.0350290
C	-2.9778641	-0.8458277	1.1046140
C	-1.6500453	-0.4974982	1.2700407
O	2.7321845	-2.2113999	0.6456732
C	1.3587379	-2.1774353	0.2408104
S	1.1347043	1.9349573	-0.3015817
C	0.3332183	3.3756868	0.4507298
C	2.7362845	2.0244053	0.5192706
C	-5.0568322	-0.7669758	-0.2079230
N	-6.1730754	-1.0522602	-0.3488323
H	2.9432585	-0.2310400	-2.0069308
H	0.4204353	-0.9879446	-1.4299085
H	0.8592801	0.3653662	1.4659175
H	-1.2115635	1.2945817	-1.6092100
H	-3.5646894	0.6918729	-1.8850751
H	-3.4838812	-1.4430325	1.8569883
H	-1.1194943	-0.8200951	2.1616668
H	1.1064511	-3.1369483	-0.2284540
H	0.7322586	-2.0384647	1.1234905
H	0.8425764	4.2699131	0.0838979
H	-0.7086710	3.3819339	0.1256013
H	0.4025781	3.2969468	1.5370900
H	3.2371094	2.9252650	0.1612704
H	3.3074571	1.1397483	0.2391017
H	2.5757385	2.0666297	1.5985193

4a_c_sy_5.log

E = -1145.536186
H = -1145.254202
G = -1145.319337

NImag=0

C	3.0120380	1.5548430	0.5419622
C	1.8037839	1.2234189	-0.2827873
C	3.8958216	0.4821721	0.5447322
O	4.9471592	0.2301945	1.1596318

C	0.5779981	0.6622215	0.4951721
C	-0.5642335	0.2059476	-0.3850617
C	-1.0729033	-1.0888849	-0.2371007
C	-2.1044307	-1.5427226	-1.0501542
C	-2.6358003	-0.6857008	-2.0208627
C	-2.1385540	0.6129667	-2.1804354
C	-1.1030950	1.0510257	-1.3636426
O	3.4342371	-0.5008001	-0.3667250
C	2.3962211	0.0870484	-1.1434223
S	-0.1554656	1.8392216	1.7311124
C	0.8849104	1.6694884	3.1943316
C	0.2609302	3.4928300	1.1452366
C	-3.7051018	-1.1449469	-2.8672881
N	-4.5658715	-1.5142943	-3.5483307
H	3.1298689	2.4073347	1.1963806
H	1.4456580	2.0280522	-0.9350376
H	0.9045426	-0.1662267	1.1356379
H	-0.6532141	-1.7486043	0.5170005
H	-2.4963912	-2.5481417	-0.9378938
H	-2.5584751	1.2666884	-2.9377019
H	-0.7169074	2.0569842	-1.5007714
H	2.8266782	0.5185974	-2.0567542
H	1.6824743	-0.6945416	-1.4193166
H	0.5153525	2.3938759	3.9232497
H	0.7402195	0.6557040	3.5722070
H	1.9275486	1.8509988	2.9398457
H	-0.1171244	4.1845114	1.9011154
H	-0.2663519	3.6575631	0.2038243
H	1.3381776	3.6012755	1.0237461

4a_c_sy_5_ts1.log

E = -1145.509045

H = -1145.229947

G = -1145.294379

NImag=1

C	-2.8772787	-0.6301006	0.8646449
C	-1.5025627	-0.6497165	1.0373418
C	-3.2632663	-1.7791290	0.0928311
O	-4.3432974	-2.1157368	-0.3723919
C	-0.4660858	0.5208031	-0.5002793
C	0.9552918	0.3085740	-0.3809580
C	1.5821928	-0.7259245	-1.1208404
C	2.9235127	-1.0194182	-0.9591966
C	3.6991967	-0.2807731	-0.0479163
C	3.1029974	0.7482900	0.6982290
C	1.7565289	1.0287489	0.5399274
O	-2.1585586	-2.5790669	-0.0993164
C	-1.0633557	-2.0381043	0.6454246
S	-0.9685296	2.2148973	-0.3758342
C	-2.4840776	2.2216416	-1.3516296
C	-1.6494106	2.5305163	1.2785188
C	5.0888414	-0.5774379	0.1203155
N	6.2161162	-0.8181551	0.2566637
H	-3.5857613	0.1383899	1.1379248
H	-0.9532357	-0.1175546	1.8071874
H	-0.9626043	0.0614799	-1.3529596
H	0.9956777	-1.2873020	-1.8433657
H	3.3842937	-1.8105751	-1.5426718
H	3.6986109	1.3159412	1.4065003
H	1.3196278	1.8158122	1.1499760
H	-0.9134631	-2.6463455	1.5465799

H	-0.1616427	-2.0918544	0.0342704
H	-2.9711854	3.1862679	-1.1984131
H	-2.2009007	2.1031549	-2.3983869
H	-3.1237620	1.4007804	-1.0222737
H	-1.9041496	3.5924547	1.2969470
H	-0.8632319	2.3312208	2.0086737
H	-2.5301042	1.9208207	1.4711373

4a_c_sy_6.log

E = -1145.541383
H = -1145.259511
G = -1145.324500

NImag=0

C	3.1219277	1.6257936	0.5480957
C	1.9627626	1.2174668	-0.3113625
C	4.0670225	0.6067249	0.5822905
O	5.1150344	0.4193955	1.2242948
C	0.7661563	0.6008995	0.4670704
C	-0.4332447	0.2089729	-0.3545275
C	-0.9257960	1.0287615	-1.3790715
C	-2.0285727	0.6351534	-2.1286748
C	-2.6433654	-0.5917369	-1.8556188
C	-2.1593404	-1.4259533	-0.8410083
C	-1.0583726	-1.0185956	-0.0987407
O	3.6897861	-0.4062159	-0.3377137
C	2.6352374	0.1092229	-1.1435533
S	0.3382272	1.7481309	1.8575922
C	-0.1597181	3.2792387	1.0514801
C	-1.2510301	1.1407493	2.4492905
C	-3.7840522	-1.0030795	-2.6307768
N	-4.7025436	-1.3339131	-3.2536089
H	3.1504613	2.4836499	1.2078028
H	1.5773858	1.9995974	-0.9738846
H	1.1325888	-0.2702838	1.0246711
H	-0.4526563	1.9786569	-1.6061307
H	-2.4097164	1.2697174	-2.9216947
H	-2.6400879	-2.3779063	-0.6418564
H	-0.6755979	-1.6613080	0.6892442
H	3.0574353	0.5474397	-2.0572232
H	1.9667997	-0.7134353	-1.4164667
H	-0.4548487	3.9632774	1.8498355
H	0.7064773	3.6825437	0.5241558
H	-0.9962139	3.0995934	0.3745401
H	-1.5478746	1.7976782	3.2694187
H	-1.1017357	0.1263546	2.8245062
H	-1.9911354	1.1625093	1.6476244

4a_c_sy_6_ts1.log

E = -1145.511051
H = -1145.231721
G = -1145.297117

NImag=1

C	-2.9900306	-0.4756320	0.9152102
C	-1.6308769	-0.7465565	0.9215355
C	-3.6435235	-1.4249682	0.0581109
O	-4.8048899	-1.5166815	-0.3143440
C	-0.5340165	0.4103821	-0.5633784
C	0.8746753	0.1614263	-0.3663220
C	1.6449320	0.7495324	0.6655224
C	2.9697270	0.3971479	0.8661684

C	3.5717567	-0.5738243	0.0517044
C	2.8241124	-1.1882030	-0.9672443
C	1.5057284	-0.8222117	-1.1689163
O	-2.7191065	-2.3596219	-0.3611390
C	-1.4808734	-2.1184224	0.3135582
S	-1.2577303	1.9971333	-0.4396734
C	-1.2623728	2.5661633	1.2825278
C	-0.1136709	3.2072572	-1.1467480
C	4.9403350	-0.9388366	0.2612493
N	6.0495237	-1.2346960	0.4307534
H	-3.5082202	0.3631251	1.3600469
H	-0.9270635	-0.4240038	1.6832431
H	-0.9709199	-0.0518924	-1.4472227
H	1.2052138	1.4834877	1.3314034
H	3.5424596	0.8650210	1.6609359
H	3.2870809	-1.9389279	-1.6002463
H	0.9408088	-1.2878011	-1.9720040
H	-1.3600211	-2.8648020	1.1089731
H	-0.6603083	-2.2263838	-0.3983289
H	-1.9492155	3.4145610	1.3142785
H	-1.6388013	1.7669765	1.9202243
H	-0.2667153	2.8827414	1.5910773
H	-0.5387811	4.1995592	-0.9793948
H	-0.0435633	3.0012942	-2.2157271
H	0.8636952	3.1198018	-0.6686007

4a_sy_c_prod_1.log

E = -667.654360

H = -667.456235

G = -667.507922

NImag=0

C	-0.2880318	-0.8113894	-1.9503016
C	1.0712126	-0.2383514	-1.7393845
C	1.3500878	0.5965112	-2.9667191
C	0.0937271	0.5078032	-3.8095369
O	-0.7470503	-0.4814977	-3.1766569
O	-0.9459267	-1.4752749	-1.1850349
C	2.1072479	-0.6741845	-2.7560454
C	1.9261914	-1.8796364	-3.6250632
C	1.5319752	-3.1067703	-3.0796092
C	1.4020341	-4.2317827	-3.8853856
C	1.6714347	-4.1267421	-5.2553623
C	2.0710099	-2.9072692	-5.8162044
C	2.1950077	-1.7921224	-4.9961893
H	3.1255282	-0.5325734	-2.4013242
H	1.3669124	0.0185464	-0.7309358
H	1.8613383	1.5483422	-2.8978954
C	1.5398234	-5.2864034	-6.0964359
N	1.4349080	-6.2202357	-6.7737422
H	0.2679088	0.1824043	-4.8376958
H	-0.4463412	1.4573542	-3.8121621
H	1.3295098	-3.1837316	-2.0150516
H	1.0968834	-5.1834824	-3.4627371
H	2.2781085	-2.8397201	-6.8791804
H	2.5050009	-0.8419938	-5.4226461

4a_sy_tr_prod_1.log

E = -667.656197

H = -667.457558

G = -667.508900

NImag=0

C	1.7705066	2.8087346	0.4829261
C	0.3015561	2.7250809	0.2610230
C	-0.3251916	3.5174981	1.3668905
C	0.8283008	4.0944399	2.1619855
O	2.0213240	3.4733109	1.6330791
O	2.6603600	2.3701585	-0.2049333
C	-0.4308141	2.0239222	1.4010585
C	-1.7258085	1.3552984	1.1108373
C	-2.6461879	1.8826642	0.1928118
C	-3.8533693	1.2410255	-0.0475734
C	-4.1526787	0.0543781	0.6347317
C	-3.2446357	-0.4858145	1.5527992
C	-2.0402143	0.1670632	1.7827724
H	0.1904010	1.5042211	2.1278217
H	-0.0757424	2.6484612	-0.7512651
H	-1.2146199	4.1165677	1.2083884
C	-5.4015591	-0.6134595	0.3887765
N	-6.4082757	-1.1516906	0.1907343
H	0.7807813	3.8656571	3.2285603
H	0.9156234	5.1735046	2.0154498
H	-2.4258139	2.8011545	-0.3441205
H	-4.5632980	1.6516468	-0.7580841
H	-3.4831945	-1.4056897	2.0766626
H	-1.3321497	-0.2484332	2.4936676

4a_tr_sy_1.log

E = -1145.539079

H = -1145.257262

G = -1145.321585

NImag=0

C	0.6121055	1.7886866	-2.9154647
C	-0.5592932	1.1589993	-2.2256190
C	1.7533494	1.0459407	-2.6568816
O	2.9721199	1.2386814	-2.8219922
C	-0.9424388	1.8429345	-0.8745719
C	-2.2809083	1.3958187	-0.3322308
C	-2.4725797	0.1716273	0.3215735
C	-3.7399822	-0.2138827	0.7416521
C	-4.8307222	0.6289176	0.4998212
C	-4.6557209	1.8541517	-0.1530287
C	-3.3815129	2.2303849	-0.5591774
O	1.3842190	-0.1620435	-2.0052939
C	-0.0341598	-0.2794459	-2.0929744
S	0.3464903	1.5811571	0.4325609
C	1.6929049	2.7131399	0.0125287
C	-0.3843688	2.5093700	1.7998364
C	-6.1449086	0.2351672	0.9330436
N	-7.2030351	-0.0809769	1.2817343
H	0.6468408	2.8197481	-3.2448421
H	-1.4978929	1.1623472	-2.7936984
H	-0.9564582	2.9281462	-1.0244757
H	-1.6375584	-0.4914576	0.5296755
H	-3.8845581	-1.1587192	1.2547749
H	-5.5063153	2.5035823	-0.3315121
H	-3.2385323	3.1832561	-1.0603894
H	-0.2971283	-0.8427956	-2.9969657
H	-0.3907593	-0.8330575	-1.2205131
H	2.2313332	2.8836381	0.9480758
H	2.3487247	2.2372850	-0.7166376
H	1.2749488	3.6460273	-0.3702281

H	0.3870526	2.5974121	2.5669451
H	-1.2303266	1.9436034	2.1904860
H	-0.6960293	3.4944562	1.4455888

4a_tr_sy_1_r.log

E = -1145.538032
H = -1145.256564
G = -1145.322058

NImag=0

C	-1.5790918	-1.7790448	-0.5666383
C	-1.2160880	-1.1929691	0.7680007
C	-0.7049955	-2.8074006	-0.8976537
O	-0.5332970	-3.5010270	-1.9157704
C	-0.4153140	0.1292640	0.6044020
C	-0.9903808	1.0830397	-0.4159805
C	-2.3371994	1.4622536	-0.3534938
C	-2.8630249	2.3427161	-1.2892894
C	-2.0312002	2.8478122	-2.2974601
C	-0.6841361	2.4781397	-2.3698358
C	-0.1706207	1.5985230	-1.4227009
O	0.1446715	-3.0674074	0.2031521
C	-0.3581108	-2.3504470	1.3252891
S	-0.4066646	1.1058422	2.1948308
C	0.5830835	0.1349272	3.3470935
C	0.7511197	2.4361881	1.8157025
C	-2.5698766	3.7600280	-3.2715154
N	-3.0025805	4.4951558	-4.0547574
H	-2.2561030	-1.3267769	-1.2785727
H	-2.0690576	-1.0024511	1.4343057
H	0.6379074	-0.0779744	0.3798164
H	-2.9845867	1.0620389	0.4227195
H	-3.9062617	2.6371210	-1.2471001
H	-0.0518171	2.8755523	-3.1567729
H	0.8742333	1.3053033	-1.4686793
H	-0.9948970	-3.0147259	1.9238093
H	0.4965335	-2.0385462	1.9284601
H	0.7919570	0.7913308	4.1948335
H	-0.0138246	-0.7126892	3.6855752
H	1.5102711	-0.1846032	2.8676706
H	0.9641536	2.9493306	2.7555245
H	0.2626763	3.1216703	1.1222529
H	1.6623074	2.0165999	1.3845180

4a_tr_sy_1_ts1.log

E = -1145.513164
H = -1145.234332
G = -1145.299771

NImag=1

C	-2.5115320	-1.4873563	1.1093282
C	-1.1958264	-1.3787506	0.6850606
C	-3.3607581	-1.5550664	-0.0415253
O	-4.5793783	-1.5544224	-0.1583607
C	-0.3952798	0.6310522	0.6941866
C	1.0038634	0.4010155	0.4081119
C	1.5807607	0.4772989	-0.8830947
C	2.9037208	0.1297615	-1.1014572
C	3.7017156	-0.3143700	-0.0359662
C	3.1512415	-0.4057293	1.2536274
C	1.8309998	-0.0538680	1.4659714
O	-2.5737277	-1.6007362	-1.1777701

C	-1.2047375	-1.7364792	-0.7804528
S	-1.2348562	1.6824426	-0.4351353
C	-2.9365646	1.7008451	0.1627893
C	-0.7482316	3.3713166	0.0180500
C	5.0700304	-0.6688104	-0.2611803
N	6.1793227	-0.9570856	-0.4432045
H	-2.8934153	-1.4045965	2.1171327
H	-0.3332987	-1.6363696	1.2920930
H	-0.6385657	0.8905937	1.7245255
H	0.9945114	0.8197381	-1.7315376
H	3.3264635	0.2021705	-2.0987276
H	3.7659738	-0.7473308	2.0807401
H	1.4158566	-0.1190221	2.4681432
H	-0.8990563	-2.7818136	-0.9139899
H	-0.5847032	-1.1064399	-1.4225692
H	-3.3768969	2.6332606	-0.1955618
H	-3.4775714	0.8588342	-0.2655881
H	-2.9412783	1.6665959	1.2539591
H	-1.3039825	4.0682170	-0.6134302
H	0.3222766	3.4603312	-0.1758572
H	-0.9683041	3.5309791	1.0756229

4a_tr_sy_1_ts1_rot1.log

E = -1145.517008

H = -1145.238116

G = -1145.303188

NImag=1

C	-1.1916285	-2.0842346	-0.5220560
C	-1.5381640	-1.5292813	0.6997105
C	0.1563100	-2.5764960	-0.4453690
O	0.8753453	-3.1087756	-1.2804811
C	-1.3115860	0.6443489	0.6807067
C	0.0827553	0.8157553	0.3616632
C	0.6077348	0.5851097	-0.9343904
C	1.9739379	0.6086094	-1.1668451
C	2.8637510	0.8633631	-0.1137834
C	2.3652374	1.1130373	1.1790754
C	1.0032708	1.0918674	1.4051941
O	0.6159531	-2.4222107	0.8467699
C	-0.4467080	-1.9249988	1.6633305
S	-2.4310782	1.1202809	-0.5839362
C	-4.0350517	0.5625455	0.0201258
C	-2.6417709	2.9100961	-0.4019353
C	4.2743138	0.8905185	-0.3560456
N	5.4184429	0.9127259	-0.5501039
H	-1.7749266	-2.1124514	-1.4326175
H	-2.5476643	-1.4257059	1.0792665
H	-1.6435047	0.9865812	1.6618658
H	-0.0573707	0.3852991	-1.7684579
H	2.3593003	0.4228762	-2.1648189
H	3.0531846	1.3276696	1.9910581
H	0.6230334	1.2916971	2.4033912
H	-0.8001117	-2.7328946	2.3162744
H	-0.0632322	-1.1119761	2.2842029
H	-4.7941768	1.1177169	-0.5338736
H	-4.1365638	-0.5019119	-0.1907028
H	-4.1125087	0.7668132	1.0901355
H	-3.3865607	3.2435642	-1.1278686
H	-1.6755965	3.3698263	-0.6178106
H	-2.9580934	3.1306330	0.6194847

4a_tr_sy_1_ts2.log

E = -1145.528959

H = -1145.249057

G = -1145.314181

NImag=1

C	-1.5294303	-1.9228657	-0.5767013
C	-1.6955794	-0.5240136	-1.0999221
C	-2.6224496	-2.2319659	0.2552964
O	-2.8734909	-3.1930612	0.9867246
C	-0.8486799	0.1078482	-0.0467783
C	0.6193768	-0.1460393	-0.0472083
C	1.3452295	-0.1631108	-1.2462197
C	2.7211423	-0.3505326	-1.2317271
C	3.3780527	-0.5238002	-0.0067592
C	2.6658123	-0.5087907	1.1988503
C	1.2911635	-0.3154248	1.1701259
O	-3.5585517	-1.1914890	0.1887440
C	-3.1970274	-0.3294030	-0.8940726
S	-0.8283475	2.3193211	-0.3431393
C	-2.3211371	2.8327139	0.5411380
C	0.4107464	2.8165716	0.8748842
C	4.8030647	-0.7198283	0.0124430
N	5.9505099	-0.8765979	0.0277312
H	-0.6514365	-2.5423715	-0.6813215
H	-1.3796177	-0.3087247	-2.1227891
H	-1.3029792	0.1354021	0.9458394
H	0.8395518	-0.0232530	-2.1970441
H	3.2870276	-0.3618539	-2.1572444
H	3.1866891	-0.6476102	2.1403489
H	0.7272309	-0.3018496	2.0985339
H	-3.7291508	-0.6465553	-1.7989107
H	-3.4992309	0.6876480	-0.6383730
H	-2.1622153	3.8456699	0.9171046
H	-3.1550697	2.8402939	-0.1610629
H	-2.5244245	2.1514151	1.3715389
H	0.3544825	3.9007604	0.9932363
H	1.3952230	2.5419537	0.4927462
H	0.2193154	2.3207693	1.8298666

4a_tr_sy_2.log

E = -1145.532897

H = -1145.251189

G = -1145.315260

NImag=0

C	0.7203464	1.8024650	-2.7008410
C	-0.5317102	1.2753998	-2.0864072
C	1.7415590	0.8706405	-2.6336383
O	2.9534729	0.8878025	-2.9177228
C	-1.0349449	2.0218563	-0.8075131
C	-2.3701645	1.5150656	-0.3078670
C	-2.4970589	0.4262918	0.5618958
C	-3.7520878	-0.0356490	0.9411821
C	-4.8957381	0.5924587	0.4372424
C	-4.7868495	1.6786015	-0.4393010
C	-3.5256322	2.1335756	-0.8013606
O	1.2362073	-0.3428303	-2.0921643
C	-0.1772474	-0.2236046	-1.9434257
S	0.1062116	2.2291418	0.6320704
C	1.1595481	0.7730605	0.8067238
C	1.3152929	3.4514033	0.0799578

C	-6.1968326	0.1180759	0.8271101
N	-7.2440694	-0.2638582	1.1412044
H	0.8681137	2.8279464	-3.0141652
H	-1.4218412	1.3636657	-2.7272950
H	-1.1574695	3.0720934	-1.0981439
H	-1.6219240	-0.0802972	0.9568289
H	-3.8459984	-0.8766488	1.6198799
H	-5.6797468	2.1617212	-0.8218373
H	-3.4339793	2.9816901	-1.4740170
H	-0.6644075	-0.7915433	-2.7437680
H	-0.4650292	-0.6685051	-0.9852006
H	1.9010676	1.0531626	1.5590488
H	0.5590507	-0.0541354	1.1860759
H	1.6383422	0.5192914	-0.1388937
H	1.9055195	3.7130474	0.9609156
H	0.7646444	4.3252663	-0.2720949
H	1.9317553	3.0272488	-0.7116795

4a_tr_sy_2_r.log

E = -1145.534954
H = -1145.253141
G = -1145.317944

NImag=0

C	1.6853756	-1.6148609	0.3021810
C	1.4297394	-0.9202090	-1.0071353
C	0.8551540	-2.7260874	0.4126177
O	0.5954549	-3.5237551	1.3293552
C	0.4493355	0.2562841	-0.7705145
C	0.9553172	1.2492331	0.2519688
C	2.2196264	1.8342658	0.1085406
C	2.6893895	2.7361751	1.0539258
C	1.8860248	3.0535778	2.1567571
C	0.6209993	2.4770254	2.3119173
C	0.1625702	1.5788692	1.3539055
O	0.1966542	-2.9363779	-0.8253423
C	0.8141015	-2.0914752	-1.7896956
S	0.0102764	1.2936903	-2.2861017
C	1.1921655	0.8377261	-3.5704784
C	-1.5219748	0.5683381	-2.9019138
C	2.3706984	3.9835512	3.1420738
N	2.7617287	4.7323427	3.9343098
H	2.1963390	-1.1723133	1.1468787
H	2.3240522	-0.5459737	-1.5168126
H	-0.5282826	-0.1335750	-0.4645622
H	2.8516322	1.5843024	-0.7400125
H	3.6690199	3.1899839	0.9464525
H	0.0094160	2.7291416	3.1718597
H	-0.8167072	1.1229746	1.4676923
H	1.6196091	-2.6416073	-2.2946792
H	0.0612032	-1.8175014	-2.5317359
H	0.9000005	1.4001112	-4.4598725
H	2.1821554	1.1597536	-3.2434643
H	1.1664472	-0.2339300	-3.7691921
H	-1.7887486	1.1219218	-3.8045254
H	-2.2821008	0.7238329	-2.1345014
H	-1.3974711	-0.4914806	-3.1218399

4a_tr_sy_2_ts1.log

E = -1145.509975
H = -1145.230949

G = -1145.295422
NImag=1

C	-2.5697632	-1.1332480	1.1961349
C	-1.1961029	-1.1055904	1.0072672
C	-3.1964825	-1.6229281	0.0050270
O	-4.3753418	-1.7353686	-0.3067680
C	-0.3482444	0.8644432	0.7390021
C	1.0394772	0.6050857	0.4438448
C	1.5782230	0.6338162	-0.8657119
C	2.8895300	0.2638320	-1.1122106
C	3.7078514	-0.1711514	-0.0573943
C	3.1910952	-0.2256792	1.2488070
C	1.8846846	0.1574646	1.4904687
O	-2.2213638	-2.0023320	-0.8945443
C	-0.9386316	-1.8562013	-0.2774066
S	-1.1632094	2.0021515	-0.3474822
C	-2.1574866	1.0676535	-1.5478739
C	-2.4730451	2.6262599	0.7213117
C	5.0611444	-0.5606580	-0.3113762
N	6.1589372	-0.8768977	-0.5162138
H	-3.1290970	-0.7886318	2.0546548
H	-0.4651563	-1.1780264	1.8063912
H	-0.5805455	1.1500397	1.7623538
H	0.9654030	0.9475495	-1.7081096
H	3.2857444	0.3016390	-2.1222013
H	3.8231719	-0.5599193	2.0658513
H	1.4984721	0.1296943	2.5058348
H	-0.5388012	-2.8531409	-0.0556997
H	-0.2608907	-1.3578417	-0.9768676
H	-2.5243944	1.8032065	-2.2670205
H	-1.5007209	0.3564774	-2.0503795
H	-2.9900770	0.5687762	-1.0549960
H	-3.1536527	3.2116705	0.1009355
H	-2.0096873	3.2611271	1.4774474
H	-2.9889192	1.7798239	1.1784369

4a_tr_sy_2_ts2.log
E = -1145.526993
H = -1145.247315
G = -1145.313160
NImag=1

C	1.2743694	1.8782619	-0.7506740
C	1.5756291	0.4268432	-1.0005484
C	2.3080703	2.4338111	0.0275612
O	2.4525129	3.5350138	0.5634290
C	0.7453469	-0.0700651	0.1377170
C	-0.7376406	0.0828923	0.0853080
C	-1.4289570	0.0429524	-1.1329739
C	-2.8133484	0.1478864	-1.1578547
C	-3.5153648	0.2883067	0.0461723
C	-2.8373874	0.3184501	1.2715128
C	-1.4533614	0.2116860	1.2820780
O	3.3285665	1.4869904	0.1784779
C	3.0800542	0.4081411	-0.7270788
S	0.8109793	-2.2948614	0.3200923
C	1.5634640	-2.7970859	-1.2426457
C	2.1654661	-2.5880817	1.4779076
C	-4.9488770	0.4018873	0.0225801
N	-6.1034422	0.4933137	0.0034823
H	0.3548922	2.3898462	-0.9910798
H	1.3171646	0.0063396	-1.9737370

H	1.1820003	0.1139625	1.1205620
H	-0.8898386	-0.0647444	-2.0693994
H	-3.3515604	0.1219356	-2.0994918
H	-3.3917657	0.4273177	2.1977098
H	-0.9168347	0.2363034	2.2266286
H	3.6193650	0.5917253	-1.6643083
H	3.4556237	-0.5091875	-0.2709787
H	1.7365950	-3.8749661	-1.2092664
H	0.8525082	-2.5687519	-2.0391057
H	2.5049537	-2.2713362	-1.4115001
H	2.3578237	-3.6621807	1.5228522
H	1.8376650	-2.2358698	2.4578514
H	3.0677732	-2.0574700	1.1710332

4a_tr_sy_3.log

E = -1145.538633

H = -1145.256944

G = -1145.322024

NImag=0

C	0.5995269	1.7385398	-3.1206236
C	-0.4662164	0.9906189	-2.3740228
C	1.8530248	1.2982071	-2.7146055
O	3.0189894	1.6807210	-2.9049128
C	-1.0328323	1.8089821	-1.1768375
C	-2.3059192	1.3368329	-0.5199622
C	-2.5929652	-0.0200125	-0.3196717
C	-3.7963067	-0.4128718	0.2548546
C	-4.7287260	0.5592183	0.6322791
C	-4.4664174	1.9185656	0.4291113
C	-3.2604646	2.2943979	-0.1484072
O	1.6841094	0.1521723	-1.8805413
C	0.3326681	-0.2758255	-2.0200550
S	0.3411908	2.1585516	0.0332080
C	-0.4265676	3.3560025	1.1421409
C	0.4414608	0.7406927	1.1424615
C	-5.9755892	0.1551806	1.2267408
N	-6.9784949	-0.1698333	1.7057706
H	0.4421111	2.6820980	-3.6281846
H	-1.3526081	0.7192921	-2.9605228
H	-1.1992634	2.8256974	-1.5524564
H	-1.8876294	-0.7877820	-0.6148610
H	-4.0152076	-1.4644749	0.4068039
H	-5.2006668	2.6647062	0.7136578
H	-3.0589588	3.3476837	-0.3228270
H	0.2572150	-0.9843186	-2.8549549
H	0.0412977	-0.7891938	-1.1019485
H	0.3364923	3.6390460	1.8698768
H	-0.7110686	4.2268892	0.5489348
H	-1.2902963	2.9166806	1.6441065
H	0.9789522	1.0925251	2.0263785
H	1.0225563	-0.0365428	0.6479676
H	-0.5570964	0.3965537	1.4194021

4a_tr_sy_3_r.log

E = -1145.540568

H = -1145.258911

G = -1145.323644

NImag=0

C	1.6576507	-1.7083165	0.6002003
C	1.4732194	-1.1240695	-0.7723752

C	0.8253873	-2.8120460	0.7551955
O	0.5165993	-3.5320534	1.7204310
C	0.4777944	0.0598261	-0.7259352
C	0.8242844	1.1698987	0.2293362
C	2.1533372	1.5726758	0.4156696
C	2.4616111	2.5975131	1.3005079
C	1.4293894	3.2256197	2.0091811
C	0.0982230	2.8309468	1.8392097
C	-0.1945912	1.8044337	0.9483435
O	0.2319718	-3.1269927	-0.4927224
C	0.8785011	-2.3474257	-1.4930270
S	0.2422971	0.7171394	-2.4659968
C	-1.0394641	1.9703660	-2.2919036
C	1.6901056	1.7415026	-2.7809424
C	1.7432919	4.2858965	2.9303610
N	1.9954144	5.1398909	3.6707653
H	2.1215563	-1.1973621	1.4331829
H	2.3965473	-0.8039156	-1.2717106
H	-0.5257203	-0.3246269	-0.5033676
H	2.9558456	1.0797469	-0.1251299
H	3.4902295	2.9091845	1.4482624
H	-0.6913870	3.3188763	2.4007342
H	-1.2247972	1.4847161	0.8161745
H	1.6902175	-2.9337856	-1.9423020
H	0.1451265	-2.1087143	-2.2701898
H	-1.1998219	2.3969208	-3.2841861
H	-1.9480594	1.4713189	-1.9503857
H	-0.7187558	2.7408784	-1.5886580
H	1.5836772	2.1200598	-3.7996161
H	2.5760431	1.1074895	-2.7155282
H	1.7335382	2.5644366	-2.0661050

4a_tr_sy_3_ts1.log

E = -1145.510896

H = -1145.231613

G = -1145.296047

NImag=1

C	2.8660570	-1.0367140	-1.0739290
C	1.4832220	-1.1837770	-1.1111340
C	3.3464650	-1.4202880	0.2188490
O	4.4638500	-1.3927080	0.7176600
C	0.4161260	0.6893050	-1.0389780
C	-0.9351110	0.4354150	-0.5999340
C	-1.4050560	0.5859250	0.7262170
C	-2.6894060	0.2060810	1.0819440
C	-3.5513450	-0.3508540	0.1256090
C	-3.1059740	-0.5199920	-1.1968070
C	-1.8269850	-0.1298380	-1.5471290
O	2.2866380	-1.9093110	0.9651120
C	1.1142960	-1.9377200	0.1439940
S	1.5029580	1.8268890	-0.2714320
C	0.6054640	3.3723980	0.0231530
C	1.8184260	1.2932480	1.4369140
C	-4.8773190	-0.7439480	0.4946480
N	-5.9524040	-1.0632130	0.7929070
H	3.5111080	-0.6414050	-1.8460080
H	0.9073990	-1.3715040	-2.0108210
H	0.5329360	0.8444580	-2.1094640
H	-0.7668210	1.0037590	1.4969740
H	-3.0302660	0.3369380	2.1043130
H	-3.7710220	-0.9487510	-1.9401640

H	-1.4944210	-0.2540120	-2.5741920
H	0.8799690	-2.9802890	-0.1016680
H	0.2766870	-1.5144100	0.7068510
H	1.2735410	4.0374960	0.5749870
H	0.3723680	3.7992380	-0.9533310
H	-0.3057110	3.1796530	0.5912170
H	2.8535970	1.5529540	1.6644590
H	1.6795680	0.2148530	1.5097690
H	1.1435040	1.8139890	2.1169590

4a_tr_sy_3_ts2.log

E = -1145.530449
H = -1145.250692
G = -1145.315892

NImag=1

C	-1.8813559	-1.6621210	-0.5929147
C	-1.8915390	-0.1968930	-0.9225085
C	-2.9828589	-1.9541881	0.2346033
O	-3.3302016	-2.9745489	0.8340729
C	-0.9361664	0.1884150	0.1526447
C	0.4928993	-0.1966584	0.0814411
C	1.1252123	-0.4422621	-1.1475769
C	2.4734692	-0.7675969	-1.1916976
C	3.2030323	-0.8436560	0.0025312
C	2.5877405	-0.6008163	1.2363905
C	1.2370304	-0.2798358	1.2671058
O	-3.7850170	-0.8137150	0.3549916
C	-3.3415170	0.1623309	-0.5927378
S	-0.8230945	2.4458352	0.0920898
C	0.2212463	2.8764883	1.4988045
C	0.3219663	2.7646065	-1.2645939
C	4.6010096	-1.1798124	-0.0395662
N	5.7269947	-1.4492575	-0.0728389
H	-1.0924216	-2.3621647	-0.8228337
H	-1.5975584	0.1143687	-1.9276665
H	-1.3610044	0.1691276	1.1572671
H	0.5637472	-0.3845879	-2.0750862
H	2.9635943	-0.9612851	-2.1400299
H	3.1619271	-0.6686529	2.1543097
H	0.7467464	-0.0982792	2.2198325
H	-3.9551653	0.0886169	-1.4979156
H	-3.4662881	1.1542398	-0.1500554
H	0.3819284	3.9568574	1.4965890
H	-0.3058790	2.5871801	2.4100869
H	1.1791702	2.3556764	1.4307538
H	0.4851441	3.8423527	-1.3356406
H	-0.1376971	2.4043337	-2.1871439
H	1.2698657	2.2515831	-1.0861778

4b.log

E = -344.460189
H = -344.349096
G = -344.386215

NImag=0

C	0.6462874	1.0590747	0.0498570
C	0.9552818	0.9434237	1.5468184
O	-0.2057034	0.3114462	2.1439290
C	-1.2802669	0.4209803	1.3417531
C	-0.8547468	1.0114078	0.0364428
O	-2.3830819	0.0678007	1.6891144

C	-1.7338537	1.4003911	-0.8837965
H	1.0544233	1.9712586	-0.3879344
H	1.0543521	0.1985018	-0.4906680
H	1.8170212	0.3168741	1.7732515
H	1.0753121	1.9221934	2.0180365
H	-2.7997811	1.2810353	-0.7079463
H	-1.4156441	1.8433133	-1.8230572

4b_sy_1.log

E = -1184.836314
H = -1184.524486
G = -1184.591825

NImag=0

C	4.7599101	2.9463255	2.1040887
C	5.9981409	2.1030569	2.4623073
C	6.7220976	2.5569691	3.7034798
C	6.0472792	2.6905401	4.9240349
C	6.7232540	3.1211937	6.0582641
C	8.0862421	3.4307418	5.9677528
C	8.7719714	3.3065647	4.7547086
C	8.0840684	2.8644240	3.6300455
C	4.0144916	2.4562453	0.9028023
C	2.6757067	1.7632595	0.9097541
C	2.4658249	1.5848319	-0.6005343
O	3.7718425	1.5549634	-1.1879793
C	4.6457294	2.2249866	-0.3059548
O	5.8116050	2.4472304	-0.7064263
S	5.4626019	0.3313068	2.6880037
C	5.5002619	-0.3753373	1.0211100
C	6.9638162	-0.4229366	3.3523859
C	8.7902265	3.8817190	7.1390074
N	9.3571985	4.2443116	8.0814137
H	4.0943219	2.9965379	2.9738252
H	5.1633866	3.9616229	1.9697122
H	6.6792666	2.0683777	1.6051873
H	4.9894682	2.4525439	4.9993254
H	6.2051796	3.2207546	7.0062449
H	9.8278192	3.5493953	4.6981711
H	8.6082875	2.7572435	2.6848146
H	2.6796426	0.7822808	1.4252224
H	1.8524847	2.3394640	1.3495864
H	1.9188895	2.4452815	-1.0104981
H	1.9426091	0.6656422	-0.8759842
H	5.7432416	-1.4333132	1.1417244
H	4.5133085	-0.2620563	0.5743579
H	6.2572242	0.1418788	0.4268984
H	6.7958182	-1.5013222	3.3615530
H	7.1107245	-0.0633450	4.3711099
H	7.8134586	-0.1672828	2.7151853

4b_sy_1_r.log

E = -1184.835794
H = -1184.524147
G = -1184.593051

NImag=0

C	-0.7063998	-1.5423874	0.0524829
C	0.0062094	-0.2482876	0.5047654
C	-0.4006576	1.0019887	-0.2356875
C	-1.7429879	1.2518906	-0.5427382
C	-2.1019729	2.4136151	-1.2141592

C	-1.1083374	3.3300405	-1.5832704
C	0.2378733	3.0883922	-1.2897140
C	0.5820611	1.9218400	-0.6157226
C	-0.6240789	-1.7104112	-1.4292781
C	0.6508613	-1.6286460	-2.2278205
C	0.0923211	-1.8626833	-3.6367881
O	-1.2674073	-1.4212789	-3.6077495
C	-1.7045530	-1.4607547	-2.2649414
O	-2.9217973	-1.2698801	-2.0563728
S	-0.3447240	0.0359915	2.3047484
C	0.4774194	-1.3691712	3.0825720
C	0.8021030	1.3601194	2.7311599
C	-1.4769815	4.5350660	-2.2782037
N	-1.7727902	5.5060151	-2.8360062
H	-0.2436258	-2.3720891	0.6038317
H	-1.7640735	-1.5063808	0.3441209
H	1.0945693	-0.3696312	0.4555706
H	-2.5079413	0.5225754	-0.2946262
H	-3.1400778	2.6103430	-1.4610144
H	0.9983126	3.8030392	-1.5863722
H	1.6249587	1.7215697	-0.3846924
H	1.1469879	-0.6409732	-2.1582466
H	1.4102945	-2.3816068	-1.9799330
H	0.1058799	-2.9356759	-3.8754870
H	0.6169704	-1.3166532	-4.4250285
H	0.5537237	-1.1400488	4.1475260
H	-0.1454079	-2.2520273	2.9389675
H	1.4668086	-1.5019982	2.6396756
H	0.7895468	1.4546611	3.8188310
H	0.4372886	2.2822069	2.2767042
H	1.8017713	1.1068129	2.3724188

4b_sy_1_ts1.log

E = -1184.805843

H = -1184.496735

G = -1184.565470

NImag=1

C	-0.9185124	-1.1485601	-0.1264955
C	0.0777014	0.6168249	0.6565115
C	1.4488715	0.2753506	0.3871018
C	2.1096918	0.5580080	-0.8345377
C	3.3946756	0.1044495	-1.0782346
C	4.0692650	-0.6588283	-0.1118264
C	3.4290047	-0.9648740	1.1024519
C	2.1472592	-0.5068119	1.3421875
C	-2.2745460	-1.1074173	-0.3759574
C	-2.9978498	-0.6654873	-1.6229238
C	-4.4099716	-1.1895441	-1.3340210
O	-4.5154452	-1.2791549	0.1023904
C	-3.2586341	-1.3569359	0.6473107
O	-3.1255069	-1.5917408	1.8414339
S	-0.6246945	1.9389241	-0.2611528
C	-2.1915566	2.1569480	0.6010930
C	0.2152919	3.4610956	0.2590882
C	5.3992892	-1.1218792	-0.3614003
N	6.4785677	-1.4985713	-0.5636416
H	-0.2324115	-1.1569687	-0.9718933
H	-0.5747406	-1.6802090	0.7585289
H	-0.2272031	0.6516748	1.7016261
H	1.6162697	1.1434522	-1.6064586
H	3.8850982	0.3392409	-2.0180336

H	3.9468319	-1.5567814	1.8509872
H	1.6616264	-0.7432239	2.2850861
H	-3.0137902	0.4287404	-1.7402362
H	-2.5922364	-1.0908115	-2.5454545
H	-4.5528363	-2.1948108	-1.7451616
H	-5.2097048	-0.5367138	-1.6856828
H	-2.7129741	2.9916233	0.1305704
H	-2.7685908	1.2394489	0.4913674
H	-1.9887415	2.3634510	1.6538965
H	-0.3157581	4.3069737	-0.1839740
H	1.2364910	3.4200635	-0.1242302
H	0.2105215	3.5154311	1.3492784

4b_sy_2.log

E = -1184.837004
H = -1184.525286
G = -1184.591934

NImag=0

C	4.7520192	2.3862870	2.3329095
C	6.2872059	2.2457204	2.4327012
C	6.8820811	2.7328921	3.7365254
C	6.2813149	2.4272563	4.9635724
C	6.8373256	2.8847852	6.1528206
C	8.0020169	3.6596751	6.1125446
C	8.6121132	3.9753497	4.8929271
C	8.0475687	3.5067795	3.7132434
C	4.1766245	2.1293469	0.9844263
C	4.5971044	2.8450562	-0.2721951
C	3.5901150	2.2544213	-1.2676616
O	3.1974278	0.9848386	-0.7355409
C	3.4304459	1.0128270	0.6557463
O	2.9770931	0.0527385	1.3259485
S	6.9348834	0.5231873	2.1854033
C	5.6705554	-0.5612928	2.8711174
C	6.7977862	0.2053971	0.4149102
C	8.5778956	4.1406875	7.3405793
N	9.0416399	4.5277031	8.3286349
H	4.2703180	1.7359720	3.0720854
H	4.5769730	3.4202559	2.6719388
H	6.7650180	2.7802725	1.6030196
H	5.3732358	1.8330973	5.0007920
H	6.3736438	2.6492022	7.1048820
H	9.5130662	4.5794348	4.8738525
H	8.5139008	3.7471188	2.7618937
H	4.5106428	3.9384680	-0.2303850
H	5.6361264	2.6213021	-0.5776877
H	3.9904140	2.0981665	-2.2724966
H	2.6992021	2.8941601	-1.3334184
H	6.0407644	-1.5787218	2.7247530
H	5.6060282	-0.3520598	3.9413630
H	4.7098592	-0.4056511	2.3643586
H	7.2176934	-0.7891214	0.2500315
H	7.4094936	0.9513481	-0.0958381
H	5.7560036	0.2575998	0.0999429

4b_sy_2_r.log

E = -1184.833907
H = -1184.521730
G = -1184.589561

NImag=0

C	-0.8065803	-0.7085609	-0.9089324
C	-0.0481345	-0.1825090	0.3187575
C	1.0077045	-1.1249511	0.8456723
C	1.9902702	-1.6578606	0.0026071
C	2.9356877	-2.5481393	0.4964839
C	2.8896992	-2.9183931	1.8462668
C	1.9085382	-2.4001879	2.6988911
C	0.9768784	-1.5013661	2.1918931
C	-1.5877409	-1.9212785	-0.4900435
C	-1.1167235	-3.3531726	-0.5631956
C	-2.3414672	-4.0534658	0.0378743
O	-2.9403488	-3.1082411	0.9311479
C	-2.5535676	-1.8238047	0.5037760
O	-3.0842726	-0.8402172	1.0655505
S	0.7374550	1.5042765	0.1081455
C	1.2914881	1.5546820	-1.6070227
C	-0.7083483	2.5791039	0.0327818
C	3.8617178	-3.8461593	2.3616067
N	4.6449795	-4.5917615	2.7760766
H	-1.4673131	0.0847770	-1.2797164
H	-0.1057071	-0.9479944	-1.7161295
H	-0.7809104	0.0278383	1.1073238
H	2.0132145	-1.3974918	-1.0517226
H	3.6981210	-2.9624067	-0.1548753
H	1.8788735	-2.7000251	3.7412058
H	0.2089389	-1.0959774	2.8450111
H	-0.9111195	-3.7287425	-1.5733345
H	-0.2156608	-3.5557117	0.0453500
H	-2.1101462	-4.9612432	0.6005282
H	-3.0671399	-4.2946467	-0.7518899
H	1.6510575	2.5702706	-1.7853078
H	2.1174833	0.8513209	-1.7214306
H	0.4649535	1.3150368	-2.2767489
H	-0.3471236	3.5896546	-0.1674211
H	-1.1937605	2.5443655	1.0096018
H	-1.3843973	2.2463714	-0.7556515

4b_sy_2_ts1.log

E = -1184.804409
H = -1184.495594
G = -1184.564051

NImag=1

C	-0.9095304	-0.9997811	-0.6042986
C	0.1313643	0.3972825	0.7699757
C	1.5238240	0.1743565	0.5038493
C	2.3167338	1.0242701	-0.3099026
C	3.6316079	0.7150145	-0.6079704
C	4.2069565	-0.4714314	-0.1223520
C	3.4362782	-1.3407458	0.6712224
C	2.1266012	-1.0225642	0.9750426
C	-2.2449284	-1.1794444	-0.3342201
C	-2.8460308	-1.8824168	0.8522784
C	-4.3230154	-1.9516754	0.4482549
O	-4.5184220	-0.9101084	-0.5324175
C	-3.3146487	-0.5431211	-1.0657250
O	-3.2824019	0.2155620	-2.0282338
S	-0.4355410	2.0650964	0.6762812
C	-1.0902600	2.3264779	-0.9937458
C	-1.9704028	1.9550741	1.6134428
C	5.5638597	-0.7934623	-0.4354295
N	6.6664395	-1.0550258	-0.6890576

H	-0.6177900	-0.4979591	-1.5255731
H	-0.1896321	-1.7147205	-0.2135100
H	-0.2962136	-0.0818535	1.6474008
H	1.9033319	1.9452344	-0.7133127
H	4.2215787	1.3875829	-1.2231487
H	3.8773542	-2.2578686	1.0497861
H	1.5445909	-1.6943048	1.6004860
H	-2.4315409	-2.8771346	1.0392550
H	-2.7185519	-1.2881197	1.7701039
H	-5.0194909	-1.7705202	1.2674921
H	-4.5637561	-2.9072185	-0.0289271
H	-1.4626837	3.3533189	-1.0222556
H	-0.2573021	2.2207648	-1.6919525
H	-1.8804599	1.6082906	-1.2211411
H	-2.5074132	2.8954565	1.4791699
H	-1.7077070	1.8171305	2.6632823
H	-2.5568900	1.1125797	1.2420123

4b_sy_3.log

E = -1184.841202
H = -1184.529434
G = -1184.596529

NImag=0

C	4.6279314	2.7519151	2.1884988
C	6.1511342	2.5491066	2.3162305
C	6.7569045	2.8234391	3.6665864
C	6.1223337	2.4276810	4.8512279
C	6.7032663	2.6930693	6.0860306
C	7.9289019	3.3660665	6.1386320
C	8.5722132	3.7770407	4.9653100
C	7.9804217	3.5019820	3.7390633
C	4.0892162	2.3274782	0.8647098
C	4.5936575	2.8130978	-0.4684147
C	3.5977164	2.1116828	-1.4017666
O	3.1208751	0.9626849	-0.6935378
C	3.3089269	1.1967596	0.6820744
O	2.7887198	0.3787076	1.4772233
S	6.5177191	0.8394353	1.6770874
C	8.2116914	0.5593315	2.2318552
C	5.6124839	-0.2654814	2.7705674
C	8.5313089	3.6445725	7.4157400
N	9.0165229	3.8679830	8.4431858
H	4.1113608	2.1930497	2.9768835
H	4.4753842	3.8206610	2.4044506
H	6.6630138	3.1601334	1.5634036
H	5.1661928	1.9152585	4.8232683
H	6.2115402	2.3866579	7.0031848
H	9.5188354	4.3042802	5.0182479
H	8.4728826	3.8183364	2.8237038
H	4.5590811	3.9013071	-0.6069840
H	5.6319582	2.4984156	-0.6868095
H	4.0287230	1.7783562	-2.3489370
H	2.7432414	2.7701668	-1.6101483
H	8.4959155	-0.4328717	1.8756466
H	8.8485975	1.3133797	1.7647179
H	8.2735170	0.6100539	3.3204758
H	5.9001637	-1.2787072	2.4797398
H	4.5434853	-0.1120132	2.5812964
H	5.8909620	-0.0790163	3.8092561

4b_sy_3_r.log

E = -1184.835577
H = -1184.523991
G = -1184.593157

NImag=0

C	-1.3326106	-1.2021818	0.0636071
C	-0.3741892	-0.1370918	0.6203433
C	-0.4550824	1.2213747	-0.0222322
C	-1.6862234	1.8006456	-0.3557286
C	-1.7386950	3.0582439	-0.9439370
C	-0.5461230	3.7429662	-1.2077984
C	0.6927066	3.1746559	-0.8905139
C	0.7277043	1.9180488	-0.2977047
C	-1.0091558	-1.4486262	-1.3802115
C	-1.7371210	-0.8761548	-2.5701115
C	-0.9326110	-1.5299626	-3.7005341
O	0.3798970	-1.7567354	-3.1761780
C	0.2653136	-1.8297493	-1.7732978
O	1.2776411	-2.1823374	-1.1267435
S	-0.5724211	-0.0547507	2.4771559
C	0.5763246	1.2351677	2.9886779
C	-2.1520267	0.7697986	2.7357350
C	-0.5958349	5.0452654	-1.8182072
N	-0.6362102	6.0940443	-2.3077290
H	-1.2079405	-2.1069422	0.6755432
H	-2.3749498	-0.8844616	0.1802431
H	0.6458011	-0.5317539	0.5330375
H	-2.6134471	1.2674992	-0.1673912
H	-2.6918473	3.5072581	-1.2025999
H	1.6104003	3.7108114	-1.1081005
H	1.6850581	1.4664109	-0.0518109
H	-2.7984730	-1.1446653	-2.6438276
H	-1.6800009	0.2261273	-2.6359185
H	-0.8435354	-0.9181071	-4.6016208
H	-1.3735327	-2.5009384	-3.9677080
H	0.4871689	1.3297242	4.0727944
H	1.5840020	0.9068636	2.7268234
H	0.3252659	2.1765276	2.4966242
H	-2.2948704	0.8386397	3.8160837
H	-2.9354702	0.1471650	2.3001602
H	-2.1358406	1.7643364	2.2872226

4b_sy_3_ts1.log

E = -1184.804612
H = -1184.495242
G = -1184.565061

NImag=1

C	1.0668272	-1.2178762	0.3416391
C	-0.0336094	0.2308932	-0.8455576
C	-1.4183652	0.0406445	-0.4952999
C	-2.1124076	0.7513804	0.5135292
C	-3.4173840	0.4334383	0.8515921
C	-4.0790123	-0.6221359	0.2055058
C	-3.4069329	-1.3566921	-0.7869472
C	-2.1084101	-1.0274488	-1.1265782
C	2.4316763	-1.2087275	0.1508448
C	3.1938968	-1.6907054	-1.0544322
C	4.6386904	-1.6020027	-0.5486482
O	4.6262100	-0.6507551	0.5364507
C	3.3505338	-0.5093194	1.0125258
O	3.1546118	0.1349374	2.0377275

S	0.8426089	1.7307303	-0.6914463
C	-0.1950620	3.0864497	-1.2990956
C	0.9866417	2.2010333	1.0505383
C	-5.4259845	-0.9503134	0.5579246
N	-6.5190558	-1.2167479	0.8435193
H	0.6717704	-0.8832176	1.3000166
H	0.4618261	-1.9631511	-0.1696186
H	0.2771135	-0.2114579	-1.7893676
H	-1.6349789	1.5643215	1.0466414
H	-3.9301364	0.9994464	1.6231876
H	-3.9127697	-2.1757165	-1.2889495
H	-1.6017283	-1.5945646	-1.9027709
H	2.9402654	-2.7079014	-1.3669618
H	3.0410515	-1.0268841	-1.9181919
H	5.3516571	-1.2468154	-1.2936773
H	4.9812348	-2.5615058	-0.1470381
H	0.3434990	4.0188713	-1.1145130
H	-0.3305206	2.9346179	-2.3707929
H	-1.1553718	3.0865967	-0.7813341
H	1.7688214	2.9626311	1.0873002
H	1.3128403	1.3255771	1.6139099
H	0.0514990	2.6128846	1.4274891

4b_sy_4_tsl.log

E = -1184.802892

H = -1184.493360

G = -1184.561105

NImag=1

C	1.3825244	-0.0834384	-1.5957826
C	-0.0144497	1.3146888	-0.7853563
C	-1.2367234	0.6182013	-0.4403859
C	-1.5912150	0.1847650	0.8585253
C	-2.7409768	-0.5549217	1.0816327
C	-3.5791415	-0.8987899	0.0100753
C	-3.2475499	-0.4841806	-1.2909120
C	-2.1023891	0.2606157	-1.5045190
C	2.0741937	-0.9160286	-0.7363483
C	1.6177158	-2.1870692	-0.0686802
C	2.9419447	-2.6920011	0.5167413
O	3.7719983	-1.5233065	0.6855722
C	3.3235912	-0.5256241	-0.1424782
O	3.9694803	0.5113389	-0.2508547
S	0.8784693	2.2951441	0.3548867
C	-0.2837061	3.3652827	1.2492095
C	1.4474379	1.2215536	1.7120647
C	-4.7659699	-1.6646096	0.2420281
N	-5.7283212	-2.2854108	0.4297852
H	0.5633716	-0.4921901	-2.1839248
H	1.9506433	0.7079523	-2.0803455
H	-0.0467918	1.8674679	-1.7214567
H	-0.9668619	0.4214235	1.7126630
H	-2.9951906	-0.8714341	2.0884889
H	-3.8947261	-0.7441021	-2.1228882
H	-1.8589576	0.5850849	-2.5127154
H	0.8906761	-1.9969445	0.7348563
H	1.1741105	-2.9183257	-0.7510786
H	3.4514535	-3.3696949	-0.1771653
H	2.8462702	-3.1745071	1.4901802
H	0.2882580	3.8989698	2.0121705
H	-0.6900739	4.0703987	0.5225202
H	-1.0786762	2.7731770	1.7039624

H	2.5034819	1.4361575	1.8760066
H	1.3156782	0.1807664	1.4190377
H	0.8642380	1.4437672	2.6070137

4b_sy_5.log

E = -1184.838755
H = -1184.527252
G = -1184.595005

NImag=0

C	6.5271303	2.0087279	0.8103903
C	7.1201518	1.2809705	2.0450109
C	7.1482554	2.1320893	3.2901915
C	5.9947086	2.4072984	4.0369559
C	6.0543450	3.2528334	5.1381160
C	7.2779871	3.8314837	5.4959549
C	8.4387359	3.5620432	4.7619399
C	8.3658268	2.7092480	3.6671235
C	5.0972456	2.4162770	0.9146458
C	4.5796915	3.7998428	1.2116983
C	3.0732442	3.5093830	1.2677087
O	2.8524457	2.3388328	0.4730884
C	4.0735306	1.6379416	0.4102851
O	4.0538087	0.4840909	-0.0851350
S	6.1276974	-0.2368493	-2.3710895
C	6.4693594	-1.2237814	0.9030094
C	7.1818181	-1.0617105	3.5817990
C	7.3446502	4.7093417	6.6340468
N	7.3985767	5.4168232	7.5494600
H	7.1824979	2.8785433	0.6625802
H	6.6863767	1.3502006	-0.0551829
H	8.1298791	0.9151078	1.8242506
H	5.0406203	1.9726174	3.7536004
H	5.1619055	3.4671649	5.7167814
H	9.3828903	4.0112267	5.0515019
H	9.2631343	2.4923457	3.0946142
H	4.9200599	4.2363876	2.1596981
H	4.8211154	4.5309361	0.4193705
H	2.4450053	4.3147751	0.8788514
H	2.7695302	3.2881520	2.3010498
H	6.1795540	-2.2488857	1.1435456
H	5.8298613	-0.8217293	0.1146412
H	7.5334753	-1.1674841	0.6635561
H	6.7639408	-2.0557373	3.7503086
H	7.1451533	-0.4854441	4.5078188
H	8.2024911	-1.1279631	3.2001353

4b_sy_5_r.log

E = -1184.834609
H = -1184.523209
G = -1184.593098

NImag=0

C	-1.4985212	-0.0473101	1.4091789
C	-0.5067096	0.9981605	0.8640549
C	0.0078107	0.7123886	-0.5255481
C	-0.8751425	0.5109764	-1.5935635
C	-0.3880467	0.2457599	-2.8669656
C	0.9958089	0.1782358	-3.0721818
C	1.8891145	0.3813659	-2.0148484
C	1.3867044	0.6537327	-0.7474845
C	-0.8533556	-1.3860268	1.5255790

C	0.1235087	-1.7669415	2.6064723
C	0.4413719	-3.2047790	2.1763626
O	-0.6951469	-3.6673192	1.4435454
C	-1.3801712	-2.5315625	0.9487699
O	-2.3110220	-2.7379273	0.1409252
S	-1.3197231	2.6678742	0.8185392
C	-1.4747942	3.0622946	2.5724306
C	0.0551273	3.7414233	0.3620167
C	1.5055142	-0.1006948	-4.3886188
N	1.9170985	-0.3241449	-5.4477877
H	-1.8651140	0.3131807	2.3841682
H	-2.3627537	-0.1172864	0.7373997
H	0.3334114	1.1278549	1.5561057
H	-1.9498825	0.5524674	-1.4374282
H	-1.0685833	0.0879005	-3.6970187
H	2.9589451	0.3270899	-2.1870557
H	2.0709791	0.8136825	0.0811559
H	1.0432458	-1.1680896	2.6448882
H	-0.3193731	-1.7348106	3.6195629
H	0.6228879	-3.8927148	3.0062330
H	1.3147015	-3.2128894	1.5084572
H	-1.6667422	4.1350324	2.6399741
H	-2.3246724	2.5108866	2.9741568
H	-0.5479577	2.7987685	3.0865237
H	-0.2842327	4.7702895	0.4964456
H	0.2878112	3.5616665	-0.6885500
H	0.9135356	3.5253405	1.0016963

4b_sy_5_ts1.log

E = -1184.809791

H = -1184.500674

G = -1184.567745

NImag=1

C	1.2432232	0.7674148	1.6391196
C	1.1678493	-1.1902795	0.7234417
C	-0.2159399	-1.2175760	0.3261845
C	-0.6902981	-0.5615812	-0.8363148
C	-2.0481969	-0.4508153	-1.0908881
C	-2.9803605	-0.9698154	-0.1808566
C	-2.5315275	-1.6283100	0.9812176
C	-1.1777235	-1.7506996	1.2215540
C	0.5421896	1.7240173	0.9345621
C	-0.8928674	2.1663055	1.0756096
C	-1.1061261	2.9564912	-0.2289027
O	0.1973473	3.1850153	-0.8062051
C	1.1187523	2.3687692	-0.2097741
O	2.2504601	2.2749168	-0.6799552
S	2.3277855	-1.2399260	-0.5962203
C	3.8565252	-0.5374844	0.0519757
C	2.8233045	-2.9798979	-0.6979839
C	-4.3823228	-0.8429142	-0.4386602
N	-5.5198148	-0.7397300	-0.6457298
H	0.8164387	0.3657435	2.5559057
H	2.3280315	0.7951455	1.6169531
H	1.4686526	-1.8395096	1.5457814
H	0.0086138	-0.1306937	-1.5474451
H	-2.3951835	0.0537807	-1.9877729
H	-3.2531272	-2.0390614	1.6807243
H	-0.8362752	-2.2561430	2.1209082
H	-1.6070594	1.3380697	1.1478202
H	-1.0421168	2.8101059	1.9515552

H	-1.5751163	3.9300533	-0.0770756
H	-1.6918899	2.3856974	-0.9565995
H	4.6572218	-0.8589191	-0.6174498
H	3.7520857	0.5479894	0.0186660
H	4.0327260	-0.9054158	1.0650487
H	3.6032233	-3.0711546	-1.4571486
H	1.9412862	-3.5498048	-0.9942310
H	3.1868531	-3.3055544	0.2788947

4b_sy_5_ts1_rot1.log

E = -1184.809658
H = -1184.500536
G = -1184.567324

NImag=1

C	1.1819505	1.7206332	-0.6215676
C	1.6180741	-0.0825412	0.3946903
C	0.3905125	-0.8380200	0.3141588
C	0.1272492	-1.8558693	-0.6350481
C	-1.1277500	-2.4226174	-0.7483436
C	-2.1777120	-1.9829332	0.0803212
C	-1.9409943	-0.9815885	1.0316851
C	-0.6777513	-0.4216048	1.1442972
C	-0.0427166	2.2192827	-0.2158905
C	-0.3513701	3.0051517	1.0326017
C	-1.8819756	2.8793250	1.1039979
O	-2.3252504	2.4898669	-0.2086085
C	-1.2709447	1.9598898	-0.9163853
O	-1.4846245	1.4300940	-2.0012684
S	3.0379033	-0.8360764	-0.3142737
C	4.2352980	0.5092145	-0.3894605
C	3.7879440	-1.8370740	0.9967549
C	-3.4789431	-2.5681990	-0.0395449
N	-4.5331261	-3.0437022	-0.1372241
H	2.0864244	2.1956733	-0.2504050
H	1.2497708	1.3112551	-1.6286522
H	1.8524315	0.3536049	1.3662509
H	0.9121544	-2.2072430	-1.2987232
H	-1.3094867	-3.2045026	-1.4790860
H	-2.7478530	-0.6475579	1.6774477
H	-0.4955239	0.3356492	1.9010302
H	0.1175520	2.5923018	1.9339781
H	-0.0447341	4.0566707	0.9569544
H	-2.3880600	3.8110393	1.3627334
H	-2.1885303	2.0980478	1.8086464
H	5.2104351	0.0568837	-0.5795524
H	3.9655408	1.1636269	-1.2185494
H	4.2381950	1.0496397	0.5592687
H	4.7313860	-2.2401700	0.6219126
H	3.0932867	-2.6491950	1.2175181
H	3.9478685	-1.2104227	1.8764828

4b_sy_6.log

E = -1184.833774
H = -1184.521757
G = -1184.588194

NImag=0

C	4.5166828	2.1803026	2.2776055
C	6.0309635	2.0395264	2.3988294
C	6.6499697	2.5627344	3.6719075
C	5.9307107	2.6162354	4.8712104

C	6.5320850	3.0862427	6.0320730
C	7.8682656	3.5030280	5.9928582
C	8.5993932	3.4592182	4.8003382
C	7.9821127	2.9912053	3.6465658
C	4.0261851	2.1091844	0.8651340
C	2.5594488	2.0509286	0.5348036
C	2.6228428	2.1248201	-0.9948232
O	3.9082670	1.6175102	-1.3640761
C	4.7586832	1.7537552	-0.2478027
O	5.9774450	1.4848649	-0.4355081
S	6.6288568	0.2669735	2.1825651
C	6.5909754	-0.3884834	3.8680756
C	5.2842978	-0.7301085	1.5012645
C	8.4950125	3.9886080	7.1938504
N	8.9992673	4.3785455	8.1606910
H	4.0128726	1.4389076	2.9264921
H	4.2774809	3.1517408	2.7378238
H	6.5112828	2.5090871	1.5393781
H	4.8964050	2.2878401	4.9060476
H	5.9772030	3.1297144	6.9633686
H	9.6316084	3.7925157	4.7809135
H	8.5394941	2.9621150	2.7137338
H	2.0867812	1.1115059	0.8781903
H	1.9587360	2.8745145	0.9416071
H	2.5519625	3.1699811	-1.3269797
H	1.8582469	1.5361251	-1.5077133
H	6.7942679	-1.4577348	3.7827305
H	7.3795990	0.0873343	4.4510523
H	5.6098895	-0.2223407	4.3184998
H	5.5834094	-1.7643548	1.6867749
H	5.2344820	-0.5289956	0.4338081
H	4.3469141	-0.5100473	2.0144102

4b_sy_7.log

E = -1184.837589

H = -1184.525885

G = -1184.593869

NImag=0

C	4.8164856	2.8013740	2.1178010
C	6.2097433	2.1919397	2.3984142
C	6.8160156	2.6471368	3.7015996
C	6.1263717	2.4830454	4.9102897
C	6.6851688	2.9210446	6.1038979
C	7.9424118	3.5383764	6.0861187
C	8.6399607	3.7126802	4.8859748
C	8.0726695	3.2601053	3.6999649
C	4.2043294	2.3982530	0.8215668
C	4.7604927	2.7463818	-0.5341537
C	3.7041339	2.0881543	-1.4306677
O	3.1383689	1.0205433	-0.6627961
C	3.3469408	1.3155347	0.7041013
O	2.7937031	0.5643152	1.5365849
S	6.0598691	0.3360500	2.4337679
C	6.2365661	-0.1614078	0.7044485
C	7.7023173	-0.1410462	3.0175241
C	8.5253848	3.9985757	7.3186510
N	8.9950214	4.3688817	8.3103225
H	4.1485468	2.5315872	2.9444410
H	4.9796987	3.8872979	2.1832668
H	6.9007161	2.3926257	1.5722196
H	5.1503904	2.0053091	4.9285305

H	6.1567358	2.7908888	7.0424742
H	9.6130715	4.1923713	4.8863620
H	8.6093296	3.3841608	2.7637472
H	4.8351295	3.8210579	-0.7434797
H	5.7622254	2.3161098	-0.7220939
H	4.0990407	1.6715853	-2.3607965
H	2.9073119	2.8060602	-1.6698238
H	6.5072283	-1.2194955	0.7202946
H	5.2817454	-0.0255803	0.1989812
H	7.0277653	0.4301118	0.2395326
H	7.7819751	-1.2213028	2.8811993
H	7.7770002	0.1024333	4.0777273
H	8.4669348	0.3805415	2.4374072

4b_sy_7_ts1.log

E = -1184.806622

H = -1184.497883

G = -1184.567714

NImag=1

C	0.8856698	-1.2310815	-0.1280929
C	-0.0754531	0.6409664	-0.7170582
C	-1.4432965	0.2981571	-0.4274956
C	-2.0627844	0.4989612	0.8317588
C	-3.3460839	0.0450732	1.0820376
C	-4.0619632	-0.6375828	0.0849124
C	-3.4640594	-0.8613713	-1.1678501
C	-2.1834271	-0.4029630	-1.4138771
C	2.2606387	-1.2938147	-0.1308106
C	3.1919763	-1.4511492	-1.3019968
C	4.5287557	-1.6717883	-0.5840166
O	4.3826822	-1.0747116	0.7222983
C	3.0515429	-0.9576685	1.0278580
O	2.7127045	-0.5906889	2.1456067
S	0.6521829	1.9039394	0.2582406
C	2.2791284	2.0713733	-0.4988597
C	-0.0837278	3.4671695	-0.2985917
C	-5.3899971	-1.1016571	0.3422764
N	-6.4678476	-1.4793875	0.5504016
H	0.3775728	-1.2162654	0.8349433
H	0.3277472	-1.6873437	-0.9431200
H	0.1976281	0.7378697	-1.7672712
H	-1.5370078	1.0196801	1.6278830
H	-3.8033460	0.2161490	2.0518546
H	-4.0129127	-1.3901613	-1.9411545
H	-1.7318949	-0.5748305	-2.3872545
H	2.9472900	-2.2888200	-1.9611233
H	3.2266594	-0.5387125	-1.9173057
H	5.3819366	-1.1979257	-1.0708127
H	4.7353003	-2.7382403	-0.4443111
H	2.7208402	2.9888836	-0.1067047
H	2.8876750	1.2167150	-0.2100846
H	2.1631487	2.1273511	-1.5831809
H	0.4256185	4.2859323	0.2149263
H	-1.1379737	3.4473594	-0.0160658
H	0.0271618	3.5480872	-1.3817401

4b_sy_8.log

E = -1184.833581

H = -1184.521560

G = -1184.587721

NImag=0

C	6.5715948	1.9848084	0.8893603
C	7.3070792	1.4108510	2.1200528
C	7.2651699	2.2292942	3.3904752
C	6.0594697	2.6481447	3.9701407
C	6.0641960	3.4177104	5.1275306
C	7.2843815	3.7722045	5.7145993
C	8.4965588	3.3605877	5.1499474
C	8.4767287	2.5898714	3.9939076
C	5.1126362	2.2929345	0.9644823
C	4.5293866	3.6752217	1.1197874
C	3.0340971	3.3364685	1.0830658
O	2.9143423	2.1163181	0.3428142
C	4.1594071	1.4662215	0.4039601
O	4.2182043	0.2892461	-0.0353889
S	6.9034474	-0.3469968	2.5607614
C	5.1532054	-0.4850238	2.9782562
C	6.9205798	-1.1853500	0.9641600
C	7.2917087	4.5690381	6.9129274
N	7.2974243	5.2105991	7.8770452
H	7.1393857	2.9016506	0.6671988
H	6.7757588	1.2996730	0.0552049
H	8.3607790	1.2742037	1.8461816
H	5.1157088	2.3852502	3.5039087
H	5.1309467	3.7440068	5.5745228
H	9.4373130	3.6414280	5.6115011
H	9.4147883	2.2678952	3.5505012
H	4.7811558	4.1944529	2.0534876
H	4.8125428	4.3521983	0.2937553
H	2.4102093	4.0949597	0.6038332
H	2.6617220	3.1599443	2.1023004
H	5.0080183	-1.5422795	3.2156331
H	4.9593046	0.1107266	3.8706399
H	4.5438597	-0.1880968	2.1233170
H	6.8021796	-2.2501850	1.1761243
H	7.8943709	-1.0072991	0.5038345
H	6.0930389	-0.8033780	0.3575704

4b_sy_8_ts1.log

E = -1184.806199
H = -1184.497384
G = -1184.564178

NImag=1

C	-1.3333777	0.4179099	-1.5792837
C	-0.9368281	-1.5099317	-0.6446655
C	0.4465741	-1.3505329	-0.2941895
C	0.8536998	-0.7952903	0.9428859
C	2.1813524	-0.4792254	1.1850124
C	3.1467539	-0.6954480	0.1909324
C	2.7669922	-1.2601908	-1.0436933
C	1.4450360	-1.5808673	-1.2756018
C	-0.8090211	1.5127208	-0.9250696
C	0.5995540	2.0567215	-0.9810742
C	0.6109300	2.9621543	0.2533445
O	-0.7647982	3.3222359	0.4922301
C	-1.5860340	2.3839847	-0.0801731
O	-2.7914862	2.4201926	0.1411380
S	-2.0255728	-1.9136989	0.6909881
C	-2.7961193	-0.3780680	1.2751312
C	-3.4175666	-2.6242100	-0.2047866
C	4.5156981	-0.3569441	0.4348299

N	5.6264365	-0.0828479	0.6310290
H	-0.8016131	0.0136396	-2.4374141
H	-2.4147549	0.2973746	-1.6091683
H	-1.1746629	-2.1374980	-1.5007197
H	0.1268637	-0.5953882	1.7263199
H	2.4750781	-0.0492875	2.1379243
H	3.5178807	-1.4400155	-1.8069722
H	1.1561001	-2.0111376	-2.2307241
H	1.3825396	1.2959388	-0.9198682
H	0.7705809	2.6439913	-1.8940654
H	1.1789054	3.8851452	0.1294759
H	0.9773426	2.4236503	1.1361858
H	-3.5093255	-0.6745497	2.0477492
H	-2.0157543	0.2466324	1.7124086
H	-3.2850091	0.1460935	0.4553026
H	-4.2338932	-2.7583765	0.5064640
H	-3.1015891	-3.5892656	-0.6027182
H	-3.7080971	-1.9437568	-1.0075174

4b_sy_9.log

E = -1184.835301
H = -1184.523717
G = -1184.590555

NImag=0

C	6.3965429	2.3823949	0.6961928
C	7.2187440	1.7000553	1.8142534
C	7.1960985	2.3381076	3.1779755
C	6.0017941	2.7003433	3.8187432
C	6.0294788	3.3271437	5.0586887
C	7.2602683	3.5934868	5.6704979
C	8.4606588	3.2332703	5.0487212
C	8.4183104	2.6067510	3.8089492
C	4.9113999	2.4621127	0.8431133
C	4.1146637	3.7248368	1.0441957
C	2.7000877	3.1334369	1.1266979
O	2.7337771	1.8909998	0.4153345
C	4.0768994	1.4606933	0.3909342
O	4.3069428	0.2931905	-0.0077818
S	6.8101285	-0.1131529	1.8430877
C	8.0857470	-0.7412180	2.9539438
C	5.3663387	-0.3417061	2.8954458
C	7.2903850	4.2445639	6.9536211
N	7.3146193	4.7687442	7.9860419
H	6.8251437	3.3905776	0.6180336
H	6.6699182	1.8562506	-0.2314237
H	8.2610706	1.6441191	1.4766588
H	5.0512470	2.4964098	3.3371724
H	5.1055021	3.6103943	5.5521414
H	9.4096426	3.4433688	5.5305722
H	9.3479567	2.3271732	3.3210710
H	4.3477083	4.2865867	1.9590420
H	4.2085892	4.4353589	0.2035902
H	1.9222162	3.7634396	0.6878741
H	2.4395672	2.9243046	2.1742492
H	7.9152929	-1.8147951	3.0583724
H	9.0561772	-0.5655873	2.4863470
H	8.0207191	-0.2483536	3.9258716
H	5.2210888	-1.4229476	2.9591590
H	4.5156431	0.1212867	2.3984212
H	5.5549322	0.0759596	3.8856918

4b_sy_9_ts1.log

E = -1184.807422

H = -1184.498061

G = -1184.564135

NImag=1

C	-1.5174596	-0.6727511	1.6448269
C	-1.0219868	1.3351572	1.0582967
C	0.3258769	1.1866668	0.5583518
C	0.6213557	0.6476368	-0.7129399
C	1.9286621	0.3688572	-1.0862732
C	2.9782362	0.6026412	-0.1883233
C	2.7086689	1.1408024	1.0843619
C	1.4055803	1.4274262	1.4422339
C	-0.9226403	-1.6572650	0.8775432
C	0.4701824	-2.2267127	1.0096784
C	0.6007900	-3.0091789	-0.3026433
O	-0.7434715	-3.2581896	-0.7609306
C	-1.6011614	-2.3647942	-0.1729846
O	-2.7680778	-2.3119713	-0.5539760
S	-2.3173922	1.9884642	0.0741495
C	-1.6245037	3.2412359	-1.0367367
C	-2.8726902	0.7751480	-1.1508602
C	4.3268989	0.3033046	-0.5691857
N	5.4192382	0.0611118	-0.8759538
H	-1.0862348	-0.4351507	2.6139144
H	-2.5987541	-0.5574979	1.5891622
H	-1.1079979	1.8241280	2.0263645
H	-0.1723961	0.4252141	-1.4166298
H	2.1395731	-0.0474828	-2.0666834
H	3.5246363	1.3291874	1.7750857
H	1.1985146	1.8395130	2.4261530
H	1.2577561	-1.4712220	1.0931285
H	0.5564767	-2.8973857	1.8755654
H	1.0994489	-3.9739091	-0.1982630
H	1.1124017	-2.4181838	-1.0709408
H	-2.4357870	3.5953684	-1.6765197
H	-1.2514139	4.0556058	-0.4142933
H	-0.8214728	2.8099354	-1.6363926
H	-3.7901917	1.1883482	-1.5762186
H	-3.0850621	-0.1674986	-0.6438229
H	-2.1301413	0.6371499	-1.9370956

4b_sy_c_1_ts2.log

E = -1184.826011

H = -1184.516195

G = -1184.585730

NImag=1

C	1.9262354	-0.1067486	-1.0519125
C	1.0183075	-0.6944559	-0.0236908
C	-0.4209525	-0.3195119	0.0184106
C	-1.1658272	-0.1432373	-1.1552086
C	-2.5250920	0.1353128	-1.0901997
C	-3.1473425	0.2469346	0.1591745
C	-2.4161365	0.0760224	1.3426592
C	-1.0612355	-0.2123058	1.2622985
C	2.0045300	1.2390553	-0.4182322
C	3.0063303	1.6820828	0.6102582
C	2.3652121	3.0029938	1.0571716
O	1.5424891	3.4432351	-0.0337887
C	1.2226963	2.3322653	-0.8186074

O	0.3758793	2.4631639	-1.7129153
S	0.9200998	-2.8422390	-0.3846361
C	2.6189846	-3.2467019	0.0743456
C	0.0567405	-3.3734762	1.1088792
C	-4.5534730	0.5393907	0.2279866
N	-5.6867609	0.7735402	0.2837671
H	2.8903648	-0.6241872	-1.0964868
H	1.4789880	-0.0823401	-2.0499621
H	1.4725018	-0.7841289	0.9654959
H	-0.6857227	-0.2237999	-2.1241625
H	-3.1044791	0.2698619	-1.9977064
H	-2.9081820	0.1679356	2.3051451
H	-0.4845142	-0.3482297	2.1733324
H	3.1286332	0.9991308	1.4598830
H	4.0086279	1.8463290	0.1809376
H	3.0824882	3.7944448	1.2838473
H	1.7196230	2.8405667	1.9302662
H	2.6719917	-4.3086531	0.3227581
H	3.2586834	-3.0417193	-0.7850470
H	2.9272760	-2.6417454	0.9314755
H	0.2025452	-4.4486791	1.2322439
H	-1.0056193	-3.1618598	0.9762243
H	0.4469094	-2.8355048	1.9769197

4b_sy_c_prod_1.log

E = -706.954852

H = -706.726336

G = -706.781326

NImag=0

C	2.6949589	1.5083449	0.0524246
O	2.1466341	2.4911268	0.9657815
C	1.0028105	2.0426271	1.5109792
C	0.6056324	0.7618646	0.8559209
C	1.5287477	0.5918687	-0.3328632
O	0.4315863	2.6375018	2.3953958
C	0.1066764	-0.3487880	1.7390009
C	-0.8707053	0.4029542	0.8887839
C	-1.5221769	-0.1747006	-0.3168006
C	-1.0060812	-1.2823318	-1.0054476
C	-1.6438247	-1.7775768	-2.1353343
C	-2.8183402	-1.1652824	-2.5908353
C	-3.3500385	-0.0604514	-1.9155334
C	-2.6985236	0.4248320	-0.7891036
C	-3.4839818	-1.6776739	-3.7571591
N	-4.0205471	-2.0903483	-4.6974988
H	3.4824385	0.9682735	0.5845324
H	3.1242437	2.0508285	-0.7890536
H	1.0465669	0.9434949	-1.2509713
H	1.8652768	-0.4351594	-0.4822873
H	0.3843664	-1.3559840	1.4434056
H	0.0740173	-0.1610133	2.8074344
H	-1.4794370	1.1326810	1.4164261
H	-0.1011061	-1.7738917	-0.6623633
H	-1.2400284	-2.6354988	-2.6628957
H	-4.2617889	0.4080585	-2.2715432
H	-3.1086763	1.2816438	-0.2625947

4b_sy_c_prod_2.log

E = -706.954584

H = -706.726125

G = -706.781051
 NImag=0

C	2.1487740	1.7624516	-0.4083961
O	1.9849103	2.5024846	0.8275868
C	1.0663346	1.9125005	1.6121844
C	0.6392374	0.6209021	0.9979696
C	1.6150678	0.3553323	-0.1272378
O	0.6847531	2.4089772	2.6468057
C	-0.0180912	-0.4016330	1.8650628
C	-0.8783022	0.3996110	0.9376465
C	-1.5132986	-0.1647264	-0.2818801
C	-1.1225252	-1.3872026	-0.8471402
C	-1.7406150	-1.8709239	-1.9932883
C	-2.7686550	-1.1295758	-2.5886015
C	-3.1757753	0.0911188	-2.0363605
C	-2.5458831	0.5621874	-0.8921827
C	-3.4133948	-1.6277619	-3.7728116
N	-3.9322728	-2.0294506	-4.7276892
H	3.2069775	1.7893578	-0.6659977
H	1.5669337	2.2758047	-1.1787236
H	1.1606358	-0.0819398	-1.0181298
H	2.4177111	-0.3040538	0.2164879
H	0.1776173	-1.4404111	1.6173975
H	-0.0941451	-0.1735570	2.9236757
H	-1.4506960	1.1987041	1.4009502
H	-0.3312203	-1.9759299	-0.3933421
H	-1.4344419	-2.8180307	-2.4252734
H	-3.9757092	0.6583005	-2.5011208
H	-2.8594270	1.5077639	-0.4592918

4b_sy_tr_2_ts2.log
 E = -1184.826876
 H = -1184.516595
 G = -1184.585464
 NImag=1

C	-1.9050379	-0.0566069	0.7111534
C	-0.9669852	-0.4919564	-0.3657609
C	0.4978274	-0.2900693	-0.2186949
C	1.1110539	-0.1880118	1.0384669
C	2.4900968	-0.0584689	1.1430468
C	3.2700415	-0.0349067	-0.0197010
C	2.6742130	-0.1362410	-1.2838710
C	1.2954175	-0.2644918	-1.3731720
C	-1.7311145	1.4131969	0.4831725
C	-0.8549945	2.3832917	1.2237405
C	-1.3820398	3.7102592	0.6527609
O	-1.9684492	3.4022653	-0.6209951
C	-2.3065550	2.0506782	-0.6271163
O	-3.0096816	1.6160558	-1.5528255
S	-1.0316781	-2.6702789	-0.6389199
C	-0.2718111	-3.2129894	0.9044980
C	-2.7673902	-3.0210677	-0.2817429
C	4.6981207	0.0967412	0.0851223
N	5.8486523	0.2017679	0.1696776
H	-2.9255556	-0.3897607	0.5071547
H	-1.6130395	-0.3773847	1.7145121
H	-1.3463127	-0.2726710	-1.3634891
H	0.5134731	-0.2065021	1.9445403
H	2.9635813	0.0222161	2.1159726
H	3.2877445	-0.1127773	-2.1783383
H	0.8242443	-0.3445062	-2.3494064

H	-0.9687047	2.3527040	2.3138402
H	0.2204984	2.2648499	1.0093885
H	-0.6074721	4.4638042	0.4974344
H	-2.1651922	4.1266010	1.2985449
H	-0.5419499	-4.2576640	1.0728618
H	0.8109315	-3.1294083	0.7976454
H	-0.6238660	-2.5926344	1.7327346
H	-2.9298366	-4.0970880	-0.3714759
H	-3.3748187	-2.4957524	-1.0215273
H	-3.0182192	-2.6848434	0.7257803

4b_sy_tr_3_ts2.log

E = -1184.828172

H = -1184.518078

G = -1184.586346

NImag=1

C	-1.8099512	0.8389395	-0.8772172
C	-0.7722560	0.9300280	0.1907327
C	0.4690224	0.1278156	0.1165080
C	1.0468835	-0.2405756	-1.1081642
C	2.2406604	-0.9508624	-1.1400706
C	2.8646301	-1.3039311	0.0625291
C	2.2963496	-0.9544409	1.2949649
C	1.1070373	-0.2405332	1.3119683
C	-2.2841567	-0.5381951	-0.5370942
C	-1.8758811	-1.8364621	-1.1721293
C	-2.8775946	-2.7910440	-0.5018496
O	-3.2796588	-2.1645309	0.7255777
C	-3.0469838	-0.7948340	0.6124928
O	-3.5012484	-0.0402444	1.4869548
S	-0.0790913	3.0270547	0.1942631
C	1.5568870	2.9792518	0.9542997
C	0.3908878	3.2080875	-1.5368607
C	4.0997701	-2.0401715	0.0320870
N	5.0951592	-2.6320470	0.0076938
H	-2.5788475	1.6084219	-0.7442223
H	-1.4093142	0.9095615	-1.8914303
H	-1.2038626	0.9837369	1.1892530
H	0.5637636	0.0184801	-2.0452516
H	2.6876090	-1.2342413	-2.0871748
H	2.7850361	-1.2405306	2.2203901
H	0.6596216	0.0390301	2.2620559
H	-1.9817470	-1.8595758	-2.2631519
H	-0.8367742	-2.1313873	-0.9437254
H	-2.4631906	-3.7725444	-0.2632360
H	-3.7688009	-2.9195089	-1.1286936
H	2.0056894	3.9713349	0.8688704
H	1.4336856	2.7223915	2.0081302
H	2.1827049	2.2370451	0.4525199
H	0.9416995	4.1442919	-1.6499642
H	-0.5213250	3.2480649	-2.1338338
H	1.0156588	2.3669761	-1.8483083

4b_sy_tr_prod_1.log

E = -706.952817

H = -706.724813

G = -706.780289

NImag=0

C	3.5831485	-2.0769097	0.1379200
O	4.8300461	-2.3908069	0.8102397

C	4.5913806	-2.8825006	2.0420423
C	3.1180231	-3.0203114	2.2344428
C	2.5203924	-2.9147728	0.8491860
O	5.4849732	-3.1470976	2.8118774
C	2.5856399	-3.8340131	3.3733360
C	2.4969935	-2.3450150	3.4524784
C	3.3287882	-1.5410271	4.3985888
C	3.7027202	-2.0377676	5.6502255
C	4.4604947	-1.2643975	6.5232984
C	4.8485632	0.0237560	6.1378039
C	4.4801341	0.5380581	4.8869882
C	3.7237667	-0.2481253	4.0287167
C	5.6318685	0.8296971	7.0349578
N	6.2626721	1.4795453	7.7574563
H	3.7127015	-2.3197267	-0.9162978
H	3.4044771	-1.0036979	0.2520398
H	1.5396150	-2.4361264	0.8354040
H	2.4408212	-3.9058409	0.3905406
H	1.6737360	-4.3923688	3.1889949
H	3.3294014	-4.3268295	3.9935289
H	1.5262255	-1.9067055	3.2290026
H	3.3992519	-3.0370232	5.9474001
H	4.7504288	-1.6500052	7.4953397
H	4.7880265	1.5377485	4.5984856
H	3.4376103	0.1403638	3.0544035

4b_sy_tr_prod_2.log

E = -706.951166

H = -706.723180

G = -706.779023

NImag=0

C	3.5702342	-3.0938901	-0.1095188
O	4.8044240	-2.8489841	0.6092945
C	4.5789502	-2.7870255	1.9369196
C	3.1081345	-2.7978101	2.1868755
C	2.4508643	-2.6442025	0.8312647
O	5.4854310	-2.7467628	2.7356342
C	2.5976572	-3.6948214	3.2942690
C	2.5274209	-2.2140960	3.4549016
C	3.3660384	-1.4644430	4.4394749
C	3.7420083	-0.1461643	4.1504239
C	4.4946721	0.5929609	5.0524237
C	4.8753112	0.0064054	6.2673430
C	4.5011821	-1.3068843	6.5742750
C	3.7476364	-2.0324144	5.6579482
C	5.6541997	0.7636965	7.2091376
N	6.2816434	1.3745682	7.9678263
H	3.5218714	-4.1644850	-0.3269003
H	3.6186500	-2.5312033	-1.0411234
H	2.1948159	-1.5956710	0.6497527
H	1.5519360	-3.2529279	0.7177147
H	1.6803489	-4.2383870	3.0941229
H	3.3536176	-4.2283713	3.8634151
H	1.5508871	-1.7655017	3.2786709
H	3.4460129	0.2995958	3.2043847
H	4.7903606	1.6121531	4.8255901
H	4.7974944	-1.7482469	7.5203472
H	3.4551972	-3.0511873	5.8939326

5a.log

E = -344.464791
H = -344.353132
G = -344.389281
NImag=0

C	-1.8293453	0.4915536	-0.6194113
C	-2.3056113	1.6748954	-0.2141424
C	-1.9999083	2.9191637	-0.9899420
C	-1.7147562	2.5465842	-2.4297099
O	-0.7261331	1.4976106	-2.5251731
C	-0.8898477	0.4033968	-1.7592038
O	-0.2220776	-0.5843722	-1.9910232
H	-2.0146806	-0.4355201	-0.0885148
H	-2.9046207	1.7453677	0.6904269
H	-1.1442641	3.4371259	-0.5366449
H	-2.8461878	3.6115428	-0.9606029
H	-1.3028525	3.3791971	-2.9994276
H	-2.6290149	2.1939556	-2.9200308

5a_sy_c_1.log
E = -1184.828479
H = -1184.516354
G = -1184.583479
NImag=0

C	-0.8818052	3.1429878	-2.2700760
C	-0.9134927	2.4852056	-0.9140865
C	-0.7947707	2.4683691	-3.4778859
O	-0.9455338	2.9301969	-4.6353129
C	-2.1039146	2.8787768	-0.0055633
C	-1.9508187	4.1616282	0.7917044
C	-1.0573126	5.1657466	0.4037644
C	-0.9385755	6.3313375	1.1530095
C	-1.7224240	6.4956306	2.2996864
C	-2.6165287	5.4974370	2.7046735
C	-2.7217418	4.3374285	1.9486849
O	-0.5164744	1.0919941	-3.4461250
C	-0.8312425	0.9566735	-1.0507618
C	0.0490675	0.6091857	-2.2344624
S	-3.7898896	3.0290523	-0.7985671
C	-3.7748390	4.4610056	-1.8988131
C	-3.9909905	1.6838837	-1.9826730
C	-1.6023992	7.7014434	3.0761584
N	-1.5066188	8.6716271	3.7010824
H	-1.0527444	4.2111535	-2.3443280
H	-0.0487848	2.7881250	-0.2983046
H	-2.3011349	2.0684463	0.7085455
H	-0.4414639	5.0448907	-0.4809590
H	-0.2435763	7.1083696	0.8528383
H	-3.2116673	5.6291463	3.6020930
H	-3.4048408	3.5551077	2.2693097
H	-1.8172689	0.5125157	-1.2179343
H	-0.4289201	0.5145703	-0.1329877
H	0.1485254	-0.4732500	-2.3521533
H	1.0539884	1.0376908	-2.1016638
H	-4.8244118	4.6755065	-2.1119226
H	-3.3313799	5.3020866	-1.3622334
H	-3.2170100	4.2290376	-2.8042865
H	-4.9491103	1.8735286	-2.4729125
H	-4.0437597	0.7469443	-1.4272980
H	-3.1719356	1.6922206	-2.7025394

5a_sy_c_1_r.log

E = -1184.827150

H = -1184.514863

G = -1184.581328

NImag=0

C	0.7907245	-1.8860058	-0.1979545
C	1.3750862	-0.6467395	-0.8394178
C	1.2589338	-2.4594217	0.9734204
O	0.7202061	-3.3311730	1.6945810
C	0.2706479	0.4344734	-0.8359502
C	-0.3776823	0.8707706	0.4696375
C	0.1688960	0.6065861	1.7319067
C	-0.4653057	1.0579313	2.8841000
C	-1.6595148	1.7795104	2.7828993
C	-2.2290565	2.0384684	1.5320100
C	-1.5857295	1.5786696	0.3900821
O	2.5153196	-2.0259455	1.4379255
C	2.7091333	-0.2337527	-0.1857535
C	3.3586408	-1.4500537	0.4505938
S	0.6746560	2.0290691	-1.7367066
C	1.9227395	2.8899765	-0.7603263
C	1.6063305	1.5150940	-3.1909614
C	-2.3116802	2.2493228	3.9762069
N	-2.8358250	2.6295725	4.9363952
H	-0.1720570	-2.2341097	-0.5624735
H	1.5702456	-0.8357830	-1.9041490
H	-0.5320064	0.0694984	-1.4898652
H	1.0754287	0.0248278	1.8383735
H	-0.0385032	0.8478077	3.8591841
H	-3.1637791	2.5840080	1.4580535
H	-2.0409485	1.7662340	-0.5791912
H	2.5740341	0.5284043	0.5863308
H	3.3966874	0.1853559	-0.9293208
H	4.2870250	-1.1757301	0.9590094
H	3.5914513	-2.2025799	-0.3167665
H	2.0101461	3.8875727	-1.1949116
H	1.5512535	2.9674803	0.2640200
H	2.8760995	2.3662410	-0.8004619
H	1.8133471	2.4235035	-3.7606165
H	0.9658889	0.8513771	-3.7751263
H	2.5348725	1.0216385	-2.9038052

5a_sy_c_1_ts1.log

E = -1184.797740

H = -1184.488015

G = -1184.554515

NImag=1

C	1.7660816	-0.8405422	1.2752276
C	1.0718163	-1.2652237	0.1457123
C	3.1699344	-0.5616352	1.2305834
O	3.7892695	0.1494722	2.0225861
C	0.0436761	0.3306804	-0.9103960
C	-1.3567238	0.2134070	-0.5694727
C	-2.0488950	1.0842549	0.3047743
C	-3.3664165	0.8471616	0.6633198
C	-4.0385594	-0.2813171	0.1711292
C	-3.3700173	-1.1679898	-0.6920927
C	-2.0585944	-0.9218433	-1.0507532
O	3.8898409	-1.1186057	0.2048205
C	1.9041656	-1.8722507	-0.9782464
C	3.2759458	-2.2410203	-0.4471265

S	0.7245381	1.9685536	-0.7673193
C	1.2788599	2.2661851	0.9442476
C	2.3207471	1.7700831	-1.5814801
C	-5.3969496	-0.5303102	0.5467493
N	-6.4985417	-0.7334545	0.8504143
H	1.2401175	-0.5011311	2.1610896
H	0.0752882	-1.6753413	0.2895338
H	0.3014637	-0.0246678	-1.9063376
H	-1.5666592	1.9712436	0.7062525
H	-3.8809955	1.5352124	1.3269287
H	-3.8887381	-2.0406672	-1.0770041
H	-1.5504713	-1.6080440	-1.7238251
H	2.0274363	-1.1798413	-1.8155036
H	1.4120619	-2.7671477	-1.3730901
H	3.9566150	-2.5239038	-1.2520672
H	3.2103254	-3.0676493	0.2705831
H	2.2198068	1.7584010	1.1542741
H	1.3974802	3.3489977	1.0151872
H	0.5000514	1.9335122	1.6305244
H	2.8600693	2.7114861	-1.4621569
H	2.1373831	1.5742148	-2.6390439
H	2.8701755	0.9490846	-1.1165596

5a_sy_c_1_ts2.log

E = -1184.817478

H = -1184.506547

G = -1184.573219

NImag=1

C	-1.6675459	1.7539339	-1.1020678
C	-2.1500520	0.4913938	-0.4332321
C	-0.9817302	2.7598123	-0.3997986
O	-0.2946602	3.6825100	-0.8642747
C	-0.9995673	-0.3414816	-0.9305982
C	0.4378287	-0.2111636	-0.5428886
C	0.9025166	0.3361591	0.6635187
C	2.2571233	0.3242511	0.9698559
C	3.1698360	-0.2494180	0.0763989
C	2.7276983	-0.7979497	-1.1327308
C	1.3728383	-0.7705332	-1.4310108
O	-1.0985971	2.7359195	0.9863201
C	-2.3595878	0.6388657	1.0865036
C	-2.2761531	2.1036776	1.4884631
S	-1.2901157	-2.5055560	-0.4932211
C	-0.4469812	-2.7534612	1.0838666
C	-3.0147644	-2.6074566	0.0308860
C	4.5704512	-0.2687357	0.4003967
N	5.6987805	-0.2855094	0.6621154
H	-1.6862234	1.8180187	-2.1836910
H	-3.0606607	0.1110610	-0.9054463
H	-1.0979052	-0.5172970	-2.0008562
H	0.2246166	0.8017618	1.3651520
H	2.6086414	0.7567777	1.9008845
H	3.4377260	-1.2340295	-1.8275085
H	1.0305722	-1.1914128	-2.3729882
H	-1.6383694	0.0491912	1.6572851
H	-3.3520603	0.2698249	1.3631547
H	-2.2391399	2.2128116	2.5749743
H	-3.1546711	2.6446943	1.1139793
H	-0.7081362	-3.7467353	1.4557892
H	0.6281409	-2.7054912	0.8996388
H	-0.7428574	-1.9896976	1.8055351

H	-3.2132985	-3.6295112	0.3608199
H	-3.6409580	-2.3769226	-0.8326351
H	-3.2103492	-1.9068680	0.8440769

5a_sy_c_2.log

E = -1184.836086
H = -1184.524042
G = -1184.590896

NImag=0

C	-0.7942905	3.0833900	-2.3805431
C	-0.9785269	2.5522794	-0.9787234
C	-0.5359710	2.3022349	-3.5015098
O	-0.4830967	2.6685144	-4.6984709
C	-2.2632061	3.0734044	-0.2648172
C	-2.0572575	4.2601405	0.6472447
C	-1.3201395	5.3743209	0.2256287
C	-1.1371341	6.4591560	1.0729969
C	-1.6934473	6.4273564	2.3580356
C	-2.4264406	5.3191615	2.7954943
C	-2.6055931	4.2426142	1.9338316
O	-0.3151479	0.9299258	-3.3177914
C	-0.9813578	1.0180086	-0.9935465
C	0.0396589	0.5294459	-2.0002316
S	-3.5111274	3.5861268	-1.5368357
C	-4.0268479	2.0344795	-2.2993592
C	-4.9521555	3.8829391	-0.4851306
C	-1.5062134	7.5494323	3.2395880
N	-1.3567090	8.4526922	3.9486879
H	-0.8536935	4.1522792	-2.5596987
H	-0.1610341	2.8713589	-0.3121769
H	-2.7553187	2.2719595	0.2985273
H	-0.8800366	5.3985335	-0.7669326
H	-0.5676065	7.3234569	0.7481293
H	-2.8488537	5.3046283	3.7946686
H	-3.1746996	3.3786178	2.2651235
H	-1.9638116	0.6305674	-1.2864712
H	-0.7567483	0.6250900	0.0039601
H	0.0935625	-0.5624013	-2.0170923
H	1.0379267	0.9215265	-1.7532192
H	-4.9238678	2.2610842	-2.8798192
H	-3.2231933	1.7050073	-2.9576353
H	-4.2452327	1.2985145	-1.5231016
H	-5.8103580	3.9900553	-1.1517778
H	-4.7922965	4.8159582	0.0565029
H	-5.0984349	3.0470410	0.2020649

5a_sy_c_2_r.log

E = -1184.834393
H = -1184.522518
G = -1184.590452

NImag=0

C	-0.5709580	-1.8568099	0.0273557
C	-1.2588705	-0.6466881	0.6056121
C	-1.1575888	-2.7600218	-0.8482246
O	-0.6208545	-3.7310248	-1.4332162
C	-0.2845081	0.5615338	0.5643531
C	0.2300287	0.9771907	-0.7954943
C	-0.5369155	1.7237953	-1.6987988
C	-0.0267625	2.0659373	-2.9464720
C	1.2640682	1.6576299	-3.2958124

C	2.0476506	0.9197195	-2.4007795
C	1.5273152	0.5923510	-1.1552039
O	-2.5234577	-2.6105198	-1.1434929
C	-2.5834137	-0.4131590	-0.1180631
C	-3.2667240	-1.7596829	-0.2843229
S	-1.0547466	2.0482996	1.3514312
C	-1.4090457	1.4804773	3.0251578
C	0.3955426	3.0793585	1.6443035
C	1.7965050	2.0099627	-4.5852192
N	2.2254698	2.2941002	-5.6227064
H	0.4715492	-2.0320169	0.2776849
H	-1.4829551	-0.7872588	1.6751675
H	0.5688252	0.3286398	1.2125422
H	-1.5399481	2.0523823	-1.4430547
H	-0.6227703	2.6447310	-3.6440711
H	3.0511038	0.6144099	-2.6779906
H	2.1335348	0.0286851	-0.4523488
H	-2.4162850	0.0029548	-1.1176753
H	-3.2402638	0.2709354	0.4339228
H	-4.2531272	-1.6493077	-0.7426028
H	-3.3933541	-2.2426916	0.6967615
H	-1.5663739	2.3774059	3.6282282
H	-2.3244551	0.8886061	3.0010524
H	-0.5659100	0.8991615	3.4036172
H	0.0687840	3.9325722	2.2415918
H	0.7612595	3.4225622	0.6751558
H	1.1546464	2.4976660	2.1710207

5a_sy_c_2_ts1.log

E = -1184.806709

H = -1184.497300

G = -1184.564583

NImag=1

C	-1.6154845	-1.2658255	-0.9170827
C	-1.0798492	-1.2460797	0.3715152
C	-3.0112021	-1.0472853	-1.1654059
O	-3.5259734	-0.7686364	-2.2455841
C	-0.1013088	0.6478734	0.8096527
C	1.2722288	0.3694850	0.4655564
C	1.7860846	0.4511626	-0.8514644
C	3.0809634	0.0528755	-1.1428018
C	3.9091953	-0.4501986	-0.1284446
C	3.4165876	-0.5535101	1.1848381
C	2.1251986	-0.1521901	1.4700094
O	-3.8629740	-1.1681771	-0.0910669
C	-2.0553923	-1.3698970	1.5326678
C	-3.3715196	-1.9280223	1.0237746
S	-0.9390319	1.7650449	-0.2565417
C	-2.5412653	1.9468753	0.5429584
C	-0.2383205	3.4007175	0.0786157
C	5.2483701	-0.8559491	-0.4287223
N	6.3344903	-1.1858266	-0.6705730
H	-0.9746001	-1.3158294	-1.7914396
H	-0.0970392	-1.6871425	0.5132710
H	-0.3070986	0.8569185	1.8593157
H	1.1714819	0.8329415	-1.6624941
H	3.4572906	0.1294477	-2.1582443
H	4.0543411	-0.9446890	1.9715834
H	1.7517751	-0.2337858	2.4872272
H	-2.2325185	-0.4058945	2.0180756
H	-1.6485809	-2.0398200	2.2968048

H	-4.1528291	-1.8750559	1.7842998
H	-3.2546183	-2.9717920	0.7078279
H	-3.0416701	2.7881737	0.0601139
H	-3.1195601	1.0364147	0.3844492
H	-2.3941762	2.1429666	1.6072131
H	-0.8039084	4.1341637	-0.5006427
H	0.8003681	3.3827790	-0.2565432
H	-0.2976502	3.6100483	1.1480306

5a_sy_c_2_ts2.log

E = -1184.819665
H = -1184.509342
G = -1184.577333

NImag=1

C	2.1201816	0.9444857	0.9889562
C	2.1952192	-0.2568815	0.0781039
C	1.5202659	2.1370055	0.5444551
O	1.1179543	3.0924154	1.2243591
C	0.8649657	-0.7750081	0.5319090
C	-0.4564612	-0.1158792	0.2932240
C	-0.9198711	0.2579657	-0.9763215
C	-2.1891587	0.8008224	-1.1341381
C	-3.0141760	0.9695886	-0.0164461
C	-2.5743183	0.5905885	1.2578371
C	-1.3061214	0.0449268	1.3986604
O	1.3542353	2.2524381	-0.8306401
C	2.3794547	0.0853000	-1.4090533
C	2.3462197	1.5945988	-1.6221697
S	0.5092705	-2.7391767	-0.4249071
C	1.8681596	-3.6465302	0.3435973
C	-0.8683118	-3.3003237	0.5988583
C	-4.3289921	1.5286613	-0.1800337
N	-5.3885338	1.9780220	-0.3117242
H	2.3269052	0.8320392	2.0463433
H	2.9637313	-0.9588563	0.4112431
H	0.9238473	-1.1914441	1.5395531
H	-0.3040355	0.1232325	-1.8568260
H	-2.5434435	1.0882563	-2.1185782
H	-3.2201454	0.7203140	2.1198238
H	-0.9582715	-0.2522624	2.3842359
H	1.6320781	-0.4189308	-2.0274046
H	3.3538079	-0.2813753	-1.7471361
H	2.1167103	1.8445384	-2.6608191
H	3.3255041	2.0229695	-1.3730390
H	1.6744050	-4.7171743	0.2518156
H	2.7844004	-3.3962096	-0.1936763
H	1.9575300	-3.3669606	1.3965343
H	-0.9727479	-4.3815489	0.4871695
H	-1.7738537	-2.8069117	0.2407830
H	-0.6849867	-3.0425451	1.6455612

5a_sy_c_3.log

E = -1184.836586
H = -1184.524480
G = -1184.590964

NImag=0

C	-0.7579192	3.0580108	-2.3642015
C	-0.8581675	2.4200212	-0.9998017
C	-0.5043216	2.3727597	-3.5503127
O	-0.4775534	2.8419958	-4.7114502

C	-2.0789117	2.8765360	-0.1629952
C	-1.9406336	4.1438316	0.6394393
C	-1.1464779	5.2126422	0.2039933
C	-1.0398665	6.3692034	0.9660182
C	-1.7329218	6.4610952	2.1788831
C	-2.5188472	5.3980529	2.6362514
C	-2.6130488	4.2460693	1.8642971
O	-0.2556352	0.9963149	-3.4923283
C	-0.9086864	0.8982021	-1.1609809
C	0.0914813	0.4745756	-2.2168761
S	-3.5379068	2.9410393	-1.3255078
C	-4.9272305	2.8211735	-0.1756198
C	-3.7354216	4.6640885	-1.8216614
C	-1.6253138	7.6587865	2.9695235
N	-1.5399684	8.6228061	3.6054633
H	-0.8267971	4.1349315	-2.4692912
H	0.0032765	2.6591250	-0.3527889
H	-2.3810264	2.0728841	0.5203138
H	-0.5981643	5.1463684	-0.7291626
H	-0.4230804	7.1955757	0.6288153
H	-3.0388669	5.4726128	3.5854253
H	-3.2054282	3.4093673	2.2246372
H	-1.9082570	0.5799944	-1.4885161
H	-0.6944911	0.4008876	-0.2088542
H	0.1182136	-0.6125692	-2.3288879
H	1.1002338	0.8178768	-1.9408976
H	-5.8374505	2.8564033	-0.7774739
H	-4.8593069	1.8602243	0.3369918
H	-4.9115933	3.6496641	0.5347355
H	-4.6725286	4.7070179	-2.3814806
H	-2.9000203	4.9326439	-2.4661740
H	-3.7871621	5.3035876	-0.9386254

5a_sy_c_3_r.log

E = -1184.831011

H = -1184.518828

G = -1184.585385

NImag=0

C	0.9425612	-1.7907646	-0.1288788
C	1.4537413	-0.5341159	-0.7824509
C	1.7040742	-2.6390952	0.6630351
O	1.3244799	-3.6425487	1.3126683
C	0.3727077	0.5760357	-0.6776432
C	-0.3147224	0.8554146	0.6368904
C	0.3703867	1.0527012	1.8444660
C	-0.3244283	1.2964403	3.0218610
C	-1.7235885	1.3470556	3.0002291
C	-2.4254213	1.1560433	1.8067389
C	-1.7146574	0.9131107	0.6367494
O	3.0805910	-2.3796494	0.7809819
C	2.8461618	-0.1927285	-0.2449155
C	3.6376483	-1.4875956	-0.1719799
S	1.0248164	2.1181244	-1.4888155
C	-0.4750788	3.0677575	-1.7988006
C	1.7768101	3.1101723	-0.1853703
C	-2.4457031	1.6004113	4.2188621
N	-3.0270658	1.8062117	5.1990303
H	-0.1089624	-2.0423618	-0.2374991
H	1.5739651	-0.6577170	-1.8735879
H	-0.4076479	0.3019145	-1.3977733
H	1.4524510	1.0220127	1.8811565

H	0.2101493	1.4454982	3.9540542
H	-3.5096038	1.1956270	1.7976410
H	-2.2581265	0.7579328	-0.2914366
H	2.8121248	0.2357391	0.7606844
H	3.3692142	0.5160281	-0.8993806
H	4.6674188	-1.3042349	0.1458620
H	3.6612971	-1.9693163	-1.1615430
H	-0.1661409	4.0178005	-2.2392237
H	-1.0811612	2.5060093	-2.5115439
H	-1.0114547	3.2326786	-0.8623726
H	2.1333792	4.0214732	-0.6704844
H	2.6209364	2.5577722	0.2291118
H	1.0371856	3.3462541	0.5808424

5a_sy_c_3_ts1.log

E = -1184.805021

H = -1184.495029

G = -1184.561146

NImag=1

C	1.2295605	-1.6131836	0.0002454
C	1.2744099	-0.8445583	-1.1652721
C	2.3468253	-1.7094239	0.8901663
O	2.3210148	-2.0901852	2.0586543
C	0.2440933	1.0004136	-0.9874286
C	-1.0847142	0.5713474	-0.5928706
C	-1.4473292	0.2671376	0.7373177
C	-2.6998487	-0.2463698	1.0412182
C	-3.6233453	-0.4924122	0.0163727
C	-3.2765148	-0.2238341	-1.3184057
C	-2.0291654	0.2994669	-1.6097730
O	3.5766669	-1.3422256	0.3934047
C	2.6525965	-0.4334283	-1.6678773
C	3.7038285	-1.3260711	-1.0353316
S	1.1334315	2.1875690	-0.0481995
C	-0.0390505	3.2770087	0.8026730
C	1.9262631	1.4063356	1.3826061
C	-4.9173098	-1.0233329	0.3290686
N	-5.9651295	-1.4525374	0.5809197
H	0.3021736	-2.0582967	0.3442896
H	0.5281457	-1.0548469	-1.9279364
H	0.3256657	1.3244759	-2.0242361
H	-0.7477775	0.4221418	1.5510476
H	-2.9630181	-0.4679815	2.0707853
H	-3.9899020	-0.4187463	-2.1129598
H	-1.7685332	0.5153150	-2.6424232
H	2.8870627	0.6100504	-1.4321474
H	2.7022238	-0.5259800	-2.7572631
H	4.7136451	-0.9645847	-1.2384270
H	3.6138259	-2.3541495	-1.4062054
H	0.5509726	4.0391092	1.3159107
H	-0.6618088	3.7387624	0.0350984
H	-0.6469526	2.7181105	1.5142956
H	2.7671706	0.8127457	1.0232162
H	1.2308321	0.7994846	1.9602970
H	2.3018577	2.2352567	1.9873158

5a_sy_c_3_ts2.log

E = -1184.818810

H = -1184.508198

G = -1184.575771

NImag=1

C	2.2481037	-0.7816327	-1.3228486
C	2.2925224	0.4243879	-0.4203418
C	1.9098508	-2.0527269	-0.8275007
O	1.5463844	-3.0522053	-1.4662451
C	0.8944301	0.8608994	-0.7365878
C	-0.3659525	0.1413977	-0.4053547
C	-0.5835717	-0.5996589	0.7692541
C	-1.8202588	-1.1766514	1.0226106
C	-2.8685152	-1.0084993	0.1092740
C	-2.6763433	-0.2699699	-1.0634724
C	-1.4319742	0.2940742	-1.3089819
O	1.9984319	-2.2145121	0.5506281
C	2.6394014	0.1071184	1.0461281
C	2.9505523	-1.3749243	1.2071358
S	0.6353109	2.8530850	0.2640823
C	-0.4325189	3.6876564	-0.9281416
C	-0.5492706	2.5729009	1.5968735
C	-4.1512132	-1.5991863	0.3797847
N	-5.1851166	-2.0736401	0.5984303
H	2.2710341	-0.6417240	-2.3971558
H	2.9675808	1.1920982	-0.8098682
H	0.8393600	1.3030756	-1.7323652
H	0.2046167	-0.7414112	1.4952521
H	-1.9789483	-1.7504365	1.9297629
H	-3.4890642	-0.1466249	-1.7713838
H	-1.2752550	0.8564614	-2.2253400
H	1.8389409	0.4136214	1.7260640
H	3.5264008	0.6742760	1.3446842
H	2.9400695	-1.6713615	2.2587845
H	3.9456537	-1.5895963	0.7968699
H	-0.7314761	4.6548808	-0.5187343
H	0.1425995	3.8389236	-1.8433838
H	-1.3155311	3.0768610	-1.1313835
H	-0.8082816	3.5396160	2.0346373
H	-0.0702061	1.9468646	2.3523777
H	-1.4446035	2.0816609	1.2081323

5a_sy_c_4.log

E = -1184.837415
H = -1184.525426
G = -1184.592573

NImag=0

C	-1.0362063	2.9067691	-3.0728986
C	-0.8023016	3.3947122	-1.6715680
C	-0.6338372	1.6719225	-3.5687404
O	-0.7237538	1.2547843	-4.7474040
C	-2.0815104	3.4778442	-0.7774802
C	-1.9697659	4.4617669	0.3585014
C	-2.1405402	4.0199121	1.6740927
C	-2.0194774	4.9048051	2.7399890
C	-1.7342137	6.2496979	2.4808587
C	-1.5660220	6.7088392	1.1681450
C	-1.6791999	5.8111415	0.1148991
O	-0.0348591	0.7578614	-2.6930585
C	0.1899876	2.4636170	-0.9654509
C	-0.1529882	1.0222217	-1.3025000
S	-3.5419988	3.9146615	-1.8413083
C	-4.1837389	2.2898633	-2.3035974
C	-4.7933416	4.3647006	-0.6173637
C	-1.6135129	7.1743009	3.5769991

N	-1.5169520	7.9182791	4.4591994
H	-1.4485075	3.5954285	-3.8052951
H	-0.3839057	4.4094101	-1.6872608
H	-2.3465312	2.4900475	-0.3848288
H	-2.3677776	2.9750796	1.8652737
H	-2.1471612	4.5616953	3.7612828
H	-1.3482056	7.7550751	0.9817466
H	-1.5491304	6.1720112	-0.9023658
H	0.1760555	2.6025082	0.1224319
H	1.2040512	2.6812245	-1.3185571
H	-1.1772180	0.7834850	-0.9759803
H	0.5271366	0.3276150	-0.8020580
H	-5.1363668	2.4568765	-2.8110650
H	-3.4587019	1.8343494	-2.9768845
H	-4.3219128	1.6937985	-1.3989228
H	-5.7458726	4.4086697	-1.1495643
H	-4.5509555	5.3486066	-0.2152254
H	-4.8264642	3.6118189	0.1730586

5a_sy_c_4_r.log

E = -1184.834335

H = -1184.522327

G = -1184.588764

NImag=0

C	-0.5020013	-0.9375907	-1.7883142
C	-1.2326735	-0.5895317	-0.5215906
C	-1.0414735	-0.8854674	-3.0685092
O	-0.5411324	-1.3240580	-4.1314487
C	-0.4029662	0.4541993	0.2962896
C	-0.4070326	1.8673546	-0.2315168
C	0.6264409	2.2454384	-1.0963526
C	0.6313185	3.5021440	-1.6903560
C	-0.4015331	4.3999797	-1.3991255
C	-1.4288515	4.0466181	-0.5164539
C	-1.4266862	2.7827454	0.0597599
O	-2.3022595	-0.2989315	-3.2362784
C	-2.6693228	-0.1558155	-0.8375469
C	-2.7391855	0.5490139	-2.1851136
S	-0.9688169	0.4753105	2.0630208
C	-0.4690442	-1.1592625	2.6423617
C	0.3071870	1.4903779	2.8371478
C	-0.4021383	5.7061122	-2.0025867
N	-0.4029656	6.7577717	-2.4876032
H	0.4678880	-1.4193336	-1.6972461
H	-1.2850293	-1.4732964	0.1302319
H	0.6286710	0.0891236	0.3591108
H	1.4290799	1.5465231	-1.3097456
H	1.4281660	3.7897759	-2.3681594
H	-2.2206215	4.7532689	-0.2911280
H	-2.2423405	2.5204038	0.7284033
H	-3.0981606	0.4848864	-0.0575173
H	-3.2981234	-1.0514917	-0.8927670
H	-2.1326483	1.4644641	-2.1875243
H	-3.7708134	0.8239100	-2.4226970
H	-0.4378315	-1.1035523	3.7323922
H	-1.2210901	-1.8848359	2.3342972
H	0.5148499	-1.4045675	2.2374448
H	0.1796275	1.3950708	3.9170165
H	0.1476498	2.5259189	2.5345614
H	1.2910164	1.1332234	2.5254483

5a_sy_c_4_ts1.log

E = -1184.810520

H = -1184.501292

G = -1184.568525

NImag=1

C	-2.3164862	-0.6772083	-1.2422920
C	-1.1461938	-1.0394873	-0.5813666
C	-3.6216091	-1.0327895	-0.7576205
O	-4.6744907	-0.8519503	-1.3667138
C	-0.1661820	0.5516897	0.5608374
C	1.2294464	0.2780316	0.3253028
C	1.9531842	-0.4753510	1.2826503
C	3.2615815	-0.8626656	1.0578485
C	3.9033017	-0.5059477	-0.1410197
C	3.2066008	0.2355791	-1.1081367
C	1.8943878	0.6137047	-0.8803973
O	-3.7215739	-1.6730452	0.4482118
C	-1.3020091	-2.0189082	0.5524119
C	-2.5713743	-1.6835717	1.3081080
S	-0.8317323	1.9832853	-0.2180023
C	-2.4058241	2.1486112	0.6404369
C	0.0440770	3.4063328	0.4816879
C	5.2604350	-0.8951354	-0.3746285
N	6.3610218	-1.2112697	-0.5639757
H	-2.2946711	-0.1561579	-2.1932590
H	-0.2322024	-1.0956514	-1.1700533
H	-0.5041851	0.4793797	1.5943529
H	1.4696306	-0.7423734	2.2183257
H	3.7994350	-1.4336380	1.8084802
H	3.6990041	0.5083306	-2.0365741
H	1.3775107	1.1771652	-1.6537144
H	-0.4481898	-2.0011181	1.2360192
H	-1.3709809	-3.0338623	0.1379350
H	-2.4826499	-0.6978010	1.7832217
H	-2.7928608	-2.4222847	2.0803332
H	-2.8563122	3.0875688	0.3145188
H	-3.0363705	1.3103744	0.3465452
H	-2.2237968	2.1538127	1.7171893
H	-0.4355466	4.3130195	0.1056006
H	1.0773536	3.3608676	0.1325310
H	-0.0009776	3.3567856	1.5710187

5a_sy_c_4_ts2.log

E = -1184.819506

H = -1184.508880

G = -1184.576287

NImag=1

C	-2.2338731	0.9585539	-0.9181368
C	-2.1460508	-0.0648298	0.1808162
C	-2.2023202	2.3558682	-0.7104909
O	-2.4159711	3.2205408	-1.5738299
C	-0.9084286	-0.6689941	-0.3961163
C	0.4942053	-0.1780590	-0.2287295
C	1.2397265	0.1150559	-1.3775945
C	2.5729312	0.4949045	-1.2858539
C	3.1771578	0.5631110	-0.0254577
C	2.4546360	0.2495063	1.1326012
C	1.1218698	-0.1241009	1.0242940
O	-1.9755121	2.8386262	0.5618609
C	-2.1002580	0.5972861	1.5531213

C	-1.3994975	1.9491854	1.5173164
S	-0.6782069	-2.7341243	0.4891317
C	-2.1309089	-3.4866331	-0.2748894
C	0.6034643	-3.3231701	-0.6398125
C	4.5592310	0.9473171	0.0814731
N	5.6721908	1.2559523	0.1678228
H	-2.5432942	0.6368695	-1.9055359
H	-2.9600691	-0.7993076	0.1529129
H	-1.0850362	-1.0898542	-1.3870176
H	0.7637919	0.0513971	-2.3519060
H	3.1436096	0.7309507	-2.1778186
H	2.9372710	0.2918206	2.1032443
H	0.5737163	-0.3807386	1.9257136
H	-1.6254650	-0.0448817	2.3031921
H	-3.1349680	0.7578731	1.8748064
H	-0.3329089	1.8510611	1.2966545
H	-1.4973687	2.4498936	2.4835367
H	-1.9880706	-4.5683727	-0.3183366
H	-2.9969429	-3.2601153	0.3486840
H	-2.2748075	-3.0853680	-1.2819420
H	0.6290821	-4.4142729	-0.6091237
H	1.5613762	-2.9258592	-0.2985879
H	0.3932225	-2.9782358	-1.6563734

5a_sy_c_5.log

E = -1184.835094

H = -1184.523116

G = -1184.589431

NImag=0

C	-0.5454705	3.0681390	-2.4205237
C	-0.5647981	2.5633528	-1.0029290
C	-0.5862987	2.2558211	-3.5495459
O	-0.4934531	2.6115156	-4.7471348
C	-1.8889331	2.8732309	-0.2260061
C	-1.8611013	4.1061262	0.6390456
C	-1.1877240	5.2644801	0.2263379
C	-1.1670316	6.3943885	1.0326718
C	-1.8227068	6.3667482	2.2703747
C	-2.4922670	5.2171947	2.7013484
C	-2.5064927	4.0944449	1.8809064
O	-0.7344760	0.8713824	-3.3915064
C	-0.2649139	1.0608139	-1.0039658
C	-1.0480073	0.3638252	-2.1007333
S	-3.2830092	2.9449797	-1.4606385
C	-4.7210726	2.8135321	-0.3712577
C	-3.4668275	4.6671801	-1.9618041
C	-1.8006316	7.5339081	3.1119766
N	-1.7841494	8.4733330	3.7889769
H	-0.3947660	4.1266790	-2.6092394
H	0.2140756	3.0541308	-0.4045175
H	-2.1935091	2.0191379	0.3920397
H	-0.6757335	5.2882996	-0.7311829
H	-0.6472752	7.2913945	0.7129282
H	-2.9884082	5.2038559	3.6660060
H	-3.0162683	3.1943462	2.2136579
H	-0.4989239	0.6012620	-0.0374025
H	0.8053251	0.9186570	-1.1922406
H	-2.1301991	0.4512007	-1.9234149
H	-0.8110157	-0.7035991	-2.1308169
H	-5.6051081	2.8781223	-1.0086168
H	-4.6877657	1.8368438	0.1147361

H	-4.7237874	3.6196727	0.3648671
H	-4.3405389	4.6924812	-2.6172762
H	-2.5732433	4.9559390	-2.5131594
H	-3.6263937	5.2983797	-1.0861609

5a_sy_c_5_r.log

E = -1184.829238
H = -1184.516871
G = -1184.582795

NImag=0

C	0.5072507	-2.0535084	-0.3605064
C	1.3310969	-0.8558126	-0.7548728
C	0.9219911	-3.0763308	0.4865424
O	0.3616145	-4.1786971	0.6905824
C	0.4497656	0.4187675	-0.5903397
C	0.0825927	0.9346374	0.7778894
C	1.0292373	1.3888227	1.7072222
C	0.6309226	1.8564508	2.9536739
C	-0.7296196	1.8702781	3.2815738
C	-1.6890672	1.4206113	2.3691228
C	-1.2747801	0.9623341	1.1243311
O	2.1073751	-2.8987307	1.2093900
C	2.6839753	-0.8928085	-0.0306947
C	2.5582678	-1.5585772	1.3317923
S	1.0388516	1.7766930	-1.7371781
C	-0.3617428	2.9114961	-1.7085877
C	2.2775968	2.7857860	-0.9035388
C	-1.1460601	2.3555159	4.5706420
N	-1.4824219	2.7474808	5.6070673
H	-0.4009271	-2.2455960	-0.9261680
H	1.5433621	-0.8782515	-1.8361392
H	-0.4824303	0.1796514	-1.1175268
H	2.0889799	1.3758454	1.4754738
H	1.3669184	2.2062331	3.6698262
H	-2.7416202	1.4331748	2.6316083
H	-2.0171945	0.6164176	0.4106385
H	3.1475716	0.0928288	0.0724469
H	3.3713408	-1.4993825	-0.6314406
H	1.8658421	-1.0084274	1.9818975
H	3.5309060	-1.6062498	1.8297359
H	-0.1073691	3.7507691	-2.3585569
H	-1.2278021	2.3809710	-2.1079206
H	-0.5424822	3.2539262	-0.6876947
H	2.5250187	3.5834216	-1.6079463
H	3.1636728	2.1783630	-0.7187895
H	1.8718813	3.2055401	0.0173457

5a_sy_c_5_ts1.log

E = -1184.807181
H = -1184.497337
G = -1184.564958

NImag=1

C	2.7794356	-0.1661831	0.9509421
C	1.4756284	-0.6383471	0.8481791
C	3.9029313	-0.8493312	0.3700346
O	5.0798732	-0.5392702	0.5441779
C	0.2594832	0.4563185	-0.6134900
C	-1.1349002	0.1734806	-0.3635699
C	-1.8833304	0.7484363	0.6913284
C	-3.1905835	0.3616353	0.9413221

C	-3.7960277	-0.6282353	0.1532242
C	-3.0699930	-1.2273150	-0.8908922
C	-1.7697167	-0.8292266	-1.1399463
O	3.6755499	-1.9712230	-0.3786398
C	1.3143591	-2.0145718	0.2580276
C	2.3391489	-2.2118821	-0.8401497
S	0.9389065	2.0652400	-0.5204881
C	-0.2155631	3.2121258	-1.3118659
C	0.8514549	2.6848296	1.1844685
C	-5.1455211	-1.0289036	0.4143192
N	-6.2391840	-1.3545319	0.6253368
H	3.0267975	0.7174569	1.5301017
H	0.7459696	-0.3427357	1.6007012
H	0.6654097	0.0157849	-1.5218410
H	-1.4406395	1.4992833	1.3358986
H	-3.7465405	0.8185678	1.7541751
H	-3.5359199	-1.9926639	-1.5038768
H	-1.2193403	-1.2870942	-1.9577276
H	0.3097021	-2.1786034	-0.1417061
H	1.4732086	-2.7543731	1.0543332
H	2.1372188	-1.5378869	-1.6822825
H	2.3387010	-3.2379099	-1.2121940
H	0.1672374	4.2241518	-1.1606712
H	-0.2344492	2.9706341	-2.3756336
H	-1.2076881	3.1032657	-0.8695909
H	1.6449298	3.4277438	1.2833730
H	1.0260426	1.8627553	1.8774446
H	-0.1185800	3.1480576	1.3655507

5a_sy_c_5_ts2.log

E = -1184.816684

H = -1184.505944

G = -1184.573704

NImag=1

C	2.5504840	-0.3908360	-1.0159819
C	2.1290769	0.7033154	-0.0738397
C	3.0216703	-1.6596137	-0.6104022
O	3.5372136	-2.5117445	-1.3498904
C	0.7658575	0.8262045	-0.6784302
C	-0.4507258	0.0180052	-0.4004582
C	-0.9501717	-0.1991063	0.8931347
C	-2.1439860	-0.8815349	1.0863606
C	-2.8565922	-1.3521715	-0.0232057
C	-2.3827368	-1.1343736	-1.3222247
C	-1.1921505	-0.4430910	-1.4993938
O	2.9694385	-1.9932947	0.7274653
C	2.2933386	0.2674360	1.3794954
C	2.0890523	-1.2321028	1.5514891
S	0.0589325	2.9541241	-0.1986560
C	-1.5239818	2.9708152	-1.0660624
C	-0.5254997	3.0358523	1.5075985
C	-4.0937321	-2.0588017	0.1746172
N	-5.0901301	-2.6273108	0.3337589
H	2.7293492	-0.1373728	-2.0545082
H	2.6699199	1.6452300	-0.2340994
H	0.8298762	1.1180071	-1.7262930
H	-0.4160902	0.1698640	1.7615997
H	-2.5265303	-1.0455769	2.0882330
H	-2.9446407	-1.4977734	-2.1761044
H	-0.8222393	-0.2614647	-2.5045950
H	1.6279884	0.8173098	2.0536036

H	3.3199975	0.5044438	1.6792565
H	1.0623194	-1.5341745	1.3249877
H	2.3103237	-1.5304962	2.5789844
H	-1.9957826	3.9456858	-0.9258100
H	-1.3273906	2.8105355	-2.1284234
H	-2.1719036	2.1798411	-0.6788665
H	-0.9203987	4.0382989	1.6893839
H	0.3234338	2.8530105	2.1687828
H	-1.3084267	2.2936227	1.6764709

5a_sy_c_6.log

E = -1184.835378
H = -1184.523405
G = -1184.590568

NImag=0

C	-1.3323604	2.3266005	-2.8860449
C	-1.0849943	3.1390121	-1.6445567
C	-0.6442245	1.1736433	-3.2455939
O	-0.8588697	0.4222935	-4.2256338
C	-2.3549011	3.3924883	-0.7941699
C	-2.1274573	4.3390018	0.3561125
C	-1.6120109	5.6249753	0.1450373
C	-1.3785895	6.4741130	1.2189466
C	-1.6565943	6.0300284	2.5179956
C	-2.1682055	4.7476027	2.7435531
C	-2.4043504	3.9112017	1.6582439
O	0.4274801	0.7634859	-2.4382584
C	-0.0823462	2.4137482	-0.7370519
C	0.9834245	1.7649612	-1.5987093
S	-3.7160699	4.0571195	-1.8892730
C	-4.6632619	2.5661324	-2.2698896
C	-4.8619485	4.8300764	-0.7279462
C	-1.4158860	6.9049737	3.6348996
N	-1.2227524	7.6085854	4.5341799
H	-2.0526040	2.6820682	-3.6185937
H	-0.6718808	4.1332675	-1.8825744
H	-2.7583568	2.4413372	-0.4293731
H	-1.3978984	5.9779654	-0.8603244
H	-0.9848751	7.4722284	1.0583606
H	-2.3793614	4.4149279	3.7543696
H	-2.8040427	2.9147880	1.8234274
H	-0.5938971	1.6265342	-0.1668025
H	0.3763362	3.1037724	-0.0209799
H	1.7380347	1.2658871	-0.9849471
H	1.4864919	2.5253738	-2.2153621
H	-5.5151914	2.8769676	-2.8777348
H	-4.0160240	1.8929274	-2.8306577
H	-4.9939339	2.1099574	-1.3348335
H	-5.7824772	5.0139787	-1.2863568
H	-4.4364872	5.7766394	-0.3943262
H	-5.0466145	4.1578358	0.1122675

5a_sy_c_6_ts1.log

E = -1184.806080
H = -1184.496717
G = -1184.564399

NImag=1

C	-2.4968061	-0.5462128	-1.1213624
C	-1.1929055	-0.8635373	-0.7475852
C	-3.6192727	-0.9682782	-0.3305767

O	-4.7385699	-0.4593821	-0.3388923
C	-0.2444682	0.6501023	0.4881933
C	1.1546185	0.3565672	0.3148179
C	1.8754566	0.6949938	-0.8579605
C	3.1878856	0.2912166	-1.0374576
C	3.8297960	-0.4747857	-0.0522230
C	3.1340815	-0.8276244	1.1187187
C	1.8268975	-0.4159262	1.2958564
O	-3.4214952	-2.0224362	0.5193749
C	-1.0092085	-2.0538828	0.1814603
C	-2.2935729	-2.8598700	0.2237562
S	-0.8487246	2.1209298	-0.2714559
C	-2.4367385	2.3230536	0.5568827
C	0.0575908	3.5010150	0.4740121
C	5.1866518	-0.8895520	-0.2362015
N	6.2871221	-1.2272775	-0.3853646
H	-2.7016983	0.1976280	-1.8851298
H	-0.4033480	-0.6739114	-1.4735101
H	-0.6506974	0.5364773	1.4929743
H	1.4035800	1.2811639	-1.6430907
H	3.7227783	0.5641921	-1.9420175
H	3.6310919	-1.4147327	1.8848924
H	1.3006621	-0.6814264	2.2085379
H	-0.7512740	-1.7358347	1.1962351
H	-0.1941577	-2.6929537	-0.1732939
H	-2.2699746	-3.6133821	1.0129310
H	-2.4729575	-3.3578222	-0.7368182
H	-2.8527644	3.2760650	0.2258490
H	-3.0885675	1.5032153	0.2536878
H	-2.2727205	2.3219538	1.6364732
H	-0.3895297	4.4290331	0.1099452
H	1.0948568	3.4326294	0.1409610
H	-0.0084277	3.4280582	1.5609793

5a_sy_c_7.log

E = -1184.832311

H = -1184.520081

G = -1184.587041

NImag=0

C	-1.4480642	2.4867197	-2.9776071
C	-1.2224155	3.4648097	-1.8574833
C	-0.6730556	1.3585957	-3.2277874
O	-0.7488437	0.5863091	-4.2132757
C	-2.2890549	3.4186142	-0.7233624
C	-2.0439390	4.3699763	0.4277491
C	-2.0369089	3.8719486	1.7350998
C	-1.7894904	4.7125507	2.8137396
C	-1.5502107	6.0712542	2.5783495
C	-1.5544571	6.5849279	1.2760323
C	-1.7987103	5.7314733	0.2069905
O	0.3291593	1.0052167	-2.3173861
C	0.1537396	3.1780788	-1.2361680
C	0.3358721	1.6802253	-1.0680923
S	-4.0355014	3.7446083	-1.2697626
C	-3.9346264	4.8499017	-2.6905071
C	-4.6242095	2.2086073	-2.0109677
C	-1.2933096	6.9511257	3.6874703
N	-1.0869375	7.6589363	4.5805630
H	-2.1740907	2.7141126	-3.7509784
H	-1.2160425	4.4981032	-2.2325878
H	-2.3753083	2.3967610	-0.3364706

H	-2.2208718	2.8153404	1.9083989
H	-1.7804544	4.3252125	3.8271674
H	-1.3642807	7.6397290	1.1076907
H	-1.7846406	6.1366026	-0.8006242
H	0.2920331	3.6767564	-0.2716501
H	0.9262682	3.5522637	-1.9175302
H	-0.4527536	1.2636169	-0.4226002
H	1.2999255	1.4525340	-0.6050219
H	-4.9613740	4.9805691	-3.0394189
H	-3.5444322	5.8085324	-2.3456293
H	-3.3110062	4.4230289	-3.4751839
H	-5.6719497	2.3803075	-2.2677962
H	-4.5531827	1.4343756	-1.2445178
H	-4.0298758	1.9513748	-2.8850418

5a_sy_c_7_ts1.log

E = -1184.804524

H = -1184.495111

G = -1184.562002

NImag=1

C	-2.8084349	-0.3713802	-0.7374389
C	-1.4490650	-0.4204367	-1.0250359
C	-3.5143925	-1.4689042	-0.1341336
O	-4.7326932	-1.5142751	0.0285287
C	-0.2908604	0.6935367	0.4770335
C	1.1184182	0.4000589	0.3602969
C	1.6868636	-0.6442673	1.1323937
C	3.0072459	-1.0198708	0.9755064
C	3.8188142	-0.3574639	0.0359365
C	3.2791798	0.6785119	-0.7423768
C	1.9517383	1.0427887	-0.5866539
O	-2.8116162	-2.5814095	0.2390842
C	-0.8013883	-1.7730072	-0.8891676
C	-1.3816051	-2.4852742	0.3143904
S	-0.6789962	2.4208047	0.3582137
C	-1.4400609	2.7842730	-1.2491336
C	-2.1291460	2.5492037	1.4216091
C	5.1877235	-0.7403997	-0.1273303
N	6.2981878	-1.0516258	-0.2589720
H	-3.4255159	0.4839229	-0.9879184
H	-1.0442684	0.2318860	-1.7952508
H	-0.7979875	0.2858734	1.3479955
H	1.0679029	-1.1535184	1.8662827
H	3.4255036	-1.8180000	1.5811890
H	3.9027063	1.1856180	-1.4723599
H	1.5526609	1.8311380	-1.2211429
H	0.2850640	-1.7122501	-0.7961524
H	-1.0161090	-2.3474262	-1.8006894
H	-1.1167897	-1.9583457	1.2397235
H	-1.0228107	-3.5135223	0.3880862
H	-1.6515169	3.8559408	-1.2383679
H	-0.7064839	2.5663307	-2.0269082
H	-2.3568076	2.2149417	-1.3956880
H	-2.5440917	3.5508137	1.2955727
H	-1.7960806	2.4047195	2.4501335
H	-2.8513157	1.7840147	1.1311192

5a_sy_c_9.log

E = -1184.837640

H = -1184.525591

G = -1184.592128
 NImag=0

C	-1.5735531	2.0938869	-2.8071059
C	-1.2700638	3.1160834	-1.7426386
C	-0.6889057	1.1192395	-3.2573194
O	-0.9082295	0.2097370	-4.0909444
C	-2.3668507	3.2092929	-0.6579763
C	-2.1361903	4.2289299	0.4266890
C	-1.6589232	5.5166506	0.1452451
C	-1.4466984	6.4295821	1.1714217
C	-1.7113837	6.0529853	2.4932773
C	-2.1805016	4.7688771	2.7921734
C	-2.3890778	3.8672782	1.7558417
O	0.6127428	1.1066973	-2.7373463
C	0.0434932	2.7492422	-1.0420282
C	1.0408302	2.2957501	-2.0904605
S	-4.0180264	3.4406553	-1.4876482
C	-5.1173599	3.8974939	-0.1363527
C	-3.8870467	5.0043983	-2.3703940
C	-1.4912170	6.9958159	3.5578665
N	-1.3144033	7.7544672	4.4147267
H	-2.5365937	2.1073001	-3.3097147
H	-1.1500891	4.1292321	-2.1607735
H	-2.5007092	2.2168158	-0.2103003
H	-1.4333444	5.8136035	-0.8741864
H	-1.0748650	7.4253690	0.9543228
H	-2.3763707	4.4851505	3.8207544
H	-2.7511408	2.8677608	1.9802079
H	-0.1255587	1.9259175	-0.3349538
H	0.4490692	3.5989329	-0.4833224
H	2.0104909	2.0664596	-1.6404910
H	1.1867658	3.0901927	-2.8384528
H	-6.1072050	4.0377129	-0.5755156
H	-5.1412523	3.0647781	0.5695046
H	-4.7713611	4.8153525	0.3418616
H	-4.8711264	5.1903671	-2.8061870
H	-3.1495622	4.8844102	-3.1658869
H	-3.6151820	5.8090817	-1.6854938

5a_sy_c_9_ts1.log
 E = -1184.803155
 H = -1184.493226
 G = -1184.560819
 NImag=1

C	2.8316151	-0.1894853	0.8281726
C	1.4956653	-0.5831360	0.8222217
C	3.8129447	-0.8418838	0.0056767
O	4.9137698	-0.3902635	-0.2999508
C	0.3100761	0.5754436	-0.5748240
C	-1.0815400	0.2348901	-0.3790274
C	-1.8498162	0.6883689	0.7194213
C	-3.1502674	0.2522142	0.9177966
C	-3.7258302	-0.6699649	0.0310031
C	-2.9786129	-1.1489582	-1.0591078
C	-1.6860639	-0.6993483	-1.2568281
O	3.4975232	-2.0853612	-0.4768230
C	1.1858869	-1.9663616	0.2713995
C	2.4613048	-2.7849317	0.2267966
S	0.9178489	2.2090040	-0.3944328
C	-0.3151566	3.3498709	-1.0665307
C	0.8703515	2.7250319	1.3441674

C	-5.0683973	-1.1226382	0.2375209
N	-6.1564006	-1.4899601	0.4044829
H	3.1556818	0.7283257	1.3087269
H	0.8408429	-0.2196532	1.6117071
H	0.7609252	0.1940636	-1.4893158
H	-1.4236729	1.3773593	1.4401839
H	-3.7229282	0.6148982	1.7658344
H	-3.4233577	-1.8604360	-1.7480609
H	-1.1203773	-1.0603738	-2.1113354
H	0.7658187	-1.9127609	-0.7375011
H	0.4477632	-2.4733444	0.9009712
H	2.3174744	-3.7228165	-0.3126069
H	2.8175806	-3.0097744	1.2396316
H	0.0338856	4.3662312	-0.8697594
H	-0.3722636	3.1711973	-2.1412134
H	-1.2815527	3.1738204	-0.5898472
H	1.5234376	3.5973725	1.4137001
H	1.2631973	1.9245058	1.9700061
H	-0.1433872	2.9950266	1.6385653

5a_sy_c_prod_1.log

E = -706.946613
H = -706.717994
G = -706.772324

NImag=0

C	0.7643039	0.1780998	3.1539701
C	-0.6781289	0.6201365	3.2500193
C	0.2092174	1.2132561	2.1916424
C	0.0090233	0.9632760	0.7299627
C	1.0055971	0.3714197	-0.0535013
C	0.8246837	0.1979938	-1.4221788
C	-0.3671665	0.6273604	-2.0154717
C	-1.3717849	1.2317663	-1.2477845
C	-1.1757571	1.3943666	0.1169276
H	0.5622306	2.2192182	2.4072366
H	1.4895975	0.5391738	3.8741053
H	-0.9171862	1.2681149	4.0862622
C	-1.7148273	-0.4354122	2.8950123
C	-1.1745205	-1.8123302	3.2153788
O	0.0658204	-2.0665459	2.5117297
C	1.0778807	-1.1973380	2.6623513
O	2.2037915	-1.5515834	2.3825973
C	-0.5631132	0.4500911	-3.4294097
N	-0.7213723	0.3078163	-4.5680948
H	1.9345391	0.0488059	0.4062748
H	1.5986555	-0.2618076	-2.0279867
H	-2.2905699	1.5643407	-1.7196784
H	-1.9510675	1.8600911	0.7192736
H	-2.6256711	-0.2727931	3.4771748
H	-1.9923867	-0.3956190	1.8369772
H	-0.9842887	-1.9247507	4.2880565
H	-1.8461998	-2.6064471	2.8883533

5a_sy_c_prod_2.log

E = -706.949332
H = -706.720584
G = -706.774549

NImag=0

C	0.8317803	0.1980925	3.1706113
C	-0.6187913	0.6065502	3.3108037

C	0.2138028	1.2138921	2.2247404
C	0.0033266	0.9818202	0.7632509
C	0.9656235	0.3358921	-0.0196761
C	0.7565818	0.1390474	-1.3803191
C	-0.4265286	0.6043900	-1.9653353
C	-1.3917593	1.2712871	-1.1982538
C	-1.1688463	1.4566180	0.1594473
H	0.5483998	2.2255907	2.4446369
H	1.5667958	0.5822487	3.8674125
H	-0.8437834	1.2542421	4.1519743
C	-1.6378673	-0.4785058	3.0502766
C	-1.1689134	-1.5253107	2.0522159
O	0.1748672	-1.9949729	2.2932354
C	1.1464778	-1.1976931	2.7603111
O	2.2602928	-1.6660122	2.8905299
C	-0.6514610	0.4019591	-3.3714431
N	-0.8331747	0.2394243	-4.5039000
H	1.8865749	-0.0190567	0.4346192
H	1.4999057	-0.3681713	-1.9865182
H	-2.3023027	1.6318451	-1.6654749
H	-1.9150943	1.9640843	0.7643894
H	-1.8643234	-0.9654339	4.0047917
H	-2.5732208	-0.0548471	2.6678810
H	-1.7886080	-2.4202191	2.1230673
H	-1.2144545	-1.1637610	1.0234259

5a_sy_tr_1.log

E = -1184.835642

H = -1184.523458

G = -1184.590991

NImag=0

C	-2.5343048	1.1056670	-2.3585337
C	-1.0882561	1.4685243	-2.1698201
C	-3.4771947	1.8914782	-3.0068535
O	-4.6170596	1.5535922	-3.4060576
C	-0.1861546	0.3528466	-2.7566367
C	1.2968299	0.5754026	-2.5800890
C	2.0170845	1.5179371	-3.3264609
C	3.3690321	1.7247842	-3.0863267
C	4.0085314	0.9893445	-2.0805370
C	3.3039094	0.0459342	-1.3260446
C	1.9535603	-0.1582008	-1.5865025
O	-3.1537982	3.2315148	-3.2565539
C	-0.8123875	2.8563108	-2.7609847
C	-2.0327053	3.7327151	-2.5413417
S	-0.6227035	0.1130243	-4.5539614
C	0.6978081	-0.9947849	-5.1036545
C	-1.9892513	-1.0738420	-4.5575429
C	5.4085747	1.2019805	-1.8251441
N	6.5353805	1.3728187	-1.6196180
H	-2.8339535	0.0858342	-2.1337049
H	-0.7901474	1.4827317	-1.1070221
H	-0.4628671	-0.6015772	-2.2951500
H	1.5342292	2.0932908	-4.1116338
H	3.9273727	2.4497535	-3.6690067
H	3.8100918	-0.5220969	-0.5526756
H	1.4021778	-0.8950167	-1.0097303
H	-0.6442334	2.7995879	-3.8441420
H	0.0717634	3.3180191	-2.3105834
H	-1.8623309	4.7466751	-2.9125943
H	-2.2740485	3.7900666	-1.4692967

H	0.4069303	-1.3565036	-6.0917293
H	1.6256365	-0.4286286	-5.1793121
H	0.7984307	-1.8254303	-4.4016092
H	-1.9754130	-1.5485340	-5.5414836
H	-2.9131143	-0.5185719	-4.4044554
H	-1.8297196	-1.8123470	-3.7695071

5a_sy_tr_10.log

E = -1184.829851
H = -1184.517733
G = -1184.584542

NImag=0

C	-1.7822370	1.6085002	-3.5893247
C	-1.5739363	0.6298884	-2.4657057
C	-2.0357452	2.9649599	-3.4288207
O	-2.1109449	3.8437648	-4.3207665
C	-0.3399791	-0.3054218	-2.5375705
C	1.0412329	0.3053904	-2.4682238
C	1.4118953	1.4159634	-3.2400930
C	2.6864300	1.9577563	-3.1236581
C	3.6032826	1.3828715	-2.2356891
C	3.2504964	0.2715450	-1.4626815
C	1.9711445	-0.2571408	-1.5849149
O	-2.2386922	3.4585796	-2.1314842
C	-1.4828797	1.3863795	-1.1329782
C	-2.5248882	2.4885649	-1.1346040
S	-0.3404891	-1.5140262	-3.9604948
C	-2.0784654	-1.7452884	-4.3819679
C	0.2964587	-0.6607356	-5.4159134
C	4.9240918	1.9419137	-2.1166041
N	5.9868933	2.3917984	-2.0206989
H	-1.7131944	1.2779571	-4.6198995
H	-2.4222829	-0.0678959	-2.3666222
H	-0.4308375	-1.0137220	-1.7051983
H	0.6976303	1.8608665	-3.9236721
H	2.9731706	2.8197286	-3.7170114
H	3.9676874	-0.1664409	-0.7766430
H	1.6882931	-1.1157449	-0.9820043
H	-0.4968396	1.8530120	-1.0188918
H	-1.6396835	0.7089327	-0.2864911
H	-2.5368006	3.0238694	-0.1813218
H	-3.5263764	2.0655656	-1.3070257
H	-2.0952858	-2.4420919	-5.2224901
H	-2.5696311	-2.1993838	-3.5197858
H	-2.5414415	-0.7954701	-4.6515443
H	0.1071155	-1.3349178	-6.2545731
H	1.3719503	-0.5390632	-5.2838179
H	-0.1988422	0.2965357	-5.5681134

5a_sy_tr_10_ts1.log

E = -1184.806991
H = -1184.496897
G = -1184.562699

NImag=1

C	-1.0397861	-1.7672486	0.9050079
C	-1.5897365	-1.5464381	-0.3619011
C	0.3028664	-2.2360875	1.0892658
O	0.9323333	-2.2448849	2.1460955
C	-1.4342927	0.4888353	-0.9507154
C	-0.0665998	0.8388406	-0.6293417

C	0.3903864	0.9885268	0.6976863
C	1.7362451	1.1834683	0.9751320
C	2.6676928	1.2123590	-0.0700209
C	2.2399500	1.0572703	-1.4001835
C	0.8943238	0.8765728	-1.6665453
O	0.9365158	-2.7706741	-0.0082342
C	-0.8530162	-2.1645020	-1.5409116
C	0.0751060	-3.2562738	-1.0455615
S	-2.7894944	1.3666099	-0.2481322
C	-3.1732865	0.7609917	1.4154644
C	-2.2427301	3.0425858	0.1607122
C	4.0587772	1.4081862	0.2175553
N	5.1842907	1.5671724	0.4483971
H	-1.5656415	-1.4878298	1.8108475
H	-2.6729726	-1.5089807	-0.4459835
H	-1.6543118	0.4284229	-2.0156772
H	-0.3057935	0.9501252	1.5273476
H	2.0717577	1.2972763	2.0011395
H	2.9629306	1.0881017	-2.2092583
H	0.5635552	0.7687329	-2.6960362
H	-0.2497565	-1.4206095	-2.0709856
H	-1.5629570	-2.5812975	-2.2623214
H	0.7356757	-3.6097412	-1.8399599
H	-0.4954941	-4.1089248	-0.6557918
H	-3.9867291	1.3976518	1.7710284
H	-3.5296128	-0.2658386	1.3346739
H	-2.3165761	0.8357119	2.0838267
H	-3.1041461	3.5713043	0.5738774
H	-1.9224683	3.5138843	-0.7695483
H	-1.4262211	3.0129654	0.8832741

5a_sy_tr_1_r.log

E = -1184.835938

H = -1184.523828

G = -1184.590648

NImag=0

C	1.1643629	-1.6120888	-0.5364948
C	1.1837921	-0.8191296	0.7472431
C	1.0353651	-2.9946032	-0.6211840
O	0.9248181	-3.6944028	-1.6545167
C	0.2258063	0.3772034	0.5889255
C	0.6001244	1.3099545	-0.5383252
C	1.9017592	1.8136766	-0.6559241
C	2.2286999	2.6807577	-1.6905042
C	1.2455359	3.0414281	-2.6202807
C	-0.0570499	2.5415693	-2.5176746
C	-0.3716794	1.6809485	-1.4719210
O	1.0201948	-3.7377322	0.5677043
C	0.7894801	-1.7297944	1.9109762
C	1.4819275	-3.0683897	1.7304254
S	0.2040608	1.4009657	2.1664828
C	-0.6077018	2.9326582	1.6591633
C	-1.1487947	0.6746709	3.1210863
C	1.5809563	3.9364341	-3.6961333
N	1.8506967	4.6577767	-4.5609473
H	1.2458477	-1.0842017	-1.4812903
H	2.1801171	-0.4024170	0.9743671
H	-0.8074265	0.0316588	0.4698611
H	2.6705730	1.5348897	0.0592551
H	3.2352466	3.0748450	-1.7835168
H	-0.8089651	2.8253190	-3.2464093

H	-1.3807393	1.2891115	-1.3817443
H	-0.2963713	-1.8949997	1.9158812
H	1.0821384	-1.3060752	2.8794597
H	1.2759368	-3.7367443	2.5705168
H	2.5707376	-2.9205343	1.6647378
H	-0.8225960	3.4839212	2.5769359
H	0.0834730	3.5025415	1.0378771
H	-1.5287507	2.6992140	1.1209440
H	-1.3898300	1.3928894	3.9075057
H	-0.8071641	-0.2575565	3.5665289
H	-2.0076583	0.5128619	2.4671724

5a_sy_tr_1_ts1.log

E = -1184.806162
H = -1184.496800
G = -1184.564227

NImag=1

C	2.5092560	-0.9922806	1.1776231
C	1.1443464	-1.0646083	0.9074194
C	3.4926151	-1.1810589	0.1506415
O	4.6644716	-0.8078054	0.1989403
C	0.2142665	0.8780978	0.7159928
C	-1.1619423	0.5560122	0.4340058
C	-1.7280367	0.5164354	-0.8649167
C	-3.0229280	0.0733246	-1.0715085
C	-3.8071409	-0.3464068	0.0150868
C	-3.2717793	-0.3080002	1.3145978
C	-1.9789588	0.1374683	1.5158538
O	3.0975410	-1.8294949	-0.9896744
C	0.7429817	-1.7269936	-0.3999965
C	1.8860763	-2.5923165	-0.8922106
S	1.0898873	1.7678978	-0.5242446
C	0.3251228	3.4115239	-0.6109107
C	2.6268846	2.2090524	0.3107479
C	-5.1466817	-0.8013407	-0.1980444
N	-6.2330604	-1.1719520	-0.3706351
H	2.8747978	-0.6008173	2.1211842
H	0.4602882	-1.1706496	1.7465269
H	0.4309868	1.2696088	1.7090434
H	-1.1520965	0.8336817	-1.7307953
H	-3.4364309	0.0522000	-2.0750963
H	-3.8782384	-0.6245808	2.1577092
H	-1.5761060	0.1721969	2.5244288
H	0.5133115	-0.9848951	-1.1734122
H	-0.1557402	-2.3375763	-0.2693899
H	1.6968662	-2.9759207	-1.8962966
H	2.0576256	-3.4377466	-0.2145921
H	0.9093270	4.0171087	-1.3074893
H	-0.6911367	3.2838193	-0.9877163
H	0.3180941	3.8504094	0.3885850
H	3.0969485	2.9840165	-0.2978219
H	3.2709528	1.3317434	0.3592509
H	2.3946739	2.5864191	1.3086389

5a_sy_tr_1_ts2.log

E = -1184.824604
H = -1184.514229
G = -1184.581885

NImag=1

C	1.6141593	-1.5376408	-0.1735764
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C	1.6041834	-0.1506202	-0.7595291
C	2.7130879	-2.0966677	0.5147489
O	2.7238844	-3.1619037	1.1497317
C	0.5457524	0.3551267	0.1564381
C	-0.8562819	-0.1200486	0.0604032
C	-1.4330922	-0.4436721	-1.1764393
C	-2.7631791	-0.8347914	-1.2496954
C	-3.5248094	-0.9062178	-0.0757186
C	-2.9621906	-0.5874258	1.1664823
C	-1.6325927	-0.1921915	1.2249111
O	3.9209969	-1.4202796	0.4663355
C	2.9476638	0.5514758	-0.5335629
C	4.0638401	-0.4713031	-0.5908070
S	0.2242791	2.5352781	-0.4421343
C	-1.3381841	2.9453262	0.3668085
C	1.3617013	3.3873523	0.6761098
C	-4.9027543	-1.3134923	-0.1472429
N	-6.0123163	-1.6406272	-0.2045830
H	0.7432562	-2.1710851	-0.2841097
H	1.3093938	-0.1031318	-1.8150488
H	0.8859855	0.5720886	1.1695425
H	-0.8464710	-0.3861040	-2.0881832
H	-3.2138139	-1.0839847	-2.2046626
H	-3.5623760	-0.6494343	2.0680302
H	-1.1846851	0.0582623	2.1825195
H	2.9721296	1.0122090	0.4614548
H	3.1108459	1.3403851	-1.2752474
H	5.0415376	-0.0063452	-0.4474344
H	4.0635674	-0.9982041	-1.5548667
H	-1.4892704	4.0248377	0.2975421
H	-2.1415386	2.4299927	-0.1628900
H	-1.3141176	2.6338784	1.4138768
H	1.0551878	4.4333902	0.7470528
H	2.3646109	3.3328978	0.2517989
H	1.3408006	2.9212140	1.6641140

5a_sy_tr_2.log

E = -1184.831928

H = -1184.520147

G = -1184.587003

NImag=0

C	-2.4748059	1.0126693	-2.0092629
C	-1.0352686	1.4305626	-2.0606187
C	-3.5575746	1.7761475	-2.4165345
O	-4.7776560	1.4999979	-2.3137211
C	-0.1340682	0.4110825	-2.8317653
C	1.3459015	0.6295609	-2.6077602
C	2.1069196	1.5517727	-3.3369601
C	3.4493522	1.7537905	-3.0389952
C	4.0372803	1.0318291	-1.9945328
C	3.2908675	0.1059661	-1.2569835
C	1.9528327	-0.0921340	-1.5730982
O	-3.3102791	3.0245274	-3.0124756
C	-0.9272796	2.8888819	-2.5212365
C	-2.0089367	3.2204819	-3.5376543
S	-0.4598066	0.3501817	-4.6531102
C	0.6679648	-0.9683517	-5.1572011
C	-2.0263762	-0.5371825	-4.8148066
C	5.4257900	1.2389508	-1.6798350
N	6.5434206	1.4054508	-1.4261392
H	-2.7085282	0.0426381	-1.5777282

H	-0.5775065	1.3701847	-1.0594444
H	-0.4033084	-0.5937481	-2.4860489
H	1.6676471	2.1195122	-4.1531369
H	4.0378872	2.4648591	-3.6089169
H	3.7571363	-0.4534931	-0.4528723
H	1.3699541	-0.8148860	-1.0091673
H	0.0569368	3.1292495	-2.9362128
H	-1.0725622	3.5378744	-1.6505343
H	-1.8939334	2.6201161	-4.4532563
H	-1.9507296	4.2723980	-3.8314307
H	0.3848819	-1.2506270	-6.1730087
H	1.6854497	-0.5777222	-5.1519669
H	0.5638599	-1.8143782	-4.4742878
H	-2.0715140	-0.8731676	-5.8535696
H	-2.8385315	0.1525801	-4.5944875
H	-2.0337169	-1.3846755	-4.1268396

5a_sy_tr_2_r.log

E = -1184.835127

H = -1184.523168

G = -1184.590051

NImag=0

C	1.6305501	-1.5432799	1.7938299
C	1.0657801	-1.1214724	0.4629129
C	2.9862911	-1.7040609	2.0669256
O	3.5074279	-2.1536286	3.1139111
C	0.4425178	0.2877805	0.6255290
C	-0.7151999	0.3117447	1.5937969
C	-1.7888233	-0.5775380	1.4571219
C	-2.8506610	-0.5416751	2.3516741
C	-2.8357658	0.3898694	3.3973484
C	-1.7694876	1.2829242	3.5470208
C	-0.7171632	1.2397684	2.6391796
O	3.9219959	-1.3553430	1.0821878
C	2.1737691	-1.1933374	-0.5875562
C	3.4511536	-0.5978672	-0.0234343
S	-0.1691459	0.9433058	-1.0368890
C	-1.3825989	2.2110500	-0.6081013
C	1.1918877	2.0258969	-1.5350169
C	-3.9321144	0.4291280	4.3287638
N	-4.8149048	0.4612633	5.0775584
H	0.9458029	-1.8202312	2.5893057
H	0.2538559	-1.7893183	0.1431313
H	1.1966376	1.0202299	0.9295344
H	-1.8085565	-1.3018907	0.6474713
H	-3.6847419	-1.2273258	2.2463724
H	-1.7685357	1.9988239	4.3622188
H	0.1142217	1.9306252	2.7456409
H	1.9059357	-0.7115890	-1.5342829
H	2.3567033	-2.2485150	-0.8198417
H	3.2913539	0.4463256	0.2878553
H	4.2550840	-0.6075196	-0.7644645
H	-1.5980539	2.7526607	-1.5317076
H	-2.2866603	1.7194449	-0.2480919
H	-0.9661806	2.8807668	0.1468670
H	0.8579981	2.5643129	-2.4240543
H	2.0620260	1.4171788	-1.7790502
H	1.4122060	2.7182494	-0.7201988

5a_sy_tr_2_ts1.log

E = -1184.807952
H = -1184.498735
G = -1184.566051

NImag=1

C	2.4804792	-1.0822186	1.1709332
C	1.1581328	-1.1382210	0.7336147
C	3.5951717	-1.3610025	0.3187076
O	4.7705797	-1.4187189	0.6809792
C	0.1871321	0.7682855	0.6443218
C	-1.2053508	0.4428636	0.4000061
C	-1.8289780	0.5004379	-0.8697846
C	-3.1299825	0.0641896	-1.0528343
C	-3.8567657	-0.4570268	0.0296620
C	-3.2594524	-0.5295822	1.2979959
C	-1.9607889	-0.0845497	1.4753367
O	3.3603412	-1.6481656	-1.0035279
C	0.9385688	-1.7348977	-0.6318836
C	2.0743539	-1.3349405	-1.5509581
S	0.8871173	1.9270818	-0.4807417
C	0.2825998	3.5537088	0.0467889
C	2.6018667	2.0671079	0.0569322
C	-5.2017848	-0.9099783	-0.1588345
N	-6.2913635	-1.2786120	-0.3118394
H	2.7245124	-0.8420659	2.2001267
H	0.3878038	-1.3482736	1.4743394
H	0.4268986	1.0529302	1.6694335
H	-1.2915743	0.8891582	-1.7306677
H	-3.5899996	0.1216950	-2.0343726
H	-3.8206409	-0.9281156	2.1376096
H	-1.5114847	-0.1302548	2.4637060
H	-0.0129762	-1.4247125	-1.0741016
H	0.9085589	-2.8279577	-0.5302781
H	2.0366546	-0.2585094	-1.7678758
H	2.0241377	-1.8641264	-2.5043924
H	0.7723072	4.3138758	-0.5664201
H	-0.7950635	3.5696244	-0.1255407
H	0.5113866	3.6906832	1.1056883
H	2.9905260	2.9839026	-0.3901649
H	3.1631083	1.2108976	-0.3136671
H	2.6402066	2.1177715	1.1468006

5a_sy_tr_3.log

E = -1184.829438
H = -1184.517166
G = -1184.582809

NImag=0

C	-2.4412621	0.9181962	-2.3090576
C	-0.9901465	1.2665962	-2.1376807
C	-3.3594710	1.6841626	-3.0063544
O	-4.5094344	1.3677648	-3.3952553
C	-0.0518263	0.1629160	-2.7077196
C	1.4162868	0.4706508	-2.5200441
C	2.1624891	1.2165763	-3.4395895
C	3.4926358	1.5270022	-3.1846533
C	4.0811453	1.0967032	-1.9899197
C	3.3466841	0.3552482	-1.0575876
C	2.0208156	0.0438861	-1.3321665
O	-2.9758923	2.9934929	-3.3502820
C	-0.6690327	2.6715796	-2.6747796
C	-1.9123041	3.5372403	-2.5780553
S	-0.3338253	-0.4067479	-4.4555668

C	-1.7775882	-1.4888855	-4.3595924
C	-1.0028223	0.9261506	-5.4773201
C	5.4568232	1.4186757	-1.7191609
N	6.5642788	1.6778736	-1.5007696
H	-2.7602188	-0.0779896	-2.0156077
H	-0.7018832	1.2467927	-1.0725140
H	-0.2832010	-0.7675077	-2.1754655
H	1.7180612	1.5715296	-4.3657109
H	4.0705689	2.1011534	-3.9009807
H	3.8131242	0.0224125	-0.1363311
H	1.4475727	-0.5396942	-0.6173475
H	-0.3542349	2.6491086	-3.7220432
H	0.1500544	3.1269944	-2.1086704
H	-1.7264709	4.5390019	-2.9746606
H	-2.2323143	3.6314247	-1.5299847
H	-1.8334897	-2.0020169	-5.3221096
H	-1.5986435	-2.2134424	-3.5633583
H	-2.6690229	-0.8935426	-4.1645210
H	-1.3209891	0.4317049	-6.3985310
H	-0.2055658	1.6340325	-5.7046085
H	-1.8472006	1.4038563	-4.9807003

5a_sy_tr_3_r.log

E = -1184.832276

H = -1184.520027

G = -1184.586730

NImag=0

C	-1.2508732	-1.5248803	0.3096274
C	-1.0349048	-0.7479829	-0.9716573
C	-1.0595826	-2.8939805	0.4640932
O	-1.1137686	-3.5624275	1.5228888
C	-0.1183687	0.4439147	-0.6389465
C	-0.6301121	1.3508278	0.4626285
C	-1.9736623	1.7405718	0.5119809
C	-2.4235352	2.5884787	1.5171964
C	-1.5203985	3.0476353	2.4828206
C	-0.1746271	2.6644572	2.4464332
C	0.2612933	1.8200784	1.4327452
O	-0.7758110	-3.6590773	-0.6748211
C	-0.4206991	-1.6734512	-2.0255538
C	-1.0663289	-3.0425567	-1.9183465
S	0.2753958	1.6382657	-2.0357334
C	1.4523253	0.8044626	-3.1212246
C	-1.2064684	1.7158059	-3.0594266
C	-1.9825698	3.9223255	3.5277347
N	-2.3543910	4.6274889	4.3677464
H	-1.5384359	-0.9870236	1.2065085
H	-1.9770811	-0.3432857	-1.3757491
H	0.8817272	0.0785160	-0.3767781
H	-2.6813168	1.3758265	-0.2268798
H	-3.4648034	2.8901849	1.5593859
H	0.5147080	3.0229032	3.2035876
H	1.3037684	1.5157448	1.3972940
H	0.6595738	-1.7800473	-1.8578457
H	-0.5743023	-1.2964516	-3.0414611
H	-0.6879221	-3.7169088	-2.6910827
H	-2.1567552	-2.9536024	-2.0409348
H	1.8214436	1.5698325	-3.8070807
H	2.2727683	0.4424102	-2.4988480
H	0.9799291	-0.0078132	-3.6698692
H	-0.9740538	2.4027000	-3.8762438

H	-2.0121259	2.1302239	-2.4510013
H	-1.4649690	0.7298434	-3.4460963

5a_sy_tr_3_ts1.log

E = -1184.802698
H = -1184.493263
G = -1184.560344

NImag=1

C	-2.4413998	-0.8387593	-1.2570439
C	-1.0797471	-0.9344211	-0.9801684
C	-3.4433401	-1.1322085	-0.2751906
O	-4.6293830	-0.8135653	-0.3295879
C	-0.1364346	0.9928467	-0.7015663
C	1.2460731	0.6834556	-0.4361296
C	1.8164202	0.6872485	0.8604423
C	3.1158190	0.2606026	1.0753122
C	3.8912282	-0.2036813	0.0003958
C	3.3448973	-0.2240656	-1.2953015
C	2.0513210	0.2148843	-1.5057968
O	-3.0414844	-1.8250317	0.8400556
C	-0.6721179	-1.7022797	0.2657799
C	-1.8260093	-2.5796309	0.7138984
S	-0.9030528	2.1524373	0.4054455
C	-2.3069963	2.6877274	-0.5917696
C	-1.7738454	1.2373856	1.7076065
C	5.2319706	-0.6513675	0.2212109
N	6.3198331	-1.0151548	0.3989906
H	-2.7955071	-0.4023426	-2.1850271
H	-0.3952661	-0.9811195	-1.8238601
H	-0.3715264	1.3119590	-1.7145676
H	1.2386581	1.0233731	1.7186906
H	3.5365746	0.2775782	2.0759563
H	3.9456191	-0.5764107	-2.1283484
H	1.6420761	0.2121090	-2.5124631
H	-0.3869084	-1.0303149	1.0811348
H	0.1999085	-2.3310740	0.0587600
H	-1.6440902	-3.0118935	1.6994617
H	-1.9959660	-3.3920413	-0.0031688
H	-2.9298771	3.3275190	0.0350096
H	-1.9127555	3.2564975	-1.4350919
H	-2.8580510	1.8087289	-0.9307858
H	-2.3562449	1.9824267	2.2545487
H	-1.0276396	0.8006359	2.3727140
H	-2.4224351	0.4721588	1.2859520

5a_sy_tr_3_ts2.log

E = -1184.822244
H = -1184.511826
G = -1184.579416

NImag=1

C	-1.3637638	-1.6247122	0.3908957
C	-1.5115115	-0.1499863	0.6713906
C	-2.3603517	-2.4114034	-0.2234149
O	-2.2337865	-3.5680858	-0.6541278
C	-0.5176904	0.2627862	-0.3638708
C	0.9302978	-0.0510581	-0.2108544
C	1.5181003	-0.1999743	1.0529348
C	2.8785388	-0.4556271	1.1701110
C	3.6607715	-0.5603761	0.0137535
C	3.0885544	-0.4065574	-1.2559861

C	1.7292043	-0.1494312	-1.3586603
O	-3.6307669	-1.8683864	-0.3357062
C	-2.9293999	0.3405403	0.3488262
C	-3.9190055	-0.7884031	0.5514082
S	-0.2693204	2.5086570	-0.4103006
C	-1.7983938	3.2238033	-1.0592452
C	-0.4285420	2.9209272	1.3405679
C	5.0687881	-0.8296423	0.1307220
N	6.2027178	-1.0460801	0.2254429
H	-0.4351607	-2.1253624	0.6315439
H	-1.2135640	0.1398719	1.6849205
H	-0.8889015	0.1987842	-1.3861823
H	0.9158002	-0.1278914	1.9530774
H	3.3345774	-0.5760445	2.1471198
H	3.7055735	-0.4902299	-2.1443572
H	1.2751193	-0.0266595	-2.3382713
H	-2.9930528	0.6549334	-0.6995542
H	-3.2004815	1.1981877	0.9728346
H	-4.9378701	-0.4706750	0.3194540
H	-3.8917858	-1.1524455	1.5874872
H	-1.6714172	4.3073477	-1.1142426
H	-1.9548626	2.8243724	-2.0631993
H	-2.6434598	2.9771329	-0.4164159
H	-0.3697714	4.0061748	1.4488416
H	0.4064246	2.4593915	1.8718177
H	-1.3794413	2.5540407	1.7322928

5a_sy_tr_4.log

E = -1184.837388

H = -1184.525564

G = -1184.593467

NImag=0

C	-1.9424081	1.6498870	-3.4996462
C	-1.6675642	0.4430872	-2.6537257
C	-2.0605849	2.9526397	-3.0262604
O	-2.4315863	3.9675014	-3.6620845
C	-0.3822541	-0.3658877	-3.0392707
C	0.9365795	0.3071747	-2.7693614
C	1.3945401	1.3852478	-3.5396694
C	2.5745628	2.0382260	-3.2040651
C	3.3038292	1.6104592	-2.0885310
C	2.8671626	0.5245921	-1.3201720
C	1.6896428	-0.1242769	-1.6715798
O	-1.7668148	3.2087899	-1.6815501
C	-1.6145001	0.8329043	-1.1691747
C	-1.0203332	2.2202013	-0.9860195
S	-0.4467326	-0.7707772	-4.8361408
C	0.7398437	-2.1252969	-4.9211967
C	-2.0015483	-1.6688851	-4.9871752
C	4.5242306	2.2862979	-1.7357322
N	5.5065119	2.8300791	-1.4515430
H	-2.2260109	1.5078118	-4.5405025
H	-2.4713479	-0.3007994	-2.7541587
H	-0.4092326	-1.3379604	-2.5324179
H	0.8256349	1.7295937	-4.3971675
H	2.9276330	2.8758226	-3.7964147
H	3.4468323	0.1943640	-0.4646389
H	1.3446997	-0.9684791	-1.0814516
H	-1.0470430	0.1043714	-0.5776697
H	-2.6381529	0.8446467	-0.7784962
H	0.0246963	2.2525951	-1.3212044

H	-1.0443306	2.5098347	0.0685354
H	0.7093652	-2.5195701	-5.9383767
H	1.7284544	-1.7112781	-4.7146310
H	0.4731296	-2.8936090	-4.1929537
H	-1.9763868	-2.1729812	-5.9552866
H	-2.8166591	-0.9443706	-4.9700540
H	-2.0906583	-2.3922560	-4.1741128

5a_sy_tr_4_ts1.log

E = -1184.811847
H = -1184.502383
G = -1184.569146

NImag=1

C	-1.5734151	1.8195500	-0.3779902
C	-1.5919012	1.1941249	0.8622312
C	-0.5651239	2.7672401	-0.7645088
O	-0.5814191	3.4226213	-1.8059233
C	-1.1786842	-0.9562096	0.6851123
C	0.2145247	-1.0473755	0.3424407
C	0.7111170	-0.7353868	-0.9497095
C	2.0730649	-0.6705736	-1.1959649
C	2.9899959	-0.9193601	-0.1633215
C	2.5203704	-1.2501391	1.1227040
C	1.1621939	-1.3162852	1.3639965
O	0.4387394	3.0547241	0.1183534
C	-0.5512575	1.6294472	1.8607783
C	0.7097870	2.1134148	1.1647654
S	-2.2872486	-1.4303965	-0.5925837
C	-2.4324431	-3.2297167	-0.4547631
C	-3.9136468	-0.9460529	0.0166287
C	4.3960356	-0.8544748	-0.4205174
N	5.5370402	-0.8016697	-0.6272830
H	-2.3825674	1.6919706	-1.0910574
H	-2.5451923	0.8993035	1.2915108
H	-1.4821552	-1.3599877	1.6519202
H	0.0256350	-0.5310617	-1.7664267
H	2.4348460	-0.4207681	-2.1888106
H	3.2291059	-1.4568702	1.9187634
H	0.8060179	-1.5723141	2.3580280
H	-0.2895357	0.8239354	2.5548542
H	-0.9830594	2.4424568	2.4600270
H	1.2674427	1.2780303	0.7321904
H	1.3645515	2.6361604	1.8650787
H	-3.1774219	-3.5689931	-1.1777964
H	-1.4550191	-3.6500296	-0.6983695
H	-2.7241955	-3.4889926	0.5648223
H	-4.6469865	-1.5129740	-0.5602215
H	-4.0539452	0.1197008	-0.1654148
H	-3.9929270	-1.1844965	1.0793189

5a_sy_tr_5.log

E = -1184.836886
H = -1184.525105
G = -1184.592249

NImag=0

C	-1.7464629	1.7882924	-3.5381086
C	-1.5468922	0.6007643	-2.6387351
C	-2.0394334	3.0755451	-3.1027881
O	-2.1251100	4.1200893	-3.7905495
C	-0.3114120	-0.2766022	-2.9799273

C	1.0407280	0.3433543	-2.7364361
C	1.5049421	1.4367146	-3.4799732
C	2.7389685	2.0089322	-3.1909325
C	3.5157465	1.4827193	-2.1527779
C	3.0690110	0.3841190	-1.4088298
C	1.8355608	-0.1799917	-1.7101088
O	-2.2742341	3.2799187	-1.7349085
C	-1.4417669	1.0694155	-1.1849746
C	-2.5149387	2.1179274	-0.9535226
S	-0.3838199	-0.7755866	-4.7576953
C	0.7637527	-2.1649987	-4.7711016
C	-1.9661065	-1.6310297	-4.8575898
C	4.7929859	2.0730118	-1.8513795
N	5.8211107	2.5472388	-1.6078091
H	-1.6241387	1.6796312	-4.6131839
H	-2.3929053	-0.1063453	-2.6770823
H	-0.3827029	-1.2223606	-2.4296898
H	0.9057811	1.8472313	-4.2858953
H	3.0996760	2.8565353	-3.7640304
H	3.6826995	-0.0201611	-0.6106489
H	1.4805103	-1.0321432	-1.1373748
H	-0.4663705	1.5335684	-0.9959122
H	-1.5643994	0.2322876	-0.4887887
H	-2.5281539	2.4493219	0.0881942
H	-3.5064117	1.7073025	-1.1983301
H	0.7044893	-2.6233131	-5.7600194
H	1.7667903	-1.7673133	-4.6070871
H	0.4878561	-2.8761969	-3.9901204
H	-1.9674227	-2.1782894	-5.8023234
H	-2.7555731	-0.8783044	-4.8652203
H	-2.0704539	-2.3135850	-4.0117392

5a_sy_tr_5_ts1.log

E = -1184.809270

H = -1184.499904

G = -1184.567367

NImag=1

C	1.0911601	-1.9098311	-0.7215559
C	1.4748160	-1.4922164	0.5523002
C	-0.2497405	-2.3320583	-1.0142122
O	-0.7334804	-2.4873113	-2.1339248
C	1.3868303	0.6710167	0.6888558
C	0.0012694	0.9631606	0.4157176
C	-0.5672059	0.8184072	-0.8733514
C	-1.9332832	0.9461328	-1.0713403
C	-2.7787306	1.2239039	0.0118441
C	-2.2369703	1.3828877	1.3005595
C	-0.8741830	1.2551572	1.4917400
O	-1.0582209	-2.6301214	0.0560898
C	0.5656603	-1.8630549	1.7084084
C	-0.3833790	-2.9653865	1.2751336
S	2.4996317	1.1835407	-0.5740447
C	2.8104797	2.9380250	-0.2544857
C	4.0883386	0.4955940	-0.0714491
C	-4.1893453	1.3591675	-0.1944733
N	-5.3327777	1.4689892	-0.3594430
H	1.7521707	-1.7996832	-1.5761608
H	2.5342796	-1.4473737	0.7837388
H	1.7624316	0.9368077	1.6783776
H	0.0631442	0.5987858	-1.7287611
H	-2.3530261	0.8235938	-2.0651159

H	-2.8897995	1.6103056	2.1375389
H	-0.4597431	1.3834395	2.4881056
H	-0.0228558	-1.0065099	2.0508763
H	1.1588641	-2.2093352	2.5608660
H	-1.1700395	-3.1295810	2.0142632
H	0.1601626	-3.9068277	1.1241936
H	3.5499892	3.2907275	-0.9767602
H	1.8644722	3.4627057	-0.4000759
H	3.1687951	3.0582822	0.7697800
H	4.8593356	1.0692340	-0.5891728
H	4.1348900	-0.5453898	-0.3904965
H	4.2007539	0.5877341	1.0109528

5a_sy_tr_6.log

E = -1184.829806
H = -1184.517629
G = -1184.583446

NImag=0

C	-1.9247911	1.5323564	-3.5293490
C	-1.6800134	0.4662212	-2.5062956
C	-1.9640616	2.8980700	-3.2748114
O	-2.2683483	3.8141063	-4.0767993
C	-0.4035032	-0.4188737	-2.6719260
C	0.9395386	0.2577984	-2.5573946
C	1.3277207	1.3098139	-3.4014111
C	2.5421200	1.9565212	-3.2073083
C	3.3781470	1.5545384	-2.1590334
C	3.0075784	0.5060086	-1.3099771
C	1.7928640	-0.1361230	-1.5191711
O	-1.6639136	3.3610577	-1.9879836
C	-1.6664461	1.0865574	-1.0981795
C	-1.0185008	2.4614521	-1.0974431
S	-0.3929369	-1.5109887	-4.1785960
C	-2.1297666	-1.9056112	-4.4610461
C	-0.0143766	-0.5199883	-5.6378010
C	4.6336776	2.2271389	-1.9534156
N	5.6439461	2.7684550	-1.7875032
H	-2.2221739	1.2443411	-4.5332710
H	-2.4967840	-0.2686941	-2.5065094
H	-0.4527071	-1.1981196	-1.9012752
H	0.6684538	1.6473844	-4.1915831
H	2.8394635	2.7734017	-3.8564729
H	3.6623604	0.2017612	-0.5003546
H	1.4971358	-0.9471469	-0.8597888
H	-1.1518990	0.4414763	-0.3755168
H	-2.7041153	1.1938365	-0.7625387
H	0.0464816	2.3972394	-1.3537856
H	-1.0949093	2.9146010	-0.1045087
H	-2.1500386	-2.6008416	-5.3025401
H	-2.5102737	-2.4012010	-3.5661149
H	-2.6969141	-1.0026950	-4.6905650
H	-0.2338447	-1.1706136	-6.4879665
H	1.0514780	-0.2920254	-5.6235528
H	-0.6245477	0.3814853	-5.6683112

5a_sy_tr_6_ts1.log

E = -1184.807480
H = -1184.497684
G = -1184.564358

NImag=1

C	-1.4932734	1.9641568	-0.0146113
C	-1.7025253	1.2533344	1.1646581
C	-0.4192076	2.8997758	-0.1933890
O	-0.2757763	3.6236053	-1.1793700
C	-1.2062486	-0.8469514	0.9709141
C	0.0941236	-0.9158598	0.3381748
C	0.3113966	-0.4973150	-0.9930514
C	1.5919060	-0.4478936	-1.5283214
C	2.6925026	-0.8088957	-0.7407494
C	2.5009819	-1.2319586	0.5874680
C	1.2218248	-1.2837704	1.1094250
O	0.4676430	3.0905371	0.8300620
C	-0.8210352	1.6352453	2.3307379
C	0.5463492	2.0807109	1.8430238
S	-2.6003276	-1.6193310	0.2214092
C	-3.3358392	-0.5692381	-1.0580310
C	-2.0095273	-2.9768983	-0.8191855
C	4.0147108	-0.7542576	-1.2914910
N	5.0856525	-0.7105701	-1.7350940
H	-2.1883156	1.9139692	-0.8444775
H	-2.7196883	0.9701200	1.4262589
H	-1.2258649	-1.1767655	2.0086884
H	-0.5246385	-0.1992549	-1.6155222
H	1.7445116	-0.1211337	-2.5523058
H	3.3555543	-1.5195143	1.1920140
H	1.0745502	-1.6068061	2.1365827
H	-0.6956878	0.8134641	3.0416907
H	-1.3086731	2.4594361	2.8689717
H	1.1121832	1.2360463	1.4386474
H	1.1257348	2.5250516	2.6549634
H	-4.1270030	-1.1754154	-1.5056360
H	-3.7806791	0.3020391	-0.5773611
H	-2.6082135	-0.2824191	-1.8163771
H	-2.8880211	-3.4517510	-1.2609526
H	-1.4877465	-3.6805724	-0.1687961
H	-1.3440703	-2.5987462	-1.5967199

5a_sy_tr_7.log

E = -1184.833221

H = -1184.521161

G = -1184.587679

NImag=0

C	-2.1448090	1.5482310	-3.3851417
C	-1.7900185	0.4730408	-2.4031712
C	-2.2641098	2.8996874	-3.0868966
O	-2.6799483	3.8153966	-3.8371535
C	-0.4980570	-0.3481851	-2.7092159
C	0.8403043	0.3318025	-2.6301344
C	1.1547254	1.4820441	-3.3713183
C	2.3898326	2.1004723	-3.2228189
C	3.3234666	1.5707952	-2.3237834
C	3.0281221	0.4251413	-1.5776010
C	1.7907017	-0.1868205	-1.7404983
O	-1.9149753	3.3432328	-1.8046385
C	-1.7146481	1.0526431	-0.9833478
C	-1.1521430	2.4646169	-0.9890051
S	-0.7678867	-1.2507800	-4.3124258
C	-0.0866653	-0.2634496	-5.6579782
C	0.4866277	-2.5410906	-4.2114067
C	4.6030055	2.2103965	-2.1677282
N	5.6332123	2.7243105	-2.0420824

H	-2.4839986	1.2581339	-4.3769998
H	-2.5698524	-0.3044810	-2.3879192
H	-0.4910559	-1.2036826	-2.0215800
H	0.4237673	1.9085492	-4.0480112
H	2.6305476	2.9913784	-3.7933913
H	3.7581804	0.0224170	-0.8834649
H	1.5551718	-1.0762801	-1.1623921
H	-1.1103507	0.4208213	-0.3209823
H	-2.7293013	1.0867330	-0.5708620
H	-0.1074795	2.4700612	-1.3248154
H	-1.1808087	2.8891630	0.0189158
H	-0.2324310	-0.8614761	-6.5607233
H	-0.6551508	0.6638825	-5.7299332
H	0.9748230	-0.0778682	-5.4892106
H	0.4752275	-3.0771134	-5.1623146
H	0.2082622	-3.2145426	-3.3993780
H	1.4649121	-2.0888809	-4.0341919

5a_sy_tr_8.log

E = -1184.833795
H = -1184.521780
G = -1184.589014

NImag=0

C	-2.0082116	1.6006974	-3.4600673
C	-1.6656051	0.6234031	-2.3682229
C	-2.2825154	2.9475575	-3.2690926
O	-2.4743500	3.8287322	-4.1409627
C	-0.4201954	-0.2656774	-2.6266551
C	0.9505127	0.3553758	-2.5722466
C	1.2457470	1.5853084	-3.1801273
C	2.5202406	2.1289888	-3.0848575
C	3.5149165	1.4394357	-2.3797718
C	3.2377198	0.2131338	-1.7674464
C	1.9567721	-0.3178295	-1.8676831
O	-2.3600559	3.4273287	-1.9515431
C	-1.4795775	1.3634778	-1.0395609
C	-2.5401964	2.4445818	-0.9414134
S	-0.7033436	-1.1901917	-4.2229397
C	0.2189304	-0.3231245	-5.5075823
C	0.3517158	-2.6357576	-4.0106170
C	4.8361459	2.0012985	-2.2808206
N	5.8994775	2.4530728	-2.2005842
H	-2.0549230	1.2576743	-4.4906226
H	-2.4746213	-0.1125473	-2.2169048
H	-0.4506234	-1.0976968	-1.9122759
H	0.4694023	2.1171234	-3.7201603
H	2.7476926	3.0815750	-3.5519673
H	4.0135238	-0.3116044	-1.2199478
H	1.7337691	-1.2656992	-1.3852261
H	-0.4987158	1.8513557	-0.9998413
H	-1.5502155	0.6731755	-0.1917912
H	-2.4804471	2.9735624	0.0135679
H	-3.5446887	2.0034399	-1.0307198
H	0.0559188	-0.8929272	-6.4250921
H	-0.1916944	0.6810277	-5.6146667
H	1.2792596	-0.2969683	-5.2514767
H	0.3181454	-3.1952358	-4.9476024
H	-0.0640339	-3.2370434	-3.2007536
H	1.3728241	-2.3192232	-3.7881249

5a_sy_tr_9.log

E = -1184.825549
H = -1184.513189
G = -1184.578730

NImag=0

C	-2.4313921	1.1600003	-1.9699324
C	-1.0267526	1.6320953	-2.2534167
C	-3.5529588	1.5424304	-2.6872126
O	-4.6820435	0.9980099	-2.7187588
C	-0.1078459	0.4105069	-2.5180654
C	1.3893841	0.6101025	-2.4042851
C	2.0653076	1.6431713	-3.0672042
C	3.4351549	1.8084679	-2.9050228
C	4.1410336	0.9300839	-2.0745948
C	3.4840297	-0.1105024	-1.4102977
C	2.1130116	-0.2617997	-1.5814549
O	-3.4413573	2.6726292	-3.5120697
C	-1.0252006	2.7308614	-3.3278320
C	-2.3260732	3.5100057	-3.2468774
S	-0.4036224	-0.6082861	-4.0674933
C	-2.0965509	-0.3800688	-4.6690276
C	0.5411820	0.1299453	-5.4174578
C	5.5603258	1.0990467	-1.9049174
N	6.7022749	1.2347890	-1.7693662
H	-2.5446409	0.2768457	-1.3457441
H	-0.5561081	2.0520309	-1.3469735
H	-0.3862638	-0.3391729	-1.7707023
H	1.5334983	2.3184449	-3.7273331
H	3.9571306	2.6091831	-3.4180852
H	4.0398983	-0.7866834	-0.7696100
H	1.5961776	-1.0656793	-1.0648482
H	-0.9520439	2.3136508	-4.3373240
H	-0.1874911	3.4211181	-3.1963740
H	-2.3524947	4.3042401	-3.9977206
H	-2.4345762	3.9667168	-2.2520560
H	-2.1417745	-0.9849833	-5.5785050
H	-2.7833923	-0.7657292	-3.9171079
H	-2.3049367	0.6672882	-4.8850784
H	0.2523575	-0.4326812	-6.3082924
H	1.6003509	-0.0307066	-5.2173828
H	0.3128019	1.1877284	-5.5432758

5a_sy_tr_9_ts1.log

E = -1184.803884
H = -1184.494072
G = -1184.561259

NImag=1

C	-2.6588743	-0.8225369	-1.2146885
C	-1.2936033	-1.0383330	-1.0102089
C	-3.6185533	-0.9388129	-0.1584487
O	-4.7741418	-0.5194767	-0.1725297
C	-0.1850232	0.7961217	-0.9656154
C	1.1698127	0.4884921	-0.5650135
C	1.6845580	0.5839956	0.7492362
C	2.9639784	0.1482599	1.0548294
C	3.7763190	-0.4126959	0.0584692
C	3.2882698	-0.5234872	-1.2549150
C	2.0154138	-0.0758593	-1.5548033
O	-3.2148251	-1.5872014	0.9869987
C	-0.8856981	-1.7213674	0.2843524
C	-2.0817355	-2.4587170	0.8565555

S	-1.2045839	2.0001795	-0.2015344
C	-1.6860345	1.4638560	1.4572447
C	-0.1949351	3.4457142	0.2102259
C	5.0958596	-0.8664916	0.3780803
N	6.1653100	-1.2353748	0.6366476
H	-3.0288383	-0.4318423	-2.1566151
H	-0.6778960	-1.2490248	-1.8807928
H	-0.3136226	0.9537413	-2.0341210
H	1.0890264	0.9999052	1.5534359
H	3.3385299	0.2369460	2.0698839
H	3.9148812	-0.9528117	-2.0305818
H	1.6501129	-0.1550719	-2.5751912
H	-0.5181102	-1.0018540	1.0238168
H	-0.0707243	-2.4297214	0.1054494
H	-1.8798257	-2.8331778	1.8617981
H	-2.3628599	-3.3019592	0.2138631
H	-2.3415346	2.2507658	1.8374696
H	-2.2488247	0.5344581	1.3750880
H	-0.8256128	1.3437397	2.1135965
H	-0.8518995	4.1711088	0.6953240
H	0.1816319	3.8506298	-0.7302831
H	0.6277494	3.1690598	0.8705083

5a_sy_tr_prod_1.log

E = -706.950863

H = -706.722074

G = -706.776810

NImag=0

C	0.5069355	-2.1959269	-0.0494030
C	-0.5953520	-2.2416657	0.9669502
C	-0.7077059	-1.2818370	-0.1858861
C	-0.5469012	0.1842108	-0.0097715
C	-1.3069952	1.0500693	-0.8075423
C	-1.1995862	2.4283035	-0.6711124
C	-0.3175617	2.9561368	0.2787118
C	0.4511999	2.1056391	1.0848041
C	0.3333266	0.7307192	0.9364325
H	-1.4235317	-1.5626358	-0.9551021
H	1.4476453	-1.7090585	0.1855681
H	-0.3664252	-1.8054201	1.9349535
C	-1.4597432	-3.4945176	0.9537071
C	-0.6522009	-4.6624531	0.4284595
O	-0.1222553	-4.3860205	-0.8915762
C	0.6286465	-3.2848012	-1.0617672
O	1.3393818	-3.1978127	-2.0397831
C	-0.1990730	4.3805005	0.4282579
N	-0.1038351	5.5289434	0.5491077
H	-1.9900617	0.6361935	-1.5436319
H	-1.7912559	3.0926351	-1.2925133
H	1.1328948	2.5240987	1.8181525
H	0.9375124	0.0837823	1.5665670
H	-1.8005687	-3.7307725	1.9650496
H	-2.3475702	-3.3514402	0.3288625
H	0.1892178	-4.8905040	1.0914250
H	-1.2575376	-5.5601662	0.3015800

5a_sy_tr_prod_2.log

E = -706.954244

H = -706.725206

G = -706.779210

NImag=0

C	0.1099381	-2.1895452	1.0736431
C	-1.3087383	-2.1875806	0.5796610
C	-0.2971978	-1.3377798	-0.1297723
C	-0.2908471	0.1422005	0.0170194
C	-0.7080152	0.7788416	1.1954929
C	-0.6922198	2.1629909	1.2980704
C	-0.2547187	2.9316451	0.2112712
C	0.1644799	2.3132133	-0.9722513
C	0.1435392	0.9269274	-1.0594399
H	0.0471643	-1.6756798	-1.1019079
H	0.3672043	-1.6458382	1.9758407
H	-2.0293177	-1.6655295	1.2028148
C	-1.7778323	-3.4779797	-0.0511006
C	-0.6523087	-4.1761415	-0.7919533
O	0.5294520	-4.3527418	0.0218094
C	0.9384244	-3.4089114	0.8844647
O	1.9580623	-3.6026041	1.5145225
C	-0.2364374	4.3651737	0.3133434
N	-0.2217012	5.5208206	0.3955766
H	-1.0497978	0.1968354	2.0467164
H	-1.0155870	2.6510799	2.2116907
H	0.5030779	2.9142815	-1.8098569
H	0.4690025	0.4433001	-1.9758423
H	-2.1631511	-4.1362304	0.7351540
H	-2.5884569	-3.2954885	-0.7636618
H	-0.9441375	-5.1865686	-1.0791239
H	-0.3636803	-3.6368908	-1.6981810

5b.log

E = -383.756315
H = -383.614988
G = -383.654836

NImag=0

C	-0.5543808	-2.8305788	-0.3237583
C	-0.0966583	-1.4108977	-0.1016110
C	1.4261135	-1.3511223	-0.1323697
C	1.9614055	-2.3131699	0.9031749
O	1.5239881	-3.6722632	0.6666735
C	0.3171077	-3.9591022	0.1571711
O	-0.0055399	-5.1267600	0.0770339
C	-1.6837240	-3.1571902	-0.9569658
H	-0.4406024	-1.0676466	0.8832050
H	-0.5490478	-0.7583341	-0.8529134
H	1.8054461	-1.6210478	-1.1250217
H	1.7863987	-0.3462972	0.1058081
H	3.0506035	-2.3698926	0.8953869
H	1.6293607	-2.0287813	1.9077936
H	-1.9712345	-4.1948947	-1.0927730
H	-2.3402351	-2.3858203	-1.3506331

5b_c_2_r2_ts2.log

E = -1224.122817
H = -1223.782487
G = -1223.853018

NImag=1

C	1.6457654	0.7775152	0.7502827
C	0.6439111	0.9538381	-0.3419876
C	-0.7033019	0.3306743	-0.2762278
C	-1.3552500	0.0146676	-1.4795386

C	-2.6383132	-0.5103603	-1.4791930
C	-3.2894602	-0.7133317	-0.2538921
C	-2.6600658	-0.3914163	0.9537686
C	-1.3707811	0.1284226	0.9394287
C	2.0469395	-0.6153931	0.3523373
C	3.1065289	-0.7766626	-0.7100730
O	1.8455170	-2.9896739	0.6850906
C	1.4727581	-1.6999578	1.0407012
O	0.6299949	-1.6359006	1.9563166
S	0.0724600	3.0836349	-0.5259754
C	-0.4737904	3.4438211	1.1555787
C	1.6952120	3.8777009	-0.5242577
C	-4.6210616	-1.2558586	-0.2387309
N	-5.6943269	-1.6921340	-0.2275461
C	3.0888229	-2.1982882	-1.2597290
C	3.0331190	-3.1590938	-0.0879392
H	2.4732225	1.4896151	0.6729724
H	1.2068179	0.8191626	1.7488250
H	1.0776851	0.9288157	-1.3412586
H	-0.8419873	0.1808382	-2.4231975
H	-3.1366955	-0.7614111	-2.4095814
H	-3.1789554	-0.5495910	1.8935694
H	-0.8817771	0.3652628	1.8759146
H	2.9597414	-0.0543779	-1.5253108
H	4.1092519	-0.5607415	-0.3028099
H	-0.5003297	4.5277454	1.2870125
H	-1.4804914	3.0405397	1.2766897
H	0.2094468	2.9921922	1.8783249
H	1.5628714	4.9498502	-0.6821049
H	2.2749983	3.4556259	-1.3484096
H	2.2015410	3.6985819	0.4253982
H	2.2048012	-2.3518689	-1.8916009
H	3.9780579	-2.4082773	-1.8631259
H	3.9077866	-3.0069774	0.5619861
H	3.0258517	-4.2026482	-0.4129223

5b_c_2_r3_ts2.log

E = -1224.124495

H = -1223.784351

G = -1223.855387

NImag=1

C	1.6686723	-0.5432791	-1.1345668
C	0.7000334	-0.9599346	-0.0813551
C	-0.6638231	-0.3754967	-0.0100514
C	-1.2270195	-0.1148231	1.2474901
C	-2.5210685	0.3752663	1.3598546
C	-3.2689196	0.5913061	0.1947005
C	-2.7239693	0.3283790	-1.0684323
C	-1.4223296	-0.1461831	-1.1651890
C	2.0457296	0.7557315	-0.4818832
C	3.1434966	0.7458653	0.5522813
O	1.6981316	3.1278689	-0.2782990
C	1.3727941	1.9225314	-0.8878425
O	0.4773451	1.9992083	-1.7507295
S	0.2682966	-3.0865372	-0.3930063
C	1.8851378	-3.7273152	0.0910381
C	-0.6692132	-3.4292409	1.1103569
C	-4.6140672	1.0899228	0.2968504
N	-5.6980120	1.4904097	0.3796064
C	3.0765810	2.0119234	1.3988434
C	2.9132247	3.1975283	0.4671533

H	2.5133253	-1.2368918	-1.2164076
H	1.1999267	-0.4109642	-2.1121963
H	1.1513690	-1.1150751	0.9002876
H	-0.6373403	-0.2908832	2.1434148
H	-2.9534553	0.5867284	2.3321344
H	-3.3167263	0.5012885	-1.9606608
H	-0.9960277	-0.3425725	-2.1426991
H	3.0679488	-0.1441720	1.1940145
H	4.1374433	0.6824490	0.0771799
H	1.7773975	-4.7752776	0.3778163
H	2.5492798	-3.6533662	-0.7711660
H	2.2825043	-3.1448707	0.9276157
H	-0.6987405	-4.5095506	1.2667223
H	-1.6838929	-3.0537018	0.9663135
H	-0.1983768	-2.9348432	1.9643414
H	2.2162058	1.9701985	2.0790849
H	3.9806451	2.1429332	2.0025917
H	3.7608351	3.2419559	-0.2330024
H	2.8698443	4.1441644	1.0119423

5b_c_2_r4_ts2.log

E = -1224.124738
H = -1223.784455
G = -1223.854489

NImag=1

C	-1.4454549	-1.3708404	0.6858664
C	-0.3779858	-1.1822772	-0.3407664
C	0.6537664	-0.1296935	-0.2272056
C	1.2174620	0.3815832	-1.4091428
C	2.2421513	1.3139037	-1.3665002
C	2.7243575	1.7366333	-0.1191671
C	2.1782458	1.2365251	1.0683116
C	1.1421857	0.3109473	1.0119669
C	-2.3158724	-0.2249938	0.2563855
C	-3.3066076	-0.4540734	-0.8592217
O	-3.0009446	2.0609160	0.5649496
C	-2.1982891	0.9934126	0.9475178
O	-1.4191082	1.2406734	1.8894162
S	0.7922417	-3.0765868	-0.3222649
C	2.4129382	-2.6376096	-0.9827492
C	1.1990405	-3.1897898	1.4309398
C	3.7933048	2.6966251	-0.0593124
N	4.6555970	3.4688426	-0.0117060
C	-3.7918644	0.8795779	-1.4159629
C	-4.1393359	1.7837873	-0.2492034
H	-1.9380351	-2.3453862	0.5766177
H	-1.0775219	-1.2568959	1.7080245
H	-0.7251787	-1.3306568	-1.3619989
H	0.8425280	0.0380234	-2.3698402
H	2.6709730	1.7119144	-2.2799989
H	2.5606557	1.5764857	2.0251414
H	0.7035615	-0.0531927	1.9320448
H	-2.8637308	-1.0583035	-1.6628996
H	-4.1759782	-1.0320895	-0.5012114
H	3.0776111	-3.4964435	-0.8651629
H	2.2960863	-2.4073187	-2.0434110
H	2.8146133	-1.7732736	-0.4476262
H	1.9340279	-3.9865654	1.5643489
H	0.2875476	-3.4396132	1.9762183
H	1.6086314	-2.2402789	1.7843342
H	-3.0022906	1.3541257	-2.0123337

H	-4.6707913	0.7527009	-2.0565380
H	-4.9173522	1.3128253	0.3701616
H	-4.5086150	2.7578066	-0.5803667

5b_sy_1.log

E = -1224.135225
H = -1223.793214
G = -1223.861724

NImag=0

C	1.3301094	-4.4298024	-2.7788769
C	0.0877460	-3.5226835	-2.8756077
C	-1.0989086	-4.1260684	-3.5997272
C	-1.3979892	-5.4888453	-3.4884980
C	-2.4889919	-6.0276851	-4.1618946
C	-3.2850696	-5.1946529	-4.9554823
C	-2.9974314	-3.8296425	-5.0772685
C	-1.9063256	-3.3057332	-4.3965167
C	2.6192806	-3.7385925	-2.4501924
C	3.2652967	-2.9249929	-3.5475963
O	4.3975261	-3.3163934	-0.8964536
C	3.1466443	-3.8736417	-1.1822307
O	2.6053856	-4.4287713	-0.1778388
S	-0.5970804	-2.9219222	-1.2570651
C	-0.5533474	-4.3624219	-0.1752360
C	0.6708669	-1.8790218	-0.5040585
C	-4.4123106	-5.7480732	-5.6583326
N	-5.3197348	-6.1928179	-6.2239413
C	4.4124283	-2.0882455	-2.9882978
C	5.1969145	-2.9454881	-2.0122018
H	1.1393556	-5.2468482	-2.0751761
H	1.3916524	-4.8885076	-3.7797187
H	0.3489873	-2.5751904	-3.3616371
H	-0.7791901	-6.1396190	-2.8785725
H	-2.7223201	-7.0838748	-4.0777959
H	-3.6202111	-3.1946002	-5.6984080
H	-1.6738692	-2.2478744	-4.4870230
H	3.6457736	-3.5704862	-4.3588138
H	2.5284342	-2.2606771	-4.0263292
H	-0.9808449	-4.0374117	0.7762176
H	-1.1886102	-5.1346837	-0.6137771
H	0.4890765	-4.6786229	-0.0608290
H	0.1776990	-1.3708915	0.3278320
H	0.9866930	-1.1467285	-1.2493520
H	1.4955108	-2.5050554	-0.1587106
H	5.0717322	-1.7215278	-3.7822686
H	4.0209257	-1.2173105	-2.4467351
H	6.0601471	-2.4148328	-1.6006287
H	5.5591491	-3.8533618	-2.5199574

5b_sy_10.log

E = -1224.138547
H = -1223.796811
G = -1223.866860

NImag=0

C	0.9430015	-2.1070206	-2.3898781
C	-0.4059288	-2.7037484	-1.9117415
C	-1.0253474	-3.6354240	-2.9243544
C	-0.6158962	-4.9669847	-3.0728941
C	-1.1556247	-5.7623165	-4.0762787
C	-2.1131200	-5.2212300	-4.9427144

C	-2.5365893	-3.8946394	-4.8022227
C	-1.9931924	-3.1133118	-3.7894214
C	2.0133940	-3.0874278	-2.7670517
C	2.2598005	-3.3837283	-4.2281509
O	3.7807928	-4.5359569	-2.0175538
C	2.7787165	-3.6027836	-1.7381100
O	2.6809649	-3.3116244	-0.5090853
S	-0.1983734	-3.5972754	-0.3106015
C	0.1962881	-2.2478608	0.8146129
C	-1.9354851	-3.8585653	0.1125715
C	-2.6722207	-6.0398235	-5.9853862
N	-3.1222605	-6.6980533	-6.8254573
C	3.6033011	-4.0886518	-4.4011452
C	3.7425686	-5.1330711	-3.3079763
H	0.6651575	-1.4921809	-3.2574332
H	1.2817918	-1.4116063	-1.6098554
H	-1.1087375	-1.8949753	-1.6777387
H	0.1384186	-5.3882423	-2.4148892
H	-0.8371011	-6.7928820	-4.1934017
H	-3.2836797	-3.4873329	-5.4753299
H	-2.3176396	-2.0830045	-3.6729373
H	1.4668487	-4.0140410	-4.6684402
H	2.2511161	-2.4513956	-4.8133560
H	0.0616087	-2.6338145	1.8271002
H	1.2424085	-2.0018749	0.6351789
H	-0.4769871	-1.4082514	0.6295373
H	-1.9663556	-4.2207449	1.1420611
H	-2.3352757	-4.6234197	-0.5553242
H	-2.4913271	-2.9238252	0.0137416
H	3.6876832	-4.5648544	-5.3839559
H	4.4276862	-3.3710454	-4.3027757
H	4.6710447	-5.7034358	-3.4025902
H	2.8979497	-5.8389754	-3.3579523

5b_sy_10_ts1.log

E = -1224.108368

H = -1223.769279

G = -1223.838480

NImag=1

C	1.2148777	0.9291665	1.5787361
C	1.4844360	-1.0858084	0.7368845
C	0.1309818	-1.3573475	0.3343443
C	-0.4332259	-0.8223745	-0.8502553
C	-1.7850971	-0.9570555	-1.1232902
C	-2.6270830	-1.6080917	-0.2092622
C	-2.0883471	-2.1484867	0.9750405
C	-0.7379669	-2.0255359	1.2342876
C	0.2469401	1.6490057	0.9042631
C	-1.1891422	1.7249291	1.3750892
O	-0.2449438	2.9444467	-1.0898782
C	0.6491990	2.2189765	-0.3604317
O	1.7799887	2.1079098	-0.8442837
S	2.6556906	-1.0102099	-0.5688580
C	4.0364420	-0.0272031	0.0459584
C	3.4456179	-2.6425008	-0.5508100
C	-4.0256132	-1.7336057	-0.4852147
N	-5.1603911	-1.8361433	-0.7073004
C	-1.8557960	2.9516914	0.7607706
C	-1.6379892	2.9155991	-0.7378542
H	0.9723591	0.5272386	2.5611601
H	2.2613373	1.1539325	1.4143047

H	1.8754329	-1.6343567	1.5936528
H	0.1943380	-0.2935463	-1.5620779
H	-2.2006687	-0.5428483	-2.0371231
H	-2.7380838	-2.6611561	1.6778273
H	-0.3281543	-2.4412297	2.1508749
H	-1.7630521	0.8330059	1.0793437
H	-1.2198282	1.7724271	2.4697051
H	4.8926225	-0.2535391	-0.5929010
H	3.7567776	1.0211197	-0.0553983
H	4.2498979	-0.2983953	1.0822102
H	4.2464124	-2.6465205	-1.2937634
H	2.6806261	-3.3730902	-0.8186488
H	3.8391025	-2.8411778	0.4484509
H	-2.9318345	2.9663139	0.9615782
H	-1.4220984	3.8726239	1.1698384
H	-2.0758396	3.7814646	-1.2389974
H	-2.0816328	2.0056030	-1.1636248

5b_sy_11.log

E = -1224.135620

H = -1223.793419

G = -1223.861248

NImag=0

C	1.2679446	-2.1621377	-2.7073177
C	-0.1908221	-2.4703701	-2.2919009
C	-0.9611589	-3.4486517	-3.1411117
C	-0.4846756	-4.7364956	-3.4292766
C	-1.2174063	-5.5958206	-4.2386231
C	-2.4413590	-5.1692585	-4.7684753
C	-2.9332904	-3.8897514	-4.4906606
C	-2.1903506	-3.0419416	-3.6774686
C	2.2747609	-3.2755912	-2.7558248
C	2.6703155	-3.8476654	-4.0969996
O	3.8924925	-4.5898968	-1.5538089
C	2.8634115	-3.6427862	-1.5629544
O	2.5432789	-3.2232832	-0.4107701
S	-0.2873429	-2.8621988	-0.4754128
C	-2.0748360	-2.7737292	-0.2255363
C	-0.0704877	-4.6412032	-0.2833602
C	-3.2024357	-6.0579796	-5.6060554
N	-3.8150685	-6.7735464	-6.2798302
C	3.5050725	-5.1092255	-3.8997905
C	4.5226106	-4.8476729	-2.8029386
H	1.1664690	-1.7101224	-3.7041691
H	1.6018144	-1.3615339	-2.0323458
H	-0.7347374	-1.5178114	-2.2912272
H	0.4670317	-5.0630861	-3.0232961
H	-0.8468441	-6.5910515	-4.4617747
H	-3.8824648	-3.5674991	-4.9055953
H	-2.5686457	-2.0472622	-3.4576252
H	1.7823482	-4.0809082	-4.7033661
H	3.2497779	-3.1222313	-4.6948760
H	-2.2641312	-3.0504198	0.8138440
H	-2.3892814	-1.7419892	-0.3928723
H	-2.5960624	-3.4567010	-0.8992345
H	-0.1313119	-4.8302481	0.7910304
H	0.9226367	-4.8973043	-0.6470481
H	-0.8652582	-5.1722165	-0.8095295
H	2.8641840	-5.9455357	-3.5894345
H	4.0193927	-5.4039789	-4.8209148
H	5.1510986	-3.9858881	-3.0776272

H 5.1764307 -5.7088066 -2.6379216

5b_sy_12.log

E = -1224.131082

H = -1223.789338

G = -1223.859022

NImag=0

C	1.3575374	-4.5016087	-2.9650290
C	0.0858977	-3.6546094	-2.8194015
C	-1.1206297	-4.1991059	-3.5539018
C	-1.8974574	-3.3271273	-4.3254060
C	-3.0076857	-3.7894619	-5.0214537
C	-3.3473585	-5.1447864	-4.9393991
C	-2.5841274	-6.0298443	-4.1690722
C	-1.4735384	-5.5526170	-3.4826792
C	2.6086169	-3.9845743	-2.3050598
C	3.5006775	-5.0048583	-1.6325729
O	4.1614315	-2.1918202	-1.9045473
C	2.9591620	-2.6561823	-2.4568610
O	2.2849898	-1.7421067	-3.0168725
S	-0.4630974	-3.3513583	-1.0699026
C	0.0253714	-4.8274961	-0.1623050
C	0.6545430	-2.1003605	-0.3973294
C	-4.4945018	-5.6346833	-5.6568355
N	-5.4178445	-6.0287818	-6.2341820
C	4.5603532	-4.3113370	-0.7831599
C	5.1457022	-3.1684401	-1.5910570
H	1.1576248	-5.5177152	-2.6002464
H	1.4581638	-4.6027825	-4.0609423
H	0.3070598	-2.6365144	-3.1539349
H	-1.6261335	-2.2767400	-4.3832870
H	-3.6054488	-3.1134225	-5.6237692
H	-2.8584480	-7.0780799	-4.1143184
H	-0.8835822	-6.2476307	-2.8925543
H	2.9093216	-5.6884002	-1.0035569
H	4.0064153	-5.6579652	-2.3661031
H	-0.2656835	-4.6635886	0.8772333
H	-0.5261501	-5.6766628	-0.5696742
H	1.1032231	-4.9670583	-0.2495194
H	0.1082535	-1.5868494	0.3951723
H	0.9122533	-1.4192150	-1.2133353
H	1.5559571	-2.5841242	-0.0219491
H	4.1090393	-3.9014336	0.1300122
H	5.3560569	-5.0025639	-0.4847838
H	5.5822794	-3.5585697	-2.5240677
H	5.9305565	-2.6394241	-1.0426483

5b_sy_13.log

E = -1224.131723

H = -1223.789706

G = -1223.857915

NImag=0

C	1.0504609	-2.2121022	-2.4419840
C	-0.4440335	-2.5257489	-2.1780401
C	-1.1352777	-3.4757135	-3.1307678
C	-0.6897767	-4.7908508	-3.3256094
C	-1.3456622	-5.6338277	-4.2137706
C	-2.4588962	-5.1600358	-4.9185001
C	-2.9155961	-3.8502511	-4.7374530
C	-2.2523984	-3.0201871	-3.8410367

C	2.0497787	-3.3162086	-2.6318401
C	2.3221563	-3.7825814	-4.0451877
O	3.8637337	-4.6136843	-1.7296590
C	2.8227536	-3.6961894	-1.5514880
O	2.6832781	-3.3280252	-0.3454668
S	-0.9086191	-3.0435894	-0.4563665
C	-0.1088888	-4.6121499	-0.0652962
C	0.0340148	-1.9146121	0.5855019
C	-3.1396395	-6.0317768	-5.8393333
N	-3.6871403	-6.7338834	-6.5799318
C	3.2014278	-5.0273667	-4.0344780
C	4.3395572	-4.7974336	-3.0572729
H	1.0014834	-1.6069196	-3.3613742
H	1.3740907	-1.5269362	-1.6490945
H	-0.9846868	-1.5715145	-2.2102800
H	0.1910328	-5.1466529	-2.8005554
H	-0.9979083	-6.6502536	-4.3671486
H	-3.7779553	-3.4916045	-5.2894425
H	-2.6054185	-2.0033673	-3.6936996
H	1.3867739	-3.9927893	-4.5813324
H	2.8238798	-2.9941218	-4.6345184
H	-0.3548015	-4.7959012	0.9841083
H	-0.5617934	-5.3922408	-0.6770929
H	0.9711916	-4.5133189	-0.1990769
H	-0.2894470	-2.1003261	1.6118750
H	-0.2302983	-0.8960322	0.2946966
H	1.0981451	-2.1293165	0.4481397
H	2.6228947	-5.9007470	-3.7045387
H	3.6049062	-5.2472777	-5.0288933
H	4.9157106	-3.9096724	-3.3621930
H	5.0233677	-5.6500894	-3.0154992

5b_sy_14.log

E = -1224.135393

H = -1223.793605

G = -1223.864315

NImag=0

C	1.4766511	-4.6778125	-1.3786580
C	0.1403994	-3.9149456	-1.4276011
C	-0.6446891	-4.1619604	-2.6901017
C	-1.1578360	-5.4306756	-2.9876102
C	-1.8316582	-5.6554250	-4.1810306
C	-1.9796338	-4.6012302	-5.0920486
C	-1.4687669	-3.3297999	-4.8092727
C	-0.8119842	-3.1162746	-3.6018945
C	2.3827192	-4.1150885	-2.4414129
C	2.5095497	-4.8401046	-3.7620997
O	3.7129228	-2.2446385	-3.1579788
C	2.8790270	-2.8425343	-2.2046708
O	2.6606780	-2.1233140	-1.1906250
S	-0.9416725	-4.3597479	0.0179297
C	-0.0674550	-3.5624956	1.3792466
C	-2.3221118	-3.2190528	-0.1976419
C	-2.6669219	-4.8290965	-6.3354758
N	-3.2206603	-5.0122244	-7.3360315
C	3.0909025	-3.9039001	-4.8186822
C	4.2080100	-3.0932676	-4.1853400
H	1.9122848	-4.5518590	-0.3801818
H	1.2917507	-5.7482135	-1.5358977
H	0.3468228	-2.8472211	-1.2936102
H	-1.0218694	-6.2566018	-2.2933780

H	-2.2314261	-6.6364310	-4.4150201
H	-1.5887980	-2.5230091	-5.5247864
H	-0.4131067	-2.1328218	-3.3694476
H	3.1486980	-5.7365444	-3.6828229
H	1.5283324	-5.2089875	-4.1003568
H	-0.7443205	-3.5610181	2.2357156
H	0.8177544	-4.1547209	1.6109133
H	0.2004846	-2.5441419	1.0906732
H	-2.9100197	-3.2428409	0.7219540
H	-2.9259387	-3.5758172	-1.0334349
H	-1.9349917	-2.2158956	-0.3897160
H	3.4728722	-4.4556813	-5.6844145
H	2.3193299	-3.2086974	-5.1756172
H	4.6974772	-2.4355963	-4.9094680
H	4.9685935	-3.7710123	-3.7659047

5b_sy_15.log

E = -1224.135189
H = -1223.793498
G = -1223.864678

NImag=0

C	1.4917127	-4.6507434	-1.3309080
C	0.1531730	-3.8970519	-1.3969170
C	-0.6028549	-4.1258392	-2.6814000
C	-1.0340435	-5.4074246	-3.0445862
C	-1.6878836	-5.6142876	-4.2526248
C	-1.9008906	-4.5274484	-5.1100590
C	-1.4735344	-3.2415435	-4.7602040
C	-0.8339679	-3.0481975	-3.5404978
C	2.3862978	-4.1227094	-2.4210010
C	2.5713844	-4.9342277	-3.6806783
O	3.6300235	-2.2472177	-3.2703104
C	2.8853549	-2.8423822	-2.2401387
O	2.7604797	-2.1188222	-1.2144110
S	-0.9675415	-4.3845872	0.0063643
C	-0.1166926	-3.6737853	1.4284743
C	-2.3216371	-3.2089180	-0.1866308
C	-2.5673478	-4.7368762	-6.3681080
N	-3.1040118	-4.9055768	-7.3804215
C	3.6764537	-4.3230441	-4.5381819
C	3.4813759	-2.8176034	-4.5642341
H	1.9319524	-4.4890355	-0.3393908
H	1.3143364	-5.7270315	-1.4522072
H	0.3424456	-2.8291930	-1.2394878
H	-0.8497394	-6.2557073	-2.3900011
H	-2.0231285	-6.6058337	-4.5378131
H	-1.6433991	-2.4093453	-5.4352560
H	-0.4985889	-2.0544551	-3.2571411
H	2.8191835	-5.9788430	-3.4381471
H	1.6451368	-4.9840021	-4.2833947
H	-0.8208856	-3.6928017	2.2625481
H	0.7443707	-4.3001493	1.6611953
H	0.1866029	-2.6507331	1.1966380
H	-2.9353071	-3.2690810	0.7142155
H	-2.9076499	-3.5108827	-1.0559380
H	-1.9123044	-2.2046081	-0.3155618
H	4.6616266	-4.5405693	-4.1063546
H	3.6610926	-4.7189600	-5.5594942
H	2.4774982	-2.5813105	-4.9536497
H	4.2199072	-2.3203714	-5.1998854

5b_sy_16.log

E = -1224.131624

H = -1223.789904

G = -1223.859344

NImag=0

C	1.3647764	-4.5168745	-3.0025048
C	0.1018212	-3.6678150	-2.8270044
C	-1.1225731	-4.2041698	-3.5371344
C	-1.4663537	-5.5606468	-3.4818406
C	-2.5979369	-6.0293447	-4.1391945
C	-3.3912929	-5.1327113	-4.8644689
C	-3.0599353	-3.7744446	-4.9309622
C	-1.9283335	-3.3207748	-4.2644707
C	2.6287320	-4.0034197	-2.3658504
C	3.5757784	-5.0490265	-1.8176331
O	4.1090853	-2.1868428	-1.8454817
C	2.9557492	-2.6660795	-2.4800365
O	2.3045112	-1.7620600	-3.0832519
S	-0.4094142	-3.3817369	-1.0612868
C	0.0923891	-4.8730114	-0.1857851
C	0.7203033	-2.1361501	-0.3953790
C	-4.5606774	-5.6140770	-5.5514316
N	-5.5018354	-6.0014747	-6.1040165
C	4.9451707	-4.4390032	-1.5311877
C	4.7351346	-3.0656571	-0.9209645
H	1.1693794	-5.5327632	-2.6344337
H	1.4463319	-4.6199561	-4.1001378
H	0.3166999	-2.6465421	-3.1576933
H	-0.8528626	-6.2635692	-2.9257641
H	-2.8660221	-7.0796771	-4.0955710
H	-3.6806362	-3.0891719	-5.4986675
H	-1.6631323	-2.2683074	-4.3105318
H	3.1894444	-5.5130556	-0.8921461
H	3.6857695	-5.8796478	-2.5323607
H	-0.1603171	-4.7157955	0.8647261
H	-0.4862256	-5.7095782	-0.5821091
H	1.1644695	-5.0279347	-0.3123130
H	0.1685408	-1.5915583	0.3721953
H	1.0087707	-1.4788866	-1.2213718
H	1.6017260	-2.6288181	0.0144996
H	5.5345550	-5.0673792	-0.8550390
H	5.5143648	-4.3196897	-2.4617043
H	5.6795360	-2.5889339	-0.6432340
H	4.1122089	-3.1515151	-0.0157584

5b_sy_1_r.log

E = -1224.132898

H = -1223.790876

G = -1223.862577

NImag=0

C	-0.5392808	-0.6103719	-0.9917698
C	0.2121388	-0.0844077	0.2371488
C	1.2257493	-1.0379913	0.8262775
C	2.2070384	-1.6427155	0.0307470
C	3.1274456	-2.5209587	0.5901151
C	3.0604815	-2.8044487	1.9593958
C	2.0834423	-2.2115717	2.7672492
C	1.1764376	-1.3279135	2.1940790
C	-1.4119831	-1.7576120	-0.5501479
C	-0.9942939	-3.1727512	-0.8768465

O	-3.3386515	-2.4485429	0.7115528
C	-2.4842067	-1.4328640	0.2647774
O	-2.7956213	-0.2805687	0.6777313
S	1.0681386	1.5616172	-0.0103263
C	1.6894274	1.5194928	-1.7018547
C	-0.3272206	2.6898096	-0.1820715
C	4.0059183	-3.7198906	2.5416513
N	4.7674808	-4.4560846	3.0099624
C	-1.7706636	-4.1595550	-0.0087059
C	-3.2185331	-3.7069872	0.0609562
H	-1.1336516	0.2097831	-1.4139008
H	0.1699348	-0.9354638	-1.7620440
H	-0.5366730	0.1833352	0.9923300
H	2.2513026	-1.4448774	-1.0362464
H	3.8873692	-2.9904776	-0.0255563
H	2.0372918	-2.4441828	3.8259142
H	0.4131289	-0.8638268	2.8123906
H	-1.1621864	-3.4190341	-1.9398722
H	0.0855050	-3.3086633	-0.7114556
H	2.0874464	2.5147340	-1.9093961
H	2.4966606	0.7873658	-1.7515361
H	0.8830937	1.2736029	-2.3933255
H	0.0839179	3.6754982	-0.4079541
H	-0.8466179	2.7145060	0.7771487
H	-0.9897562	2.3545346	-0.9805139
H	-1.7163904	-5.1791565	-0.4053597
H	-1.3618644	-4.1719039	1.0102639
H	-3.8374450	-4.4028060	0.6347504
H	-3.6348418	-3.6339145	-0.9564619

5b_sy_1_ts1.log

E = -1224.100343

H = -1223.761279

G = -1223.831375

NImag=1

C	-0.7274766	-0.9173315	-0.5875287
C	0.3769225	0.4525949	0.7926637
C	1.7584806	0.1812342	0.5224158
C	2.5947933	1.0238504	-0.2555968
C	3.8962861	0.6666365	-0.5581478
C	4.4154396	-0.5611117	-0.1129197
C	3.6026674	-1.4213465	0.6481674
C	2.3068949	-1.0558721	0.9571327
C	-2.0826014	-1.0121056	-0.3451793
C	-2.5718151	-1.7118580	0.9068502
O	-4.3412621	-0.5335577	-1.0749456
C	-3.0025747	-0.3646675	-1.2592068
O	-2.6780951	0.3340973	-2.2210064
S	-0.1396465	2.1379883	0.7293882
C	-0.7204737	2.4591930	-0.9564371
C	-1.7160397	2.0213784	1.5961943
C	5.7578559	-0.9329346	-0.4319149
N	6.8488614	-1.2354589	-0.6903983
C	-4.0308249	-1.3706764	1.1872962
C	-4.8044196	-1.4884511	-0.1076797
H	-0.3724418	-0.4750538	-1.5155790
H	-0.0650963	-1.6502003	-0.1319551
H	-0.0666961	-0.0240129	1.6634041
H	2.2276660	1.9779485	-0.6248900
H	4.5199997	1.3340393	-1.1450947
H	4.0006482	-2.3692809	0.9975658

H	1.6934330	-1.7211275	1.5590994
H	-2.4673362	-2.8016868	0.8102422
H	-1.9415685	-1.4134701	1.7557988
H	-1.1103562	3.4799941	-0.9618647
H	0.1458848	2.3960998	-1.6179267
H	-1.4808468	1.7324697	-1.2496992
H	-2.2256462	2.9802274	1.4885246
H	-1.5021245	1.8235344	2.6476630
H	-2.3014563	1.2128696	1.1529456
H	-4.4614536	-2.0434547	1.9349675
H	-4.1242971	-0.3442091	1.5638133
H	-5.8669460	-1.2726096	0.0187725
H	-4.6997574	-2.4962907	-0.5308654

5b_sy_2.log

E = -1224.134619

H = -1223.792561

G = -1223.860940

NImag=0

C	1.3304487	-4.4860009	-2.8220183
C	0.1058760	-3.5512300	-2.8767001
C	-1.1077757	-4.1151174	-3.5873055
C	-1.9113488	-3.2641284	-4.3552759
C	-3.0259385	-3.7528035	-5.0241521
C	-3.3410030	-5.1131832	-4.9195605
C	-2.5491187	-5.9765456	-4.1547134
C	-1.4344117	-5.4728928	-3.4931158
C	2.6319836	-3.8182818	-2.4968348
C	3.2902300	-3.0116400	-3.5918445
O	4.3538551	-3.3161494	-0.9015837
C	3.1623668	-3.9743466	-1.2321378
O	2.6820862	-4.6474489	-0.2710638
S	-0.5317247	-2.9769846	-1.2276906
C	-0.4744804	-4.4402809	-0.1773037
C	0.7588997	-1.9576975	-0.4785507
C	-4.4920937	-5.6307726	-5.6108951
N	-5.4185998	-6.0468605	-6.1672938
C	4.7286102	-2.6689005	-3.2139950
C	4.7499791	-2.2501833	-1.7557745
H	1.1350358	-5.3133073	-2.1319038
H	1.3677305	-4.9235183	-3.8327576
H	0.3782907	-2.5987536	-3.3468248
H	-1.6572759	-2.2102032	-4.4325226
H	-3.6458718	-3.0942758	-5.6233167
H	-2.8040172	-7.0287485	-4.0839919
H	-0.8184086	-6.1472139	-2.9062921
H	3.2743999	-3.5716993	-4.5398644
H	2.7449476	-2.0726938	-3.7973613
H	-0.8696685	-4.1294001	0.7926624
H	-1.1330408	-5.1948920	-0.6123913
H	0.5659299	-4.7754805	-0.0992603
H	0.2796368	-1.4460559	0.3592463
H	1.0818792	-1.2267325	-1.2218912
H	1.5772374	-2.5937363	-0.1391806
H	5.3751431	-3.5472831	-3.3341508
H	5.1323619	-1.8656392	-3.8397127
H	4.0741775	-1.3929065	-1.6046953
H	5.7513722	-1.9577120	-1.4270816

5b_sy_2_r.log

```

E = -1224.132985
H = -1223.791114
G = -1223.862451
NImag=0
C -0.6020874 -0.5697018 -0.9463436
C 0.1542711 -0.0777297 0.2889512
C 1.1740190 -1.0396822 0.8564620
C 1.2895488 -1.1687517 2.2458801
C 2.2205534 -2.0342684 2.8057417
C 3.0537235 -2.7775858 1.9608110
C 2.9553604 -2.6564511 0.5700220
C 2.0155647 -1.7887824 0.0253914
C -1.4189127 -1.7732888 -0.5475850
C -1.0598296 -3.1295309 -1.1055576
O -3.2069498 -2.6343429 0.8106130
C -2.4575562 -1.5469448 0.3406433
O -2.8338204 -0.4298170 0.7931188
S 1.0307858 1.5611556 0.0733927
C 1.7704496 1.4589022 -1.5662581
C -0.3249598 2.7136152 -0.2187896
C 4.0228446 -3.6766615 2.5287785
N 4.8036440 -4.3996352 2.9860031
C -2.1714808 -4.1308756 -0.8013051
C -2.6275217 -3.9202013 0.6315925
H -1.2330483 0.2492314 -1.3156628
H 0.0970634 -0.8319907 -1.7480466
H -0.5865368 0.1761005 1.0571665
H 0.6358911 -0.5901110 2.8932596
H 2.3024202 -2.1397140 3.8824510
H 3.6065125 -3.2387326 -0.0735158
H 1.9386390 -1.7067515 -1.0545284
H -0.8976029 -3.0717887 -2.1927181
H -0.1120028 -3.5142068 -0.6870165
H 2.2570768 2.4185049 -1.7514564
H 2.5198441 0.6655182 -1.5485649
H 1.0010496 1.2640130 -2.3140064
H 0.1215243 3.6992809 -0.3636127
H -0.9503588 2.7170154 0.6758778
H -0.8959067 2.4154117 -1.0983381
H -3.0284436 -3.9660009 -1.4667385
H -1.8332275 -5.1637668 -0.9377230
H -1.7696216 -4.0319516 1.3144484
H -3.3955834 -4.6410629 0.9264324

```

```

5b_sy_2_r2.log
E = -1224.132990
H = -1223.790921
G = -1223.861002
NImag=0
C -0.6393358 -0.4448649 -0.5245128
C 0.7825178 -0.8203776 -0.9776691
C 0.9091394 -1.5964395 -2.2691328
C 2.0289881 -2.4117114 -2.4674511
C 2.1991128 -3.1049524 -3.6605262
C 1.2303625 -2.9784853 -4.6618662
C 0.0995749 -2.1732548 -4.4713596
C -0.0594210 -1.4840231 -3.2746330
C -1.5556059 -1.6352649 -0.4710489
C -1.2176996 -2.7388712 0.5038195
O -3.5756927 -2.7055570 -1.2027405
C -2.6561399 -1.6518055 -1.3128600

```

O	-2.9545208	-0.8175722	-2.2136216
S	1.9078289	0.6554015	-1.1822162
C	1.1956250	1.5622402	-2.5669402
C	1.4884109	1.7359514	0.1996746
C	1.3956093	-3.6899699	-5.9016445
N	1.5296068	-4.2613413	-6.9001903
C	-2.1051349	-3.9576072	0.2635483
C	-3.5175195	-3.4769506	-0.0110526
H	-0.5359972	0.0191649	0.4670877
H	-1.0713249	0.3010516	-1.1991353
H	1.3042165	-1.3652774	-0.1823258
H	2.7722004	-2.5098591	-1.6800487
H	3.0665150	-3.7377128	-3.8158900
H	-0.6477772	-2.0965460	-5.2545640
H	-0.9582467	-0.8908927	-3.1114173
H	-0.1623540	-3.0411254	0.4102483
H	-1.3326779	-2.4037792	1.5503632
H	1.6762440	2.5429883	-2.5701782
H	1.4445760	1.0269697	-3.4838887
H	0.1161979	1.6633821	-2.4430710
H	2.1824190	2.5774395	0.1541739
H	1.6465199	1.1752259	1.1228686
H	0.4574060	2.0792021	0.1134838
H	-1.7535874	-4.5162058	-0.6133729
H	-2.0976262	-4.6391086	1.1209989
H	-3.8770455	-2.8707383	0.8359031
H	-4.2129284	-4.3088675	-0.1558004

5b_sy_2_r3.log

E = -1224.133619

H = -1223.791666

G = -1223.861552

NImag=0

C	-0.5274419	-0.5749990	-1.9760998
C	0.7475061	-0.7038780	-1.1056783
C	1.5111127	-1.9954173	-1.2607235
C	2.0852959	-2.5941441	-0.1354088
C	2.8044340	-3.7793296	-0.2533940
C	2.9455435	-4.3641052	-1.5158788
C	2.3653023	-3.7790370	-2.6501128
C	1.6448652	-2.5990532	-2.5176470
C	-1.3882802	-1.8024459	-1.9242079
C	-1.9534278	-2.2045281	-0.5824669
O	-2.3966575	-3.6545905	-3.0694488
C	-1.5491636	-2.5357779	-3.0894964
O	-1.0130151	-2.3329808	-4.2143483
S	1.9004692	0.6711412	-1.5672236
C	0.9666895	2.1343533	-1.0760690
C	3.1416950	0.6236533	-0.2607044
C	3.6903851	-5.5880465	-1.6506376
N	4.2914336	-6.5721794	-1.7588394
C	-2.5349013	-3.6144505	-0.6482398
C	-3.2790639	-3.7655751	-1.9618705
H	-1.0621959	0.3145582	-1.6111714
H	-0.2456758	-0.3900934	-3.0191279
H	0.5265058	-0.5258892	-0.0471962
H	1.9649333	-2.1333356	0.8414803
H	3.2501137	-4.2472344	0.6180490
H	2.4703307	-4.2559701	-3.6191361
H	1.1435380	-2.1749880	-3.3852146
H	-1.1735347	-2.1741199	0.1965471

H	-2.7338491	-1.5018091	-0.2398178
H	1.6689468	2.9701857	-1.0713679
H	0.1904789	2.3096784	-1.8207844
H	0.5400362	1.9776096	-0.0831822
H	3.7444094	1.5286014	-0.3618582
H	3.7679512	-0.2549643	-0.4211353
H	2.6476729	0.5899995	0.7124108
H	-1.7283447	-4.3587459	-0.6203008
H	-3.2075250	-3.8161190	0.1923929
H	-4.0619072	-2.9937978	-2.0377115
H	-3.7555508	-4.7461424	-2.0527551

5b_sy_2_r4.log

E = -1224.134822
H = -1223.792714
G = -1223.862744

NImag=0

C	0.5147581	-1.4477845	-2.6462412
C	0.7718773	-0.7653852	-1.2824183
C	1.2437448	-1.6528670	-0.1632514
C	0.8920787	-1.3432753	1.1554340
C	1.3266025	-2.1369057	2.2119320
C	2.1178154	-3.2570369	1.9373393
C	2.4619988	-3.5896276	0.6199994
C	2.0199966	-2.7900412	-0.4266309
C	-0.3826000	-2.6438250	-2.5380126
C	-1.7866524	-2.4275030	-2.0253008
O	-0.7057881	-5.0007656	-2.8560816
C	0.1407286	-3.8824790	-2.8760117
O	1.3281202	-4.1576583	-3.2061262
S	1.9603976	0.6282842	-1.6135671
C	2.1194732	1.4913890	-0.0415599
C	3.5685982	-0.1734036	-1.7277728
C	2.5749050	-4.0865174	3.0208159
N	2.9448236	-4.7532612	3.8926572
C	-2.4602410	-3.7648146	-1.7269259
C	-2.1022705	-4.7403480	-2.8322945
H	0.0906877	-0.6666742	-3.2981723
H	1.4637957	-1.7678811	-3.0892681
H	-0.1188696	-0.2112140	-0.9631996
H	0.2662905	-0.4778245	1.3572377
H	1.0544574	-1.8974993	3.2344779
H	3.0606976	-4.4731841	0.4237401
H	2.2424135	-3.0781366	-1.4526319
H	-1.7812096	-1.8169856	-1.1075996
H	-2.4012296	-1.8612089	-2.7477743
H	2.8256813	2.3087061	-0.2023368
H	1.1390742	1.8941832	0.2188635
H	2.4879258	0.8102069	0.7270883
H	4.2977237	0.6197152	-1.9059455
H	3.5506128	-0.8537761	-2.5806761
H	3.7906361	-0.7022474	-0.7995389
H	-2.0930360	-4.1709603	-0.7756212
H	-3.5481127	-3.6625337	-1.6508003
H	-2.4158135	-4.3321570	-3.8065296
H	-2.5877964	-5.7110559	-2.6958112

5b_sy_2_ts1.log

E = -1224.101024
H = -1223.762213

```

G = -1223.833044
NImag=1
C -0.7186900 -0.8302325 -0.7102648
C 0.3615188 0.4234217 0.7802925
C 1.7462909 0.1634578 0.5147957
C 2.2905237 -1.0917492 0.8987929
C 3.5903557 -1.4416914 0.5888098
C 4.4104015 -0.5473730 -0.1236596
C 3.8936929 0.6972537 -0.5222881
C 2.5881626 1.0391817 -0.2190576
C -2.0608534 -0.9932795 -0.4374033
C -2.4903377 -1.8559914 0.7270804
O -4.3537941 -0.3757135 -0.9244974
C -3.0312744 -0.2670020 -1.2337649
O -2.7665444 0.4203447 -2.2211510
S -0.1443242 2.1116751 0.7980675
C -0.7631995 2.5168733 -0.8575497
C -1.6983236 1.9848617 1.7015965
C 5.7569051 -0.9033224 -0.4437876
N 6.8512386 -1.1928347 -0.7030405
C -3.9639967 -2.2265879 0.6160247
C -4.7457212 -0.9633136 0.3266291
H -0.4073015 -0.2654792 -1.5857137
H -0.0224511 -1.5933552 -0.3689493
H -0.1020658 -0.1059150 1.6090482
H 1.6699963 -1.7844008 1.4613977
H 3.9857736 -2.4040329 0.8996371
H 4.5219788 1.3893146 -1.0747617
H 2.2208149 2.0057491 -0.5548159
H -1.8595314 -2.7514311 0.7767829
H -2.3345267 -1.3133369 1.6748392
H -1.1207342 3.5483048 -0.8099628
H 0.0833156 2.4546611 -1.5445142
H -1.5549080 1.8290867 -1.1592255
H -2.1939375 2.9553865 1.6454011
H -1.4595493 1.7424487 2.7382034
H -2.3110239 1.2044525 1.2456445
H -4.1234725 -2.9443161 -0.1977275
H -4.3342721 -2.6772482 1.5418941
H -4.5920272 -0.2247385 1.1246907
H -5.8170195 -1.1491937 0.2290361

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```

5b_sy_3.log
E = -1224.139800
H = -1223.797640
G = -1223.866229
NImag=0
C 1.5445365 -4.4692742 -3.0729513
C 0.2866391 -3.5763834 -2.9829647
C -0.9738110 -4.1387999 -3.5861952
C -1.3256378 -5.4861124 -3.4268433
C -2.4805452 -5.9888781 -4.0145849
C -3.2911547 -5.1377245 -4.7746407
C -2.9514588 -3.7913080 -4.9495545
C -1.7952385 -3.3031484 -4.3537114
C 2.8026086 -3.7992279 -2.6091823
C 3.5583971 -2.9326717 -3.5890107
O 4.3377941 -3.3832134 -0.8095702
C 3.1460800 -3.9446749 -1.2778877
O 2.4740000 -4.5419687 -0.3865074
S 0.0746903 -3.0642338 -1.2097135

```


C	-1.4292741	-2.0704700	-1.2842233
C	-0.5554194	-4.5279164	-0.3745926
C	-4.4854660	-5.6548910	-5.3885464
N	-5.4469410	-6.0708667	-5.8822313
C	4.5990018	-2.0926451	-2.8521804
C	5.2661072	-2.9639520	-1.8021445
H	1.3676747	-5.3946943	-2.5127720
H	1.6132678	-4.7444060	-4.1355826
H	0.5088672	-2.6086902	-3.4488248
H	-0.6982237	-6.1540661	-2.8449642
H	-2.7527876	-7.0318637	-3.8912914
H	-3.5846244	-3.1420075	-5.5449102
H	-1.5223834	-2.2599122	-4.4877243
H	4.0625398	-3.5358191	-4.3641316
H	2.8696989	-2.2696164	-4.1361903
H	-1.6373475	-1.7376183	-0.2652051
H	-1.2294324	-1.2039168	-1.9176297
H	-2.2645895	-2.6559919	-1.6717634
H	-0.7085978	-4.2389623	0.6677303
H	0.2310564	-5.2800806	-0.4338734
H	-1.4963262	-4.8501453	-0.8234732
H	5.3528650	-1.6884210	-3.5363026
H	4.1171872	-1.2470578	-2.3447687
H	6.0563010	-2.4285393	-1.2680712
H	5.7122460	-3.8496306	-2.2817157

5b_sy_3_r.log

E = -1224.134609

H = -1223.792660

G = -1223.863511

NImag=0

C	-0.5386619	-1.1952299	-0.9379122
C	0.0910014	-0.4894751	0.2723645
C	1.0065399	-1.3214532	1.1300921
C	1.9518272	-2.1934907	0.5737315
C	2.7824728	-2.9504992	1.3914469
C	2.6656294	-2.8377665	2.7817977
C	1.7252701	-1.9739300	3.3548108
C	0.9051308	-1.2210898	2.5234303
C	-1.4736579	-2.2701771	-0.4505395
C	-1.0865692	-3.7204387	-0.6210144
O	-3.5383900	-2.7903429	0.6669117
C	-2.6137544	-1.8423463	0.2102035
O	-2.9334179	-0.6482171	0.4695645
S	0.8985178	1.0916232	-0.3072033
C	1.7267330	1.7389657	1.1551267
C	2.3087252	0.5611694	-1.2930428
C	3.5197593	-3.6239973	3.6318280
N	4.2078733	-4.2564069	4.3157676
C	-1.9769635	-4.6049568	0.2478845
C	-3.4067010	-4.1050311	0.1420102
H	-1.0650823	-0.4303594	-1.5278243
H	0.2393633	-1.6227690	-1.5816200
H	-0.7351254	-0.0915849	0.8736023
H	2.0398906	-2.2963482	-0.5034473
H	3.5125430	-3.6276128	0.9608100
H	1.6394546	-1.8998059	4.4337067
H	0.1682703	-0.5518573	2.9592984
H	-1.1685533	-4.0496074	-1.6718095
H	-0.0325752	-3.8789064	-0.3460691
H	2.2263818	2.6624612	0.8551561

H	0.9611492	1.9574014	1.9020798
H	2.4498364	1.0120747	1.5293201
H	2.8128289	1.4689747	-1.6309391
H	1.9309203	0.0077556	-2.1544249
H	2.9833486	-0.0489978	-0.6902057
H	-1.9251178	-5.6559581	-0.0564091
H	-1.6643022	-4.5424707	1.2984431
H	-4.1009356	-4.7282499	0.7131353
H	-3.7261038	-4.1110018	-0.9123894

5b_sy_4.log

E = -1224.136769
H = -1223.794690
G = -1223.864097

NImag=0

C	1.4566243	-4.3279423	-3.1779368
C	0.1407472	-3.5994395	-2.8264180
C	-1.0626587	-4.1969285	-3.5131936
C	-1.3950724	-5.5463537	-3.3343539
C	-2.4896167	-6.0943296	-3.9907694
C	-3.2538300	-5.2860669	-4.8418570
C	-2.9298752	-3.9384424	-5.0340221
C	-1.8372574	-3.4011287	-4.3627812
C	2.7125006	-3.6889861	-2.6706426
C	3.3154764	-2.5609811	-3.4741859
O	4.3757188	-3.5628270	-0.9453553
C	3.1759885	-4.0903545	-1.4341814
O	2.6014444	-4.8807269	-0.6291427
S	-0.1838934	-3.6494685	-0.9946784
C	0.8314619	-2.3195180	-0.3095313
C	-1.7853944	-2.8090412	-0.9427325
C	-4.3879085	-5.8483280	-5.5258231
N	-5.3011298	-6.3003148	-6.0762647
C	4.3668221	-1.8293407	-2.6433155
C	5.1823857	-2.8604437	-1.8828994
H	1.3757520	-5.3643545	-2.8305934
H	1.4580342	-4.3563316	-4.2782048
H	0.2128629	-2.5304662	-3.0563138
H	-0.8035150	-6.1772891	-2.6763311
H	-2.7525681	-7.1375095	-3.8507625
H	-3.5304274	-3.3230588	-5.6957193
H	-1.5828242	-2.3541064	-4.4998701
H	3.7758841	-2.9220038	-4.4103099
H	2.5344455	-1.8494616	-3.7873973
H	0.3250844	-1.9983410	0.6037266
H	1.8071051	-2.7383696	-0.0750946
H	0.8893543	-1.4971114	-1.0255400
H	-1.9985686	-2.5987653	0.1071202
H	-2.5439593	-3.4829096	-1.3420696
H	-1.7388725	-1.8827769	-1.5200926
H	5.0245536	-1.2154880	-3.2679004
H	3.8820221	-1.1681632	-1.9129780
H	5.9869399	-2.4002186	-1.3023473
H	5.6312631	-3.5771130	-2.5885371

5b_sy_5.log

E = -1224.139418
H = -1223.797554
G = -1223.866171

NImag=0

C	0.9766961	-2.1395009	-2.3593923
C	-0.3902114	-2.7094323	-1.8944465
C	-1.0098405	-3.6369770	-2.9100463
C	-1.9512841	-3.1052024	-3.7977464
C	-2.4799137	-3.8818936	-4.8216848
C	-2.0679660	-5.2133749	-4.9508669
C	-1.1388448	-5.7647492	-4.0601242
C	-0.6146828	-4.9746666	-3.0444008
C	2.0167402	-3.1429003	-2.7554545
C	2.1679568	-3.5047742	-4.2152236
O	3.7692441	-4.6272234	-2.0458239
C	2.7559748	-3.7156905	-1.7395736
O	2.6108111	-3.5077857	-0.4972270
S	-0.2372390	-3.5989923	-0.2847225
C	0.2136082	-2.2641290	0.8354167
C	-1.9917346	-3.7584676	0.1191801
C	-2.6107174	-6.0260015	-6.0066760
N	-3.0476621	-6.6794256	-6.8573750
C	3.0055123	-4.7726961	-4.3525258
C	4.1882047	-4.6739464	-3.4044713
H	0.7160274	-1.4996877	-3.2145289
H	1.3335394	-1.4686745	-1.5669847
H	-1.0799987	-1.8845053	-1.6780975
H	-2.2641632	-2.0701432	-3.6919889
H	-3.2055917	-3.4667630	-5.5132096
H	-0.8296413	-6.7991961	-4.1685517
H	0.1191265	-5.4040592	-2.3686612
H	1.1843101	-3.6572842	-4.6853094
H	2.6461711	-2.6933765	-4.7915833
H	0.0343419	-2.6298387	1.8485754
H	1.2750555	-2.0803293	0.6761049
H	-0.4043048	-1.3876868	0.6277571
H	-2.0557466	-4.1238729	1.1459889
H	-2.4285613	-4.4946019	-0.5578280
H	-2.4905321	-2.7921142	0.0196677
H	2.4098683	-5.6537703	-4.0779992
H	3.3629927	-4.9151003	-5.3781248
H	4.7743927	-3.7703921	-3.6352663
H	4.8502621	-5.5408745	-3.4847758

5b_sy_5_r.log

E = -1224.133617

H = -1223.791672

G = -1223.861610

NImag=0

C	-1.2585731	-0.0126480	1.2927308
C	-0.5805679	1.2230718	0.6503426
C	-0.5296028	2.4584939	1.5143740
C	-0.7253098	3.7140385	0.9312901
C	-0.6713417	4.8698136	1.7039368
C	-0.4178707	4.7579286	3.0746914
C	-0.2313223	3.5039153	3.6730541
C	-0.2936490	2.3574735	2.8914333
C	-2.5618215	0.3220509	1.9555788
C	-3.6648283	0.8815605	1.0886558
O	-3.8800568	0.4284300	3.9580120
C	-2.6506429	0.1728096	3.3307893
O	-1.7395335	-0.1710331	4.1343556
S	1.1686917	0.7686648	0.2412644
C	0.9495508	-0.5272225	-0.9943591
C	1.7125203	2.1300877	-0.8078187

C	-0.3555635	5.9468191	3.8832217
N	-0.3037564	6.9040613	4.5332023
C	-4.7892278	1.4464949	1.9529068
C	-5.0218917	0.5003984	3.1161194
H	-1.3883388	-0.7480397	0.4848238
H	-0.5899832	-0.4536988	2.0410530
H	-1.0297861	1.4641348	-0.3197178
H	-0.9267764	3.7887226	-0.1340660
H	-0.8237993	5.8454344	1.2545884
H	-0.0527540	3.4347362	4.7411426
H	-0.2080086	1.3804611	3.3626895
H	-3.2807549	1.6802195	0.4324180
H	-4.0763286	0.1170872	0.4056425
H	1.9183684	-0.6692887	-1.4772047
H	0.6559200	-1.4424561	-0.4805472
H	0.1945297	-0.2154583	-1.7190774
H	2.6696238	1.8339720	-1.2423217
H	1.8511902	3.0086279	-0.1762068
H	0.9692673	2.3111934	-1.5868700
H	-4.5014304	2.4261349	2.3563470
H	-5.7144718	1.5771211	1.3814120
H	-5.2614695	-0.5057940	2.7361001
H	-5.8469369	0.8303648	3.7542572

5b_sy_5_ts1.log

E = -1224.109021

H = -1223.769822

G = -1223.838310

NImag=1

C	1.2289189	0.8010506	1.6074920
C	1.3570608	-1.2350035	0.7219764
C	-0.0134468	-1.3947834	0.3243955
C	-0.9190890	-2.0508580	1.1987258
C	-2.2755767	-2.0727496	0.9467903
C	-2.7854098	-1.4417532	-0.2061283
C	-1.9072661	-0.8058087	-1.0967312
C	-0.5482522	-0.7711567	-0.8305777
C	0.3794152	1.6348441	0.9091818
C	-1.0798640	1.8036042	1.2951127
O	0.1973654	3.1814770	-0.9441913
C	0.9146302	2.2218051	-0.2987713
O	1.9881819	1.8972899	-0.8138241
S	2.5307064	-1.2030255	-0.5806356
C	3.9934926	-0.3955737	0.0972414
C	3.1628493	-2.9027165	-0.6464862
C	-4.1902675	-1.4604329	-0.4746183
N	-5.3310587	-1.4753196	-0.6902394
C	-1.8422553	2.5808752	0.2246998
C	-0.9624965	3.7063641	-0.2799019
H	0.8880687	0.3809339	2.5523018
H	2.3013590	0.9217878	1.5117725
H	1.7104562	-1.8276806	1.5657952
H	-0.5310955	-2.5360847	2.0902983
H	-2.9535380	-2.5756903	1.6297639
H	-2.3008819	-0.3224870	-1.9861105
H	0.1096522	-0.2479497	-1.5189397
H	-1.5450987	0.8219749	1.4531387
H	-1.1575443	2.3454387	2.2480949
H	4.8334948	-0.6698013	-0.5441795
H	3.8204851	0.6787573	0.0522560
H	4.1623845	-0.7440174	1.1185535

H	3.9678181	-2.9444108	-1.3839261
H	2.3352355	-3.5421457	-0.9579184
H	3.5244300	-3.1924061	0.3425483
H	-2.0953416	1.9327391	-0.6228531
H	-2.7753171	2.9917956	0.6223002
H	-0.6365624	4.3496093	0.5485613
H	-1.4638139	4.3255341	-1.0259976

5b_sy_5_ts1_rot1.log

E = -1224.105940
H = -1223.766663
G = -1223.836293

NImag=1

C	0.9603812	1.7997049	-0.6568958
C	1.7230905	0.0691485	0.3835540
C	0.6647725	-0.9081398	0.3228656
C	-0.4774775	-0.6718885	1.1264597
C	-1.5950091	-1.4874105	1.0518403
C	-1.6077272	-2.5764772	0.1685989
C	-0.4767265	-2.8429867	-0.6271217
C	0.6317669	-2.0225926	-0.5526060
C	-0.3473196	2.0567544	-0.2798124
C	-0.6392867	2.7876740	1.0158699
O	-2.6998410	1.8405594	-0.8125224
C	-1.4024369	1.5174693	-1.1093148
O	-1.2424738	0.8028851	-2.0980035
S	3.2580406	-0.3949963	-0.3238458
C	4.1722536	1.1566139	-0.3994705
C	4.1975164	-1.2327040	0.9812904
C	-2.7566515	-3.4256053	0.0899186
N	-3.6881965	-4.1153470	0.0254556
C	-2.1061946	2.6415082	1.4066603
C	-2.9523047	2.8537247	0.1688423
H	1.7467963	2.4144389	-0.2256136
H	1.1467032	1.4204233	-1.6584501
H	1.8642904	0.5685581	1.3422631
H	-0.4643282	0.1539267	1.8310553
H	-2.4613470	-1.2879673	1.6760409
H	-0.4809000	-3.6945593	-1.3005329
H	1.4837239	-2.2517603	-1.1864424
H	0.0085797	2.3994817	1.8145550
H	-0.4018832	3.8573477	0.9220824
H	5.2161168	0.9022770	-0.5923492
H	3.7785364	1.7482099	-1.2259181
H	4.0724701	1.6850344	0.5509686
H	5.1997158	-1.4440065	0.6012847
H	3.6755791	-2.1648559	1.2049160
H	4.2357855	-0.5875430	1.8614341
H	-2.3071844	1.6377576	1.8014721
H	-2.3891916	3.3681543	2.1746211
H	-2.7450105	3.8374700	-0.2748203
H	-4.0216437	2.7886771	0.3806866

5b_sy_5_ts1_rot2.log

E = -1224.102673
H = -1223.763734
G = -1223.835418

NImag=1

C	-0.7480760	-0.9997103	-0.2440262
C	0.3180075	0.6731396	0.6653100

C	1.6699527	0.2887456	0.3587009
C	2.3211610	-0.6261310	1.2255776
C	3.5757009	-1.1286844	0.9358532
C	4.2357496	-0.7354092	-0.2420454
C	3.6083979	0.1623931	-1.1212383
C	2.3507625	0.6603283	-0.8278911
C	-2.1253282	-0.9437148	-0.3639768
C	-2.7782596	-0.3688301	-1.6090180
O	-4.2591433	-1.4688140	0.6511121
C	-2.9042317	-1.3544902	0.7844275
O	-2.4462376	-1.6110477	1.8973444
S	-0.3042333	2.1173800	-0.1097289
C	-1.9122787	2.2717428	0.6861866
C	0.5403056	3.5378335	0.6425240
C	5.5371373	-1.2460892	-0.5433559
N	6.5933423	-1.6612296	-0.7880419
C	-4.2725971	-0.1523757	-1.3896666
C	-4.8287861	-1.3579780	-0.6606265
H	-0.1477815	-0.8943416	-1.1476582
H	-0.3131659	-1.6161747	0.5380721
H	0.0072567	0.6111217	1.7070862
H	1.8200720	-0.9316557	2.1402273
H	4.0566419	-1.8239487	1.6171585
H	4.1140111	0.4656124	-2.0330257
H	1.8937658	1.3503869	-1.5326960
H	-2.2969912	0.5790018	-1.8884259
H	-2.6366062	-1.0453156	-2.4635402
H	-2.3900015	3.1711852	0.2952583
H	-2.4976536	1.3883604	0.4320380
H	-1.7666178	2.3421468	1.7661874
H	0.0573603	4.4486901	0.2803257
H	1.5813291	3.5112355	0.3152003
H	0.4705227	3.4561046	1.7289414
H	-4.4532962	0.7405013	-0.7776699
H	-4.7986719	-0.0187797	-2.3396748
H	-4.6185404	-2.2798246	-1.2196130
H	-5.9062362	-1.2867795	-0.4999870

5b_sy_6.log

E = -1224.139000

H = -1223.796894

G = -1223.865618

NImag=0

C	1.5362359	-4.4456279	-3.1146978
C	0.2757385	-3.5616337	-2.9737353
C	-0.9917442	-4.1099625	-3.5748446
C	-1.3330286	-5.4646162	-3.4609466
C	-2.4957853	-5.9514521	-4.0467102
C	-3.3255583	-5.0766307	-4.7577050
C	-2.9969612	-3.7222756	-4.8862422
C	-1.8323032	-3.2504186	-4.2937891
C	2.8040993	-3.7945726	-2.6479644
C	3.6287147	-3.0073770	-3.6400025
O	4.3120373	-3.3695267	-0.8239277
C	3.1541799	-3.9767824	-1.3222145
O	2.5235199	-4.6600708	-0.4633773
S	0.0886236	-3.1183040	-1.1795310
C	-1.4202575	-2.1301320	-1.1828973
C	-0.5138375	-4.6185196	-0.3897824
C	-4.5285134	-5.5770485	-5.3686562
N	-5.4970305	-5.9793184	-5.8599216

C	5.0142441	-2.7262733	-3.0628331
C	4.8585274	-2.3171384	-1.6092271
H	1.3670747	-5.3904743	-2.5842315
H	1.5899498	-4.6823837	-4.1866737
H	0.4843702	-2.5761302	-3.4068549
H	-0.6917850	-6.1512952	-2.9172705
H	-2.7596371	-7.0001526	-3.9592301
H	-3.6449251	-3.0543966	-5.4439955
H	-1.5675505	-2.2011695	-4.3925053
H	3.7258263	-3.5631564	-4.5851145
H	3.1549638	-2.0474068	-3.9110541
H	-1.6092901	-1.8438593	-0.1460242
H	-1.2357398	-1.2358619	-1.7814676
H	-2.2601992	-2.7031156	-1.5791266
H	-0.6521017	-4.3698395	0.6649819
H	0.2793743	-5.3594935	-0.4906016
H	-1.4588880	-4.9328009	-0.8357348
H	5.6342651	-3.6307881	-3.1048117
H	5.5328515	-1.9371631	-3.6180745
H	4.2037873	-1.4337024	-1.5391434
H	5.8193525	-2.0671296	-1.1501612

5b_sy_6_r.log

E = -1224.134755

H = -1223.792959

G = -1223.863392

NImag=0

C	-0.8538732	-0.8720973	-0.7978587
C	-0.0300695	-0.1864424	0.3007905
C	0.9555915	-1.0574539	1.0323480
C	1.7282778	-2.0153818	0.3626798
C	2.6332300	-2.8064347	1.0599775
C	2.7656866	-2.6411091	2.4439036
C	1.9984984	-1.6922755	3.1296182
C	1.1004094	-0.9069310	2.4172711
C	-1.6950704	-1.9570920	-0.1792401
C	-1.4144068	-3.3993783	-0.5267230
O	-3.4515401	-2.5116641	1.3667137
C	-2.6830189	-1.5467399	0.7006782
O	-2.9956862	-0.3565763	0.9830671
S	0.7704685	1.3397982	-0.4170925
C	1.7431100	2.0168951	0.9391408
C	2.0720299	0.7117260	-1.4911711
C	3.7008937	-3.4589648	3.1695053
N	4.4549507	-4.1164863	3.7529366
C	-2.5484574	-4.2892976	-0.0240808
C	-2.9304426	-3.8344909	1.3732800
H	-1.4656943	-0.0957326	-1.2809389
H	-0.1956445	-1.2916606	-1.5678882
H	-0.7402282	0.2581137	1.0084896
H	1.6234855	-2.1543901	-0.7089956
H	3.2308475	-3.5490849	0.5419298
H	2.1047669	-1.5783111	4.2032006
H	0.4954250	-0.1725362	2.9422969
H	-1.2987925	-3.5214335	-1.6146019
H	-0.4639003	-3.7552276	-0.0887822
H	2.2506040	2.9042465	0.5551651
H	1.0524744	2.3000106	1.7357118
H	2.4672194	1.2778211	1.2863429
H	2.5673241	1.5827085	-1.9250742
H	1.6046568	0.1224475	-2.2819718

H	2.7807205	0.1153673	-0.9141664
H	-3.4277961	-4.1928748	-0.6735412
H	-2.2566313	-5.3449851	-0.0067827
H	-2.0471823	-3.8751699	2.0312755
H	-3.7112382	-4.4642524	1.8094688

5b_sy_6_ts1.log

E = -1224.101417

H = -1223.761809

G = -1223.832618

NImag=1

C	-0.8478608	-1.2151361	-0.2732899
C	0.2713242	0.2599493	0.8938559
C	1.6510042	0.0588847	0.5405117
C	2.3470206	0.7595525	-0.4750460
C	3.6482732	0.4302858	-0.8153424
C	4.3060264	-0.6251105	-0.1642960
C	3.6328231	-1.3473599	0.8369070
C	2.3377018	-1.0082577	1.1785184
C	-2.2209401	-1.1047263	-0.1518188
C	-2.9025992	-1.5543948	1.1220455
O	-4.2969919	-0.2579253	-1.0681818
C	-2.9585734	-0.4710682	-1.2253914
O	-2.4892676	-0.1425596	-2.3165833
S	-0.6188764	1.7409557	0.6789521
C	0.3799958	3.1279630	1.2809748
C	-0.7087344	2.1571436	-1.0833510
C	5.6497367	-0.9634741	-0.5180173
N	6.7406059	-1.2384676	-0.8045356
C	-4.4104744	-1.6529256	0.9254687
C	-4.8779415	-0.3878200	0.2381105
H	-0.3726742	-0.9699614	-1.2203685
H	-0.3222700	-1.9496967	0.3335648
H	-0.0436177	-0.1607397	1.8459204
H	1.8734405	1.5739526	-1.0099231
H	4.1622669	0.9881452	-1.5920911
H	4.1357406	-2.1651869	1.3438437
H	1.8303243	-1.5661947	1.9608623
H	-2.4854228	-2.5150276	1.4474445
H	-2.7010347	-0.8374108	1.9344292
H	-0.1626125	4.0470341	1.0473169
H	0.4773843	3.0118891	2.3611732
H	1.3588897	3.1241479	0.7991649
H	-1.5732378	2.8147955	-1.1957141
H	-0.8750175	1.2381862	-1.6476258
H	0.1951415	2.6757949	-1.4018457
H	-4.6653632	-2.5160903	0.2985468
H	-4.9322976	-1.7633391	1.8809789
H	-4.6074379	0.4955724	0.8325866
H	-5.9568724	-0.3771968	0.0720208

5b_sy_7_ts1.log

E = -1224.103166

H = -1223.764246

G = -1223.835392

NImag=1

C	-0.8793319	-0.4429035	1.4674044
C	0.3079970	1.2395960	0.6195328
C	1.5963067	0.6555757	0.3696625
C	2.5374944	0.6212580	1.4314362

C	3.7579618	-0.0125646	1.2971548
C	4.0953490	-0.6424841	0.0855791
C	3.1798696	-0.6251869	-0.9801666
C	1.9574021	0.0068426	-0.8390285
C	-1.8829508	-0.9385470	0.6529613
C	-1.5452092	-1.8804638	-0.4872252
O	-4.2557329	-1.0720063	0.1905141
C	-3.2406013	-0.5027656	0.8996173
O	-3.5760292	0.3574832	1.7179665
S	-0.6772407	1.6631651	-0.7664087
C	-1.9959375	2.5948906	0.0279331
C	0.1743910	3.0121528	-1.6267449
C	5.3580485	-1.2963039	-0.0607290
N	6.3834896	-1.8280338	-0.1789640
C	-2.7159334	-1.9916594	-1.4560614
C	-3.9795152	-2.2030739	-0.6495089
H	0.0626227	-0.9836575	1.5173230
H	-1.1502062	0.1187374	2.3568956
H	0.2466346	1.9895243	1.4061385
H	2.2881886	1.1084288	2.3701795
H	4.4614914	-0.0229941	2.1242663
H	3.4344980	-1.1112666	-1.9170846
H	1.2713378	-0.0080474	-1.6826098
H	-0.6505153	-1.5206443	-1.0090246
H	-1.3015902	-2.8824333	-0.1043576
H	-2.6877095	2.9159509	-0.7525816
H	-2.4980603	1.9319180	0.7363579
H	-1.5558479	3.4555765	0.5362027
H	-0.4905086	3.3802552	-2.4115496
H	1.0817227	2.6003941	-2.0724308
H	0.4154238	3.8001474	-0.9112911
H	-2.8199510	-1.0720058	-2.0459613
H	-2.5822963	-2.8254326	-2.1519840
H	-3.8881121	-3.0963557	-0.0173575
H	-4.8642500	-2.3122345	-1.2797148

5b_sy_8.log

E = -1224.135715
H = -1223.793674
G = -1223.863432

NImag=0

C	1.4474405	-4.3238175	-3.2140527
C	0.1387948	-3.6098308	-2.8074773
C	-1.0776608	-4.1804707	-3.4939828
C	-1.8726329	-3.3496117	-4.2896519
C	-2.9782898	-3.8596417	-4.9606795
C	-3.2942870	-5.2158880	-4.8234245
C	-2.5096402	-6.0592127	-4.0267577
C	-1.4026474	-5.5377993	-3.3694761
C	2.7147759	-3.6941118	-2.7218112
C	3.3864877	-2.6485477	-3.5797270
O	4.3241959	-3.4911309	-0.9484962
C	3.1793606	-4.0954359	-1.4861108
O	2.6563928	-4.9604178	-0.7242239
S	-0.1544646	-3.7366846	-0.9722028
C	0.8669165	-2.4348034	-0.2404066
C	-1.7584019	-2.9077096	-0.8557574
C	-4.4413086	-5.7507131	-5.5078535
N	-5.3649385	-6.1804404	-6.0587498
C	4.7888191	-2.3572566	-3.0514923
C	4.7207559	-2.2583028	-1.5384008

H	1.3752812	-5.3701681	-2.8942214
H	1.4221153	-4.3207579	-4.3135280
H	0.2064229	-2.5324254	-2.9945481
H	-1.6237815	-2.2966353	-4.3846895
H	-3.5947291	-3.2168710	-5.5803959
H	-2.7669872	-7.1085490	-3.9287444
H	-0.7958687	-6.1959730	-2.7534091
H	3.4438377	-2.9864137	-4.6257754
H	2.8138426	-1.7038327	-3.6066691
H	0.3546624	-2.1358644	0.6770335
H	1.8360975	-2.8695827	-0.0067953
H	0.9392094	-1.5924340	-0.9312688
H	-1.9544736	-2.7476711	0.2061735
H	-2.5205778	-3.5662890	-1.2731730
H	-1.7253444	-1.9553606	-1.3899415
H	5.4730112	-3.1728857	-3.3175486
H	5.1945728	-1.4286391	-3.4673032
H	4.0054556	-1.4710300	-1.2497250
H	5.6924857	-2.0137900	-1.0999357

5b_sy_8_ts1.log

E = -1224.103061
H = -1223.763899
G = -1223.835509

NImag=1

C	0.7399814	-0.9007599	0.5313663
C	-0.3193895	0.6752494	-0.5426704
C	-1.6910196	0.2769158	-0.3229412
C	-2.2571154	-0.6919963	-1.1887618
C	-3.5224144	-1.2070766	-0.9716510
C	-4.2772171	-0.7712967	0.1302977
C	-3.7331537	0.1783708	1.0110594
C	-2.4642202	0.6851643	0.7919779
C	2.0771141	-1.0726056	0.2230208
C	2.4815232	-1.7458496	-1.0689068
O	4.3863481	-0.6646405	0.8294491
C	3.0623699	-0.5308755	1.1310826
O	2.8128734	0.0311660	2.1997054
S	0.1161235	2.2618066	0.0479764
C	1.9156673	2.2952438	-0.0243567
C	-0.2572105	3.4097477	-1.3057500
C	-5.5891748	-1.2943424	0.3571307
N	-6.6536718	-1.7190452	0.5413257
C	3.9269627	-2.2230266	-0.9939123
C	4.7758497	-1.0752249	-0.4906437
H	0.4611561	-0.5352281	1.5169984
H	0.0177517	-1.5628657	0.0570841
H	0.0834768	0.4972274	-1.5397461
H	-1.6824554	-1.0302983	-2.0469623
H	-3.9371057	-1.9438332	-1.6528832
H	-4.3097805	0.5095927	1.8692888
H	-2.0662966	1.4071392	1.4991635
H	1.8017968	-2.5799734	-1.2812976
H	2.3885976	-1.0461717	-1.9155836
H	2.2078069	3.3470837	-0.0205613
H	2.2964350	1.7967852	0.8672746
H	2.2558025	1.8041682	-0.9393782
H	0.0735271	4.4082028	-1.0107094
H	-1.3390603	3.3988530	-1.4486153
H	0.2584511	3.0746169	-2.2083045
H	4.0194219	-3.0703501	-0.3035865

H	4.2958228	-2.5427530	-1.9734437
H	4.6902185	-0.2116230	-1.1638442
H	5.8307014	-1.3437722	-0.4051387

5b_sy_9.log

E = -1224.135248
H = -1223.793312
G = -1223.863493

NImag=0

C	1.5343253	-4.1641144	-3.4552792
C	0.2266497	-3.6912613	-2.8098239
C	-1.0289150	-4.2139156	-3.4585312
C	-1.2070810	-5.5827678	-3.6993397
C	-2.3701466	-6.0479223	-4.2993130
C	-3.3629449	-5.1325809	-4.6717952
C	-3.1985399	-3.7625167	-4.4413461
C	-2.0325145	-3.3138222	-3.8312447
C	2.7723123	-3.8272217	-2.6689520
C	3.7744005	-4.9310140	-2.4085631
O	4.1397762	-2.1383872	-1.6410281
C	3.0140527	-2.4926467	-2.3909417
O	2.2898554	-1.5101343	-2.7173451
S	0.2926767	-4.2117884	-1.0119676
C	0.9878698	-2.7846035	-0.1329057
C	-1.4402294	-4.0309440	-0.5187363
C	-4.5678797	-5.6082162	-5.2989758
N	-5.5374816	-5.9909915	-5.8034097
C	5.1129026	-4.3388795	-1.9758493
C	4.8438897	-3.2002479	-1.0088346
H	1.4846249	-5.2504658	-3.5990948
H	1.5213116	-3.7160135	-4.4629995
H	0.2123800	-2.5989707	-2.7630028
H	-0.4416794	-6.2978807	-3.4107498
H	-2.5123988	-7.1078913	-4.4813811
H	-3.9747963	-3.0634405	-4.7342774
H	-1.8982852	-2.2527803	-3.6417401
H	3.4228892	-5.6317947	-1.6312805
H	3.9164019	-5.5421411	-3.3129673
H	0.3260417	-2.5594071	0.7050562
H	1.9775551	-3.0695877	0.2222557
H	1.0637989	-1.9425310	-0.8262288
H	-1.4707296	-4.1631345	0.5641920
H	-2.0270910	-4.8132332	-1.0003941
H	-1.8018422	-3.0383669	-0.7968887
H	5.7538652	-5.0893759	-1.5010992
H	5.6510130	-3.9364373	-2.8434728
H	5.7685119	-2.7604678	-0.6244455
H	4.2574510	-3.5711039	-0.1526992

5b_sy_9_ts1.log

E = -1224.103900
H = -1223.765034
G = -1223.836508

NImag=1

C	-0.9581004	-0.2032247	1.5677318
C	0.2459503	1.3998271	0.6146881
C	1.5077980	0.7684685	0.3452799
C	1.8134008	0.0716835	-0.8516801
C	3.0118755	-0.6015345	-1.0077731
C	3.9583892	-0.6131583	0.0306549

C	3.6769266	0.0659143	1.2298768
C	2.4801123	0.7400249	1.3792743
C	-1.7907150	-0.9015929	0.7117614
C	-1.2366272	-1.9768630	-0.1984286
O	-4.0387217	-1.2489730	-0.1271401
C	-3.2000257	-0.5636091	0.7001819
O	-3.7372278	0.2764298	1.4258016
S	-0.7740811	1.7957750	-0.7504259
C	-2.1042332	2.6976462	0.0595567
C	0.0318797	3.1573342	-1.6343145
C	5.1965832	-1.3088073	-0.1312025
N	6.2021122	-1.8745417	-0.2621567
C	-2.3430493	-2.9340667	-0.6245633
C	-3.4987547	-2.1065814	-1.1449825
H	-0.0053488	-0.6459177	1.8484892
H	-1.4000959	0.4713384	2.2959707
H	0.2304034	2.1757771	1.3781565
H	1.1033289	0.0533943	-1.6748008
H	3.2243158	-1.1237318	-1.9357908
H	4.4048166	0.0610143	2.0356930
H	2.2742222	1.2647294	2.3083021
H	-0.7983788	-1.5336728	-1.1048313
H	-0.4229797	-2.5072866	0.3120372
H	-1.6724180	3.5246946	0.6271683
H	-2.7692480	3.0685299	-0.7223888
H	-2.6365048	2.0001758	0.7103749
H	-0.6474169	3.4980111	-2.4189376
H	0.9467333	2.7629753	-2.0806212
H	0.2574985	3.9603694	-0.9305275
H	-2.0038073	-3.6149877	-1.4112854
H	-2.6837213	-3.5385618	0.2250034
H	-4.3390974	-2.7223430	-1.4715876
H	-3.1737530	-1.4836941	-1.9892205

5b_sy_c_prod_1.log

E = -746.250103

H = -745.991712

G = -746.049796

NImag=0

C	4.8095565	1.1437029	2.6980785
O	4.2233227	2.4326599	2.9967380
C	3.9231695	3.3265662	2.0439640
C	4.0685545	2.9404180	0.6040497
C	4.7404686	1.6186391	0.2848192
C	4.3672259	0.6039644	1.3569006
O	3.4980471	4.4110338	2.3912189
C	2.9152774	3.4109211	-0.2647363
C	4.2226593	4.1170914	-0.3528280
C	5.1543629	3.9787064	-1.5107852
C	4.7346838	3.5188632	-2.7632995
C	5.6361784	3.3995801	-3.8160031
C	6.9766748	3.7464676	-3.6153472
C	7.4143396	4.2140377	-2.3685232
C	6.5011850	4.3262963	-1.3295021
C	7.9131397	3.6255843	-4.6996914
N	8.6677681	3.5276076	-5.5732856
H	5.8980275	1.2634007	2.7277455
H	4.5031453	0.5032285	3.5262952
H	4.4393586	1.2813108	-0.7111196
H	5.8314269	1.7458362	0.2716031
H	3.2850416	0.4260921	1.3606079

H	4.8673158	-0.3541216	1.1879476
H	2.6290961	2.7296137	-1.0602405
H	2.1024961	3.9328776	0.2278699
H	4.2736731	5.0774106	0.1534246
H	3.6939534	3.2575013	-2.9260962
H	5.3067955	3.0454296	-4.7874392
H	8.4559226	4.4815120	-2.2235792
H	6.8332338	4.6863685	-0.3593862

5b_sy_c_prod_2.log

E = -746.250315
H = -745.991930
G = -746.051214

NImag=0

C	4.9386519	1.1278809	2.4479539
O	4.4224790	2.4129906	2.8711143
C	3.8026635	3.2615337	2.0382858
C	3.7793943	2.9571848	0.5724771
C	4.1708058	1.5574332	0.1501707
C	5.3557008	1.1088500	0.9944590
O	3.3269514	4.2774892	2.5058270
C	2.8041503	3.7500020	-0.2521826
C	4.2344288	4.1704349	-0.2633984
C	5.1579187	3.9803908	-1.4171647
C	4.7188595	3.5854759	-2.6861498
C	5.6213949	3.4161257	-3.7308146
C	6.9831682	3.6474605	-3.5079967
C	7.4410095	4.0495589	-2.2459521
C	6.5269617	4.2123880	-1.2145771
C	7.9208170	3.4770266	-4.5845213
N	8.6767856	3.3393894	-5.4515791
H	5.7725534	0.9297912	3.1229479
H	4.1520341	0.3882918	2.6322207
H	3.3256721	0.8756848	0.3094900
H	4.4044635	1.5381308	-0.9179892
H	5.6680265	0.0915129	0.7410027
H	6.2116500	1.7767231	0.8350262
H	2.4084592	3.2312168	-1.1200502
H	2.1057046	4.3883689	0.2771455
H	4.4706015	5.0381819	0.3465067
H	3.6631394	3.4140811	-2.8704548
H	5.2762176	3.1117461	-4.7135014
H	8.4986523	4.2301274	-2.0836048
H	6.8747850	4.5255282	-0.2337906

5b_sy_c_prod_4.log

E = -746.250173
H = -745.991571
G = -746.049317

NImag=0

C	4.9976960	1.0470667	2.5279172
O	4.5450206	2.3540571	2.9518136
C	4.2153386	3.3174138	2.0807331
C	4.1980854	3.0104879	0.6132045
C	4.6988946	1.6510108	0.1599459
C	4.3625901	0.6166891	1.2257811
O	3.9017493	4.4049476	2.5237715
C	3.0448268	3.6594080	-0.1245163
C	4.4094154	4.2384084	-0.2755142
C	5.2395037	4.1206204	-1.5072952

C	4.8193219	3.4347624	-2.6540742
C	5.6405967	3.3464612	-3.7721049
C	6.9007968	3.9552891	-3.7521670
C	7.3362094	4.6514729	-2.6172272
C	6.5042076	4.7279166	-1.5087565
C	7.7515864	3.8713708	-4.9078603
N	8.4377443	3.8031741	-5.8389419
H	6.0883173	1.0895373	2.4335695
H	4.7412220	0.3849160	3.3560309
H	4.2475443	1.3884354	-0.8003312
H	5.7871431	1.6794630	0.0153695
H	3.2765308	0.5277133	1.3496482
H	4.7543666	-0.3683942	0.9564141
H	2.6263956	3.0760250	-0.9386717
H	2.3346275	4.2292708	0.4642144
H	4.5935013	5.1451025	0.2932175
H	3.8398164	2.9684328	-2.6866468
H	5.3085185	2.8159951	-4.6585883
H	8.3126476	5.1249912	-2.6111889
H	6.8358853	5.2688549	-0.6268466

5b_sy_tr_prod_1.log

E = -746.248951

H = -745.990772

G = -746.048930

NImag=0

C	2.9207190	-0.5288732	2.5017430
O	3.2425904	-0.9632838	3.8453742
C	3.1441826	-2.2417954	4.2452826
C	2.4053346	-3.2068380	3.3714340
C	2.2420900	-2.8216915	1.9162762
C	1.8351445	-1.3563436	1.8495439
O	3.6048065	-2.5393627	5.3282013
C	2.4568146	-4.6549718	3.7726667
C	1.2113866	-3.8833974	4.0553892
C	0.7792008	-3.5236460	5.4392472
C	1.0683442	-4.3393699	6.5368999
C	0.6300649	-3.9971054	7.8113851
C	-0.1076025	-2.8209533	7.9906361
C	-0.4082139	-1.9926736	6.9008314
C	0.0361257	-2.3517179	5.6354369
C	-0.5644157	-2.4604538	9.3056219
N	-0.9328600	-2.1701815	10.3650309
H	2.6347383	0.5181992	2.6109723
H	3.8462925	-0.5823434	1.9182116
H	3.1899554	-2.9674243	1.3819701
H	1.4976038	-3.4738655	1.4501152
H	1.7199405	-1.0147093	0.8165643
H	0.8790297	-1.2051248	2.3655511
H	2.4383798	-5.3772156	2.9627701
H	3.0956061	-4.8982361	4.6153695
H	0.3821177	-4.0284377	3.3651137
H	1.6414046	-5.2506464	6.3955801
H	0.8543824	-4.6313376	8.6629165
H	-0.9805793	-1.0831304	7.0514126
H	-0.1910838	-1.7141692	4.7846522

5b_sy_tr_prod_2.log

E = -746.246987

H = -745.988866

G = -746.046869
 NImag=0

C	3.2035213	-0.6247474	2.1754046
O	3.4807642	-0.9489468	3.5572460
C	2.9941082	-2.0465160	4.1583570
C	2.1449152	-2.9952188	3.3698592
C	1.8400305	-2.6476704	1.9222444
C	3.0001780	-1.8616412	1.3301320
O	3.2968468	-2.2371310	5.3191944
C	2.3480542	-4.4532893	3.7533338
C	1.0802853	-3.7742484	4.1304933
C	0.7003582	-3.4797723	5.5451232
C	1.0297033	-4.3560726	6.5830039
C	0.6294519	-4.0936211	7.8881029
C	-0.1135340	-2.9380401	8.1581291
C	-0.4570926	-2.0522253	7.1277894
C	-0.0497339	-2.3319399	5.8303098
C	-0.5317023	-2.6588365	9.5049162
N	-0.8693727	-2.4337704	10.5902361
H	2.3108656	0.0100878	2.1549656
H	4.0627293	-0.0345513	1.8532404
H	1.6447726	-3.5679420	1.3636853
H	0.9318790	-2.0335128	1.8719185
H	3.9161896	-2.4647865	1.3202125
H	2.7871604	-1.5522834	0.3027831
H	2.3319849	-5.1692787	2.9381150
H	3.0656969	-4.6412002	4.5454237
H	0.2230392	-3.9846982	3.4920168
H	1.6080869	-5.2500146	6.3691937
H	0.8864816	-4.7737019	8.6937943
H	-1.0335810	-1.1598780	7.3493558
H	-0.3091866	-1.6485525	5.0258200

5b_sy_tr_prod_3.log
 E = -746.248288
 H = -745.989724
 G = -746.046959
 NImag=0

C	2.2869119	-0.7238666	3.2594281
O	3.2399484	-1.2935731	4.1865338
C	3.3099096	-2.6330968	4.2462814
C	2.3937752	-3.3588082	3.3096291
C	2.3798272	-2.8183260	1.8840692
C	2.5257620	-1.2839972	1.8702201
O	4.0683524	-3.1563457	5.0338509
C	2.1171685	-4.7961923	3.5838756
C	1.0576926	-3.7918890	3.9381488
C	0.6897737	-3.4288041	5.3342520
C	1.3837395	-3.8958870	6.4592017
C	1.0036817	-3.5097066	7.7392815
C	-0.0863924	-2.6481024	7.9073863
C	-0.7959015	-2.1747867	6.7960713
C	-0.4026676	-2.5674967	5.5244179
C	-0.4854419	-2.2532372	9.2306552
N	-0.8074882	-1.9350901	10.2972140
H	1.2740163	-0.9398903	3.6183053
H	2.4571930	0.3516745	3.3070220
H	3.1962419	-3.2819408	1.3212676
H	1.4445385	-3.1312921	1.4105986
H	3.5335310	-0.9965117	1.5544058
H	1.8199771	-0.8228434	1.1741300

H	1.9255204	-5.4285692	2.7226001
H	2.6730490	-5.2638177	4.3901901
H	0.2287915	-3.7034466	3.2402050
H	2.2261880	-4.5691570	6.3455469
H	1.5433781	-3.8771139	8.6060472
H	-1.6431686	-1.5109152	6.9336207
H	-0.9528072	-2.2067708	4.6596436

5b_sy_tr_prod_5.log

E = -746.243114
H = -745.984816
G = -746.042902

NImag=0

C	4.1267429	-1.8185276	2.0635387
O	3.9722809	-1.3518309	3.4218719
C	2.9378045	-1.8317948	4.1364830
C	2.0368273	-2.7705442	3.3953950
C	1.6918438	-2.3697824	1.9615793
C	2.8391290	-1.5874231	1.2999403
O	2.8299686	-1.5071911	5.2989121
C	2.3217081	-4.2329910	3.7004952
C	1.0334138	-3.6145427	4.1437891
C	0.6639169	-3.4172696	5.5785413
C	1.2540235	-4.1565294	6.6075101
C	0.8671427	-3.9692017	7.9299054
C	-0.1323293	-3.0361363	8.2283150
C	-0.7485769	-2.3006707	7.2058988
C	-0.3494778	-2.5011986	5.8924746
C	-0.5369404	-2.8366497	9.5929895
N	-0.8630742	-2.6753808	10.6931907
H	4.9588237	-1.2408896	1.6605264
H	4.4048071	-2.8784147	2.0825161
H	1.4716620	-3.2848242	1.4030658
H	0.7784314	-1.7668520	1.9674058
H	2.9758699	-1.8890287	0.2579497
H	2.6281636	-0.5131856	1.3069233
H	2.3079782	-4.9199414	2.8601962
H	3.0722791	-4.4377770	4.4588437
H	0.1726421	-3.8439497	3.5173488
H	2.0252243	-4.8857241	6.3798672
H	1.3293378	-4.5422796	8.7272873
H	-1.5275695	-1.5844226	7.4463553
H	-0.8215530	-1.9331461	5.0952845

5b_tr_1_ts2.log

E = -1224.125656
H = -1223.785315
G = -1223.856115

NImag=1

C	1.5508100	0.5075769	0.9652211
C	0.6520416	0.8207856	-0.1828532
C	-0.7719721	0.3865795	-0.1701835
C	-1.5344270	0.3920033	1.0063114
C	-2.8734157	0.0202701	0.9822259
C	-3.4599970	-0.3589342	-0.2306471
C	-2.7141715	-0.3626687	-1.4174445
C	-1.3797080	0.0150486	-1.3783524
C	1.6962327	-0.9512395	0.6148086
C	0.9286488	-1.9956946	1.3830935
O	2.7907471	-2.5786256	-0.7825403

C	2.5790062	-1.2538762	-0.4380475
O	3.2038399	-0.4230407	-1.1309398
S	0.4065232	2.9967276	-0.3968002
C	0.4034172	3.5105477	1.3324113
C	2.0861418	3.4451155	-0.8813512
C	-4.8444369	-0.7469468	-0.2588454
N	-5.9597044	-1.0592217	-0.2815345
C	0.9401131	-3.3164707	0.6204064
C	2.3525037	-3.5804525	0.1356177
H	2.4918127	1.0619170	0.9179992
H	1.0817366	0.6564494	1.9411760
H	1.1481490	0.7119148	-1.1463525
H	-1.0850721	0.6859336	1.9499868
H	-3.4628912	0.0232492	1.8930794
H	-3.1795838	-0.6590185	-2.3516151
H	-0.7924479	0.0165839	-2.2926187
H	1.3624512	-2.1510290	2.3852201
H	-0.1071169	-1.6735317	1.5570116
H	0.4223049	4.6014766	1.3733156
H	-0.5206421	3.1470096	1.7868379
H	1.2711983	3.0976932	1.8502801
H	2.1842948	4.5322093	-0.8523144
H	2.2383703	3.0919960	-1.9031293
H	2.8113531	2.9823193	-0.2096373
H	0.6062395	-4.1474664	1.2502376
H	0.2710246	-3.2591284	-0.2480043
H	2.4321570	-4.5278943	-0.4032565
H	3.0439424	-3.6099950	0.9908074

5b_tr_2_ts2.log

E = -1224.125901

H = -1223.785485

G = -1223.856194

NImag=1

C	1.5619748	0.5415958	0.9589643
C	0.6493862	0.8542649	-0.1778942
C	-0.7579749	0.3713599	-0.1693736
C	-1.3854784	0.0888140	-1.3920285
C	-2.7068021	-0.3311852	-1.4343540
C	-3.4205379	-0.4629516	-0.2348944
C	-2.8131575	-0.1780878	0.9933572
C	-1.4871031	0.2375822	1.0204530
C	1.7170582	-0.9129529	0.5999422
C	1.0045219	-1.9723394	1.4028340
O	2.7624725	-2.5097882	-0.8657350
C	2.6040372	-1.1969955	-0.4559158
O	3.2938259	-0.3614921	-1.0764721
S	0.3322387	3.0249885	-0.3342910
C	0.3069130	3.4762676	1.4119225
C	1.9944536	3.5507144	-0.8002683
C	-4.7917231	-0.8946862	-0.2660428
N	-5.8965393	-1.2421421	-0.2912595
C	1.5995755	-3.3457062	1.0975420
C	1.8002690	-3.4561892	-0.4013723
H	2.4967314	1.1057029	0.9052526
H	1.1013275	0.6773493	1.9405361
H	1.1424356	0.7843359	-1.1470961
H	-0.8240024	0.1960243	-2.3163340
H	-3.1871664	-0.5566367	-2.3807403
H	-3.3764379	-0.2826318	1.9147851
H	-1.0227026	0.4544667	1.9774513

H	1.0863870	-1.7530210	2.4768414
H	-0.0766308	-2.0020202	1.1850842
H	0.2503827	4.5635475	1.4932006
H	-0.5862131	3.0321460	1.8570624
H	1.2047451	3.1056277	1.9098975
H	2.0567774	4.6380151	-0.7224284
H	2.1553298	3.2488671	-1.8370678
H	2.7365850	3.0822451	-0.1512357
H	2.5715702	-3.4648139	1.5917408
H	0.9435551	-4.1502643	1.4451085
H	0.8464960	-3.2856792	-0.9234993
H	2.1844171	-4.4360283	-0.6954177

5b_tr_3_ts2.log

E = -1224.127013

H = -1223.786647

G = -1223.856848

NImag=1

C	1.4523761	1.1478374	0.8958051
C	0.4299192	1.0733245	-0.1866021
C	-0.7022049	0.1206440	-0.1233474
C	-1.3015769	-0.2524785	1.0897057
C	-2.3976036	-1.1072143	1.1023047
C	-2.9020037	-1.5980609	-0.1075170
C	-2.3166410	-1.2362945	-1.3287917
C	-1.2269555	-0.3783690	-1.3268004
C	2.1727626	-0.1209510	0.5264604
C	1.9524530	-1.3755005	1.3301504
O	3.7747245	-1.1646833	-0.9364148
C	3.0372896	-0.0467827	-0.5803803
O	3.2101675	0.9525526	-1.3104466
S	-0.5432470	3.0602356	-0.2339646
C	-2.1582720	2.7783101	-0.9880579
C	-1.0349698	3.2375819	1.4918969
C	-4.0329626	-2.4862953	-0.0961545
N	-4.9438853	-3.2017187	-0.0872441
C	2.4975544	-2.5836606	0.5747547
C	3.8602389	-2.2272891	0.0129856
H	2.0700099	2.0471004	0.7960517
H	1.0268349	1.1067388	1.9022705
H	0.8675213	1.1836338	-1.1765676
H	-0.9147144	0.1198221	2.0328428
H	-2.8608064	-1.3953437	2.0401237
H	-2.7146567	-1.6259145	-2.2597298
H	-0.7673813	-0.0884111	-2.2679351
H	2.4435310	-1.3087050	2.3155091
H	0.8839142	-1.5218224	1.5432503
H	-2.7333183	3.7050858	-0.9293044
H	-2.0007618	2.5111690	-2.0347795
H	-2.6823434	1.9742038	-0.4651566
H	-1.6775103	4.1162681	1.5803818
H	-0.1331005	3.3846472	2.0880960
H	-1.5735585	2.3470419	1.8246837
H	2.5841953	-3.4592219	1.2263007
H	1.8295170	-2.8447649	-0.2561660
H	4.3164003	-3.0640124	-0.5219702
H	4.5364092	-1.9276084	0.8275137

5b_tr_4_ts2.log

E = -1224.127615

H = -1223.787294
G = -1223.858876
NImag=1

C	1.5179439	0.4064664	1.3042761
C	0.6313567	0.8617066	0.1975199
C	-0.7702730	0.3680853	0.1135604
C	-1.5958532	0.3314477	1.2457589
C	-2.9074338	-0.1144554	1.1482270
C	-3.3997321	-0.5298757	-0.0955910
C	-2.5899267	-0.4940433	-1.2376429
C	-1.2823149	-0.0383033	-1.1255560
C	1.7721604	-0.9467063	0.6951136
C	1.0119286	-2.1563036	1.1750592
O	2.9915540	-2.1883984	-0.9696295
C	2.7054419	-0.9804501	-0.3565335
O	3.3110679	0.0079922	-0.8254571
S	0.3579943	3.0189818	0.3549849
C	2.0714960	3.4573032	-0.0107796
C	-0.3899416	3.2974122	-1.2635941
C	-4.7561708	-0.9969268	-0.2005713
N	-5.8486466	-1.3724507	-0.2846058
C	1.1107217	-3.2726826	0.1400215
C	2.5532216	-3.3805140	-0.3169428
H	2.4195747	1.0193294	1.3926020
H	1.0079599	0.3494127	2.2695455
H	1.1456461	0.9299609	-0.7609632
H	-1.2151963	0.6579771	2.2092967
H	-3.5485452	-0.1427842	2.0230290
H	-2.9835854	-0.8202214	-2.1945336
H	-0.6424598	-0.0098215	-2.0034030
H	1.4040140	-2.5196281	2.1395321
H	-0.0423291	-1.9057850	1.3594108
H	2.0925238	4.4500561	-0.4646813
H	2.6225691	3.4756242	0.9304427
H	2.5060222	2.7137486	-0.6869040
H	-0.3048120	4.3563931	-1.5148301
H	-1.4438765	3.0210663	-1.1991366
H	0.1173788	2.6871811	-2.0164032
H	0.7828949	-4.2332082	0.5506651
H	0.4797314	-3.0423817	-0.7283836
H	2.6942486	-4.1828621	-1.0454346
H	3.2068962	-3.5777993	0.5455933

5b_tr_6_ts2.log

E = -1224.127318
H = -1223.787017
G = -1223.857505
NImag=1

C	-1.4660561	-1.1895380	0.8695136
C	-0.4362973	-1.1114735	-0.2059816
C	0.6771972	-0.1384414	-0.1368755
C	1.2127075	0.3002425	1.0838757
C	2.2903929	1.1776522	1.1078161
C	2.8389248	1.6278981	-0.0985659
C	2.3141382	1.2041524	-1.3276533
C	1.2424767	0.3241887	-1.3366987
C	-2.1650941	0.0953091	0.5202606
C	-1.9692123	1.3177967	1.3796387
O	-3.6593071	1.2150862	-0.9968427
C	-3.0245832	0.0518571	-0.5931674
O	-3.2952324	-0.9609733	-1.2717003

S	0.5596312	-3.0845788	-0.2202997
C	2.1825667	-2.7962264	-0.9550332
C	1.0293800	-3.2203434	1.5153183
C	3.9508452	2.5393525	-0.0763683
N	4.8469041	3.2732442	-0.0588358
C	-3.0277015	2.3676524	1.0473724
C	-3.1677143	2.4428598	-0.4606546
H	-2.0933677	-2.0799745	0.7523081
H	-1.0450417	-1.1681411	1.8784334
H	-0.8620157	-1.2321241	-1.2005459
H	0.7876570	-0.0367094	2.0239242
H	2.7037631	1.5164289	2.0519527
H	2.7443627	1.5644664	-2.2560831
H	0.8299284	-0.0127057	-2.2839671
H	-2.0227295	1.0465392	2.4436678
H	-0.9708940	1.7674787	1.2367764
H	2.7650242	-3.7166776	-0.8740855
H	2.0385863	-2.5457365	-2.0077575
H	2.6909266	-1.9799893	-0.4356706
H	1.7139277	-4.0643796	1.6233570
H	0.1262783	-3.4071766	2.0982008
H	1.5164954	-2.3000233	1.8475386
H	-3.9975962	2.0876420	1.4764440
H	-2.7538197	3.3502262	1.4448714
H	-2.1936307	2.6717617	-0.9191677
H	-3.8833929	3.2081978	-0.7709734

dimethylsulfide.log

E = -477.935305

H = -477.853025

G = -477.885651

NImag=0

S	-0.5213679	0.4129884	0.0001686
C	-0.9604508	2.1713240	-0.0001168
H	-0.5733566	2.6659317	-0.8949189
H	-2.0504574	2.2446397	0.0017798
H	-0.5701714	2.6670194	0.8926972
C	1.2826781	0.5860343	-0.0031440
H	1.7156401	-0.4169797	-0.0033030
H	1.6180926	1.1171687	-0.8978744
H	1.6212702	1.1182559	0.8897417

e_pent_sr_oe_1_ts1.log

E = -1110.795242

H = -1110.470677

G = -1110.539754

NImag=1

C	-2.6943402	-1.1638568	0.8372876
C	-1.3711223	-0.8127927	1.1100484
C	-3.0945231	-2.0906398	-0.1765240
O	-4.2909987	-2.3524617	-0.4122950
C	-2.0250803	-2.7730860	-1.0170528
C	-1.0467879	-0.0949245	2.3959490
C	-0.5432249	0.5528760	-0.3246481
S	-1.0531513	2.1915808	0.0385135
C	0.8836389	0.3125954	-0.2682668
C	-0.8106052	3.1445913	-1.4856392
C	-2.8502579	2.0792115	0.0354376
C	1.7946003	1.0634271	0.5137632
C	3.1291297	0.7053157	0.6055790

C	3.6051921	-0.4248545	-0.0777911
C	2.7199116	-1.1912966	-0.8540427
C	1.3885637	-0.8273392	-0.9426604
C	4.9848036	-0.7942568	0.0158687
N	6.1031397	-1.0949311	0.0921307
H	-3.4998131	-0.6439160	1.3542348
H	-0.5948359	-1.4998665	0.7732376
H	-1.2182090	-3.1908686	-0.4068934
H	-2.4871027	-3.5721389	-1.5999870
H	-1.5727884	-2.0522774	-1.7085490
H	-0.0502793	0.3563009	2.3813660
H	-1.0704963	-0.8142871	3.2233092
H	-1.7874433	0.6803384	2.6207121
H	-1.0528943	0.1742595	-1.2103784
H	-1.2059151	4.1505661	-1.3262744
H	0.2640204	3.1885141	-1.6713742
H	-1.3275113	2.6410479	-2.3049685
H	-3.2270601	3.1020269	-0.0223698
H	-3.1699728	1.6158744	0.9678137
H	-3.1779106	1.4945075	-0.8268106
H	1.4602273	1.9433057	1.0566168
H	3.8111305	1.2991836	1.2062333
H	3.0842768	-2.0656762	-1.3844908
H	0.7113004	-1.4233903	-1.5486331

e_pent_sr_oe_2_ts1.log

E = -1110.790301

H = -1110.465579

G = -1110.534896

NImag=1

C	1.7923580	-1.7711137	0.1397215
C	1.5191701	-1.0670904	1.3108653
C	3.0063176	-1.6868861	-0.6170087
O	3.2036217	-2.3720307	-1.6381475
C	4.1302422	-0.7705505	-0.1522999
C	0.5049741	-1.6347605	2.2702951
C	0.4339671	0.8285233	1.0251025
S	1.4593741	1.9816548	0.1947949
C	-0.8812899	0.4881932	0.5201233
C	1.8681711	1.3812012	-1.4681847
C	0.4360490	3.4060790	-0.2694955
C	-1.1215164	0.1037538	-0.8192276
C	-2.3794248	-0.3113416	-1.2334225
C	-3.4371670	-0.3693270	-0.3162977
C	-3.2198260	-0.0102871	1.0257008
C	-1.9654597	0.4100380	1.4276985
C	-4.7358740	-0.7956764	-0.7445997
N	-5.7884157	-1.1404207	-1.0901399
H	1.0439319	-2.4664349	-0.2397876
H	2.3347162	-0.5258770	1.7867767
H	3.7892910	0.1194309	0.3832216
H	4.7886497	-1.3281019	0.5239891
H	4.7168952	-0.4644734	-1.0214061
H	0.1843236	-0.9131408	3.0254407
H	0.9619709	-2.4857041	2.7898172
H	-0.3776149	-2.0067890	1.7398195
H	0.4615430	1.1302227	2.0713495
H	2.8264844	1.8278202	-1.7390974
H	1.9499805	0.2957128	-1.4412429
H	1.0929186	1.6895717	-2.1703710
H	1.0520615	4.0727798	-0.8779846

H	0.1335097	3.9054343	0.6521892
H	-0.4335742	3.0592053	-0.8315814
H	-0.3192378	0.1108669	-1.5473925
H	-2.5442539	-0.6006971	-2.2667175
H	-4.0389956	-0.0544852	1.7367231
H	-1.8048012	0.6949994	2.4638682

e_pent_sr_oe_3_ts1.log

E = -1110.788381
H = -1110.463604
G = -1110.532292

NImag=1

C	0.9113795	-1.6950389	0.8094673
C	1.3708042	-0.5558123	1.4703208
C	1.6387288	-2.5435029	-0.0883594
O	1.0816698	-3.4543913	-0.7331111
C	3.1525331	-2.4436895	-0.2071007
C	0.7666163	-0.2004331	2.8068011
C	0.6468991	1.2783841	0.4924266
S	1.5651259	1.8337761	-0.9204159
C	-0.7206602	0.9272365	0.1885768
C	2.7055372	3.0134075	-0.1770095
C	2.7422213	0.5466161	-1.3986023
C	-1.0483896	0.1664032	-0.9575870
C	-2.3466910	-0.2609226	-1.1913431
C	-3.3565385	0.0387291	-0.2663183
C	-3.0505547	0.7735185	0.8938183
C	-1.7556078	1.2082196	1.1111956
C	-4.6976677	-0.4051435	-0.5010504
N	-5.7849914	-0.7636544	-0.6901845
H	-0.1273138	-1.9886188	0.9676986
H	2.4212783	-0.2880178	1.3673614
H	3.6065155	-1.6629283	0.4037797
H	3.5674985	-3.4078356	0.1049025
H	3.4332122	-2.2932715	-1.2548736
H	1.0259081	0.8078294	3.1382259
H	1.1455365	-0.9084212	3.5541953
H	-0.3234982	-0.3007204	2.7896327
H	0.7972087	1.9981847	1.2940954
H	3.4409850	3.2855235	-0.9358768
H	2.1307324	3.8903401	0.1227706
H	3.1892583	2.5471310	0.6837992
H	3.4321662	0.3431872	-0.5801084
H	3.2746711	0.9259284	-2.2736326
H	2.1686959	-0.3401942	-1.6715818
H	-0.2771690	-0.1009732	-1.6769687
H	-2.5817398	-0.8377341	-2.0805400
H	-3.8353036	1.0073555	1.6065506
H	-1.5273905	1.7889734	2.0006869

e_pent_sr_oe_4_ts1.log

E = -1110.790716
H = -1110.466098
G = -1110.535082

NImag=1

C	-2.6302595	-0.8984029	1.0569531
C	-1.2344885	-0.9087436	1.0644781
C	-3.4620423	-1.5510059	0.0912415
O	-4.7057468	-1.4646862	0.1183890
C	-2.8271272	-2.3315899	-1.0476885

C	-0.5047955	-0.4345975	2.2947894
C	-0.3981610	0.3171258	-0.5187563
S	-1.0078200	1.9791546	-0.6239212
C	1.0334878	0.1738846	-0.4490778
C	-2.6018594	1.7154240	-1.4244127
C	-1.5570170	2.4800771	1.0279480
C	1.8983366	1.1474416	0.1095318
C	3.2532808	0.9075349	0.2551922
C	3.7961680	-0.3280738	-0.1349190
C	2.9565615	-1.3154078	-0.6806439
C	1.6059260	-1.0649546	-0.8361697
C	5.1952342	-0.5799198	0.0232112
N	6.3307456	-0.7843144	0.1517404
H	-3.1535366	-0.2713693	1.7781640
H	-0.7264945	-1.7156402	0.5378308
H	-1.8694092	-2.7896495	-0.7900881
H	-3.5224668	-3.1052453	-1.3810192
H	-2.6568794	-1.6482896	-1.8898722
H	0.5081584	-0.0845403	2.0774113
H	-0.4153335	-1.2792265	2.9893396
H	-1.0545651	0.3578981	2.8088639
H	-0.8966909	-0.2706133	-1.2857348
H	-3.1330165	2.6688669	-1.4215674
H	-2.4074925	1.3955678	-2.4491135
H	-3.1560533	0.9561285	-0.8698221
H	-1.9697628	3.4858741	0.9236492
H	-0.6779807	2.5071873	1.6737438
H	-2.3057548	1.7843638	1.4040755
H	1.5077229	2.1074076	0.4394224
H	3.8991265	1.6710727	0.6777821
H	3.3746973	-2.2695897	-0.9866057
H	0.9666182	-1.8279455	-1.2728662

e_pent_sr_oe_5_ts1.log

E = -1110.796443

H = -1110.471905

G = -1110.540730

NImag=1

C	1.2146579	-1.8526355	0.4425328
C	1.3025376	-0.9054358	1.4596564
C	2.2180661	-2.1644197	-0.5348392
O	1.9988374	-2.9534085	-1.4738006
C	3.6188202	-1.5747581	-0.4394569
C	0.3686232	-0.9960709	2.6371478
C	0.5681827	1.0505270	0.7412364
S	1.6973359	1.3505639	-0.5706341
C	-0.7782561	0.7347103	0.3448683
C	1.1729365	2.8871596	-1.3765876
C	3.1453358	1.9524453	0.3145877
C	-1.0867033	0.0365015	-0.8493165
C	-2.3838500	-0.3635483	-1.1322194
C	-3.4207990	-0.0780352	-0.2328484
C	-3.1400143	0.6188082	0.9581440
C	-1.8465550	1.0158146	1.2344727
C	-4.7602482	-0.4859485	-0.5276392
N	-5.8472110	-0.8176817	-0.7640074
H	0.2700258	-2.3807457	0.3134541
H	2.2785596	-0.4877462	1.6986468
H	3.8384992	-1.0771760	0.5063820
H	4.3361994	-2.3890573	-0.5775727
H	3.7741056	-0.8650354	-1.2594280

H	0.3186744	-0.0616600	3.2023816
H	0.7296719	-1.7810555	3.3131070
H	-0.6425940	-1.2712200	2.3205290
H	0.6891025	1.7768701	1.5453512
H	1.9355118	3.1604420	-2.1094259
H	0.2276405	2.6820546	-1.8826525
H	1.0501855	3.6666887	-0.6225280
H	3.8890560	2.2387988	-0.4309059
H	3.5331655	1.1442250	0.9341621
H	2.8577694	2.8088961	0.9278181
H	-0.3054279	-0.1964805	-1.5675195
H	-2.5998468	-0.8985574	-2.0520435
H	-3.9435496	0.8468666	1.6516478
H	-1.6367493	1.5551725	2.1541394

e_pent_sr_oz_1_ts1.log

E = -1110.801483

H = -1110.477189

G = -1110.546201

NImag=1

C	0.5393130	-1.8995689	0.9943846
C	1.2976904	-0.9223747	1.6186991
C	0.9269314	-2.3942586	-0.2917923
O	1.9409067	-1.9813470	-0.8932247
C	0.0515935	-3.4301319	-0.9690259
C	0.9268150	-0.4165145	2.9843967
C	1.0023073	1.0134325	0.4913866
S	2.0841085	1.0958083	-0.8879313
C	-0.3938373	0.8905021	0.1816127
C	2.4291703	2.8688474	-1.0601812
C	3.6994438	0.5660324	-0.2882185
C	-1.3552160	1.4124855	1.0843674
C	-2.7077692	1.1884506	0.9091888
C	-3.1581273	0.4304825	-0.1882044
C	-2.2270624	-0.1043621	-1.0912822
C	-0.8714135	0.1105776	-0.9016581
C	-4.5574175	0.2037460	-0.3795571
N	-5.6933543	0.0202201	-0.5338045
H	-0.4418191	-2.1631510	1.3836869
H	2.3493597	-0.8666827	1.3552035
H	-0.8358100	-3.6784292	-0.3819167
H	-0.2587169	-3.0565919	-1.9506943
H	0.6352667	-4.3418630	-1.1359200
H	1.4789362	0.4868491	3.2535463
H	1.1574501	-1.1851771	3.7324003
H	-0.1467570	-0.2080923	3.0498048
H	1.2857437	1.7309773	1.2608403
H	3.1683799	3.0024774	-1.8534030
H	1.4914198	3.3544437	-1.3355781
H	2.8016870	3.2589720	-0.1104932
H	4.4383622	0.9246976	-1.0077229
H	3.6901708	-0.5228020	-0.2645701
H	3.8838738	0.9986662	0.6976509
H	-1.0164827	2.0085861	1.9274966
H	-3.4268644	1.6036967	1.6087567
H	-2.5717989	-0.6987277	-1.9324122
H	-0.1677072	-0.3239251	-1.6057634

e_pent_sr_oz_2_ts1.log

E = -1110.796298

H = -1110.471929
G = -1110.542684
NImag=1

C	-2.6235910	-1.1923042	0.7563365
C	-1.3060279	-0.9402884	1.1083608
C	-2.9159512	-1.8530912	-0.4826969
O	-2.0366293	-2.1679742	-1.3085994
C	-4.3652518	-2.1607688	-0.8098937
C	-0.9339873	-0.4183570	2.4672933
C	-0.4566688	0.6126898	-0.2286164
S	-0.8696316	2.1949271	0.3764976
C	0.9388779	0.2684232	-0.2668613
C	-0.6792830	3.3502001	-1.0117128
C	-2.6674048	2.1481813	0.4700817
C	1.9536502	0.9017967	0.4946806
C	3.2602342	0.4458646	0.4699390
C	3.6074289	-0.6675015	-0.3133955
C	2.6159131	-1.3217760	-1.0664511
C	1.3121953	-0.8647188	-1.0382844
C	4.9585646	-1.1347094	-0.3412338
N	6.0553898	-1.5149564	-0.3639096
H	-3.4435419	-0.8034976	1.3551974
H	-0.5602491	-1.5658848	0.6197054
H	-5.0492007	-1.8702296	-0.0090644
H	-4.6474740	-1.6353021	-1.7285915
H	-4.4719695	-3.2334573	-1.0010866
H	0.0690767	0.0200297	2.4762615
H	-0.9330500	-1.2488143	3.1841770
H	-1.6530195	0.3239986	2.8293569
H	-1.0639841	0.3148041	-1.0814651
H	-1.0190958	4.3363447	-0.6864869
H	0.3829436	3.3819326	-1.2607861
H	-1.2662807	2.9873826	-1.8578471
H	-3.0040191	3.1809870	0.5767401
H	-2.9548759	1.5694750	1.3468073
H	-3.0670427	1.7015410	-0.4430608
H	1.7219786	1.7672567	1.1096664
H	4.0226288	0.9511058	1.0550680
H	2.8792227	-2.1866308	-1.6679492
H	0.5424163	-1.3790161	-1.6087578

e_pent_sr_oz_3_ts1.log

E = -1110.788832
H = -1110.464026
G = -1110.532474
NImag=1

C	0.6465659	-1.6077958	1.2654660
C	1.4005196	-0.5583930	1.7537641
C	1.0136796	-2.2841325	0.0546801
O	2.0209048	-1.9827667	-0.6191491
C	0.1205184	-3.4027397	-0.4442688
C	1.0612635	0.0951183	3.0639959
C	0.9623723	1.3039076	0.4591692
S	2.1956934	1.7043795	-0.7602077
C	-0.3996981	1.0070582	0.1137032
C	3.6953289	0.7935658	-0.3230458
C	1.8359649	0.8935903	-2.3271128
C	-1.4253556	1.5695757	0.9225861
C	-2.7516087	1.2129473	0.7774916
C	-3.1215920	0.2716119	-0.2021483
C	-2.1318022	-0.3149614	-1.0023924

C	-0.7987200	0.0279584	-0.8324338
C	-4.4944747	-0.0926741	-0.3709876
N	-5.6092191	-0.3869741	-0.5074585
H	-0.3219449	-1.8335917	1.7073350
H	2.4336489	-0.4976428	1.4300081
H	-0.7926980	-3.5077970	0.1461533
H	-0.1425582	-3.2175925	-1.4909016
H	0.6760679	-4.3465017	-0.4092337
H	1.6425511	1.0045813	3.2313356
H	1.2742313	-0.5968190	3.8883645
H	-0.0050372	0.3444211	3.1147843
H	1.0610157	2.1009088	1.1964230
H	4.4640026	1.1077299	-1.0328409
H	3.9850963	1.0920621	0.6862089
H	3.4915936	-0.2771925	-0.3909483
H	2.6396522	1.2029032	-2.9990524
H	0.8823934	1.2611552	-2.7066414
H	1.8433938	-0.1903365	-2.1927270
H	-1.1549851	2.3102620	1.6703424
H	-3.5120995	1.6669319	1.4054990
H	-2.4084289	-1.0599193	-1.7427730
H	-0.0622477	-0.4798441	-1.4404431

e_pent_sr_oz_4_ts1.log

E = -1110.792300

H = -1110.467524

G = -1110.536466

NImag=1

C	1.9988106	-1.7495960	0.1345005
C	1.4880471	-1.2093583	1.3054966
C	3.2720939	-1.3226705	-0.3745930
O	3.9456098	-0.4128203	0.1440427
C	3.7865346	-1.9773566	-1.6412675
C	0.3852251	-1.9082072	2.0478207
C	0.3674963	0.7268993	1.0406843
S	1.4642205	1.8470686	0.2638912
C	-0.9503574	0.4451676	0.5242785
C	1.8482389	1.2887236	-1.4214883
C	0.5128096	3.3398087	-0.1422731
C	-1.2397292	0.2423608	-0.8472436
C	-2.5083993	-0.1240947	-1.2706694
C	-3.5378280	-0.3122959	-0.3377638
C	-3.2767931	-0.1229994	1.0316627
C	-2.0126008	0.2496252	1.4451707
C	-4.8455372	-0.6940621	-0.7764392
N	-5.9061711	-1.0040124	-1.1315259
H	1.4329577	-2.4971482	-0.4169772
H	2.1887818	-0.6379134	1.9113349
H	3.2545156	-2.8994018	-1.8870467
H	3.6600223	-1.2710081	-2.4718934
H	4.8562835	-2.1821969	-1.5442005
H	-0.0709558	-1.2761236	2.8130506
H	0.8084848	-2.7871504	2.5497164
H	-0.3976171	-2.2593535	1.3673318
H	0.4163860	0.9456212	2.1056102
H	2.8827087	1.5708667	-1.6199215
H	1.7408495	0.2060065	-1.4632457
H	1.1716860	1.7733070	-2.1267222
H	1.1677506	4.0066259	-0.7087559
H	0.2244449	3.8061467	0.8010919
H	-0.3676114	3.0711053	-0.7293916

H	-0.4690998	0.3627491	-1.5987082
H	-2.7053117	-0.2727219	-2.3280238
H	-4.0726618	-0.2602876	1.7572203
H	-1.8237171	0.4057675	2.5036286

e_pent_sr_oz_5_ts1.log

E = -1110.792847
H = -1110.468019
G = -1110.538800

NImag=1

C	-2.7900737	-0.9990891	0.8766762
C	-1.4081592	-1.1647918	0.9349997
C	-3.5149154	-1.3945890	-0.2929779
O	-2.9678040	-1.8877668	-1.3000722
C	-5.0149821	-1.1666985	-0.3196643
C	-0.6516395	-0.9333250	2.2125015
C	-0.4845439	0.1936352	-0.5152493
S	-1.3832745	1.6827633	-0.3897331
C	0.9436139	0.0764900	-0.4038563
C	-1.3566291	2.2667160	1.3215517
C	-0.4732403	3.0054063	-1.2279088
C	1.7993993	0.9645226	0.2945215
C	3.1529790	0.7060286	0.4289315
C	3.7106879	-0.4594458	-0.1199145
C	2.8832673	-1.3626257	-0.8110528
C	1.5352697	-1.0945720	-0.9500007
C	5.1086357	-0.7248307	0.0228716
N	6.2433743	-0.9406832	0.1394218
H	-3.3083544	-0.4520931	1.6609691
H	-0.9874775	-1.9284767	0.2823067
H	-5.4089722	-0.8391297	0.6453542
H	-5.2470472	-0.4043736	-1.0719956
H	-5.5186097	-2.0898160	-0.6225303
H	0.3894317	-0.6476369	2.0351298
H	-0.6353517	-1.8727624	2.7792920
H	-1.1283349	-0.1760622	2.8403452
H	-0.9529612	-0.3835451	-1.3098754
H	-1.7302155	3.2927428	1.2989742
H	-2.0476798	1.6391343	1.8839270
H	-0.3572648	2.2332781	1.7520474
H	-1.0857890	3.9072968	-1.1662210
H	-0.3627236	2.6996104	-2.2696438
H	0.5012569	3.1699233	-0.7689238
H	1.4111879	1.8700394	0.7460676
H	3.7869093	1.4059366	0.9647342
H	3.3084798	-2.2648317	-1.2400743
H	0.9066327	-1.7941025	-1.4946549

e_pent_ss_oe_1_ts1.log

E = -1110.786641
H = -1110.462317
G = -1110.531790

NImag=1

C	2.5675072	-1.0608548	-0.7262451
C	1.3863902	-0.7843627	-1.4105694
C	2.6219988	-1.7772501	0.5093333
O	3.6760581	-1.9080258	1.1616726
C	1.3404758	-2.3835431	1.0628810
C	1.4659826	-0.3534808	-2.8566677
C	0.2856539	0.9448237	-0.6826647

S	1.1479281	2.0707072	0.3916619
C	-0.9975237	0.4828920	-0.2011750
C	2.1632206	1.1416824	1.5879074
C	2.4366300	2.6624975	-0.7206503
C	-1.9046693	-0.0619997	-1.1460415
C	-3.1129782	-0.6084778	-0.7570826
C	-3.4682528	-0.6302041	0.6035334
C	-2.5883645	-0.0969840	1.5585553
C	-1.3758093	0.4418800	1.1627445
H	0.5140304	-1.3905190	-1.1683849
C	-4.7193727	-1.1906108	1.0120129
N	-5.7350376	-1.6450774	1.3426799
H	3.5009511	-0.6148331	-1.0697525
H	0.5528142	-1.6276804	1.1583714
H	0.9590702	-3.1671204	0.3987351
H	1.5441075	-2.8160807	2.0441113
H	0.5004405	-0.0275671	-3.2507188
H	1.8028733	-1.2053096	-3.4596672
H	2.1906291	0.4564159	-2.9891887
H	0.2623350	1.4301543	-1.6563364
H	2.4514970	1.8758212	2.3427682
H	1.5437041	0.3678355	2.0438173
H	3.0378974	0.7097565	1.1067193
H	3.1141241	3.2849349	-0.1336888
H	1.9583159	3.2588639	-1.4990079
H	2.9606081	1.8034372	-1.1431879
H	-1.6421103	-0.0424725	-2.2005145
H	-3.7930038	-1.0160285	-1.4988750
H	-2.8613302	-0.1084763	2.6092957
H	-0.7198327	0.8379976	1.9337044

e_pent_ss_oe_2_ts1.log

E = -1110.795386

H = -1110.470904

G = -1110.541174

NImag=1

C	-2.5300947	-1.2751955	0.7713745
C	-1.2832552	-0.9761536	1.3206275
C	-2.7764819	-1.8658301	-0.5115542
O	-3.9322829	-2.0797076	-0.9268988
C	-1.6239327	-2.2597622	-1.4222814
C	-1.1747135	-0.7005711	2.7983196
C	-0.4458184	0.9513202	0.6789444
S	-1.5229418	1.3426127	-0.6529158
C	0.9126700	0.6149248	0.3461571
C	-2.9323634	2.0107826	0.2452919
C	-0.8873409	2.8629885	-1.4058697
C	1.9169551	0.7534238	1.3376479
C	3.2165692	0.3399301	1.1119624
C	3.5695578	-0.2280066	-0.1253481
C	2.5936774	-0.3754203	-1.1241579
C	1.2920658	0.0327754	-0.8898809
H	-0.4093643	-1.4522596	0.8801831
C	4.9146580	-0.6505092	-0.3664844
N	6.0063689	-0.9936738	-0.5614095
H	-3.4241305	-0.9966004	1.3294515
H	-0.6444158	-2.2579618	-0.9412028
H	-1.8258988	-3.2575258	-1.8225221
H	-1.5914486	-1.5667723	-2.2704430
H	-0.2047757	-0.2734518	3.0665466
H	-1.2910319	-1.6420499	3.3495829

H	-1.9646574	-0.0189297	3.1296105
H	-0.5933700	1.6310794	1.5172569
H	-3.6684601	2.3388554	-0.4902055
H	-3.3419263	1.2076345	0.8572001
H	-2.5937815	2.8463274	0.8613772
H	-1.6140140	3.1959305	-2.1506482
H	0.0576346	2.6179631	-1.8946070
H	-0.7406001	3.6176388	-0.6314375
H	1.6572713	1.2043675	2.2913751
H	3.9699053	0.4599680	1.8846450
H	2.8624265	-0.8139792	-2.0803147
H	0.5578784	-0.1044131	-1.6803857

e_pent_ss_oe_3_ts1.log

E = -1110.795054

H = -1110.470158

G = -1110.538157

NImag=1

C	-1.1511828	-2.1642412	-0.2650035
C	-1.6393844	-1.5282718	0.8751558
C	0.1862344	-2.6315744	-0.4895346
O	0.5181436	-3.1777078	-1.5611726
C	1.2484206	-2.5327286	0.5929345
C	-3.1250898	-1.5373190	1.1502982
C	-1.2955462	0.6120912	0.9038712
S	-2.5523678	1.4257614	-0.0067684
C	0.1027246	0.7591795	0.5676221
C	-1.9496056	3.0678690	-0.4828048
C	-2.7201508	0.6866933	-1.6544617
C	0.5939445	0.6509016	-0.7522285
C	1.9555354	0.6878044	-1.0171415
C	2.8701973	0.8119719	0.0369405
C	2.4070252	0.9000868	1.3621482
C	1.0480690	0.8740457	1.6144008
H	-1.0235572	-1.5533139	1.7715269
C	4.2769007	0.8420724	-0.2350975
N	5.4159833	0.8667354	-0.4535397
H	-1.8315789	-2.3264680	-1.1012333
H	0.8916871	-2.1480679	1.5489148
H	1.6714686	-3.5307841	0.7457730
H	2.0578499	-1.8856214	0.2368384
H	-3.4122235	-0.8038709	1.9085386
H	-3.4098475	-2.5295013	1.5213594
H	-3.7078165	-1.3559187	0.2404255
H	-1.5389678	0.7762705	1.9527407
H	-2.7088926	3.5229479	-1.1233543
H	-1.8297315	3.6478848	0.4332611
H	-1.0004229	2.9754643	-1.0138925
H	-3.7321799	0.9160605	-1.9926669
H	-2.5881132	-0.3910793	-1.5685439
H	-1.9897287	1.1139963	-2.3421332
H	-0.0890789	0.5276150	-1.5851722
H	2.3156133	0.6054369	-2.0380335
H	3.1172321	0.9944092	2.1777911
H	0.6931528	0.9464592	2.6390068

e_pent_ss_oe_4_ts1.log

E = -1110.789144

H = -1110.463924

G = -1110.532308

NImag=1

C	2.7774397	-1.6131670	-0.1956668
C	1.5689550	-1.4654759	0.4841157
C	3.9959724	-0.9005463	0.0430881
O	5.0066134	-1.0646926	-0.6689090
C	4.1167527	0.0775848	1.2016357
C	0.5412460	-2.5643020	0.4118527
C	0.3602512	0.0176330	-0.5946334
S	1.3342519	1.4683819	-0.4598486
C	-1.0719058	0.0209915	-0.3621725
C	0.4620072	2.8219985	-1.2896778
C	1.2839928	2.0853658	1.2453360
C	-1.7129925	0.7008555	0.6996132
C	-3.0752931	0.5737659	0.9196758
C	-3.8503469	-0.2481502	0.0881116
C	-3.2380553	-0.9400317	-0.9708502
C	-1.8799770	-0.7997875	-1.1886596
H	1.5651118	-0.9151507	1.4230931
C	-5.2571078	-0.3820988	0.3181540
N	-6.3973035	-0.4912975	0.5041905
H	2.8027937	-2.2944652	-1.0467681
H	3.2944167	0.0391176	1.9175521
H	5.0509393	-0.1331635	1.7303798
H	4.1938621	1.0958178	0.8036158
H	-0.4225616	-2.2591197	0.8247364
H	0.9020822	-3.4193030	0.9966435
H	0.3932686	-2.9050496	-0.6183286
H	0.6546889	-0.4403978	-1.5373203
H	1.0289131	3.7393353	-1.1147477
H	0.4414561	2.5883197	-2.3551508
H	-0.5499760	2.9089723	-0.8891425
H	2.1932063	2.6716609	1.3913470
H	1.2745975	1.2370960	1.9298230
H	0.4071411	2.7160733	1.3930739
H	-1.1434372	1.3220875	1.3800305
H	-3.5447880	1.1049873	1.7417847
H	-3.8350394	-1.5739859	-1.6192145
H	-1.4164085	-1.3308207	-2.0153398

e_pent_ss_oe_6_ts1.log

E = -1110.786268
H = -1110.461746
G = -1110.531902

NImag=1

C	2.2731989	1.2876974	0.9185581
C	1.3733630	0.4588840	1.5813502
C	1.9304189	2.3238747	-0.0042090
O	2.7990272	2.9345587	-0.6589515
C	0.4786785	2.7033741	-0.2523725
C	1.8636209	-0.3640801	2.7491077
C	0.6022699	-1.1974397	0.3724899
S	1.5229192	-1.6693533	-1.0719977
C	-0.7903958	-0.8911739	0.1512022
C	2.2007327	-0.1938787	-1.9025947
C	3.0287247	-2.3107717	-0.3184063
C	-1.6662123	-0.9193998	1.2677975
C	-2.9853054	-0.5225845	1.1625986
C	-3.4897782	-0.0815805	-0.0746051
C	-2.6456113	-0.0487552	-1.1954490
C	-1.3219863	-0.4398259	-1.0812197
H	0.3429299	0.7946971	1.6749991

C	-4.8552491	0.3283252	-0.1896056
N	-5.9636954	0.6606437	-0.2816531
H	3.3378840	1.0619775	0.9902381
H	-0.2433977	2.2101551	0.4008631
H	0.3799497	3.7875221	-0.1390241
H	0.2284659	2.4622653	-1.2916608
H	1.1190474	-1.0859770	3.0927761
H	2.0831509	0.3114135	3.5850354
H	2.7859570	-0.8990468	2.5032074
H	0.8056796	-1.9546154	1.1264598
H	2.5682602	-0.5610201	-2.8629117
H	1.3916548	0.5191513	-2.0652133
H	3.0024014	0.2522502	-1.3187149
H	3.7255523	-2.5387054	-1.1267374
H	2.7711574	-3.2217636	0.2238111
H	3.4410294	-1.5537744	0.3509350
H	-1.2863355	-1.2632861	2.2264707
H	-3.6368784	-0.5533416	2.0305696
H	-3.0327034	0.2870921	-2.1526019
H	-0.6998000	-0.3920774	-1.9711431

e_pent_ss_oe_8_ts1.log

E = -1110.795453

H = -1110.471026

G = -1110.539325

NImag=1

C	0.9452149	2.1719454	-0.2739884
C	1.3597087	1.5538786	0.9028086
C	-0.3951344	2.5576848	-0.6159973
O	-0.6637501	3.1091015	-1.7015487
C	-1.5201963	2.4147634	0.3978993
C	2.7807236	1.7470278	1.3728695
C	1.3230730	-0.6291486	0.6944679
S	2.4011976	-0.9324321	-0.6716363
C	-0.0782217	-0.8289185	0.4474128
C	3.9930096	-1.1955328	0.1368633
C	2.0890973	-2.6393981	-1.2057729
C	-0.9303477	-1.1233903	1.5426879
C	-2.3014783	-1.1765269	1.3947148
C	-2.8796248	-0.9392418	0.1317907
C	-2.0587064	-0.6590970	-0.9686967
C	-0.6817090	-0.6044921	-0.8137257
H	0.6345936	1.4481005	1.7081971
C	-4.3009838	-0.9901358	-0.0279671
N	-5.4540286	-1.0298504	-0.1553108
H	1.6987431	2.4103987	-1.0253947
H	-1.3789214	1.5967769	1.1064801
H	-1.5972541	3.3506093	0.9648678
H	-2.4623046	2.2692631	-0.1365067
H	3.1024910	0.9755986	2.0771768
H	2.8498930	2.7155149	1.8839187
H	3.4777522	1.7825752	0.5285387
H	1.7237918	-1.0566374	1.6133887
H	4.6643265	-1.6092978	-0.6177065
H	4.3775048	-0.2400586	0.4872238
H	3.8606021	-1.8955604	0.9639914
H	2.8206616	-2.8844694	-1.9788969
H	1.0817070	-2.6810640	-1.6224587
H	2.1821128	-3.3042594	-0.3450413
H	-0.4885880	-1.3029291	2.5192163
H	-2.9373237	-1.4027434	2.2451546

H	-2.5048476	-0.4763538	-1.9418278
H	-0.0735436	-0.3826209	-1.6865144

e_pent_ss_oe_9_ts1.log

E = -1110.797873
H = -1110.473538
G = -1110.543228

NImag=1

C	-0.6109141	2.2068221	0.8534074
C	-1.1402632	2.4655704	2.1168809
C	-0.6714150	3.1186241	-0.2502971
O	-0.2176084	2.8429265	-1.3771046
C	-1.3099050	4.4848477	-0.0381385
C	-0.7100511	1.6027196	3.2753823
C	-3.2439240	2.0227211	2.0817375
S	-4.0002207	2.3118564	3.6403800
C	-3.2956084	0.6623857	1.5972564
C	-3.4295409	3.9674030	4.0690061
C	-5.7430903	2.6775302	3.2995451
C	-3.1739623	0.4567296	0.2018596
C	-3.0720912	-0.8166344	-0.3349161
C	-3.0944424	-1.9350902	0.5112106
C	-3.2150457	-1.7570018	1.9007714
C	-3.3075416	-0.4824892	2.4307177
H	-1.3536936	3.5044847	2.3608949
C	-2.9978093	-3.2539689	-0.0372986
N	-2.9183236	-4.3233809	-0.4810324
H	-0.1912138	1.2235259	0.6440763
H	-2.3621180	4.3871591	0.2522576
H	-0.8029396	5.0429147	0.7558488
H	-1.2507614	5.0538052	-0.9676140
H	-1.3095749	1.7615856	4.1773948
H	0.3315992	1.8310104	3.5306561
H	-0.7594748	0.5411100	3.0102661
H	-3.5441780	2.7899529	1.3678744
H	-4.0530439	4.3207577	4.8922242
H	-2.3913148	3.9016125	4.3963507
H	-3.5297658	4.6215443	3.1999286
H	-6.2226110	2.9635382	4.2383072
H	-6.1929079	1.7623911	2.9106621
H	-5.8009606	3.4833126	2.5648492
H	-3.1765708	1.3175886	-0.4603174
H	-2.9822145	-0.9525824	-1.4083707
H	-3.2307412	-2.6225918	2.5557525
H	-3.3857469	-0.3744100	3.5090152

e_pent_ss_oz_10_ts1.log

E = -1110.794199
H = -1110.469833
G = -1110.540323

NImag=1

C	1.4870806	-1.8462295	0.9422190
C	1.3935781	-0.5290108	1.3581064
C	2.5257031	-2.2376407	0.0307150
O	3.3562853	-1.4312631	-0.4311036
C	2.5710476	-3.6813623	-0.4289957
C	0.3889123	-0.1161336	2.3927671
C	0.6840780	0.5879187	-0.4507544
S	1.2530334	2.2549137	-0.6214016
C	-0.7292278	0.3693606	-0.4563633

C	1.6854213	2.8872627	1.0223396
C	2.9039123	1.9474523	-1.2777977
C	-1.6700817	1.3129304	0.0330457
C	-3.0150358	1.0076487	0.1247059
C	-3.4770488	-0.2669703	-0.2510699
C	-2.5642430	-1.2217947	-0.7336589
C	-1.2227739	-0.9054778	-0.8443837
H	2.3042839	0.0614088	1.2848850
C	-4.8662833	-0.5863326	-0.1490913
N	-5.9952162	-0.8455484	-0.0650068
H	0.7075797	-2.5609849	1.1947853
H	3.6049298	-4.0378787	-0.4217674
H	1.9525739	-4.3364381	0.1891214
H	2.2096838	-3.7362013	-1.4626681
H	0.1800337	0.9559534	2.3716435
H	0.7767513	-0.3591557	3.3900419
H	-0.5552851	-0.6554419	2.2601580
H	1.3109742	-0.0530026	-1.0642648
H	2.1746760	3.8505515	0.8609316
H	0.7587141	3.0403129	1.5769613
H	2.3507403	2.1976223	1.5420185
H	3.4725537	2.8754242	-1.2037936
H	2.7904926	1.6558118	-2.3230962
H	3.3643005	1.1405726	-0.7012461
H	-1.3404561	2.2975845	0.3578120
H	-3.7178221	1.7469265	0.4968708
H	-2.9208201	-2.2024250	-1.0345879
H	-0.5296994	-1.6377478	-1.2480794

e_pent_ss_oz_1_ts1.log

E = -1110.792437

H = -1110.467856

G = -1110.538884

NImag=1

C	2.7891833	-1.5977947	-0.2124990
C	1.5186246	-1.5850694	0.3405803
C	3.8352319	-0.7526453	0.2904537
O	3.6728912	0.0590885	1.2211133
C	5.2023061	-0.8476221	-0.3596820
C	0.5347471	-2.6787847	0.0392372
C	0.3393705	0.0670604	-0.6719390
S	1.3495071	1.4685995	-0.4014817
C	-1.0800563	0.0530607	-0.4124503
C	0.4765436	2.9147586	-1.0644380
C	1.3478795	1.9200439	1.3534235
C	-1.6984036	0.6550981	0.7108583
C	-3.0568414	0.5205219	0.9465656
C	-3.8553812	-0.2319843	0.0717051
C	-3.2661767	-0.8493891	-1.0463548
C	-1.9123248	-0.7036477	-1.2792580
H	1.4079584	-1.0968273	1.3076525
C	-5.2578792	-0.3718628	0.3167595
N	-6.3959897	-0.4858578	0.5147455
H	2.9940334	-2.2234007	-1.0784066
H	5.9671531	-0.9583314	0.4148509
H	5.2780090	-1.6763225	-1.0672864
H	5.4066035	0.0888310	-0.8911558
H	-0.4789497	-2.4246650	0.3554310
H	0.8359415	-3.5816273	0.5852104
H	0.5239044	-2.9245881	-1.0276876
H	0.6369561	-0.3419640	-1.6346451

H	1.0606864	3.8025067	-0.8102028
H	0.4263842	2.7948662	-2.1476563
H	-0.5248220	2.9764279	-0.6336347
H	2.2682351	2.4821017	1.5189991
H	1.3781593	1.0055797	1.9429467
H	0.4786329	2.5353472	1.5875731
H	-1.1103251	1.2190673	1.4246324
H	-3.5061995	0.9918050	1.8153217
H	-3.8799233	-1.4307612	-1.7277018
H	-1.4682167	-1.1773567	-2.1504480

e_pent_ss_oz_2_ts1.log

E = -1110.799715

H = -1110.475324

G = -1110.546509

NImag=1

C	0.5660725	-2.1306237	0.8875969
C	1.4200854	-1.0867937	1.2071848
C	0.8320406	-2.9840859	-0.2356895
O	1.8306911	-2.8612994	-0.9691456
C	-0.1785948	-4.0690201	-0.5612782
C	1.2030865	-0.2911551	2.4642824
C	1.0813056	0.4639727	-0.3402736
S	2.0671456	1.8732291	-0.0345380
C	-0.3432517	0.6380475	-0.2904913
C	3.7172175	1.1829041	0.1944664
C	2.3125763	2.6889162	-1.6371150
C	-1.1473181	-0.3185595	-0.9616096
C	-2.5282249	-0.3064875	-0.8532864
C	-3.1607759	0.6689867	-0.0678226
C	-2.3852177	1.6284974	0.6096120
C	-1.0072169	1.6086423	0.5031430
H	2.4388527	-1.1666244	0.8344238
C	-4.5869084	0.6916424	0.0406747
N	-5.7442512	0.7101501	0.1301329
H	-0.3900016	-2.2258456	1.3972080
H	0.3290274	-5.0382256	-0.5998006
H	-0.9942935	-4.1185920	0.1639475
H	-0.5983224	-3.8806291	-1.5556864
H	1.8069981	0.6203814	2.5044271
H	1.4743854	-0.8992954	3.3358791
H	0.1489303	-0.0125716	2.5714604
H	1.4780742	-0.1408343	-1.1555019
H	4.4241847	2.0127422	0.1371189
H	3.7691355	0.7226978	1.1816702
H	3.9141778	0.4520730	-0.5928528
H	3.0146973	3.5143244	-1.4992696
H	1.3401156	3.0704164	-1.9529171
H	2.6957922	1.9593406	-2.3535190
H	-0.6666220	-1.0595961	-1.5933627
H	-3.1242926	-1.0456347	-1.3803561
H	-2.8736214	2.3823776	1.2193572
H	-0.4346042	2.3547628	1.0473038

e_pent_ss_oz_3_ts1.log

E = -1110.795402

H = -1110.471317

G = -1110.542361

NImag=1

C	-2.5132105	-1.1654923	0.8635313
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C	-1.3176207	-0.8100584	1.4681401
C	-2.5286035	-1.8734102	-0.3900229
O	-1.5021282	-2.1590922	-1.0310851
C	-3.8789694	-2.2616062	-0.9639969
C	-1.2675070	-0.3431987	2.8956335
C	-0.3976825	1.0652662	0.5773684
S	-1.4861122	1.2748694	-0.7787773
C	0.9398768	0.6270017	0.3020373
C	-2.8722409	2.0810035	0.0397226
C	-0.8498256	2.6742825	-1.7401210
C	1.9823830	0.9699972	1.2014441
C	3.2722163	0.5058586	1.0221052
C	3.5768196	-0.3218539	-0.0735642
C	2.5567762	-0.6905781	-0.9682680
C	1.2645950	-0.2364505	-0.7772373
H	-0.4315800	-1.3165649	1.0881599
C	4.9113820	-0.7948257	-0.2692517
N	5.9959592	-1.1782768	-0.4281508
H	-3.4623569	-0.8794412	1.3116289
H	-3.8399271	-3.2914935	-1.3301017
H	-4.6912292	-2.1599090	-0.2404789
H	-4.0943704	-1.6142712	-1.8223592
H	-0.3089090	0.1234625	3.1380253
H	-1.3984118	-1.2044478	3.5632801
H	-2.0715112	0.3687440	3.1081975
H	-0.5205440	1.8597275	1.3122123
H	-3.6212747	2.3089618	-0.7201702
H	-3.2765619	1.3787107	0.7683086
H	-2.5169562	2.9928531	0.5245769
H	-1.5886192	2.9214479	-2.5061908
H	0.0786467	2.3488420	-2.2137491
H	-0.6707203	3.5212110	-1.0756782
H	1.7605447	1.6235948	2.0406940
H	4.0561803	0.7876098	1.7185814
H	2.7858094	-1.3452406	-1.8038747
H	0.4785373	-0.5785622	-1.4464544

e_pent_ss_oz_4_ts1.log

E = -1110.792524

H = -1110.467933

G = -1110.538931

NImag=1

C	2.7869237	-1.6027449	-0.2082240
C	1.5175366	-1.5862883	0.3473224
C	3.8347053	-0.7562404	0.2890047
O	3.6751326	0.0588079	1.2172152
C	5.1998731	-0.8537522	-0.3647327
C	0.5312108	-2.6793952	0.0519579
C	0.3393187	0.0639621	-0.6702971
S	1.3522816	1.4646239	-0.4063916
C	-1.0802029	0.0537872	-0.4111673
C	0.4819166	2.9095534	-1.0754587
C	1.3512125	1.9239401	1.3464133
C	-1.6973171	0.6601478	0.7105425
C	-3.0561212	0.5291969	0.9463454
C	-3.8559125	-0.2248631	0.0739374
C	-3.2678093	-0.8471000	-1.0419926
C	-1.9137182	-0.7044095	-1.2754085
H	1.4092236	-1.0937080	1.3124507
C	-5.2586124	-0.3615622	0.3195142
N	-6.3968508	-0.4728813	0.5182486

H	2.9892082	-2.2315264	-1.0724269
H	5.9668232	-0.9634286	0.4078752
H	5.2729411	-1.6840310	-1.0707538
H	5.4034028	0.0814353	-0.8987085
H	-0.4816560	-2.4218126	0.3680448
H	0.8311673	-3.5803446	0.6017265
H	0.5187647	-2.9300076	-1.0138313
H	0.6360681	-0.3498182	-1.6312634
H	1.0662603	3.7976565	-0.8228697
H	0.4336192	2.7863356	-2.1584002
H	-0.5201731	2.9730944	-0.6466219
H	2.2719438	2.4861730	1.5094049
H	1.3807552	1.0120120	1.9399132
H	0.4823698	2.5408082	1.5779359
H	-1.1080972	1.2251913	1.4225359
H	-3.5047003	1.0040839	1.8135396
H	-3.8825522	-1.4297927	-1.7213155
H	-1.4704028	-1.1817706	-2.1450085

e_pent_ss_oz_7_ts1.log

E = -1110.792911

H = -1110.468821

G = -1110.538552

NImag=1

C	0.6973660	2.1757813	-0.2841143
C	1.3859894	1.6835725	0.8137190
C	-0.7250560	2.4006977	-0.2487339
O	-1.4235478	2.3082526	0.7749573
C	-1.3927346	2.8536483	-1.5379180
C	2.8594129	1.9385955	0.9884446
C	1.3924835	-0.5469577	0.7091133
S	2.4748873	-0.8757771	-0.6496401
C	-0.0023692	-0.7853827	0.4667628
C	4.0704845	-1.1191334	0.1576979
C	2.1737355	-2.5962655	-1.1488085
C	-0.8506956	-1.0903476	1.5621056
C	-2.2168119	-1.1880863	1.4086043
C	-2.7956464	-0.9869160	0.1386946
C	-1.9784030	-0.7101695	-0.9641663
C	-0.6044548	-0.6121719	-0.8036734
H	0.8112213	1.6050075	1.7358871
C	-4.2132840	-1.0877457	-0.0274450
N	-5.3637758	-1.1698524	-0.1601057
H	1.2261457	2.3644231	-1.2170025
H	-1.5693039	3.9347414	-1.4904481
H	-0.7890701	2.6410490	-2.4242688
H	-2.3668800	2.3648182	-1.6314276
H	3.3112688	1.2803762	1.7348206
H	2.9971616	2.9713070	1.3329596
H	3.4031597	1.8457837	0.0410590
H	1.8057722	-0.9295271	1.6420696
H	4.7309062	-1.5717149	-0.5840671
H	4.4683735	-0.1544606	0.4646162
H	3.9373957	-1.7832971	1.0138228
H	2.9023414	-2.8491388	-1.9222203
H	1.1639512	-2.6559367	-1.5570379
H	2.2793043	-3.2431537	-0.2759412
H	-0.4080309	-1.2405091	2.5433131
H	-2.8507279	-1.4207637	2.2588739
H	-2.4243527	-0.5683843	-1.9442921
H	0.0019707	-0.4003712	-1.6802315

e_pent_ss_oz_9_ts1.log

E = -1110.793003

H = -1110.468527

G = -1110.537945

NImag=1

C	0.9383541	-2.1625469	0.2260745
C	1.6184155	-1.6134594	-0.8513783
C	-0.4653660	-2.4740370	0.1461394
O	-1.1428404	-2.3828994	-0.8915006
C	-1.1418437	-2.9953031	1.4039949
C	3.1177379	-1.7046943	-0.9774315
C	1.3612420	0.5817953	-0.9010292
S	2.6409865	1.3135989	0.0404498
C	-0.0317857	0.7720005	-0.5703195
C	2.1329051	2.9940407	0.4963928
C	2.7071537	0.5755738	1.6974321
C	-0.5341880	0.6304521	0.7425140
C	-1.8974290	0.6843483	0.9976721
C	-2.7997605	0.8726151	-0.0561758
C	-2.3227313	1.0237250	-1.3722685
C	-0.9651802	0.9735534	-1.6155376
H	1.0727444	-1.6182105	-1.7937089
C	-4.2068481	0.9224605	0.2076239
N	-5.3470166	0.9629757	0.4200437
H	1.4466250	-2.3262738	1.1738946
H	-1.3570139	-4.0629543	1.2806963
H	-0.5312430	-2.8634502	2.3009204
H	-2.0993229	-2.4817088	1.5359845
H	3.5186357	-0.9864424	-1.6980211
H	3.3782320	-2.7089543	-1.3346042
H	3.6244172	-1.5663146	-0.0163034
H	1.6265939	0.7417222	-1.9450275
H	2.8917441	3.3968113	1.1717068
H	2.0934549	3.5815953	-0.4218938
H	1.1566870	2.9645582	0.9843052
H	3.7322921	0.6964118	2.0516235
H	2.4575703	-0.4818717	1.6203398
H	2.0157168	1.0881475	2.3671225
H	0.1383969	0.4624017	1.5755131
H	-2.2681663	0.5683765	2.0117556
H	-3.0241685	1.1813225	-2.1858277
H	-0.5989312	1.0861522	-2.6325410

e_pentenone_1.log

E = -270.451269

H = -270.324733

G = -270.363874

NImag=0

C	-0.9707749	2.2759810	-0.2626491
C	0.4412793	2.4800984	-0.6567463
O	0.7125269	2.7393357	-1.8226089
H	-1.6949708	2.3746264	-1.0701755
C	1.5271344	2.3655465	0.3851386
H	2.4950448	2.5457623	-0.0836721
H	1.3669263	3.0939514	1.1860017
H	1.5192683	1.3690650	0.8374624
C	-2.7930094	1.7830553	1.3871947
H	-3.4733961	1.8931624	0.5392944
H	-2.9224062	0.7849671	1.8205712

H	-3.0741212	2.5017619	2.1651400
C	-1.3706979	1.9897177	0.9839214
H	-0.6274074	1.8959299	1.7755724

e_pentenone_2.log

E = -270.450203
H = -270.323838
G = -270.363528

NImag=0

C	0.2826329	-0.5694403	0.0225924
C	-1.1561512	-0.1984753	-0.0376791
O	-1.7485811	-0.0458695	-1.0966970
H	0.7271237	-0.6841974	1.0097144
C	-1.8462335	-0.0210207	1.2886643
H	-2.8930611	0.2485209	1.1446260
H	-1.7745800	-0.9488894	1.8668054
H	-1.3354490	0.7567556	1.8670142
C	2.4559307	-1.1295124	-1.1036430
H	2.8605842	-1.2342384	-0.0939888
H	2.5970505	-2.0728065	-1.6433567
H	3.0355820	-0.3715368	-1.6426205
C	1.0115344	-0.7571796	-1.0848745
H	0.5176179	-0.6296945	-2.0486166

sy_1.log

E = -840.355846
H = -840.159278
G = -840.212336

NImag=0

C	-1.3829606	0.7429653	0.0412540
C	-0.0082717	0.4247907	0.0212764
C	0.5319224	-0.8983921	-0.0415589
C	1.8911289	-1.1267858	-0.0574160
C	2.8072370	-0.0561436	-0.0119478
C	2.3030377	1.2604721	0.0504374
C	0.9460058	1.4913085	0.0664098
S	-2.5907470	-0.4601193	-0.0088824
C	-3.7126159	-0.0083922	-1.3581369
C	-3.7019147	-0.1333726	1.3845396
C	4.2093317	-0.2985481	-0.0286471
N	5.3557420	-0.4965890	-0.0422978
H	-1.7259171	1.7717229	0.0900533
H	-0.1364541	-1.7533864	-0.0781379
H	2.2629799	-2.1464756	-0.1056469
H	2.9941440	2.0980814	0.0861084
H	0.5806283	2.5134717	0.1147337
H	-3.1637921	-0.1411144	-2.2913086
H	-4.5777426	-0.6745161	-1.3283540
H	-4.0178224	1.0328182	-1.2335648
H	-3.1458824	-0.3501682	2.2974787
H	-4.5674532	-0.7943713	1.3010192
H	-4.0077970	0.9147199	1.3575526

sy_2.log

E = -840.354449
H = -840.157694
G = -840.210628

NImag=0

C	-1.2652149	0.5735965	-0.0594590
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C	-0.4068833	0.8501953	1.0314815
C	-0.6581586	0.5084452	2.3927205
C	0.2393256	0.8189430	3.3969019
C	1.4411112	1.4882996	3.1068782
C	1.7178874	1.8396922	1.7684086
C	0.8237483	1.5302261	0.7687981
S	-2.7735625	-0.2115660	-0.0482776
C	-3.9207917	0.5891272	1.1128567
C	-2.6549596	-1.8482061	0.7345935
C	2.3632592	1.8062118	4.1461424
N	3.1160702	2.0659921	4.9931483
H	-0.9850866	0.8744336	-1.0614153
H	-1.5690572	-0.0081854	2.6719923
H	0.0140802	0.5427216	4.4230003
H	2.6426979	2.3571617	1.5295926
H	1.0538475	1.8086989	-0.2560149
H	-4.0551744	1.6140531	0.7645014
H	-4.8680368	0.0479775	1.0581770
H	-3.5350635	0.5770165	2.1318819
H	-1.9538115	-2.4318945	0.1366157
H	-3.6485106	-2.3001918	0.6936186
H	-2.3129432	-1.7763933	1.7666873

z_pent_sr_oe_1_ts1.log

E = -1110.786849

H = -1110.462291

G = -1110.531722

NImag=1

C	2.5705298	-1.4405756	0.8005425
C	1.2328532	-1.3993124	0.3839752
C	3.7755455	-1.3547417	0.0305567
O	4.8969584	-1.3885710	0.5784246
C	3.7374239	-1.2034182	-1.4831823
C	0.7413293	-1.7196089	-1.0100323
C	0.3039763	0.5291943	0.6666143
S	1.0907578	1.7221636	-0.3653228
C	-1.1017811	0.3043151	0.4158193
C	0.3297822	3.3278825	0.0072351
C	2.6690341	1.9568574	0.4717024
C	-1.7522241	0.5840894	-0.8113647
C	-3.0751133	0.2362398	-1.0196397
C	-3.8026568	-0.4084848	-0.0056298
C	-3.1811003	-0.6942482	1.2216553
C	-1.8597609	-0.3398179	1.4251381
C	-5.1717789	-0.7654838	-0.2191434
N	-6.2820339	-1.0560392	-0.3925527
H	2.7433357	-1.4645651	1.8756239
H	0.5331359	-1.7198259	1.1562679
H	3.1855918	-0.3048446	-1.7825515
H	4.7629248	-1.1236935	-1.8486260
H	3.2529180	-2.0597321	-1.9611802
H	-0.3498468	-1.7515996	-1.0284815
H	1.1081933	-2.7073293	-1.3110987
H	1.0716230	-1.0025478	-1.7659707
H	0.5808024	0.6833530	1.7091761
H	0.9074009	4.0980059	-0.5096443
H	-0.6926421	3.3106539	-0.3731752
H	0.3412968	3.4817692	1.0879375
H	3.1870596	2.7674801	-0.0430415
H	3.2416840	1.0339775	0.3977973
H	2.4819733	2.2132288	1.5165376

H	-1.2171210	1.0706738	-1.6231859
H	-3.5542452	0.4610237	-1.9675760
H	-3.7425029	-1.1874500	2.0092100
H	-1.3892178	-0.5562909	2.3804252

z_pent_sr_oe_2_ts1.log

E = -1110.791650
H = -1110.466426
G = -1110.533101

NImag=1

C	1.0367038	-2.0922250	-0.4188877
C	1.5688385	-1.6208965	0.7903589
C	-0.2982811	-2.5057141	-0.7441759
O	-0.5792468	-2.9342173	-1.8832654
C	-1.4142103	-2.4863157	0.2901281
C	0.9905565	-1.9024009	2.1615346
C	1.4436043	0.5018968	0.9528234
S	2.8020213	1.2007645	0.0792044
C	0.0778481	0.7939052	0.5748002
C	3.1653959	0.2734286	-1.4330987
C	2.2720216	2.7696372	-0.6519717
C	-0.3866362	0.6911163	-0.7546147
C	-1.7351438	0.8282874	-1.0548223
C	-2.6592579	1.0607409	-0.0284055
C	-2.2210991	1.1723863	1.3037373
C	-0.8750540	1.0409292	1.5916591
C	-4.0528087	1.1934280	-0.3376089
N	-5.1809120	1.3006692	-0.5855728
H	1.7079564	-2.1219830	-1.2748249
H	2.6586829	-1.6038292	0.8044791
H	-1.4855038	-1.5257248	0.8059211
H	-2.3587624	-2.6928833	-0.2181248
H	-1.2484687	-3.2600106	1.0482292
H	1.6593380	-1.5236391	2.9384324
H	0.8826893	-2.9839179	2.3031939
H	0.0068758	-1.4513311	2.3130029
H	1.6695286	0.6617616	2.0055986
H	3.9679484	0.8301051	-1.9222548
H	3.5313726	-0.7127092	-1.1492512
H	2.2994425	0.2042385	-2.0898982
H	3.1362905	3.1932657	-1.1678269
H	1.9668975	3.4210834	0.1683354
H	1.4485033	2.6081826	-1.3486383
H	0.3051292	0.4931979	-1.5649803
H	-2.0782654	0.7413685	-2.0811543
H	-2.9387390	1.3624377	2.0956074
H	-0.5366017	1.1276622	2.6206334

z_pent_sr_oe_3_ts1.log

E = -1110.789976
H = -1110.465272
G = -1110.532492

NImag=1

C	0.9111032	-2.0841652	-0.1642298
C	1.4725430	-1.3894912	0.9096158
C	-0.4339748	-2.5532012	-0.3656201
O	-0.7400203	-3.1923349	-1.3918737
C	-1.5208543	-2.3301906	0.6741401
C	0.9295017	-1.3648345	2.3205168
C	1.3831367	0.7654612	0.6193785

S	2.5032284	1.3158794	-0.6416422
C	-0.0069770	0.9842238	0.3214386
C	3.9650517	1.7080009	0.3370164
C	3.1537002	-0.0939960	-1.5813422
C	-0.5409639	0.6796155	-0.9530776
C	-1.9047075	0.7515844	-1.1949373
C	-2.7788849	1.1183249	-0.1621567
C	-2.2706461	1.4297022	1.1142054
C	-0.9103871	1.3606973	1.3460754
C	-4.1882887	1.1831112	-0.4073146
N	-5.3308300	1.2360017	-0.6038655
H	1.5586837	-2.2856578	-1.0148913
H	2.5606530	-1.3467260	0.8894550
H	-1.3106228	-2.9078671	1.5809650
H	-1.6049944	-1.2792212	0.9617934
H	-2.4725312	-2.6661260	0.2566717
H	1.6041316	-0.8079600	2.9757795
H	0.8538122	-2.3892697	2.7039426
H	-0.0625754	-0.9143790	2.3944923
H	1.7474889	1.1229916	1.5804468
H	4.7770117	1.9341345	-0.3557033
H	3.7327231	2.5834572	0.9444589
H	4.2158076	0.8503546	0.9647705
H	3.9295411	0.3239632	-2.2270672
H	2.3470809	-0.4964342	-2.1942581
H	3.5699797	-0.8541793	-0.9202191
H	0.1164698	0.3722308	-1.7630330
H	-2.3004851	0.5101077	-2.1768044
H	-2.9496196	1.7260336	1.9077291
H	-0.5196410	1.6050880	2.3301595

z_pent_sr_oe_4_ts1.log

E = -1110.782538

H = -1110.457586

G = -1110.525927

NImag=1

C	-2.5146126	-1.0801486	-0.9770885
C	-1.1608543	-1.1964420	-0.6258704
C	-3.7058696	-1.2442984	-0.1982449
O	-4.8265897	-0.9611294	-0.6741515
C	-3.6771274	-1.8365362	1.2053273
C	-0.6419838	-1.7914743	0.6593896
C	-0.1865925	0.7117444	-0.7038532
S	-0.9040500	2.0656891	0.1982085
C	1.2154301	0.4755903	-0.4427918
C	-2.2572847	2.5374006	-0.8956445
C	-1.8485013	1.3666572	1.5747673
C	1.8361053	0.7409355	0.8017772
C	3.1507476	0.3814854	1.0405204
C	3.8913969	-0.2776762	0.0450429
C	3.2944096	-0.5606078	-1.1951988
C	1.9840970	-0.1853934	-1.4323842
C	5.2487649	-0.6569377	0.2928556
N	6.3497009	-0.9643925	0.4943150
H	-2.7165688	-0.7603996	-1.9992186
H	-0.4987729	-1.4007888	-1.4678533
H	-3.2621508	-1.1381541	1.9406019
H	-4.7043436	-2.0661737	1.4957562
H	-3.0772508	-2.7490712	1.2497923
H	0.4440819	-1.6871633	0.7184788
H	-0.8686204	-2.8644698	0.6774326

H	-1.0819107	-1.3432424	1.5514363
H	-0.4524688	0.8451794	-1.7503716
H	-2.8668457	3.2714189	-0.3658726
H	-1.8191899	2.9856172	-1.7885284
H	-2.8376755	1.6466729	-1.1439457
H	-2.3502870	2.2026805	2.0662496
H	-1.1429475	0.9001523	2.2636652
H	-2.5676353	0.6490758	1.1879021
H	1.2832718	1.2280272	1.6016903
H	3.6110021	0.6006167	1.9990884
H	3.8677406	-1.0645124	-1.9672913
H	1.5353107	-0.3920556	-2.4002224

z_pent_sr_oe_5_ts1.log

E = -1110.794017
H = -1110.469431
G = -1110.537694

NImag=1

C	0.9171778	-2.1648707	-0.3460901
C	1.4139850	-1.5900077	0.8276613
C	-0.4217839	-2.5612196	-0.6862180
O	-0.6813567	-3.0583804	-1.8008408
C	-1.5627656	-2.4483904	0.3153153
C	0.7686000	-1.6463060	2.1920712
C	1.4278867	0.5799260	0.6611042
S	2.5353989	0.8669219	-0.6760432
C	0.0467261	0.8681747	0.3769866
C	2.8241518	2.6548169	-0.6884044
C	4.1276284	0.3036014	-0.0467581
C	-0.5363212	0.6555871	-0.8973276
C	-1.9027009	0.7877100	-1.0915727
C	-2.7356547	1.1340859	-0.0187658
C	-2.1784714	1.3656041	1.2539660
C	-0.8161038	1.2371564	1.4407587
C	-4.1469854	1.2657718	-0.2192197
N	-5.2915651	1.3718079	-0.3798315
H	1.6246232	-2.2919408	-1.1655576
H	2.4995435	-1.6066924	0.9006805
H	-1.6618154	-1.4364248	0.7170224
H	-2.4913359	-2.7241464	-0.1894277
H	-1.4046222	-3.1285052	1.1594285
H	1.3953819	-1.1325934	2.9257108
H	0.6692938	-2.6924439	2.5060475
H	-0.2261240	-1.1988059	2.2230081
H	1.8334779	0.9585079	1.5998494
H	3.5619808	2.8755474	-1.4627718
H	1.8728253	3.1319099	-0.9313287
H	3.1761998	2.9689081	0.2961068
H	4.8968244	0.7936172	-0.6466874
H	4.1953186	-0.7755278	-0.1814785
H	4.2222930	0.5818479	1.0048327
H	0.0818534	0.3821920	-1.7463575
H	-2.3322009	0.6136315	-2.0736629
H	-2.8217976	1.6470579	2.0818977
H	-0.3910326	1.4164946	2.4246897

z_pent_sr_oz_1_ts1.log

E = -1110.793767
H = -1110.469501
G = -1110.539544

NImag=1

C	0.8462386	-2.1515313	-0.2853957
C	1.4413319	-1.6049228	0.8510179
C	-0.5332922	-2.5344434	-0.4045631
O	-1.3501555	-2.5929107	0.5337599
C	-1.0154268	-2.9533680	-1.7874923
C	0.8196845	-1.6420603	2.2208502
C	1.4439357	0.6004193	0.6465806
S	2.5338049	0.8681355	-0.7047030
C	0.0581344	0.8668852	0.3771709
C	2.8138914	2.6577109	-0.7585201
C	4.1379240	0.3305357	-0.0825758
C	-0.7908252	1.2586669	1.4446686
C	-2.1539867	1.3900846	1.2720818
C	-2.7280859	1.1356780	0.0107539
C	-1.9098483	0.7631342	-1.0647314
C	-0.5419215	0.6286358	-0.8854826
C	-4.1395251	1.2784142	-0.1775316
N	-5.2845256	1.3949255	-0.3290623
H	1.4487911	-2.2170232	-1.1889167
H	2.5289529	-1.6024068	0.8669918
H	-0.2645546	-2.8098398	-2.5683619
H	-1.3062927	-4.0094268	-1.7642704
H	-1.9105269	-2.3750355	-2.0392282
H	1.4369375	-1.0993717	2.9421220
H	0.7354818	-2.6846284	2.5513722
H	-0.1926908	-1.2347911	2.2156383
H	1.8583460	0.9867418	1.5779672
H	3.5428897	2.8663857	-1.5445544
H	1.8574675	3.1247572	-1.0010073
H	3.1739809	2.9932322	0.2160618
H	4.8963816	0.8156653	-0.6999186
H	4.2144449	-0.7502712	-0.1965866
H	4.2411157	0.6300591	0.9623234
H	-0.3521852	1.4566755	2.4190579
H	-2.7859742	1.6924079	2.1014355
H	-2.3525892	0.5758518	-2.0385775
H	0.0655164	0.3434987	-1.7386578

z_pent_sr_oz_2_ts1.log

E = -1110.792782
H = -1110.468236
G = -1110.538747

NImag=1

C	2.3802928	-1.5933459	0.4912856
C	1.1917182	-1.3139068	-0.1850907
C	3.7088585	-1.4025972	-0.0081060
O	3.9948220	-0.8957756	-1.1124208
C	4.8552665	-1.8432397	0.8870353
C	1.0974958	-1.0736108	-1.6687823
C	0.2211152	0.5417583	0.5549922
S	0.8639852	1.9295222	-0.2879253
C	-1.1851023	0.2743025	0.3668046
C	0.5057076	3.3723796	0.7519851
C	2.6391172	1.7993933	-0.0200840
C	-1.9324197	0.6728440	-0.7696437
C	-3.2527485	0.2909606	-0.9330720
C	-3.8810686	-0.5133752	0.0315617
C	-3.1595702	-0.9297369	1.1634205
C	-1.8420308	-0.5418615	1.3230126
C	-5.2466992	-0.9048971	-0.1374307

N	-6.3544901	-1.2232355	-0.2747869
H	2.2944033	-1.9933471	1.4983010
H	0.3071071	-1.7840432	0.2430715
H	4.5262891	-2.4182378	1.7553338
H	5.5637958	-2.4377996	0.3028135
H	5.3875905	-0.9513556	1.2381873
H	0.0761664	-0.8050116	-1.9540969
H	1.3618984	-1.9998230	-2.1953004
H	1.7938877	-0.3102003	-2.0182387
H	0.5960521	0.4791698	1.5753169
H	0.9847032	4.2455136	0.3029845
H	-0.5779330	3.5020560	0.7616064
H	0.8850480	3.1882064	1.7591820
H	3.0717776	2.7579603	-0.3138555
H	3.0266738	0.9978681	-0.6522247
H	2.8321686	1.5966501	1.0361286
H	-1.4768193	1.2916808	-1.5375363
H	-3.8065216	0.6129652	-1.8096808
H	-3.6409224	-1.5516055	1.9120097
H	-1.2939287	-0.8627468	2.2049297

z_pent_sr_oz_3_ts1.log

E = -1110.789926

H = -1110.465630

G = -1110.535578

NImag=1

C	-0.8299791	2.0549354	-0.1888550
C	-1.5178079	1.4398131	0.8539084
C	0.5407164	2.4887112	-0.1465500
O	1.2581657	2.5130035	0.8697859
C	1.1445519	2.9947223	-1.4498947
C	-1.0457119	1.4555510	2.2839598
C	-1.4050361	-0.7614243	0.6116586
S	-2.4970938	-1.3397674	-0.6570496
C	-0.0094293	-0.9695205	0.3512405
C	-3.9880203	-1.6829992	0.2954988
C	-3.1080278	0.0449060	-1.6600879
C	0.8783083	-1.2881411	1.4097707
C	2.2408453	-1.3711486	1.2042542
C	2.7718883	-1.1324898	-0.0794524
C	1.9152735	-0.8180552	-1.1436562
C	0.5484374	-0.7261629	-0.9274339
C	4.1832937	-1.2234045	-0.2995323
N	5.3280209	-1.2989140	-0.4765543
H	-1.3347306	2.1533689	-1.1454252
H	-2.5987523	1.3762604	0.7461563
H	0.4640116	2.9146165	-2.3009760
H	1.4433388	4.0415495	-1.3285480
H	2.0524545	2.4200648	-1.6629307
H	-1.7335822	0.8998222	2.9268064
H	-0.9969147	2.4916830	2.6398704
H	-0.0372034	1.0481921	2.3793778
H	-1.7927353	-1.0745421	1.5783962
H	-4.7859292	-1.9190945	-0.4101037
H	-3.7831223	-2.5425113	0.9347283
H	-4.2418503	-0.8032234	0.8905590
H	-3.8558128	-0.3891410	-2.3278545
H	-2.2761865	0.4317599	-2.2490630
H	-3.5523464	0.8220140	-1.0382457
H	0.4711684	-1.4818351	2.3985115
H	2.9059525	-1.6265125	2.0234332

H	2.3269506	-0.6337453	-2.1314984
H	-0.0933766	-0.4641591	-1.7656697

z_pent_sr_oz_4_ts1.log

E = -1110.791960
H = -1110.466948
G = -1110.534964

NImag=1

C	0.8969805	-2.0615681	-0.4635282
C	1.5896648	-1.6981092	0.6952893
C	-0.4947918	-2.4036445	-0.5246704
O	-1.2483482	-2.5460931	0.4570808
C	-1.0812975	-2.6577746	-1.9078177
C	1.0997313	-2.0255220	2.0841553
C	1.4903679	0.4560074	0.9389904
S	2.8381460	1.1460968	0.0513221
C	0.1200925	0.7637380	0.6032410
C	3.1206531	0.2749752	-1.5126268
C	2.3452789	2.7634645	-0.5982262
C	-0.3693356	0.7526934	-0.7217536
C	-1.7208175	0.9226039	-0.9887812
C	-2.6257201	1.0910033	0.0662147
C	-2.1632458	1.1063564	1.3954844
C	-0.8151866	0.9455057	1.6502035
C	-4.0214472	1.2622207	-0.2099517
N	-5.1516984	1.4016704	-0.4320426
H	1.4184357	-1.9875815	-1.4138114
H	2.6756754	-1.6822954	0.6084397
H	-0.4118279	-2.3640296	-2.7204041
H	-1.3121392	-3.7241884	-2.0114842
H	-2.0246705	-2.1099793	-2.0000040
H	1.8065063	-1.6703838	2.8387592
H	0.9974252	-3.1124137	2.1868609
H	0.1116617	-1.5999022	2.2701007
H	1.7469567	0.5591887	1.9911946
H	3.9483989	0.8049295	-1.9891733
H	3.4278677	-0.7460654	-1.2887579
H	2.2426224	0.2942359	-2.1567370
H	3.2057700	3.1742354	-1.1305625
H	2.0972999	3.3918569	0.2584235
H	1.4902382	2.6629126	-1.2678657
H	0.3061352	0.6140565	-1.5577456
H	-2.0807470	0.9138687	-2.0131344
H	-2.8657851	1.2485713	2.2107270
H	-0.4586410	0.9617766	2.6766206

z_pent_sr_oz_5_ts1.log

E = -1110.789497
H = -1110.464619
G = -1110.535227

NImag=1

C	-2.7742094	-1.0769127	-0.8904812
C	-1.3976719	-1.3300917	-0.9070076
C	-3.6281011	-1.1758010	0.2534129
O	-3.2457282	-1.4598634	1.4081188
C	-5.1094171	-0.9108168	0.0408563
C	-0.6587932	-2.0243091	0.2071690
C	-0.2407385	0.5632290	-1.0343755
S	-1.3130055	1.7637849	-0.3540465
C	1.1123429	0.3411616	-0.5928960

C	-1.7166782	1.3426426	1.3617249
C	-0.3750354	3.2905357	-0.0945936
C	1.5716040	0.5120194	0.7353380
C	2.8599556	0.1611543	1.1028274
C	3.7416972	-0.3838790	0.1565255
C	3.3104308	-0.5647340	-1.1699969
C	2.0272296	-0.2030541	-1.5319965
C	5.0706722	-0.7503796	0.5384314
N	6.1491328	-1.0483803	0.8475997
H	-3.2407104	-0.7865897	-1.8281514
H	-0.9765819	-1.5118597	-1.8931932
H	-5.3800742	-0.8040705	-1.0118951
H	-5.6917717	-1.7233913	0.4856700
H	-5.3788990	0.0118556	0.5682881
H	0.3839315	-2.1974106	-0.0691131
H	-1.1350582	-2.9940256	0.3953916
H	-0.6905163	-1.4741937	1.1493918
H	-0.3713732	0.6238099	-2.1121321
H	-2.6460672	1.8691284	1.5910252
H	-1.8834176	0.2669253	1.4319975
H	-0.9271932	1.6771206	2.0345131
H	-1.0365881	3.9975488	0.4114108
H	-0.0976606	3.6723480	-1.0781003
H	0.5118789	3.0924531	0.5094534
H	0.9139316	0.9087601	1.5001419
H	3.1890386	0.3011464	2.1279700
H	3.9905742	-0.9819470	-1.9063540
H	1.7042469	-0.3416098	-2.5603082

z_pent_ss_oe_1_ts1.log

E = -1110.783853

H = -1110.459435

G = -1110.529109

NImag=1

C	-2.8189920	-0.5979550	-0.9202550
C	-1.4481340	-0.6265480	-1.1822180
C	-3.5985230	-1.4686940	-0.0836770
O	-4.8273930	-1.3100990	0.0440380
C	-2.9377830	-2.5952670	0.6913510
C	-0.5751400	-1.8599730	-1.1715280
C	-0.3637200	0.4353370	0.4104050
S	-0.8602130	2.1373090	0.4524940
C	1.0651290	0.2403680	0.3384050
C	-1.5255630	2.6256110	-1.1644280
C	-2.3833200	2.0612170	1.4138340
C	1.6595610	-0.8599000	1.0070740
C	3.0068600	-1.1383750	0.8817610
C	3.8230640	-0.3170290	0.0815830
C	3.2600510	0.7824830	-0.5859600
C	1.9071220	1.0492970	-0.4640270
H	-1.1247750	0.1004670	-1.9259390
C	5.2192470	-0.5982120	-0.0491540
N	6.3525930	-0.8264640	-0.1551770
H	-3.3895070	0.2434710	-1.3084770
H	-2.0880030	-2.2289930	1.2776050
H	-3.6759100	-3.0380960	1.3627750
H	-2.5625660	-3.3701820	0.0152910
H	0.4256590	-1.6186780	-1.5364450
H	-1.0075690	-2.6114600	-1.8428560
H	-0.4716810	-2.3168150	-0.1855920
H	-0.8822900	-0.1008390	1.2023190

H	-1.7850620	3.6826950	-1.0736660
H	-0.7291940	2.5061320	-1.9009650
H	-2.4016800	2.0354370	-1.4277850
H	-2.8516550	3.0461450	1.3689850
H	-2.1104910	1.8194530	2.4419640
H	-3.0336890	1.2947220	0.9880650
H	1.0381140	-1.4920630	1.6355950
H	3.4427290	-1.9832170	1.4062640
H	3.8874910	1.4160480	-1.2054600
H	1.4953380	1.8907070	-1.0166520

z_pent_ss_oe_2_ts1.log

E = -1110.788299

H = -1110.463812

G = -1110.534080

NImag=1

C	-2.4475718	-0.9822038	-1.0498724
C	-1.2295769	-1.2681832	-0.4228716
C	-3.7884833	-1.1332784	-0.5564752
O	-4.7739587	-0.8748485	-1.2736803
C	-4.0477899	-1.6016503	0.8663424
C	-1.0223228	-2.2444917	0.7116769
C	-0.2865743	0.4258805	0.6009695
S	-1.0355141	1.7755693	-0.2502124
C	1.1191710	0.2228113	0.3546673
C	-2.5675054	1.9685464	0.6747021
C	-0.1713701	3.2712889	0.2963092
C	1.9176128	-0.3901510	1.3532116
C	3.2462602	-0.6968947	1.1286587
C	3.8371576	-0.3968886	-0.1122177
C	3.0681853	0.2074226	-1.1189369
C	1.7355629	0.5059850	-0.8901562
H	-0.3857477	-1.2417112	-1.1134289
C	5.2146119	-0.7044061	-0.3464857
N	6.3322091	-0.9544828	-0.5358505
H	-2.3965826	-0.5468381	-2.0466083
H	-3.4987559	-0.9945644	1.5945624
H	-5.1179118	-1.5256168	1.0686015
H	-3.7341059	-2.6417258	1.0005158
H	0.0394218	-2.3060438	0.9637639
H	-1.3495241	-3.2441051	0.3996823
H	-1.5702694	-1.9806312	1.6166650
H	-0.6067130	0.3979207	1.6423547
H	-3.0655207	2.8626172	0.2962707
H	-3.1837007	1.0909380	0.4878412
H	-2.3305640	2.0701675	1.7357953
H	-0.7018812	4.1322907	-0.1171170
H	0.8426034	3.2339470	-0.1057938
H	-0.1558429	3.3022244	1.3871522
H	1.4715210	-0.6163434	2.3178484
H	3.8395818	-1.1617096	1.9100829
H	3.5204043	0.4369473	-2.0789356
H	1.1636080	0.9638435	-1.6939675

z_pent_ss_oe_3_ts1.log

E = -1110.785720

H = -1110.460391

G = -1110.528312

NImag=1

C	-1.1573116	-1.7567446	0.5537667
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C	-1.4597739	-0.7036998	1.4349209
C	-1.9711750	-2.4412449	-0.4076839
O	-1.4871019	-3.3236862	-1.1479753
C	-3.4687759	-2.1830856	-0.5254951
C	-2.8531787	-0.2264949	1.7787946
C	-0.5583620	1.1362150	0.9025570
S	-1.6023272	2.0566197	-0.1653010
C	0.7926577	0.7722763	0.5228203
C	-0.6217774	3.3377059	-0.9936451
C	-2.0348979	1.0001856	-1.5787365
C	1.1647169	0.3736432	-0.7791251
C	2.4426448	-0.0951731	-1.0490569
C	3.3849315	-0.1962756	-0.0172665
C	3.0332461	0.1782430	1.2909706
C	1.7603031	0.6547031	1.5479557
H	-0.7835733	-0.6504196	2.2875870
C	4.7036536	-0.6834191	-0.2952071
N	5.7716238	-1.0772201	-0.5188609
H	-0.1318195	-2.1235017	0.5797810
H	-3.6861764	-1.1767295	-0.8972213
H	-3.8833950	-2.9084924	-1.2282826
H	-3.9716666	-2.2912510	0.4395104
H	-2.8042764	0.6438623	2.4386652
H	-3.3937212	-1.0196638	2.3091399
H	-3.4479127	0.0400771	0.9014962
H	-0.6490886	1.6004714	1.8833192
H	-1.2805623	3.8356852	-1.7093005
H	-0.2968388	4.0413953	-0.2258641
H	0.2337155	2.8897004	-1.5009163
H	-3.0965490	1.1433981	-1.7827787
H	-1.8301304	-0.0338135	-1.3003657
H	-1.4393970	1.2876117	-2.4466634
H	0.4572630	0.4258141	-1.5993062
H	2.7120169	-0.3918489	-2.0579336
H	3.7626811	0.0987174	2.0910309
H	1.4942365	0.9481462	2.5598951

z_pent_ss_oe_4_ts1.log

E = -1110.786007

H = -1110.460950

G = -1110.530420

NImag=1

C	-2.8521031	-0.5640462	-1.0105929
C	-1.5282737	-1.0030855	-0.9161145
C	-3.9848638	-0.9155106	-0.1998853
O	-5.1132366	-0.4378154	-0.4236591
C	-3.8341182	-1.8719998	0.9710921
C	-1.0698495	-2.3434309	-0.3886608
C	-0.3878773	0.1736957	0.5355006
S	-1.2141783	1.7169899	0.4600492
C	1.0377097	0.0432795	0.3432974
C	-0.1955993	2.9410533	1.3185624
C	-1.1282117	2.3760123	-1.2316012
C	1.7819037	0.7714273	-0.6165002
C	3.1331970	0.5359831	-0.8124037
C	3.7944688	-0.4479836	-0.0623972
C	3.0772876	-1.1925241	0.8915570
C	1.7322555	-0.9452297	1.0879327
H	-0.8900628	-0.6433077	-1.7241086
C	5.1894125	-0.6917549	-0.2670126
N	6.3209961	-0.8900141	-0.4327743

H	-3.0619786	0.2306781	-1.7252926
H	-3.0221967	-1.5613415	1.6371759
H	-4.7717905	-1.8908830	1.5298168
H	-3.6087177	-2.8853120	0.6234527
H	0.0149213	-2.4335885	-0.4817023
H	-1.5239293	-3.1396633	-0.9911996
H	-1.3379270	-2.5199294	0.6534389
H	-0.7860340	-0.3347306	1.4122044
H	-0.6687293	3.9163179	1.1822038
H	-0.1862280	2.6712884	2.3756913
H	0.8158987	2.9418694	0.9079761
H	-2.0200458	2.9882061	-1.3750898
H	-1.1286203	1.5468953	-1.9378279
H	-0.2319684	2.9858050	-1.3473954
H	1.3020882	1.5271001	-1.2280953
H	3.6823709	1.1091881	-1.5530930
H	3.5856206	-1.9523776	1.4772020
H	1.1887265	-1.5187590	1.8339921

z_pent_ss_oe_7_ts1.log

E = -1110.786640

H = -1110.462316

G = -1110.531785

NImag=1

C	2.4493108	-1.1789337	-0.8665472
C	1.4192595	-0.5178228	-1.5311087
C	2.2386031	-2.1955308	0.1158105
O	3.1707878	-2.6869792	0.7815255
C	0.8197886	-2.6803177	0.3770402
C	1.7426301	0.2601366	-2.7854574
C	0.5204309	1.1272910	-0.4275011
S	1.4092819	1.7483440	0.9830062
C	-0.8683490	0.7980186	-0.1939240
C	2.1116067	0.3641180	1.9399112
C	2.9017507	2.3660318	0.1834784
C	-1.4131787	0.4665035	1.0703296
C	-2.7341977	0.0741122	1.2054587
C	-3.5622425	-0.0153060	0.0754419
C	-3.0434008	0.3013638	-1.1928274
C	-1.7261970	0.6999046	-1.3195828
H	0.4398968	-0.9952187	-1.5368602
C	-4.9259591	-0.4244020	0.2137112
N	-6.0328444	-0.7558160	0.3251958
H	3.4760608	-0.8374269	-0.9984815
H	0.1542714	-1.8453598	0.6236230
H	0.4053498	-3.1746152	-0.5086552
H	0.8308860	-3.3882419	1.2077571
H	0.8955693	0.8507320	-3.1424828
H	2.0146745	-0.4473214	-3.5780539
H	2.5951662	0.9287118	-2.6280000
H	0.6928810	1.8497400	-1.2227690
H	2.4154826	0.8048760	2.8913658
H	1.3274894	-0.3753343	2.1097958
H	2.9608239	-0.0776490	1.4233380
H	3.5905642	2.6746985	0.9716487
H	2.6220983	3.2249647	-0.4283266
H	3.3331551	1.5685012	-0.4238968
H	-0.8033379	0.5161765	1.9687798
H	-3.1326915	-0.1656609	2.1864845
H	-3.6821965	0.2375529	-2.0684161
H	-1.3361903	0.9501668	-2.3026902

z_pent_ss_oe_8_fr_ts1.log

E = -1110.795242

H = -1110.470413

G = -1110.537716

NImag=1

C	-0.2523780	2.4933497	-0.5231505
C	-1.2461488	1.8511157	0.2271492
C	1.1525594	2.6380787	-0.2681201
O	1.8896765	3.2664627	-1.0560693
C	1.7929346	2.0761492	0.9933109
C	-1.1716226	1.5619186	1.7092582
C	-1.4692914	-0.1300757	-0.5243117
S	-2.7804191	-0.9854735	0.2791182
C	-0.1531094	-0.7043646	-0.3686364
C	-4.1742950	0.1401379	0.0791361
C	-3.2979104	-2.3000226	-0.8582793
C	0.2609371	-1.4625108	0.7543482
C	1.5828607	-1.8334351	0.9212393
C	2.5461164	-1.4480363	-0.0285779
C	2.1588517	-0.7099341	-1.1562973
C	0.8308029	-0.3522579	-1.3239369
H	-2.2529728	2.0942633	-0.1087439
C	3.9175825	-1.8202482	0.1502306
N	5.0285841	-2.1213007	0.2973022
H	-0.5589108	2.9013124	-1.4855966
H	1.4527649	2.6267701	1.8773300
H	1.5509507	1.0210312	1.1447599
H	2.8763135	2.1866212	0.9082208
H	-2.1267944	1.1740926	2.0772149
H	-0.9589416	2.4833319	2.2632172
H	-0.3947255	0.8371141	1.9649795
H	-1.7567489	0.1345367	-1.5420646
H	-5.0788569	-0.4258502	0.3092856
H	-4.0649703	0.9609257	0.7884584
H	-4.1980587	0.5059103	-0.9495127
H	-4.1833694	-2.7837404	-0.4398145
H	-2.4740800	-3.0129443	-0.9217582
H	-3.5111747	-1.8619114	-1.8354930
H	-0.4582282	-1.7588789	1.5129652
H	1.8819020	-2.4135773	1.7886623
H	2.9009505	-0.4217685	-1.8947236
H	0.5347366	0.2046034	-2.2070829

z_pent_ss_oz_1_ts1.log

E = -1110.787994

H = -1110.463052

G = -1110.534438

NImag=1

C	2.8215228	-0.6528717	0.9304239
C	1.4955376	-1.0781916	0.8641717
C	3.8796048	-1.0873227	0.0613401
O	3.7492377	-1.8996281	-0.8724475
C	5.2571606	-0.4874233	0.2985752
C	1.0631475	-2.3904268	0.2654021
C	0.3450581	0.1838177	-0.5748445
S	1.1948503	1.7051249	-0.4514047
C	-1.0736277	0.0528368	-0.3605129
C	0.1932013	2.9843579	-1.2493413
C	1.1474330	2.3028992	1.2655863

C	-1.8066829	0.7798017	0.6100602
C	-3.1555298	0.5457623	0.8211239
C	-3.8283677	-0.4343813	0.0758095
C	-3.1230693	-1.1776169	-0.8882321
C	-1.7799958	-0.9331453	-1.0992892
H	0.8507052	-0.7315501	1.6724260
C	-5.2212932	-0.6748620	0.2947241
N	-6.3517651	-0.8705699	0.4717425
H	3.0683019	0.1405364	1.6317966
H	5.5124532	0.1583761	-0.5493129
H	5.3160527	0.1009663	1.2170161
H	5.9997327	-1.2902399	0.3336712
H	-0.0256805	-2.4807813	0.2662865
H	1.4667127	-3.2034882	0.8831759
H	1.4509405	-2.5265034	-0.7435177
H	0.7418463	-0.3209455	-1.4528911
H	0.6861344	3.9439062	-1.0766269
H	0.1716378	2.7587235	-2.3165024
H	-0.8153238	2.9876042	-0.8318088
H	2.0589029	2.8821188	1.4219251
H	1.1289119	1.4484155	1.9407885
H	0.2720865	2.9352053	1.4154962
H	-1.3193633	1.5329555	1.2188394
H	-3.6948027	1.1181629	1.5697243
H	-3.6394967	-1.9346913	-1.4704551
H	-1.2466689	-1.5049425	-1.8539224

z_pent_ss_oz_2_ts1.log

E = -1110.785855

H = -1110.461551

G = -1110.532473

NImag=1

C	2.7804232	-0.6683202	0.9151485
C	1.4260997	-0.6693099	1.2378541
C	3.4135679	-1.6030039	0.0270429
O	2.8261380	-2.5271692	-0.5640230
C	4.8996963	-1.4134989	-0.2321307
C	0.5568380	-1.8973822	1.1901610
C	0.3400952	0.4341711	-0.3842119
S	0.8466085	2.1264635	-0.3987647
C	-1.0851236	0.2360932	-0.3264249
C	1.5641910	2.5827418	1.2053293
C	2.3414383	2.0675817	-1.4050134
C	-1.6697589	-0.8768891	-0.9850157
C	-3.0193011	-1.1510641	-0.8795710
C	-3.8504208	-0.3143375	-0.1107313
C	-3.2973512	0.7959402	0.5480293
C	-1.9423750	1.0586553	0.4473073
H	1.1175088	0.0615944	1.9839155
C	-5.2484302	-0.5922544	-0.0002886
N	-6.3839445	-0.8178740	0.0889694
H	3.3970717	0.1555955	1.2632140
H	5.0354069	-1.0439691	-1.2553759
H	5.3662055	-0.7065909	0.4578457
H	5.4076529	-2.3798051	-0.1627523
H	-0.4594585	-1.6707714	1.5202995
H	0.9775473	-2.6488253	1.8705114
H	0.5315333	-2.3455208	0.1964601
H	0.8858508	-0.1225243	-1.1416917
H	1.8378960	3.6369224	1.1212400
H	0.7861721	2.4662169	1.9616654

H	2.4371857	1.9752206	1.4381421
H	2.8177002	3.0482100	-1.3499769
H	2.0393858	1.8506459	-2.4304162
H	2.9995059	1.2875451	-1.0160554
H	-1.0381282	-1.5214120	-1.5899794
H	-3.4459269	-2.0053977	-1.3963670
H	-3.9348986	1.4410572	1.1449682
H	-1.5393026	1.9089962	0.9925022

z_pent_ss_oz_3_ts1.log

E = -1110.793031
H = -1110.468581
G = -1110.539616

NImag=1

C	-1.8622635	-1.5599724	-0.3128028
C	-1.1290244	-1.2444655	0.8319793
C	-3.2894888	-1.5010620	-0.4444001
O	-4.0725153	-1.1200319	0.4490049
C	-3.8838636	-1.9391569	-1.7723083
C	-1.7164621	-1.1047725	2.2130922
C	-0.2030955	0.8031366	0.7142271
S	-1.1665176	1.5412759	-0.5441105
C	1.1569239	0.4752522	0.3900060
C	-2.7209139	1.8396273	0.3107864
C	-0.5726754	3.2444976	-0.7165888
C	2.0731651	0.2530484	1.4510489
C	3.3650830	-0.1739773	1.2130257
C	3.8006294	-0.3995725	-0.1059528
C	2.9112258	-0.1937023	-1.1726696
C	1.6161822	0.2310197	-0.9294708
H	-0.1026036	-1.6052663	0.8227919
C	5.1390256	-0.8350386	-0.3582251
N	6.2257122	-1.1897100	-0.5614254
H	-1.3052900	-1.8833562	-1.1884499
H	-4.3337767	-1.0670513	-2.2605286
H	-3.1469992	-2.3783578	-2.4481341
H	-4.6856290	-2.6609042	-1.5892881
H	-0.9332370	-0.8661200	2.9374359
H	-2.1750210	-2.0589798	2.5030601
H	-2.5001987	-0.3487565	2.2646248
H	-0.3953772	1.2424143	1.6917292
H	-3.3468612	2.4343240	-0.3571917
H	-3.1930737	0.8751419	0.5091732
H	-2.5171853	2.3836514	1.2358197
H	-1.2309302	3.7614486	-1.4188818
H	0.4398718	3.1978478	-1.1220812
H	-0.5772587	3.7303931	0.2606726
H	1.7467597	0.4281884	2.4726369
H	4.0493269	-0.3323229	2.0411018
H	3.2424247	-0.3696737	-2.1916221
H	0.9533996	0.3758296	-1.7787747

z_pent_ss_oz_6_ts1.log

E = -1110.795465
H = -1110.470924
G = -1110.539590

NImag=1

C	0.1587420	-2.4356926	-0.5256883
C	1.2569959	-1.9016147	0.1523988
C	-1.1781554	-2.5232889	-0.0135048

O	-1.5225118	-2.2703763	1.1574468
C	-2.2536225	-3.0172741	-0.9729094
C	1.2662631	-1.6714014	1.6412901
C	1.4730153	0.1408728	-0.5517496
S	2.8012933	0.9407755	0.2722839
C	0.1633031	0.7080883	-0.3572638
C	4.1865875	-0.1656391	-0.0512744
C	3.2851813	2.3394625	-0.7771400
C	-0.2299805	1.4431043	0.7889172
C	-1.5428949	1.8332925	0.9746993
C	-2.5201363	1.4941622	0.0204756
C	-2.1544849	0.7770922	-1.1281997
C	-0.8358598	0.3943366	-1.3120083
H	2.2271585	-2.1325233	-0.2844467
C	-3.8799157	1.8989866	0.2122467
N	-4.9820417	2.2277585	0.3683505
H	0.3022623	-2.7263450	-1.5634885
H	-3.0989471	-2.3218783	-0.9456819
H	-1.9013168	-3.1151352	-2.0027790
H	-2.6224259	-3.9910413	-0.6314301
H	2.2321200	-1.2839850	1.9816288
H	1.0798827	-2.6165689	2.1638039
H	0.4697919	-0.9872495	1.9433773
H	1.7461272	-0.0993591	-1.5792320
H	5.0988683	0.3775018	0.2019398
H	4.0903571	-1.0418435	0.5902995
H	4.1838778	-0.4462754	-1.1066230
H	4.1845193	2.7916326	-0.3529598
H	2.4602416	3.0538696	-0.7576676
H	3.4639383	1.9793161	-1.7922295
H	0.5003807	1.7082548	1.5485020
H	-1.8251462	2.3971062	1.8584047
H	-2.9058815	0.5284497	-1.8717497
H	-0.5551153	-0.1387100	-2.2148809

z_pent_ss_oz_9_ts1.log

E = -1110.791776

H = -1110.466907

G = -1110.536726

NImag=1

C	-1.1697692	-1.6914926	0.6791286
C	-1.4306025	-0.6384261	1.5573078
C	-2.0906474	-2.2760904	-0.2501352
O	-3.2714748	-1.9085415	-0.4175734
C	-1.5785832	-3.4269763	-1.0998752
C	-2.8090757	-0.1592628	1.9383832
C	-0.5338331	1.2579989	0.8624417
S	-1.6190840	2.0767136	-0.2303042
C	0.7930858	0.8302216	0.4908848
C	-0.6621576	3.1694100	-1.3172449
C	-2.2791098	0.9280744	-1.4657114
C	1.1303591	0.3046045	-0.7768614
C	2.3943297	-0.2066258	-1.0325694
C	3.3618106	-0.2284862	-0.0192200
C	3.0452757	0.2685546	1.2579696
C	1.7870089	0.7868219	1.5002349
H	-0.6977414	-0.5262568	2.3549216
C	4.6653643	-0.7594003	-0.2824937
N	5.7219792	-1.1893862	-0.4949430
H	-0.1675659	-2.1115387	0.6934653
H	-1.4907142	-3.0819794	-2.1369604

H	-0.6054285	-3.8004069	-0.7736169
H	-2.3071774	-4.2428880	-1.0865896
H	-2.7470104	0.7241110	2.5794392
H	-3.3120347	-0.9547216	2.5037106
H	-3.4437210	0.0553858	1.0784703
H	-0.6140367	1.7677709	1.8199547
H	-1.3663305	3.6342365	-2.0108973
H	-0.1996070	3.9283675	-0.6848688
H	0.0944238	2.6020693	-1.8605984
H	-3.0163039	1.5038727	-2.0303887
H	-2.7700232	0.1027713	-0.9472007
H	-1.5018822	0.5638000	-2.1372826
H	0.4025520	0.2856882	-1.5791915
H	2.6331071	-0.6002585	-2.0157951
H	3.7922869	0.2492809	2.0456209
H	1.5509162	1.1747353	2.4875577

z_pentenone_1.log

E = -270.444870
H = -270.318028
G = -270.357441

NImag=0

C	-0.9665714	2.1951186	-0.3124226
C	-1.4700192	1.8548770	0.8862951
C	0.4407546	2.4584489	-0.7037180
O	0.6940137	2.6256513	-1.8908361
H	-1.6581461	2.3059247	-1.1452241
H	-2.5531989	1.7404753	0.9180238
C	1.5378763	2.5444180	0.3258116
H	2.4241246	2.9805068	-0.1378490
H	1.2319874	3.1424884	1.1878754
H	1.7851182	1.5394526	0.6846742
C	-0.7798172	1.6078209	2.1949098
H	-0.6493985	2.5512738	2.7397037
H	-1.3993832	0.9594790	2.8186540
H	0.2017447	1.1463136	2.0854122

z_pentenone_2.log

E = -270.446077
H = -270.319551
G = -270.359906

NImag=0

C	0.2035076	-0.8864519	0.0909151
C	0.8367243	-1.5404241	-0.8972380
C	-0.9676227	0.0089218	-0.0823360
O	-1.2981795	0.4666039	-1.1682053
H	0.5375335	-1.0334077	1.1156421
H	1.6796361	-2.1652954	-0.6029121
C	-1.7290807	0.3368543	1.1766645
H	-2.5826791	0.9768225	0.9505163
H	-2.0686419	-0.5863543	1.6584035
H	-1.0630928	0.8426636	1.8845959
C	0.5225575	-1.5265525	-2.3599534
H	1.1186074	-0.7527803	-2.8606287
H	0.7947506	-2.4847340	-2.8101870
H	-0.5267716	-1.3053222	-2.5565521

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