



Supporting Information

Chiral Phosphoric Acid Catalyzed Conversion of Epoxides into Thiiranes: Mechanism, Stereochemical Model, and New Catalyst Design

M. Duan, C. D. Díaz-Oviedo, Y. Zhou, X. Chen, P. Yu, B. List, K. N. Houk*, Y. Lan**

Supporting Information

Table of contents

1.	Distortion/Interaction Analysis	2
2.	Computational and Experimental Results with Aliphatic Substrates	2
3.	Benchmark for Various DFT Methods	3
4.	Theoretically Predicted Enantioselectivities at the M06-2X/6-311+ G(d,p)-SMD//M06-2X/6-31G(d)-SMD Level of Theory.....	3
5.	Absolute Calculation Energies, Enthalpies, and Free Energies.....	4
6.	General Experimental Methods.....	8
7.	Preparation of 3,3'-disubstituted BINOL <i>S7</i> (precursor of (<i>R</i>)- <i>C7</i>).....	9
8.	Preparation of Chiral Phosphoric Acids (<i>R</i>)- <i>C5</i> , (<i>R</i>)- <i>C6</i> and (<i>R</i>)- <i>C7</i>	13
9.	General Procedure for the CPA-catalyzed Epoxide Thionation	16
10.	B3LYP Geometries for All the Optimized Compounds and Transition States	18
11.	M062X Geometries for All the Optimized Compounds and Transition States	140
12.	Complete Reference for Gaussian 09.....	163
13.	Copies of NMR Spectra	164
14.	GC Traces.....	168
15.	References.....	175

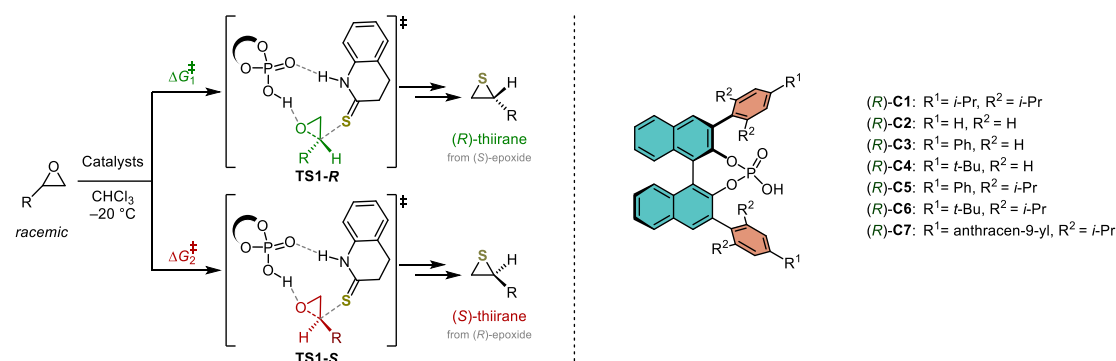
1. Distortion/Interaction Analysis

Table S1. Distortion/Interaction analysis for the enantioselectivity-determining transition states **TS1-R** and **TS1-S**. Energy differences are given in kcal/mol.

	$\Delta E(\text{dist-catalyst})$	$\Delta E(\text{dist-epoxide})$	$\Delta E(\text{dist-thiolactam})$	$\Delta E(\text{int})$
TS1-R	57.9	24.6	1.0	-102.2
TS1-S	63.8	25.6	1.2	-107.2

2. Computational and Experimental Results with Aliphatic Substrates

Table S2. Theoretically predicted and experimentally observed enantioselectivities for the reactions with aliphatic substrates.



Catalyst	$\Delta\Delta G_{\text{calc}}^{\ddagger} / \Delta\Delta G_{\text{exp}}^{\ddagger}$ ^a	$ee_{\text{calc}} / ee_{\text{exp}}$ ^d	Catalyst	$\Delta\Delta G_{\text{calc}}^{\ddagger} / \Delta\Delta G_{\text{exp}}^{\ddagger}$ ^b	$ee_{\text{calc}} / ee_{\text{exp}}$ ^d
R = <i>n</i>-hexyl			R = cyclohexyl		
(R)-C1	1.1/1.2	73/76	(R)-C1	1.2/0.6	77/48
(R)-C5	1.4/0.6	83/45	(R)-C5	1.3/0.3	80/22
(R)-C6	1.4/1.0	83/67	(R)-C6	0.7/0.6	53/45
(R)-C7	0.8/0.6	59/46	(R)-C7	0.8/0.6	59/46

^a $\Delta\Delta G_{\text{calc}}^{\ddagger} = \Delta G_{\text{TS2}}^{\ddagger} - \Delta G_{\text{TS1}}^{\ddagger}$, where $\Delta G_{\text{TS1}}^{\ddagger}$ and $\Delta G_{\text{TS2}}^{\ddagger}$ were obtained by theoretical calculations. ^b $\Delta\Delta G_{\text{exp}}^{\ddagger}$ is extrapolated by experimentally observed ee ($\Delta\Delta G^{\ddagger} = -RT \ln(1-ee)/(1+ee)$). ^c ee value obtained by theoretical calculations. ^d ee value obtained by experiment.

We also using the new designed CPA catalysts for the thionation reaction of aliphatic epoxides with thiolactam **3a** (Table S2). Both computational and experimental results

demonstrated that the reactions proceed with low enantioselectivity. Based on the first enantioselectivity-determining model (Figure 4a), the phenyl group on the epoxide **1** (*rac*-styrene oxide) is much closer to the *para*-substituents of the catalyst in the unfavorable transition state **TS1-S**. When the phenyl group of the substrate is replaced by a cyclohexyl or *n*-hexyl group, the attractive dispersion interactions between the catalyst and aliphatic groups favour transition state **TS1-S**. Therefore, the enantioselectivity is reduced.

3. Benchmark for Various DFT Methods

Table S3. Benchmark for various DFT methods using the def2-TZVP basis set (Except for PWPB95-D3BJ with the def2-TZVPP basis set). All numbers are given in kcal/mol.

	ω B97X- D3	ω B97M- V	ω B97M- D3BJ	ω B97M- D4	PWPB95- D3BJ	AVERAGE $\Delta\Delta G^\ddagger$
(<i>R</i>)-C1	2.0	2.0	1.8	1.9	1.8	1.9(+/-0.1)
(<i>R</i>)-C2	1.4	1.4	1.3	1.5	1.2	1.4(+/-0.2)
(<i>R</i>)-C3	0.3	0.3	0.6	0.6	0.3	0.4(+/-0.2)
(<i>R</i>)-C4	-0.2	-0.3	0.0	0.0	-0.8	-0.3(+/-0.4)
(<i>R</i>)-C5	2.2	2.2	2.0	2.1	2.5	2.2(+/-0.3)
(<i>R</i>)-C6	3.4	3.3	3.3	3.4	3.1	3.3(+/-0.2)
(<i>R</i>)-C7	4.7	4.6	4.1	4.1	3.6	4.2(+/-0.6)

4. Theoretically Predicted Enantioselectivities at the M06-2X/6-311+G(d,p)-SMD//M06-2X/6-31G(d)-SMD Level of Theory

Table S4. Theoretically predicted enantioselectivities $\Delta\Delta G^\ddagger$ of various CPAs. Free energies are given in kcal/mol.

	M06-2X/6-311+G(d,p)-SMD //M06-2X/6-31G(d)-SMD ¹	M06-2X/6-311+G(d,p)-SMD //B3LYP/6-31G(d) ²
(<i>R</i>)-C1	2.1	1.9
(<i>R</i>)-C2	0.8	1.0
(<i>R</i>)-C3	0.6	0.7
(<i>R</i>)-C4	0.4	0.4
(<i>R</i>)-C5	1.9	3.1
(<i>R</i>)-C6	2.3	3.6
(<i>R</i>)-C7	5.4	4.2

¹ Geometry optimizations were performed with the SMD solvation model at the M06-2X/6-31G(d) level of theory, then single-point energies were computed with the SMD solvation model at the M06-2X/6-311+G(d,p) level of theory using the gas-phase-optimized structures. ² Geometry optimizations were performed at the B3LYP/6-31G(d) level of theory, then single-point energies were computed with the SMD solvation model at the M06-2X/6-311+G(d,p) level of theory using the gas-phase-optimized structures.

5. Absolute Calculation Energies, Enthalpies, and Free Energies

Table S5. Absolute calculation energies, enthalpies, and free energies at the M06-2X/6-311+G(d,p)-SMD//B3LYP/6-31G(d) level of theory.

Geometry	$E_{(\text{elec-B3LYP})}^1$	$G_{(\text{corr-B3LYP})}^2$	$H_{(\text{corr-B3LYP})}^3$	$E_{(\text{solv,M06-2X})}^4$	IF ⁵
(R)-1	-384.838385	0.107234	0.147439	-384.797634	-
(R)-2	-707.829279	0.103705	0.145456	-707.789269	-
(S)-1	-384.838385	0.107234	0.147439	-384.797634	-
(S)-2	-707.829268	0.103748	0.145473	-707.789266	-
3a	-801.328581	0.128062	0.171808	-801.282923	-
4b	-478.372673	0.130835	0.173468	-478.330015	-
(R)-C1	-2582.023457	0.863614	1.010433	-2581.746428	-
(R)-C2	-1874.384407	0.386487	0.474888	-1874.252716	-
(R)-C3	-2336.490156	0.534907	0.646404	-2336.301198	-
(R)-C4	-2188.889585	0.599755	0.712154	-2188.696522	-
(R)-C5	-2808.243702	0.854926	1.003486	-2807.961600	-
(R)-C6	-2660.642497	0.919062	1.069224	-2660.356020	-
(R)-C7	-3422.780704	1.026695	1.201139	-3422.426021	-
(R)-5-CP-R	-3994.465768	1.134108	1.325618	-3994.105059	-
(R)-6-CP-R	-3846.861144	1.201905	1.393681	-3846.502351	-
(R)-7-CP-R	-4609.000978	1.309183	1.525515	-4608.574826	-
I	-3383.380155	1.012685	1.183981	-3383.050064	-
II-R	-3768.241979	1.146294	1.334732	-3767.892049	-
II-S	-3768.239270	1.147066	1.334762	-3767.890006	-

III-R	-1186.195853	0.259490	0.322335	-1186.118205	-
III-S	-1186.195225	0.259984	0.322387	-1186.118584	-
IV-R	-3768.244116	1.141848	1.332666	-3767.887233	-
IV-S	-3768.245260	1.143364	1.332704	-3767.889634	-
V	-3060.431647	1.016200	1.185931	-3060.101657	-
TS1-R	-3768.210454	1.140934	1.331839	-3767.843933	-280.21
TS1-S	-3768.207928	1.141020	1.332129	-3767.841045	-289.01
TS2-R	-3768.225135	1.146449	1.330690	-3767.875002	-476.55
TS2-S	-3768.222764	1.149263	1.330921	-3767.874746	-506.40
TS3-R	-3768.225293	1.144196	1.329858	-3767.868668	-329.88
TS3-S	-3768.230195	1.143742	1.329596	-3767.872807	-732.76
TS4-R	-3768.222541	1.139288	1.330113	-3767.853917	-336.24
TS4-S	-3768.221490	1.140131	1.330087	-3767.853403	-351.50
TS5-R	-3060.571912	0.660645	0.796285	-3060.346224	-272.42
TS5-S	-3060.570449	0.661309	0.796325	-3060.345367	-297.88
(R)-3-TS1-R	-3522.679010	0.809555	0.967861	-3522.396868	-266.04
(R)-3-TS1-S	-3522.676305	0.810147	0.967756	-3522.396343	-273.57
(R)-4-TS1-R	-3375.076785	0.874600	1.033557	-3374.791212	-277.36
(R)-4-TS1-S	-3375.075176	0.874805	1.033429	-3374.790762	-292.07
(R)-5-TS1-R	-3994.431089	1.130710	1.325022	-3994.061364	-271.59
(R)-5-TS1-S	-3994.430578	1.132424	1.325409	-3994.058135	-276.28
(R)-6-TS1-R	-3846.829603	1.194972	1.390487	-3846.454661	-284.04
(R)-6-TS1-S	-3846.827123	1.197058	1.390904	-3846.451052	-292.68
(R)-7-TS1-R	-4608.970440	1.305851	1.522772	-4608.527206	-271.05
(R)-7-TS1-S	-4608.967570	1.306759	1.523494	-4608.521444	-256.89
(R)-5-TS4-R	-3994.444193	1.130636	1.323266	-3994.071373	-341.07
(R)-6-TS4-R	-3846.841738	1.195664	1.389080	-3846.463654	-335.47
(R)-7-TS4-R	-4608.981485	1.305343	1.520958	-4608.534474	-342.65
TS1-R-cyclohexyl-	-4612.595341	1.595301	1.377458	-4612.139243	-280.78

anthryl					
TS1-R-cyclohexyl-iPr	-3771.836644	1.40442	1.212466	-3771.45761	-292.29
TS1-R-cyclohexyl-Ph	-3998.057382	1.397574	1.202315	-3997.673808	-282.91
TS1-R-cyclohexyl-tBu	-3850.455773	1.463532	1.268953	-3850.066667	-289.87
TS1-R-n-hexyl-anthryl	-4613.800361	1.617045	1.392344	-4613.333946	-303.06
TS1-R-n-hexyl-iPr	-3773.040542	1.426145	1.227131	-3772.649651	-308.56
TS1-R-n-hexyl-Ph	-3999.26025	1.419494	1.216433	-3998.866816	-317.5
TS1-R-n-hexyl-tBu	-3851.65841	1.484869	1.280627	-3851.259552	-326.69
TS1-S-cyclohexyl-anthryl	-4612.594389	1.59552	1.378873	-4612.139353	-295.67
TS1-S-cyclohexyl-iPr	-3771.833922	1.404302	1.212047	-3771.455325	-304.33
TS1-S-cyclohexyl-Ph	-3998.055073	1.397523	1.202713	-3997.672155	-300.94
TS1-S-cyclohexyl-tBu	-3850.453047	1.463449	1.268519	-3850.065128	-300.43
TS1-S-n-hexyl-anthryl	-4613.79692	1.616918	1.394361	-4613.334763	-329.26

TS1-S-<i>n</i>-hexyl-iPr	-3773.036781	1.425939	1.227741	-3772.648477	-333.76
TS1-S-<i>n</i>-hexyl-Ph	-3999.259326	1.419164	1.219149	-3998.867376	-333.25
TS1-S-<i>n</i>-hexyl-tBu	-3851.65624	1.484851	1.280567	-3851.257247	-346.93

¹The electronic energy calculated by B3LYP in gas phase. ²The thermal correction to Gibbs free energy calculated by B3LYP in gas phase. ³The thermal correction to enthalpy calculated by B3LYP in gas phase. ⁴The electronic energy calculated by M06-2X in chloroform solvent. ⁵The B3LYP calculated imaginary frequencies for the transition states.

Table S6. Absolute calculation energies, enthalpies, and free energies at the M06-2X/6-311+G(d,p)-SMD//M06-2X/6-31G(d)-SMD level of theory.

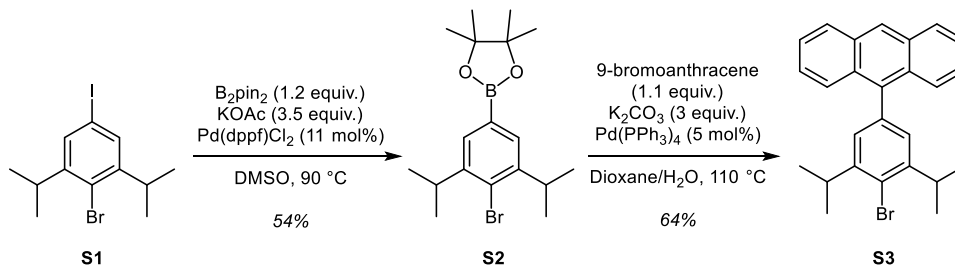
Geometry	$E_{(\text{elec-M06-2X})}^1$	$G_{(\text{corr-M06-2X})}^2$	$H_{(\text{corr-M06-2X})}^3$	$E_{(\text{solv,M06-2X})}^4$	IF ⁵
M-(R)-3-TS1-R	-3521.587375	0.826963	0.977399	-3522.40453	-412.3
M-(R)-3-TS1-S	-3521.586741	0.827276	0.977549	-3522.403816	-429.62
M-(R)-4-TS1-R	-3374.011132	0.894083	1.043733	-3374.79929	-432.66
M-(R)-4-TS1-S	-3374.009631	0.893649	1.044246	-3374.798233	-428.36
M-(R)-5-TS1-R	-3993.124007	1.151734	1.336827	-3994.071676	-434.6
M-(R)-5-TS1-S	-3993.120209	1.151906	1.336307	-3994.068748	-426.27
M-(R)-6-TS1-R	-3845.545007	1.217501	1.402279	-3846.463843	-417.83
M-(R)-6-TS1-S	-3845.540527	1.216938	1.402381	-3846.459611	-441.77
M-(R)-7-TS1-R	-4607.443755	1.330685	1.536785	-4608.540887	-379.79
M-(R)-7-TS1-S	-4607.43831	1.333283	1.537983	-4608.534916	-413.34
M-TS1-R	-3766.9583	1.161951	1.343057	-3767.854728	-437.3
M-TS1-S	-3766.95455	1.162221	1.343657	-3767.851612	-434.88
M-TS5-R	-3059.654476	0.67595	0.804332	-3060.354217	-435
M-TS5-S	-3059.653607	0.675649	0.804789	-3060.352678	-433.94

¹The electronic energy calculated by M06-2X in gas phase. ²The thermal correction to Gibbs free energy calculated by M06-2X in gas phase. ³The thermal correction to enthalpy calculated by M06-2X in gas phase. ⁴The electronic energy calculated by M06-2X in chloroform solvent. ⁵The M06-2X calculated imaginary frequencies for the transition states.

6. General Experimental Methods

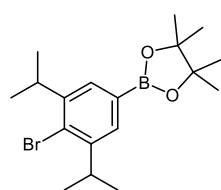
Unless otherwise stated, all reagents were purchased from commercial suppliers and used without further purification. *rac*-Styrene oxide was distilled under reduced pressure and stored under argon before use. All solvents used in the reactions were distilled from appropriate drying agents before use. Reactions were monitored by thin-layer chromatography (TLC) on silica gel pre-coated plastic sheets (0.2 mm, Macherey-Nagel) or glass plates (SIL G-25 UV₂₅₄, 0.25 mm, Macherey-Nagel). Visualization was accomplished by irradiation with UV light at 254/366 nm and/or with the following stains: CAM (10 g ammonium molybdate + 4 g ceric ammonium sulfate, dissolved in 360 mL distilled water and treated with 40 mL concentrated H₂SO₄), PMA (10 g phosphomolybdic acid dissolved in 100 mL absolute ethanol), KMnO₄ (1.5 g KMnO₄ + 10 g Na₂CO₃, dissolved in 200 mL distilled water and treated with 1.25 mL aq. NaOH 10%). Column chromatography was performed on Merck silica gel (60, particle size 0.040–0.063 mm). Preparative TLC was performed on Macherey-Nagel SIL G-25 UV₂₅₄ plates (silica gel 60, 0.25 mm layer, 20 cm x 20 cm, with fluorescence indicator). NMR spectra were recorded on a Bruker AV-500 spectrometer in deuterated solvents. Proton chemical shifts are reported in ppm (δ) relative to tetramethylsilane (TMS) with the solvent resonance employed as the internal standard (CDCl₃ δ 7.26 ppm; CD₂Cl₂ δ 5.32 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, sext = sextet, hept = heptet, m = multiplet, br = broad), coupling constants (Hz) and integration. ¹³C chemical shifts are reported in ppm from tetramethylsilane (TMS) with the solvent resonance as the internal standard (CDCl₃ δ 77.16 ppm; CD₂Cl₂ δ 53.84 ppm). High-resolution mass spectra were determined on a Bruker APEX III FTMS (7 T magnet). Enantiomeric ratios (e.r.) were determined by GC analysis employing a chiral stationary phase column specified in the individual experiment, by comparing the samples with the appropriate racemic mixtures.

7. Preparation of 3,3'-disubstituted BINOL **S7** (precursor of (*R*)-**C7**)



The synthesis of **S3** has previously been reported by using a Suzuki cross-coupling reaction of **S1** with 9-anthracenyl boronic acid [3]. However, we observed that the latter readily undergoes protodeboronation with traces of water to produce anthracene, which co-elutes with the desired product **S3** during column chromatography. Instead, the proposed inversed-polarity two-step sequence easily provides **S3** with high purity.

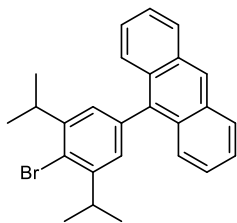
2-(4-bromo-3,5-diisopropylphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (S2):



Adapted from Ref. [1]: An oven-dried 50 mL Schlenk flask was charged with 2-bromo-5-iodo-1,3-diisopropylbenzene [2] (**S1**, 2.50 g, 6.81 mmol, 1 equiv.), bis-(pinacolato)-diboron (2.11 g, 8.30 mmol, 1.2 equiv.), Pd(dppf)Cl₂·CH₂Cl₂ (612 mg, 0.75 mmol, 0.11 equiv.), and DMSO (21 mL). The mixture was purged with argon for 5 min, followed by addition of potassium acetate (2.34 g, 23.8 mmol, 3.5 equiv.). The reaction mixture was stirred vigorously at 90 °C for 16 h. After cooling to room temperature, the reaction was diluted with MTBE (50 mL) and filtered over a short pad of Celite. The filtered mixture was washed with water (1 x 30 mL) and the aqueous layer was further extracted with MTBE (2 x 20 mL). The combined organic phases were washed with brine (1 x 30 mL), dried over anhydrous Na₂SO₄, filtered and concentrated in vacuo, and the crude product was purified by column chromatography (silica gel, *iso*-hexane/CH₂Cl₂ mixture, gradient from 100:0 to 80:20 v/v) to give **S2** (1.347 g, 54% yield) as a white solid.

¹H NMR (CD₂Cl₂, 501 MHz): δ 7.50 (s, 2H), 3.50 (hept, *J* = 6.8 Hz, 2H), 1.33 (s, 12H), 1.28 (d, *J* = 6.8 Hz, 12H). ¹³C NMR (CD₂Cl₂, 126 MHz): δ 147.5 (C), 130.70 (C), 130.66 (CH), 84.3 (C), 34.0 (CH), 25.1 (CH₃), 23.2 (CH₃). ¹¹B NMR (CD₂Cl₂, 161 MHz): δ 30.9. HRMS (ESI): calculated for C₁₈H₂₈O₂BBrNa⁺ ([M+Na]⁺): 389.1258, found: 389.1260.

9-(4-bromo-3,5-diisopropylphenyl)anthracene (**S3**):

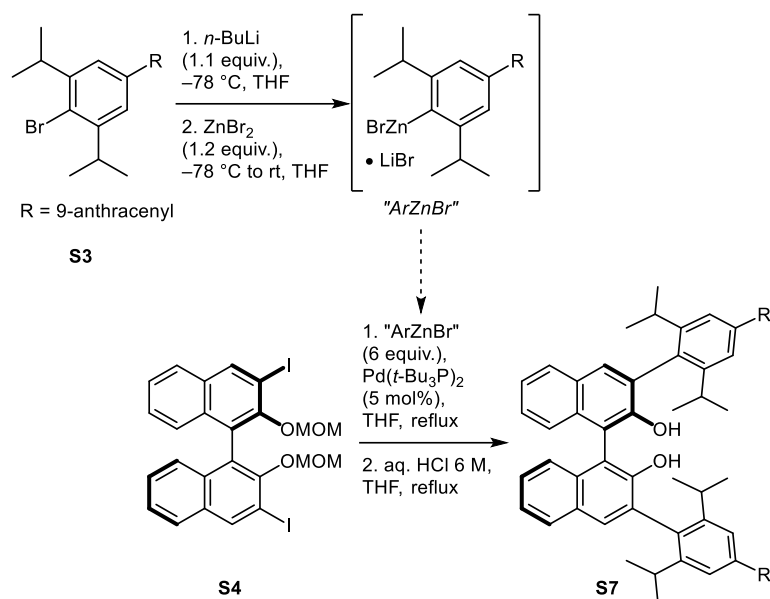


An oven-dried 50 mL Schlenk flask was charged with 2-(4-bromo-3,5-diisopropylphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**S2**, 1.34 g, 3.65 mmol, 1 equiv.), 9-bromoanthracene (1.03 g, 4.02 mmol, 1.1 equiv.), and K_2CO_3 (1.51 g, 11.0 mmol, 3 equiv.). The flask was evacuated and back-filled with argon, then 1,4-dioxane (18 mL) and distilled water (4 mL) were added and the mixture was degassed by bubbling argon for 5 min, followed by addition of $Pd(PPh_3)_4$ (211 mg, 0.18 mmol, 0.05 equiv.) The reaction mixture was stirred vigorously at 110 °C for 72 h. After cooling to room temperature, the reaction was diluted with MTBE (70 mL) and water (30 mL), and the aqueous phase was further extracted with MTBE (2 x 30 mL). The combined organic phases were washed with brine (1 x 30 mL), dried over anhydrous Na_2SO_4 , filtered and concentrated in vacuo, and the crude product was purified by column chromatography (silica gel, *iso*-hexane; mass ratio silica/sample 150:1, height/diameter ratio \approx 3:1) to give **S3** (968 mg, 64% yield) as an off-white solid (photosensitive, kept under dark and under argon, in a vial covered with aluminum foil).

1H NMR (CD_2Cl_2 , 501 MHz): δ 8.52 (s, 1H), 8.06 (d, $J = 8.7$ Hz, 2H), 7.66 (dd, $J = 8.8$ Hz, 1.1 Hz, 2H), 7.48 (br t, $J = 7.5$ Hz, 2H), 7.37 (ddd, $J = 8.8$ Hz, 6.5 Hz, 1.3 Hz, 2H), 7.21 (s, 2H), 3.64 (hept, $J = 6.9$ Hz, 2H), 1.27 (d, $J = 6.9$ Hz, 12H). ^{13}C NMR (CD_2Cl_2 , 126 MHz): δ 148.1 (C), 138.0 (C), 137.0 (C), 131.6 (C), 130.3 (C), 128.6 (CH), 127.5 (CH), 127.0 (CH), 126.8 (C), 125.9 (C), 125.8 (CH), 125.5 (CH), 34.0 (CH), 23.2 (CH_3). HRMS (APPI): calculated for $C_{26}H_{26}Br^+$ ($[M+H]^+$): 417.1212, found: 417.1210. The analytical data matches those reported in the literature [3].

The installation of 2,6-diisopropyl-4-substituted-phenyl (“4-R-DIP”) substituents on the 3,3’-positions of the BINOL moiety was performed by cross-coupling reactions. With the substituent in position 4 being either phenyl or *tert*-butyl, reported procedures using Kumada coupling were followed ([4] and [5], respectively), leading to BINOLs **S5** and **S6**, respectively.

With the 9-anthracenyl substituent, the reported Kumada coupling ([3]) presented reproducibility issues, whereas the following Negishi coupling performed satisfactorily, giving thus access to the BINOL **S7**.



Preparation of organozinc coupling partner:

An oven-dried 10 mL Schlenk flask was purged with argon and flame-dried under vacuum. Using "argon trousers", anhydrous ZnBr₂ was added to the previously weighed Schlenk flask and further dried under vacuum (120 °C, 10⁻³ mbar) for 2 h. After cooling to room temperature, the mass of dry ZnBr₂ was determined and dissolved in the corresponding volume of dry THF to generate a 1 M solution.

Another oven-dried 25 mL Schlenk flask, previously purged with argon, was charged with the aryl bromide **S3** (2 mmol, 1 equiv.) and dry THF (6.5 mL). After cooling to -78 °C, *n*-BuLi (2.2 mmol, 1.1 equiv., freshly titrated) was added dropwise over 2 min and the mixture is stirred vigorously for 1 h.

After checking completion of lithium-halogen exchange by ¹H NMR (comparison of aliquot quenching with CH₃OH and with CD₃OD), ZnBr₂ 1 M solution (1.2 equiv.) was added at -78 °C. The mixture was further stirred at -78 °C for 30 min, then gradually warmed to room temperature and further stirred for 1 h. The solvent was removed under vacuum, using a liquid N₂ trap in between, giving the desired organozinc derivative (yield is assumed quantitative for the next step).

Negishi cross-coupling and MOM deprotection:

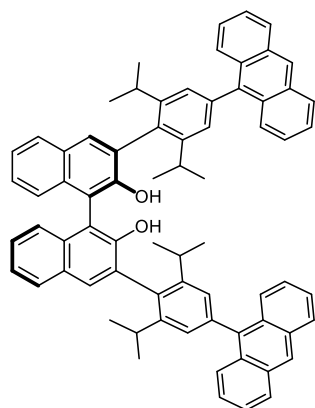
The Schlenk flask, containing the previously prepared organozinc derivative (2 mmol, 6 equiv.), was charged with **S4** ([6]) (208 mg, 0.33 mmol, 1 equiv.) and Pd(*t*-Bu₃P)₂ (8.5 mg, 0.017 mmol, 0.05 equiv.). The flask was evacuated and back-filled with argon (×3), then dry THF (2.5 mL) was added and the reaction mixture was stirred vigorously

at 80 °C for 24 h. After cooling to room temperature, the reaction was diluted with MTBE (30 mL) and water (20 mL), and the aqueous phase was further extracted with MTBE (2 x 30 mL). The combined organic phases were washed with brine (1 x 30 mL), dried over anhydrous Na₂SO₄, filtered and concentrated in vacuo.

This crude product was redissolved in THF (5 mL), and treated with methanol (0.5 mL) and aq. HCl 6 M (2.5 mL), then the flask was closed and the mixture was heated at 80 °C for 12 h.

After cooling to room temperature, the reaction was diluted with MTBE (40 mL) and water (30 mL), and the aqueous phase was further extracted with MTBE (2 x 30 mL). The combined organic phases were washed with brine (1 x 30 mL), dried over anhydrous Na₂SO₄, filtered and concentrated in vacuo, and the crude product was purified by column chromatography (silica gel, pentane-CH₂Cl₂ mixture, gradient from 100:0 to 80:20).

(*R*)-3,3'-bis(4-(anthracen-9-yl)-2,6-diisopropylphenyl)-[1,1'-binaphthalene]-2,2'-diol (S7**):**

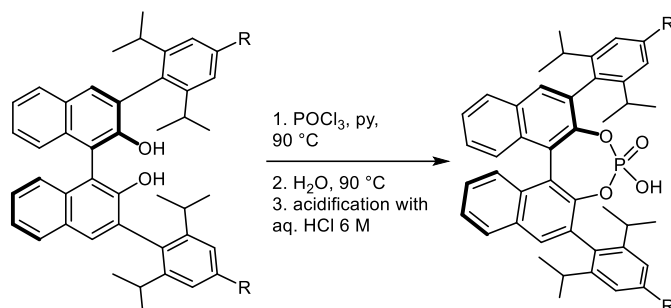


Starting from 417 mg (1.0 mmol) of aryl bromide **S3** and 102 mg (0.16 mmol) of diiodo derivative **S4**, the corresponding 3,3'-disubstituted BINOL **S7** was obtained in 65% yield (100.8 mg, 0.105 mmol) as an off-white solid.

¹H NMR (CD₂Cl₂, 501 MHz): δ 7.08 (d, *J* = 1.5 Hz, 2H), 6.92 (br t, *J* = 1.6 Hz, 1H), 2.88 (hept, *J* = 6.9 Hz, 2H), 1.32 (s, 9H), 1.25 (d, *J* = 6.9 Hz, 12H). ¹³C NMR (CD₂Cl₂, 126 MHz): δ 151.2 (C), 148.71 (C), 148.67 (C), 139.4 (C), 138.2

(C), 134.0 (C), 132.7 (C), 131.9 (C), 131.4 (CH), 130.6 (C), 130.5 (C), 129.8 (C), 129.4 (C), 128.9 (CH), 128.8 (CH), 128.7 (CH), 127.33 (CH), 127.29 (CH), 126.8 (CH), 126.7 (CH), 125.83 (CH), 125.79 (CH), 125.56 (CH), 124.7 (CH), 124.4 (CH), 113.7 (C), 31.5 (CH), 24.5 (CH₃), 24.4 (CH₃), 24.1 (CH₃), 24.0 (CH₃). ESI-HRMS: calculated for C₇₂H₆₁O₂⁻ ([M-H]⁻): 957.4677, found: 957.4667. The analytical data matches those reported in the literature [3].

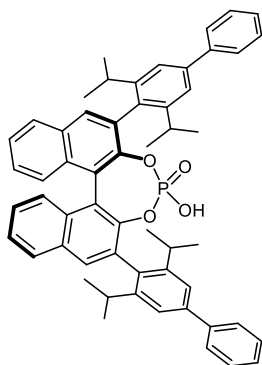
8. Preparation of Chiral Phosphoric Acids (*R*)-C5, (*R*)-C6 and (*R*)-C7



General Procedure for the synthesis of BINOL-derived phosphoric acids:

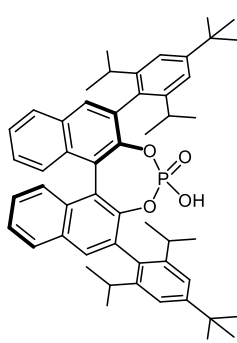
An oven-dried 10 mL Schlenk flask was charged with 3,3'-disubstituted (*R*)-BINOL (0.1 mmol) and dry pyridine (2.5 mL). To this solution, POCl₃ (17 μ L, 0.18 mmol, 1.8 equiv.) was added dropwise; then, the flask was closed under argon and the mixture was stirred at 90 °C for 24 h. After cooling to room temperature and checking full conversion by TLC, distilled water (0.20 mL, 11.1 mmol, 111 equiv.) was added and the mixture was further stirred at 90 °C for 24 h. After cooling to room temperature, the mixture was diluted with CH₂Cl₂ (30 mL), water (20 mL) and aq. HCl 6 M (10 mL); the aqueous layer was further extracted with CH₂Cl₂ (2 x 20 mL), and the combined organic layers were washed with aq. HCl 1 M (1 x 20 mL) and brine (1 x 20 mL), dried over anhydrous Na₂SO₄, filtered and concentrated in vacuo. The crude product was purified by column chromatography (silica gel, *iso*-hexane-EtOAc mixture, gradient from 90:10 to 70:30) and concentrated in vacuo. The product was dissolved in CH₂Cl₂ (20 mL), treated with aq. HCl 6 M (15 mL) and stirred vigorously for 30 min; the organic layer was diluted with toluene (20 mL) and concentrated under reduced pressure, then dissolved again in toluene and concentrated (this cycle is repeated 3x). The acidified BINOL-derived phosphoric acid was dried on high vacuum (room temperature, 10⁻³ mbar) overnight.

(*R*)-2,6-bis(3,5-diisopropyl-[1,1'-biphenyl]-4-yl)-4-hydroxydinaphtho[2,1-*d*:1',2'-*f*][1,3,2]dioxaphosphepine 4-oxide ((*R*)-C5)



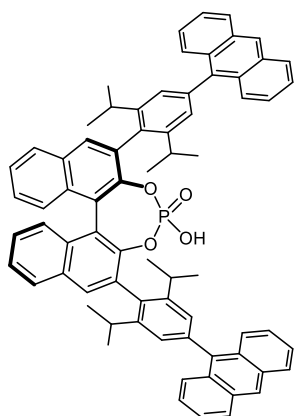
Starting from 50.0 mg (0.066 mmol) of the corresponding 3,3'-disubstituted BINOL (**S5** [4]), 34.1 mg of phosphoric acid (*R*)-**C5** are obtained (63% yield). ¹H NMR (CD₂Cl₂, 501 MHz): δ 7.94 (d, *J* = 8.2 Hz, 2H), 7.83 (s, 2H), 7.56 (d, *J* = 7.5 Hz, 4H), 7.52 (t, *J* = 8.0 Hz, 2H), 7.39 (t, *J* = 7.6 Hz, 4H), 7.35–7.27 (m, 10H), 2.69–2.55 (m, 4H), 1.12 (d, *J* = 6.8 Hz, 6H), 1.00 (d, *J* = 6.6 Hz, 6H), 0.89 (d, *J* = 6.9 Hz, 6H), 0.83 (d, *J* = 6.5 Hz, 6H). ³¹P NMR (CD₂Cl₂, 203 MHz): δ 2.94. ESI-HRMS: calculated for C₅₆H₅₂O₄P⁻ ([M-H]⁻): 819.3609, found: 819.3613. The analytical data matches those reported in the literature [7].

(*R*)-2,6-bis(4-(*tert*-butyl)-2,6-diisopropylphenyl)-4-hydroxydinaphtho[2,1-*d*:1',2'-*f*][1,3,2]dioxaphosphepine 4-oxide ((*R*)-C6)



Starting from 71 mg (0.1 mmol) of the corresponding 3,3'-disubstituted BINOL (**S6** [5]), 68 mg of phosphoric acid (*R*)-**C6** are obtained (87% yield). ¹H NMR (CD₂Cl₂, 501 MHz): δ 7.90 (d, *J* = 7.9 Hz, 2H), 7.79 (s, 2H), 7.50 (t, *J* = 7.6 Hz, 2H), 7.30 (t, *J* = 7.6 Hz, 4H), 7.17–7.08 (m, 4H), 2.64–2.50 (m, 4H), 1.28 (s, 18H), 1.05 (br s, 6H), 0.98 (d, *J* = 6.9 Hz, 6H), 0.89 (d, *J* = 6.8 Hz, 6H), 0.74 (br s, 6H). ³¹P NMR (CD₂Cl₂, 203 MHz): δ 2.64. ESI-HRMS: calculated for C₅₂H₆₀O₄P⁻ ([M-H]⁻): 779.4235, found: 779.4243. The analytical data matches those reported in the literature [8].

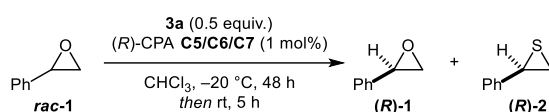
(R)-2,6-bis(4-(anthracen-9-yl)-2,6-diisopropylphenyl)-4-hydroxydinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepine 4-oxide ((R)-C7)




Starting from 60.0 mg (0.062 mmol) of the corresponding 3,3'-disubstituted BINOL (**S7**), 55.2 mg of phosphoric acid (**R-C7**) are obtained (86% yield). ^1H NMR (CD_2Cl_2 , 501 MHz): δ 8.42 (s, 2H), 8.07–8.02 (m, 6H), 7.89–7.64 (m, 8H), 7.58 (t, $J = 7.5$ Hz, 2H), 7.46 (t, $J = 7.4$ Hz, 2H), 7.40–7.35 (m, 4H), 7.32 (t, $J = 7.7$ Hz, 2H), 7.27–7.11 (m, 6H), 2.84–2.72 (m, 4H), 1.08 (br s, 6H), 1.00 (br s, 6H), 0.92–0.80 (m, 12H). ^{31}P NMR (CD_2Cl_2 , 203 MHz): δ 3.81. ESI-HRMS: calculated for $\text{C}_{72}\text{H}_{60}\text{O}_4\text{P}^-$ ($[\text{M}-\text{H}]^-$): 1019.4235, found:


1019.4227. The analytical data matches those reported in the literature [3].

9. General Procedure for the CPA-catalyzed Epoxide Thionation



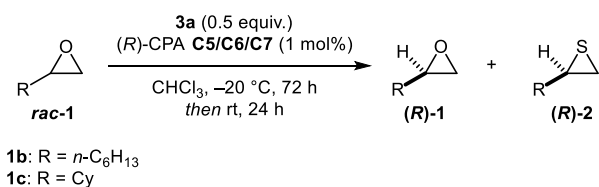
Following the previously reported procedure [9]: Styrene oxide *rac*-1 (0.05 mmol, 6.0 mg, 5.7 μ L) was weighed into a glass vial, and dissolved with 0.4 mL of dry CHCl₃. The vial was cooled at -20 °C for 20 min, and then sulfur donor **3a** [9] (0.025 mmol, 4.1 mg, 0.50 equiv.) was added, followed by the addition of the CPA catalyst (**R**)-C5/C6/C7 (0.0025 mmol, 5 mol%, as 0.1 mL of a stock solution in dry CHCl₃). Until the complete consumption of the sulfur donor, the reaction was then warmed up to room temperature and stirred for another five hours (to ensure all the intermediates were converted to the product). The crude ¹H NMR indicated an almost 1:1 ratio of the epoxide and thiirane product and both products in around 50% NMR yields (with Ph₃CH as an internal standard). The reaction was then neutralized with Et₃N (50 μ L) and concentrated under reduced pressure, leaving a residue which was subjected to preparative TLC on silica gel (eluted with pentane-MTBE 90:10 v/v mixture). The pure epoxide and thiirane product were obtained as a colorless liquids upon the removal of the eluent (used to extract the compounds from the scratched silica) under reduced pressure (400 mbar, in 40 °C water bath, 20–30 min), and kept in the freezer (-20 °C).

 (**R**)-1: Colorless liquid. ¹H NMR (500 MHz, CD₂Cl₂): δ 7.37–7.26 (m, 5H), 3.83 (dd, *J* = 4.1, 2.5 Hz, 1H), 3.11 (dd, *J* = 5.5, 4.1 Hz, 1H), 2.80 (dd, *J* = 5.5, 2.6 Hz, 1H). The enantiomeric ratio was determined by chiral GC analysis using a BGB-176 column (0.25 mm x 30 m): 70 °C for 40 min, *t*₁ = 33.4 min, *t*₂ = 35.8 min.

 (**R**)-2: Colorless liquid. ¹H NMR (500 MHz, CD₂Cl₂): δ 7.32–7.22 (m, 5H), 3.91 (dd, *J* = 6.6, 5.6 Hz, 1H), 2.87 (dd, *J* = 6.6, 1.6 Hz, 1H), 2.66 (dd, *J* = 5.6, 1.5 Hz, 1H). The enantiomeric ratio was determined by chiral GC analysis using a Hydrodex- β -TBDAc column (0.4 mm x 25 m): 100 °C for 25 min, *t*₁ = 21.8 min, *t*₂ = 22.8 min.

The analytical data of both compounds matches those reported in the literature [9].

As shown in Table S1, catalysts (*R*)-**C5**, (*R*)-**C6** and (*R*)-**C7** were also tested for the epoxide thionation reaction with two racemic aliphatic substrates, namely 2-(*n*-hexyl)oxirane (commercially available) and 2-cyclohexyloxirane (prepared by epoxidation of vinylcyclohexane with *m*-CPBA, following a reported procedure [10]).



The analytical data of these aliphatic epoxides and thiiranes matches those reported in literature [9].

10.B3LYP Geometries for All the Optimized Compounds and Transition States

3a E= -801.328580760

C	-1.130161	0.199574	-0.084241
C	0.266501	0.267737	-0.115155
C	0.933709	1.497522	0.021789
C	0.169951	2.649346	0.209877
C	-1.225933	2.593496	0.245219
C	-1.873195	1.365956	0.092357
H	-1.627978	-0.761411	-0.190462
H	0.677726	3.604466	0.322974
H	-1.802583	3.502152	0.390565
H	-2.957736	1.311233	0.117527
C	2.440692	1.492375	-0.082429
H	2.736784	1.575716	-1.138906
H	2.868153	2.360199	0.431547
C	3.021098	0.194153	0.501530
H	4.097274	0.121032	0.338349
H	2.856103	0.175536	1.589501
C	2.356135	-1.045418	-0.066918
S	3.145266	-2.484320	-0.327463
N	1.026964	-0.904492	-0.306504
H	0.544583	-1.742480	-0.613716

4b E= -478.372673225

C	-1.384581	-1.495110	0.022402
C	-0.309085	-0.606903	-0.086207
C	-0.529514	0.782817	-0.117986
C	-1.838790	1.253494	-0.016884
C	-2.919030	0.374114	0.093195
C	-2.686347	-1.001968	0.106310
H	-1.198801	-2.566408	0.047290
H	-2.013198	2.327096	-0.033411

H	-3.931133	0.760791	0.167486
H	-3.516883	-1.697296	0.190800
C	0.670600	1.683652	-0.301835
H	0.890009	1.783717	-1.375893
H	0.456437	2.692976	0.066217
C	1.905824	1.107254	0.406847
H	2.814970	1.666248	0.172739
H	1.766263	1.152028	1.496661
C	2.157000	-0.351122	0.047659
N	1.009396	-1.087679	-0.180899
H	1.161586	-2.079216	-0.323290
O	3.263565	-0.862943	-0.007913

III-R E= -1186.19585334

C	3.331900	1.693330	0.873488
C	2.733753	0.492207	0.458295
C	3.365197	-0.299361	-0.522162
C	4.587428	0.130480	-1.046013
C	5.185021	1.321534	-0.634222
C	4.545600	2.103916	0.330523
H	2.840394	2.296899	1.633848
H	5.074327	-0.485364	-1.799822
H	6.134896	1.633694	-1.058214
H	4.992931	3.036002	0.665615
C	2.692499	-1.568310	-1.004718
H	2.180311	-1.379542	-1.959769
H	3.442206	-2.342055	-1.208582
C	1.678457	-2.093929	0.015700
H	1.070533	-2.898720	-0.404354
H	2.195422	-2.484989	0.901138
C	0.747472	-0.988418	0.512052

S	-0.437839	-0.382587	-0.880824	H	1.698887	6.998672	0.078709
N	1.531644	0.079970	1.055827	C	0.373914	5.703686	-1.033206
H	0.985063	0.834999	1.452366	H	-0.056910	6.449638	-1.704781
C	-1.923500	-0.939491	0.066791	H	1.217571	5.226219	-1.547440
C	-1.398394	-0.956443	1.511101	C	-0.662906	4.607826	-0.790635
H	-1.385109	0.064117	1.922419	S	-2.325924	5.330274	-0.145569
H	-2.015570	-1.584165	2.160592	N	-0.116280	3.628373	0.102626
O	-0.103873	-1.535046	1.499103	H	-0.736049	2.849041	0.289328
H	-2.152593	-1.967164	-0.231779	C	-3.276647	4.620766	-1.573802
C	-3.153135	-0.078632	-0.124592	C	-2.321913	3.526658	-2.082512
C	-4.380759	-0.687830	-0.415257	H	-2.428118	2.620631	-1.467536
C	-3.115137	1.315622	0.028353	H	-2.513958	3.266030	-3.126353
C	-5.545552	0.071760	-0.541603	O	-0.990060	4.022132	-2.033169
H	-4.424406	-1.766964	-0.544463	H	-4.166410	4.147663	-1.147174
C	-4.277058	2.075779	-0.096185	C	-3.708322	5.643262	-2.603720
H	-2.165305	1.805522	0.223259	C	-5.030900	6.105293	-2.600160
C	-5.497220	1.456633	-0.380441	C	-2.825794	6.142682	-3.574420
H	-6.487650	-0.419645	-0.769578	C	-5.465371	7.046558	-3.535128
H	-4.228865	3.155079	0.021972	H	-5.727842	5.725898	-1.855719
H	-6.401116	2.051195	-0.481741	C	-3.260384	7.077830	-4.513160
III-S E= -1186.19522471				H	-1.797856	5.793924	-3.592278
C	0.978712	3.037788	2.182911	C	-4.580305	7.535866	-4.496339
C	0.679732	3.996088	1.200582	H	-6.495428	7.392632	-3.513737
C	1.211824	5.296288	1.309280	H	-2.564782	7.450941	-5.260463
C	2.043855	5.592226	2.392516	H	-4.915294	8.266444	-5.227705
C	2.345024	4.642115	3.368054	II-R E= -3768.24197925			
C	1.802463	3.359466	3.257275	H	-0.434078	-2.373528	-2.423381
H	0.566749	2.034938	2.090293	C	0.276408	-0.167182	3.332432
H	2.457019	6.596040	2.470996	C	0.273398	-1.561411	3.437460
H	2.993362	4.897795	4.200988	C	0.825734	-2.217999	4.548091
H	2.023014	2.603850	4.006679	C	1.368511	-1.442773	5.572124
C	0.843365	6.342349	0.277591	C	1.370642	-0.047750	5.487089
H	0.046132	6.990724	0.670320	C	0.830265	0.586687	4.366528

H	-0.136794	0.303684	2.448238	C	-0.684273	2.401130	-0.026102
H	1.796693	-1.936803	6.440916	C	1.746147	4.325033	2.081982
H	1.797576	0.540666	6.294078	C	-0.701548	4.287790	2.035903
H	0.840636	1.669584	4.288185	C	-1.939782	2.832436	0.501275
C	0.832839	-3.727509	4.545271	C	1.713297	5.188868	3.155687
H	1.728129	-4.097965	4.024802	H	2.699042	3.984195	1.693618
H	0.873644	-4.122368	5.565405	C	-0.700629	5.196368	3.129190
C	-0.423753	-4.251280	3.838643	C	-1.914848	3.789717	1.495058
H	-0.403567	-5.338279	3.728058	C	0.479263	5.642256	3.679762
H	-1.316497	-4.001778	4.431462	H	2.644615	5.524638	3.604064
C	-0.604789	-3.592707	2.485481	H	-1.656694	5.523213	3.531616
N	-0.279829	-2.328406	2.365541	H	-2.854115	4.160211	1.897504
H	-0.473880	-1.761625	1.480083	H	0.466919	6.331639	4.519616
C	-0.339028	-3.903703	-1.235837	C	-3.240884	2.300372	-0.023905
C	-1.583185	-3.710206	-0.332458	C	-3.669404	2.644471	-1.330646
H	0.534204	-3.462524	-0.730904	C	-4.067890	1.494783	0.794668
H	-1.690221	-2.650337	-0.092273	C	-4.904311	2.173376	-1.785462
C	2.153178	1.270188	-0.538664	C	-5.297320	1.053450	0.287115
C	1.778695	2.599404	-0.383447	C	-5.736849	1.374388	-0.996885
C	2.598793	3.619490	-0.982169	H	-5.227054	2.443921	-2.787763
C	3.840860	3.241289	-1.586392	H	-5.937170	0.437825	0.916046
C	4.211838	1.872793	-1.612869	C	3.831183	-0.560947	-1.191452
C	3.388171	0.874469	-1.135759	C	4.457311	-1.137321	-0.060950
H	1.267835	5.294855	-0.623928	C	3.692446	-1.312619	-2.382054
C	2.222832	4.991133	-1.036050	C	4.935205	-2.449455	-0.142403
C	4.673030	4.239256	-2.161922	C	4.188185	-2.622833	-2.407110
H	5.174949	1.604277	-2.038567	C	4.811089	-3.212513	-1.306241
C	4.288820	5.560285	-2.175951	H	5.425776	-2.882719	0.726099
C	3.043562	5.933007	-1.617391	H	4.083153	-3.207274	-3.317193
H	5.617200	3.932704	-2.606103	O	-0.700351	1.451672	-1.028725
H	4.929409	6.313916	-2.625768	O	1.339933	0.281926	-0.011269
H	2.727374	6.972175	-1.652376	P	-0.119462	-0.061308	-0.722103
C	0.532116	2.950436	0.359927	O	-0.917364	-0.705671	0.402688
C	0.545719	3.858213	1.476198	C	-2.855525	3.551638	-2.253752

H	-1.914060	3.795263	-1.754648	H	2.769648	-2.512541	-4.898652
C	-3.584228	4.888273	-2.501203	C	4.139093	-0.168901	-4.594454
H	-3.800409	5.403420	-1.558148	H	4.824781	-0.963968	-4.913536
H	-4.536028	4.737107	-3.024136	H	4.735815	0.616354	-4.119565
H	-2.966756	5.552196	-3.118457	H	3.675850	0.256825	-5.493050
C	-2.495437	2.857476	-3.580994	C	5.331536	-4.642574	-1.382658
H	-1.941339	1.932175	-3.399519	H	5.139128	-5.000508	-2.403181
H	-1.869885	3.516883	-4.194974	C	6.851838	-4.719536	-1.146594
H	-3.390519	2.613599	-4.165862	H	7.211153	-5.749199	-1.264710
C	-7.080601	0.872734	-1.509580	H	7.115739	-4.389192	-0.134751
H	-7.518924	0.254874	-0.713155	H	7.394150	-4.084817	-1.855902
C	-8.059141	2.031353	-1.781436	C	4.575977	-5.577295	-0.418470
H	-9.037878	1.647067	-2.093821	H	4.926532	-6.611487	-0.523666
H	-7.688456	2.686103	-2.579107	H	3.498518	-5.559595	-0.617023
H	-8.202632	2.645984	-0.885880	H	4.729265	-5.277433	0.625546
C	-6.924841	-0.020982	-2.754887	C	4.669611	-0.356501	1.235928
H	-6.252030	-0.863405	-2.559204	H	4.121643	0.587033	1.158685
H	-6.510546	0.541575	-3.599756	C	4.110367	-1.096068	2.464408
H	-7.896666	-0.422409	-3.067624	H	4.650605	-2.030265	2.660958
C	-3.684274	1.083051	2.216575	H	3.052309	-1.336873	2.322772
H	-2.655526	1.406413	2.395938	H	4.197841	-0.470470	3.360755
C	-4.577627	1.775665	3.265058	C	6.156620	-0.001189	1.433719
H	-4.522028	2.867031	3.184259	H	6.539161	0.582687	0.589185
H	-4.271156	1.494782	4.280477	H	6.772991	-0.904301	1.520716
H	-5.629095	1.489592	3.141630	H	6.296029	0.590592	2.347127
C	-3.709489	-0.445476	2.406042	O	0.027883	-0.742825	-2.042453
H	-3.060732	-0.925317	1.668466	S	-1.312386	-4.625328	1.298847
H	-4.720947	-0.855431	2.302581	O	-0.565199	-3.350720	-2.498146
H	-3.350922	-0.706565	3.410241	C	-2.880909	-4.246695	-0.895754
C	3.058162	-0.729769	-3.645661	C	-2.971631	-5.535766	-1.439441
H	2.410705	0.097656	-3.340672	C	-4.027821	-3.441691	-0.866855
C	2.173043	-1.735640	-4.403795	C	-4.183408	-6.009521	-1.941878
H	1.612998	-1.212562	-5.187562	H	-2.091361	-6.171457	-1.485219
H	1.452644	-2.221940	-3.743092	C	-5.239086	-3.913659	-1.373402

H	-3.966635	-2.435648	-0.459381	C	0.453425	4.892488	-1.441370
C	-5.320703	-5.199908	-1.910174	C	1.666571	4.180384	-1.264673
H	-4.236986	-7.009000	-2.364944	C	1.702085	2.907704	-0.734358
H	-6.117606	-3.274427	-1.350825	H	-2.930419	4.565951	-0.987685
H	-6.263301	-5.567879	-2.306395	C	-1.983339	5.010131	-1.269968
H	-0.135582	-4.973438	-1.365385	C	0.436987	6.168043	-2.068086
II-S E= -3768.23926980				H	2.594913	4.647312	-1.583646
H	0.347278	-2.454842	-2.043486	C	-0.746549	6.833712	-2.288606
C	-0.498484	-0.431535	3.712986	C	-1.968032	6.237702	-1.895880
C	0.412393	-1.482014	3.865840	H	1.382994	6.601156	-2.384617
C	0.992695	-1.777279	5.109806	H	-0.748148	7.805182	-2.775346
C	0.627564	-1.003877	6.211112	H	-2.905527	6.749804	-2.095579
C	-0.288294	0.042959	6.077303	C	-1.977130	2.413803	0.226112
C	-0.845742	0.328322	4.829385	C	-2.779232	3.104275	1.200816
H	-0.908065	-0.222041	2.731101	C	-2.389618	1.154289	-0.191221
H	1.066553	-1.223421	7.181342	C	-2.357875	4.301527	1.844214
H	-0.562655	0.634036	6.946267	C	-4.045518	2.548491	1.575078
H	-1.552166	1.145162	4.716808	C	-3.664137	0.600061	0.137395
C	2.006307	-2.894303	5.175622	C	-3.154448	4.925851	2.779686
H	3.011415	-2.506633	4.953699	H	-1.387954	4.718368	1.598160
H	2.049145	-3.326295	6.180597	C	-4.851941	3.227823	2.528423
C	1.642121	-3.985081	4.160747	C	-4.469493	1.327506	0.989925
H	2.404659	-4.765973	4.113630	C	-4.420831	4.393551	3.119512
H	0.696721	-4.464890	4.454833	H	-2.805335	5.834769	3.262511
C	1.414888	-3.387119	2.786660	H	-5.816288	2.798588	2.790555
N	0.789563	-2.237480	2.711213	H	-5.456499	0.946593	1.239173
H	0.432343	-1.827760	1.789058	H	-5.043788	4.900528	3.851460
C	0.439604	-3.952351	-0.806121	C	-4.140958	-0.693143	-0.456413
C	1.784514	-3.517208	-0.173549	C	-4.459307	-0.759145	-1.836602
H	0.404039	-5.045348	-0.883202	C	-4.329057	-1.833696	0.359533
C	0.468857	2.340502	-0.295072	C	-4.950829	-1.956959	-2.362837
C	-0.740371	3.022398	-0.347303	C	-4.831428	-3.005526	-0.221337
C	-0.776612	4.304500	-1.001874	C	-5.144824	-3.095950	-1.576782
				H	-5.192840	-1.998985	-3.421815

H	-4.977160	-3.883346	0.404647	H	-3.501681	-0.911456	2.100592
C	3.006136	2.174272	-0.610899	C	-5.285131	-1.929563	2.709618
C	3.655863	2.096705	0.644409	H	-5.962605	-1.094499	2.499083
C	3.619673	1.617197	-1.757247	H	-5.038005	-1.905003	3.778395
C	4.902726	1.469616	0.728297	H	-5.836221	-2.857477	2.514686
C	4.872146	1.003060	-1.615837	C	-3.033042	-2.986600	2.222814
C	5.533517	0.915592	-0.389621	H	-2.120104	-2.909522	1.626090
H	5.400778	1.424815	1.693925	H	-3.475993	-3.975453	2.055599
H	5.353837	0.588605	-2.498736	H	-2.763357	-2.921213	3.284827
O	-1.573323	0.429066	-1.039388	C	2.991036	1.694706	-3.149330
O	0.509544	1.088714	0.292122	H	1.964643	2.054313	-3.034842
P	-0.177936	-0.223022	-0.450978	C	2.903789	0.324187	-3.846515
O	-0.480611	-1.172712	0.695743	H	2.410654	0.435661	-4.820005
C	-4.326797	0.441032	-2.774655	H	2.316762	-0.375708	-3.247391
H	-3.907105	1.276838	-2.208911	H	3.894826	-0.107978	-4.032760
C	-5.706002	0.901905	-3.288039	C	3.743556	2.710626	-4.033462
H	-6.377121	1.149075	-2.457427	H	4.782370	2.398841	-4.198709
H	-6.191935	0.124303	-3.889307	H	3.765489	3.706920	-3.577479
H	-5.601054	1.793446	-3.918471	H	3.260168	2.797133	-5.014126
C	-3.362981	0.159920	-3.943257	C	6.907699	0.265048	-0.288585
H	-2.374592	-0.127352	-3.573535	H	7.144871	-0.142116	-1.281543
H	-3.249937	1.057318	-4.563869	C	7.998071	1.298736	0.055277
H	-3.734149	-0.644158	-4.590267	H	8.989373	0.829124	0.067032
C	-5.670815	-4.395634	-2.171760	H	7.826078	1.741273	1.043852
H	-5.740491	-5.121505	-1.349482	H	8.014470	2.114394	-0.675888
C	-7.085017	-4.230190	-2.760301	C	6.929417	-0.909842	0.707100
H	-7.463258	-5.189132	-3.135227	H	7.916827	-1.387408	0.718510
H	-7.087023	-3.522011	-3.597511	H	6.186909	-1.669759	0.440531
H	-7.787046	-3.856719	-2.006421	H	6.714332	-0.571247	1.727846
C	-4.700788	-4.975708	-3.219067	C	3.060715	2.718076	1.907733
H	-3.700247	-5.117825	-2.796879	H	2.063444	3.094815	1.664215
H	-4.603105	-4.307062	-4.082409	C	2.886451	1.685447	3.036165
H	-5.061407	-5.944483	-3.586408	H	3.849983	1.280397	3.369096
C	-4.005339	-1.850060	1.853875	H	2.260865	0.851912	2.702827

H	2.402494	2.145585	3.906173	C	-5.145786	3.138723	1.125466
C	3.895021	3.924678	2.381706	H	-6.849929	0.190193	1.056207
H	3.973318	4.683999	1.595646	H	-7.215840	2.600115	1.501414
H	4.913137	3.624073	2.657064	H	-5.298897	4.190544	1.351049
H	3.434391	4.391998	3.261025	C	-1.223818	1.730797	-0.215044
O	0.616420	-0.709616	-1.622580	C	-1.333067	2.779982	-1.195108
S	2.041324	-4.347983	1.498988	C	-0.018137	1.596970	0.457007
O	0.323996	-3.438996	-2.101364	C	-2.437326	2.898193	-2.083962
H	-0.377267	-3.629010	-0.145548	C	-0.267490	3.729940	-1.314066
H	1.764460	-2.441441	0.005699	C	1.043018	2.543840	0.383257
C	3.005070	-3.874961	-0.993898	C	-2.497018	3.914304	-3.012575
C	3.276779	-5.202202	-1.355821	H	-3.235483	2.166814	-2.036223
C	3.877930	-2.863104	-1.412904	C	-0.369369	4.778072	-2.268849
C	4.404071	-5.512981	-2.115508	C	0.875457	3.604216	-0.483718
H	2.601401	-5.998901	-1.052952	C	-1.460944	4.873804	-3.100662
C	5.000264	-3.174177	-2.182463	H	-3.346504	3.976014	-3.687265
H	3.666351	-1.827945	-1.159570	H	0.443677	5.496801	-2.337302
C	5.269755	-4.498751	-2.530743	H	1.653573	4.359889	-0.549430
H	4.601687	-6.545809	-2.389401	H	-1.524436	5.674544	-3.832232
H	5.660173	-2.376801	-2.512734	C	2.269566	2.433310	1.241298
H	6.144833	-4.739662	-3.128330	C	2.184448	2.714981	2.627559
				C	3.518655	2.105469	0.664977
				C	3.347818	2.666539	3.400664
				C	4.652570	2.079281	1.487359
				C	4.595271	2.352414	2.853740
				H	3.276592	2.888293	4.462593
				H	5.615779	1.831995	1.047097
				C	-3.062839	-2.973001	-0.007033
				C	-2.800253	-3.525458	-1.285223
				C	-3.173513	-3.823992	1.119421
				C	-2.649927	-4.909858	-1.407067
				C	-3.018824	-5.204208	0.935643
				C	-2.754099	-5.770814	-0.310796
				H	-2.452423	-5.327781	-2.391314
IE= -3383.38015461							
C	-2.205764	-0.561099	0.005197				
C	-2.364953	0.814071	0.078385				
C	-3.654128	1.324640	0.468359				
C	-4.746245	0.408187	0.607011				
C	-4.525361	-0.977573	0.403843				
C	-3.273087	-1.494669	0.142368				
H	-3.072675	3.401863	0.701348				
C	-3.893381	2.696809	0.758377				
C	-6.030525	0.899409	0.967497				
H	-5.369757	-1.656382	0.485075				
C	-6.231773	2.236841	1.218555				

H	-3.102338	-5.861956	1.797313	H	4.414233	0.192568	-2.114251
O	0.153721	0.519088	1.331415	C	-3.474211	-3.306330	2.527701
O	-0.949506	-1.078303	-0.312553	H	-3.378644	-2.216935	2.515979
P	0.296908	-0.971648	0.718425	C	-2.481315	-3.830825	3.582287
O	1.550106	-1.312385	-0.008386	H	-2.686334	-3.363070	4.552715
C	0.874046	3.107889	3.310410	H	-1.450640	-3.597429	3.303925
H	0.074175	3.076973	2.565152	H	-2.560244	-4.915531	3.718874
C	0.930957	4.555072	3.839583	C	-4.921165	-3.642265	2.944796
H	1.160538	5.262979	3.035026	H	-5.078025	-4.727073	2.982958
H	1.699141	4.670160	4.613338	H	-5.653593	-3.227860	2.243123
H	-0.031901	4.840718	4.280482	H	-5.138229	-3.236490	3.940387
C	0.486767	2.120872	4.428530	C	-2.577629	-7.276358	-0.460009
H	0.407729	1.100866	4.040456	H	-2.740912	-7.720156	0.531548
H	-0.481756	2.398553	4.862060	C	-3.616401	-7.891034	-1.416890
H	1.224318	2.120537	5.239918	H	-3.507230	-8.981573	-1.457905
C	5.854264	2.312676	3.709885	H	-3.496632	-7.506907	-2.436911
H	6.681517	2.012178	3.052216	H	-4.637365	-7.662081	-1.092152
C	6.200981	3.701670	4.280372	C	-1.143793	-7.636928	-0.894996
H	7.140933	3.665277	4.844439	H	-1.013966	-8.725064	-0.943402
H	5.418173	4.058557	4.960426	H	-0.409224	-7.233557	-0.188828
H	6.310630	4.442329	3.480487	H	-0.917072	-7.227325	-1.886715
C	5.753898	1.263968	4.833869	C	-2.720920	-2.670917	-2.550558
H	5.538714	0.269021	4.429451	H	-2.816803	-1.620484	-2.262294
H	4.955889	1.515365	5.542545	C	-1.368037	-2.820065	-3.272071
H	6.693549	1.209565	5.397001	H	-1.213456	-3.843049	-3.635308
C	3.686483	1.781768	-0.819600	H	-0.537556	-2.565892	-2.606622
H	2.689686	1.699494	-1.262756	H	-1.325720	-2.152239	-4.141199
C	4.433122	2.910524	-1.558480	C	-3.894232	-2.979307	-3.502737
H	3.916834	3.871591	-1.454888	H	-4.858976	-2.825528	-3.006146
H	4.515150	2.683491	-2.628552	H	-3.862539	-4.017348	-3.854408
H	5.448558	3.037029	-1.163818	H	-3.856258	-2.326783	-4.383627
C	4.386763	0.427969	-1.042834	O	-0.019496	-1.826391	2.006611
H	3.849627	-0.372036	-0.526665	H	0.573665	-2.641239	2.086338
H	5.423128	0.438023	-0.685165	C	3.355523	-3.271292	-2.313114

C	3.150397	-4.297671	-1.384804	H	4.493032	-1.460382	5.004260
C	3.519166	-5.622273	-1.670669	C	3.613648	-2.611120	3.394367
C	4.123794	-5.892693	-2.898436	H	4.516562	-3.047498	2.961067
C	4.345792	-4.875826	-3.830558	H	3.200887	-3.348874	4.098577
C	3.954702	-3.567731	-3.536378	C	2.596363	-2.445560	2.296036
H	3.044457	-2.259850	-2.070477	N	1.640584	-1.559548	2.412196
H	4.418582	-6.914287	-3.127601	H	0.875912	-1.400767	1.663603
H	4.818632	-5.105281	-4.781128	C	2.594820	-3.125209	-1.142605
H	4.118194	-2.772443	-4.257989	C	1.841699	-3.449796	0.147434
C	3.195374	-6.679811	-0.642323	H	2.745711	-2.044666	-1.200837
H	2.177475	-7.061465	-0.813236	H	0.953832	-2.827520	0.258190
H	3.871178	-7.536635	-0.738130	O	2.757070	-3.271373	1.302163
C	3.284419	-6.097188	0.775658	S	1.465545	-3.571358	-2.549524
H	2.941731	-6.807853	1.529194	H	1.570109	-4.504814	0.198841
H	4.332594	-5.855602	1.008903	C	3.925029	-3.836531	-1.275930
C	2.498876	-4.806980	0.915927	C	4.026486	-5.232746	-1.194974
S	1.706114	-4.429105	2.352296	C	5.090340	-3.089539	-1.488802
N	2.529093	-3.996097	-0.149723	C	5.264103	-5.864010	-1.319095
H	2.122378	-3.053835	-0.062488	H	3.132631	-5.833832	-1.046526
IV-R E= -3768.24411627				C	6.330297	-3.719155	-1.613069
H	0.704016	-2.453582	-2.407692	H	5.021453	-2.007054	-1.568899
C	0.292174	-0.083258	3.791585	C	6.421098	-5.109076	-1.526428
C	1.506645	-0.739263	3.577742	H	5.324275	-6.947497	-1.258457
C	2.585498	-0.601447	4.463380	H	7.223278	-3.122767	-1.780653
C	2.413045	0.193557	5.596834	H	7.384620	-5.601935	-1.624641
C	1.200158	0.844729	5.834774	C	-0.194702	2.404677	-0.578187
C	0.146084	0.710347	4.929214	C	-1.512595	2.841723	-0.621810
H	-0.507462	-0.190206	3.066602	C	-1.826198	3.994496	-1.425571
H	3.238846	0.306631	6.295024	C	-0.755315	4.731053	-2.027718
H	1.082484	1.459267	6.722511	C	0.579811	4.286096	-1.852026
H	-0.794661	1.223715	5.103334	C	0.884874	3.125839	-1.171900
C	3.886662	-1.282936	4.110728	H	-3.985961	3.857003	-1.278057
H	4.478436	-0.631176	3.451156	C	-3.157815	4.423373	-1.687184
				C	-1.048126	5.882148	-2.808061

H	1.384356	4.869805	-2.291737	C	5.015195	1.886976	-0.772570
C	-2.347149	6.281838	-3.021496	H	4.888481	2.750622	1.190841
C	-3.410195	5.533289	-2.463888	H	4.817637	1.166475	-2.778115
H	-0.220306	6.433566	-3.247880	O	-1.885907	0.071702	-0.930598
H	-2.559571	7.158859	-3.626813	O	0.108313	1.263124	0.143206
H	-4.437399	5.832485	-2.654607	P	-0.339666	-0.221947	-0.441995
C	-2.575778	2.102530	0.121860	O	-0.346955	-1.109369	0.799078
C	-3.434529	2.762635	1.069046	C	-4.747249	-0.703181	-2.341763
C	-2.759279	0.742563	-0.095673	H	-4.480704	0.274010	-1.930559
C	-3.220524	4.097964	1.511899	C	-6.228524	-0.619374	-2.761970
C	-4.538829	2.039252	1.625414	H	-6.873998	-0.406464	-1.902090
C	-3.869492	0.010967	0.424340	H	-6.573106	-1.557662	-3.212880
C	-4.065996	4.690563	2.424716	H	-6.372369	0.177710	-3.501642
H	-2.369434	4.649946	1.129979	C	-3.834561	-0.944639	-3.559170
C	-5.402924	2.685316	2.550769	H	-2.782715	-0.957695	-3.259717
C	-4.745563	0.687528	1.248218	H	-3.970133	-0.146970	-4.299947
C	-5.177402	3.984803	2.943233	H	-4.063861	-1.896765	-4.052980
H	-3.874818	5.709214	2.751777	C	-4.996712	-5.565897	-0.968761
H	-6.243140	2.123873	2.952912	H	-4.809179	-6.162399	-0.064940
H	-5.615668	0.165664	1.638287	C	-6.475867	-5.764523	-1.351136
H	-5.841613	4.466186	3.655922	H	-6.687835	-6.823406	-1.543801
C	-4.114143	-1.424242	0.058729	H	-6.730721	-5.203870	-2.258359
C	-4.538806	-1.755536	-1.252496	H	-7.141079	-5.422535	-0.550486
C	-3.979386	-2.444936	1.029040	C	-4.064260	-6.098445	-2.073542
C	-4.813889	-3.091207	-1.560120	H	-3.011775	-5.987245	-1.791033
C	-4.276644	-3.765320	0.666978	H	-4.213551	-5.557467	-3.015435
C	-4.690735	-4.115770	-0.617497	H	-4.258446	-7.160875	-2.265499
H	-5.141489	-3.335903	-2.567719	C	-3.522205	-2.173048	2.462735
H	-4.177637	-4.551357	1.412626	H	-3.211713	-1.126155	2.523511
C	2.309353	2.669850	-1.034073	C	-4.672049	-2.375987	3.469503
C	3.012220	2.931717	0.167090	H	-5.527299	-1.730487	3.240325
C	2.965286	2.031310	-2.112011	H	-4.338647	-2.147526	4.489645
C	4.348724	2.535164	0.272032	H	-5.029287	-3.412809	3.458830
C	4.305673	1.652528	-1.950932	C	-2.300671	-3.027027	2.852685

H	-1.488081	-2.869903	2.138739			
H	-2.541290	-4.096478	2.880195	IV-S E= -3768.24526049		
H	-1.946582	-2.744880	3.852778	H	-1.497409	-0.966058 -2.758950
C	2.284553	1.797543	-3.461164	C	0.065026	-1.643344 3.393359
H	1.206569	1.912016	-3.315987	C	0.012391	-2.914352 2.815553
C	2.506385	0.383022	-4.024161	C	0.368448	-4.064542 3.536447
H	1.945858	0.266873	-4.959558	C	0.760434	-3.917565 4.867288
H	2.146068	-0.370847	-3.321897	C	0.806584	-2.655846 5.464321
H	3.560838	0.187331	-4.254400	C	0.463804	-1.522907 4.724911
C	2.739926	2.859067	-4.485068	H	-0.195618	-0.776203 2.796316
H	3.818061	2.783787	-4.674408	H	1.034662	-4.801184 5.438518
H	2.535418	3.876997	-4.135942	H	1.113123	-2.559887 6.501826
H	2.220256	2.717820	-5.440563	H	0.506358	-0.538101 5.180161
C	6.474984	1.468250	-0.645788	C	0.347189	-5.394666 2.821191
H	6.746006	0.955289	-1.579039	H	1.309961	-5.561205 2.315500
C	7.409033	2.685387	-0.502900	H	0.216543	-6.219248 3.528658
H	8.459067	2.369407	-0.470717	C	-0.780996	-5.415331 1.783358
H	7.199107	3.241444	0.418689	H	-0.735217	-6.288672 1.129445
H	7.286015	3.376865	-1.343457	H	-1.760282	-5.430228 2.283943
C	6.694728	0.469314	0.506522	C	-0.749281	-4.177509 0.926774
H	7.743254	0.149979	0.550193	N	-0.395345	-3.028385 1.445020
H	6.072682	-0.424473	0.379846	H	-0.466893	-2.085423 0.922626
H	6.444740	0.919745	1.475154	C	-2.534416	-2.629566 -1.383091
C	2.372224	3.706513	1.319206	C	-1.190879	-3.365552 -1.377136
H	1.290194	3.716416	1.160164	C	2.414540	1.401272 -0.340232
C	2.613502	3.060778	2.693949	C	2.081088	2.740640 -0.189228
H	3.672148	3.081235	2.979884	C	2.914554	3.727774 -0.824708
H	2.275892	2.020148	2.703209	C	4.127749	3.305386 -1.458891
H	2.058042	3.602535	3.468589	C	4.461012	1.926805 -1.476545
C	2.845969	5.174436	1.311072	C	3.621425	0.961395 -0.962082
H	2.610158	5.661255	0.358438	H	1.642203	5.444304 -0.453221
H	3.930975	5.238612	1.459638	C	2.575277	5.108294 -0.889717
H	2.360331	5.743971	2.113338	C	4.968860	4.270924 -2.075439
O	0.439304	-0.629638	-1.649014	H	5.400980	1.624849 -1.931079

C	4.620318	5.601637	-2.100475	H	5.238488	-2.958537	0.977973
C	3.403282	6.017684	-1.511218	H	4.192098	-3.127263	-3.162703
H	5.890566	3.931366	-2.542262	O	-0.457782	1.654282	-0.747134
H	5.267309	6.329914	-2.581852	O	1.579675	0.439721	0.205406
H	3.114733	7.064569	-1.553936	P	0.128910	0.130740	-0.528216
C	0.867270	3.129489	0.588744	O	-0.677427	-0.601887	0.537777
C	0.941702	4.051562	1.691060	C	-2.617625	3.850376	-1.865590
C	-0.373721	2.600456	0.256524	H	-1.649552	4.062219	-1.404140
C	2.172880	4.509263	2.238414	C	-3.329720	5.206373	-2.046604
C	-0.273649	4.511115	2.294513	H	-3.486055	5.704236	-1.082715
C	-1.598017	3.062128	0.828343	H	-4.310529	5.085285	-2.521748
C	2.198619	5.393968	3.294602	H	-2.731463	5.872147	-2.680763
H	3.103798	4.143760	1.820633	C	-2.332320	3.185104	-3.225133
C	-0.213091	5.438286	3.370105	H	-1.795622	2.241471	-3.091425
C	-1.516229	4.026761	1.811316	H	-1.715711	3.845085	-3.847606
C	0.995293	5.876499	3.861312	H	-3.256910	2.978962	-3.777588
H	3.153113	5.721288	3.698257	C	-6.838767	1.198193	-1.006682
H	-1.146464	5.786590	3.806476	H	-7.263195	0.592598	-0.193365
H	-2.432192	4.419961	2.244778	C	-7.812223	2.363715	-1.265427
H	1.028898	6.580846	4.688100	H	-8.802087	1.985434	-1.548908
C	-2.928935	2.558867	0.351106	H	-7.456972	3.006509	-2.079719
C	-3.407077	2.935945	-0.928669	H	-7.927701	2.989509	-0.373335
C	-3.732224	1.748768	1.187541	C	-6.718889	0.289335	-2.245181
C	-4.665556	2.489625	-1.341365	H	-6.045547	-0.553275	-2.056105
C	-4.989460	1.337765	0.725188	H	-6.320705	0.840764	-3.105032
C	-5.476026	1.686817	-0.534094	H	-7.700887	-0.109049	-2.529204
H	-5.024200	2.779819	-2.325745	C	-3.289874	1.302174	2.581359
H	-5.612641	0.719694	1.368154	H	-2.237847	1.574935	2.704331
C	3.991545	-0.492691	-1.015300	C	-4.089463	2.023483	3.685015
C	4.491511	-1.127984	0.146964	H	-3.981730	3.111469	3.614505
C	3.883428	-1.218139	-2.224996	H	-3.744763	1.712937	4.679423
C	4.852804	-2.477181	0.082096	H	-5.159225	1.792363	3.613658
C	4.268033	-2.565667	-2.234605	C	-3.380338	-0.225363	2.759940
C	4.746686	-3.218349	-1.098185	H	-2.802852	-0.731957	1.981384

H	-4.417038	-0.580557	2.717197	H	-0.356797	-2.666265	-1.292816
H	-2.974998	-0.518918	3.736350	H	-1.070116	-3.972005	-2.273581
C	3.408012	-0.576284	-3.528924	C	-3.737120	-3.540699	-1.249109
H	2.941791	0.381150	-3.280472	C	-4.658954	-3.320289	-0.217593
C	2.339709	-1.408413	-4.261496	C	-3.956507	-4.608538	-2.132011
H	1.998843	-0.866861	-5.152299	C	-5.771245	-4.151231	-0.064205
H	1.475892	-1.572208	-3.614156	H	-4.508258	-2.484709	0.462087
H	2.728621	-2.376597	-4.600602	C	-5.065668	-5.439649	-1.979354
C	4.603965	-0.291397	-4.461544	H	-3.264266	-4.783336	-2.951479
H	5.108988	-1.222001	-4.749230	C	-5.976126	-5.215218	-0.943299
H	5.348516	0.354267	-3.982678	H	-6.478073	-3.962838	0.739660
H	4.265552	0.204802	-5.379403	H	-5.222486	-6.261085	-2.673510
C	5.142368	-4.688806	-1.153885	H	-6.841591	-5.862101	-0.827129
H	4.980698	-5.027668	-2.186345	O	-1.114011	-4.382135	-0.306307
C	6.632797	-4.899984	-0.826926	S	-2.626052	-1.692455	-2.985610
H	6.907883	-5.957187	-0.927598				
H	6.862331	-4.591954	0.200087				
H	7.269984	-4.315748	-1.499637	(R)-1 E= -384.838385433			
C	4.251284	-5.554596	-0.241987	C	0.636528	0.539994	-0.074112
H	4.512421	-6.616093	-0.334122	C	0.980021	1.929960	0.293241
H	3.193068	-5.438673	-0.503854	H	1.100265	2.180239	1.347512
H	4.370385	-5.271100	0.811086	H	1.533457	2.557075	-0.407055
C	4.697286	-0.375642	1.461870	O	-0.346692	1.583123	-0.107665
H	4.319557	0.642551	1.333987	H	0.951865	0.196378	-1.061554
C	3.908774	-1.003605	2.624868	C	0.470422	-0.534481	0.948314
H	4.247536	-2.023814	2.843345	C	1.206427	-1.720848	0.839349
H	2.840259	-1.040983	2.394058	C	-0.405563	-0.369632	2.028820
H	4.039460	-0.410865	3.538722	C	1.083918	-2.720582	1.805226
C	6.195822	-0.257072	1.805084	H	1.878211	-1.862047	-0.004852
H	6.748481	0.235835	0.997392	C	-0.530199	-1.370744	2.991729
H	6.649740	-1.242274	1.966521	H	-0.997948	0.538282	2.090910
H	6.335851	0.329998	2.721180	C	0.216007	-2.547309	2.885325
O	0.274628	-0.483744	-1.884680	H	1.661466	-3.636360	1.710568
H	-2.539078	-1.891760	-0.578084	H	-1.216405	-1.235451	3.823717
				H	0.116241	-3.327257	3.635408

(R)-2 E= -707.829278605

C	2.167104	-0.061089	1.097392
C	1.214996	-0.725380	0.167760
H	1.800679	0.788911	1.669105
H	2.886901	-0.682235	1.626307
H	1.367910	-1.794028	0.031137
C	-0.214615	-0.309623	0.061621
C	-0.616417	1.033269	0.126714
C	-1.195827	-1.299900	-0.080671
C	-1.966548	1.370716	0.068020
H	0.135144	1.814927	0.196010
C	-2.549269	-0.962000	-0.141405
H	-0.897076	-2.344097	-0.140486
C	-2.939221	0.374828	-0.064328
H	-2.261679	2.415507	0.118057
H	-3.295461	-1.744385	-0.251292
H	-3.991310	0.642031	-0.113549
S	2.553354	0.273653	-0.659119

(R)-3-TS1-R E= -3522.67900972

H	0.175879	-1.815606	-2.227237
C	-0.458696	1.078136	3.361154
C	-0.613638	-0.237787	3.811646
C	-0.517135	-0.553144	5.177170
C	-0.284231	0.480490	6.084694
C	-0.135521	1.799632	5.649015
C	-0.217909	2.093558	4.285896
H	-0.522974	1.288399	2.298885
H	-0.213687	0.245929	7.144603
H	0.046672	2.591583	6.369978
H	-0.097017	3.114766	3.935821
C	-0.638113	-2.005880	5.569169
H	0.346169	-2.493374	5.499160

H	-0.962186	-2.104062	6.611171
C	-1.624427	-2.726325	4.639120
H	-1.652101	-3.800790	4.826963
H	-2.641021	-2.341429	4.812369
C	-1.311525	-2.491095	3.171663
N	-0.848087	-1.270113	2.870160
H	-0.697423	-1.021574	1.880376
C	-0.037685	-3.496749	-1.074415
C	-1.404114	-3.003385	-0.936394
H	0.709039	-3.037826	-0.428561
H	-1.483639	-1.996928	-0.536882
C	2.616067	1.676976	-0.743505
C	2.236357	2.998593	-0.928706
C	3.071559	3.848128	-1.732195
C	4.315613	3.330562	-2.220519
C	4.679344	1.993672	-1.924509
C	3.853447	1.144043	-1.213299
H	1.747751	5.564561	-1.781409
C	2.703734	5.170208	-2.106369
C	5.156946	4.164044	-3.007133
H	5.641174	1.627950	-2.274499
C	4.779802	5.446423	-3.332760
C	3.533825	5.946453	-2.885708
H	6.103308	3.759946	-3.358973
H	5.428107	6.071082	-3.941123
H	3.225710	6.950744	-3.163880
C	0.955144	3.478589	-0.329156
C	0.911976	4.575006	0.599396
C	-0.224940	2.809710	-0.623586
C	2.077951	5.236530	1.076169
C	-0.358786	4.999236	1.109750
C	-1.500105	3.214276	-0.123649
C	1.989124	6.277390	1.974802
H	3.050692	4.905655	0.731875

C	-0.416934	6.087954	2.023219	H	-1.708656	-5.622663	-1.729401
C	-1.533777	4.313746	0.713698	C	-5.009890	-3.571891	-1.749490
C	0.730127	6.718681	2.447122	H	-3.812462	-1.915767	-1.071241
H	2.895875	6.761332	2.327514	C	-5.008628	-4.917385	-2.127103
H	-1.390635	6.405780	2.388827	H	-3.822032	-6.698463	-2.411140
H	-2.491155	4.665455	1.089225	H	-5.932828	-3.000014	-1.751834
H	0.673806	7.545930	3.149332	H	-5.936788	-5.396457	-2.427041
C	-2.750801	2.484238	-0.457571	H	0.133723	-4.559878	-1.231082
C	-3.058507	2.081624	-1.768094	H	-3.467565	2.487965	1.575926
C	-3.689562	2.207729	0.550060	H	-2.350966	2.270612	-2.567439
C	-4.257149	1.434638	-2.053773	H	3.705696	-0.293470	1.125026
C	-4.887484	1.560034	0.262829	H	4.896259	-0.606033	-2.990664
C	-5.199430	1.158685	-1.046808	C	-6.475528	0.464647	-1.355678
H	-4.455838	1.118389	-3.074081	C	-7.157727	0.705582	-2.561503
H	-5.598791	1.379422	1.063903	C	-7.039079	-0.453231	-0.450659
C	4.255167	-0.264126	-0.961810	C	-8.354546	0.052430	-2.853326
C	4.130449	-0.861011	0.304416	H	-6.757641	1.430722	-3.264423
C	4.823099	-1.029628	-1.993045	C	-8.237829	-1.105738	-0.741030
C	4.563778	-2.164591	0.526352	H	-6.521996	-0.672716	0.479367
C	5.252971	-2.334749	-1.769937	C	-8.900942	-0.856977	-1.945025
C	5.134640	-2.932164	-0.504114	H	-8.866312	0.261852	-3.789039
H	4.487611	-2.584276	1.525685	H	-8.651170	-1.812817	-0.026304
H	5.653324	-2.911142	-2.599328	H	-9.835108	-1.363779	-2.171378
O	-0.168857	1.699596	-1.449587	C	5.592166	-4.323896	-0.263786
O	1.762035	0.831579	-0.051617	C	6.743993	-4.825893	-0.894728
P	0.406268	0.290006	-0.815531	C	4.887329	-5.179327	0.601333
O	-0.494666	-0.265015	0.251089	C	7.174040	-6.133190	-0.670830
O	0.762634	-0.563570	-2.015519	H	7.320695	-4.175298	-1.546221
S	-1.604319	-3.687575	2.024891	C	5.317686	-6.486247	0.827376
O	-0.242930	-2.801166	-2.323684	H	3.980501	-4.822751	1.081994
C	-2.614470	-3.690433	-1.353587	C	6.463055	-6.970174	0.191757
C	-2.627473	-5.045240	-1.735148	H	8.072178	-6.495445	-1.164452
C	-3.819372	-2.961766	-1.365384	H	4.751710	-7.130379	1.495493
C	-3.818164	-5.652269	-2.119333	H	6.798471	-7.988752	0.367430

(R)-3-TS1-S E= -3522.67630518

H	0.484100	-1.722275	-2.150723	H	5.590097	2.606610	-1.726801
C	-1.403783	1.183152	3.178270	C	4.172070	6.215842	-2.910281
C	-2.132185	0.005902	3.385294	C	2.819400	6.483590	-2.592912
C	-2.806287	-0.226402	4.595901	H	5.769483	4.791041	-2.787429
C	-2.759683	0.757491	5.583762	H	4.755794	6.949431	-3.459596
C	-2.049526	1.944035	5.383861	H	2.366755	7.418848	-2.911287
C	-1.368206	2.150270	4.182180	C	0.475850	3.584503	-0.283879
H	-0.872375	1.324150	2.243263	C	0.129981	4.661942	0.603252
H	-3.283707	0.587922	6.521853	C	-0.527409	2.718395	-0.694834
H	-2.026613	2.700278	6.163374	C	1.098284	5.514757	1.202836
H	-0.811183	3.067897	4.017256	C	-1.248397	4.863284	0.943674
C	-3.509751	-1.551459	4.764525	C	-1.906512	2.908891	-0.377975
H	-2.802515	-2.300943	5.150965	C	0.723260	6.525840	2.060861
H	-4.317004	-1.474494	5.501264	H	2.148103	5.354688	0.986217
C	-4.068747	-2.033168	3.418690	C	-1.602727	5.926737	1.818646
H	-4.482914	-3.040165	3.487392	C	-2.232872	3.988399	0.419687
H	-4.885165	-1.366486	3.100720	C	-0.641176	6.744765	2.366080
C	-3.025575	-2.001036	2.315435	H	1.483707	7.158657	2.510503
N	-2.164662	-0.976427	2.364682	H	-2.653793	6.072673	2.056646
H	-1.514780	-0.830504	1.577817	H	-3.275895	4.172878	0.663714
C	-1.380844	-2.574694	-1.900545	H	-0.924152	7.550211	3.038278
C	-0.718470	-3.245996	-0.786136	C	-2.953256	1.973075	-0.865351
H	-2.051303	-3.146362	-2.539501	C	-3.014587	1.564348	-2.208517
C	2.470301	2.108501	-0.493691	C	-3.932643	1.486372	0.015093
C	1.879518	3.341149	-0.734114	C	-4.013543	0.699987	-2.647293
C	2.625477	4.329828	-1.464520	C	-4.925622	0.614098	-0.424295
C	3.983530	4.045231	-1.823236	C	-4.985410	0.198174	-1.764015
C	4.549303	2.793917	-1.475650	H	-4.027460	0.388466	-3.688414
C	3.823545	1.809290	-0.833369	H	-5.675124	0.259202	0.277800
H	1.029979	5.784209	-1.664161	C	4.448081	0.498214	-0.517645
C	2.067579	5.567469	-1.889732	C	4.342263	-0.089356	0.754144
C	4.736631	5.018920	-2.534465	C	5.214118	-0.168509	-1.486798
				C	4.984367	-1.289720	1.041815
				C	5.850934	-1.372573	-1.198906

C	5.751191	-1.959630	0.072890	C	-8.013879	-2.544603	-3.116904
H	4.870067	-1.728478	2.029376	H	-8.130019	-1.292272	-4.870096
H	6.448742	-1.855550	-1.966942	H	-7.659190	-3.588704	-1.262469
O	-0.182508	1.619429	-1.461047	H	-8.778566	-3.237284	-3.458296
O	1.726332	1.122403	0.135189	C	6.426934	-3.245039	0.381485
P	0.543277	0.342991	-0.703044	C	7.021160	-3.467600	1.636106
O	-0.348502	-0.300862	0.317867	C	6.491435	-4.275491	-0.572809
O	1.111084	-0.499219	-1.826444	C	7.656702	-4.674557	1.925708
S	-3.020611	-3.169185	1.102879	H	7.006407	-2.676036	2.380250
O	-0.018618	-2.641358	-2.376491	C	7.127807	-5.482282	-0.284342
H	-1.743464	-1.567814	-1.701077	H	6.015625	-4.136114	-1.539509
H	-0.272201	-2.572532	-0.063311	C	7.713687	-5.687984	0.966544
C	-0.501208	-4.675869	-0.645001	H	8.116720	-4.819685	2.899888
C	-1.138097	-5.625339	-1.465671	H	7.158559	-6.266690	-1.036299
C	0.381925	-5.119597	0.357357	H	8.210184	-6.628158	1.191445
C	-0.895077	-6.982801	-1.284756				
H	-1.822074	-5.302121	-2.243617				
C	0.622752	-6.477980	0.536552	(R)-4-TS1-R E= -3375.07678543			
H	0.873228	-4.388267	0.992975	H	0.392552	1.994801	-2.272756
C	-0.015525	-7.411057	-0.285059	C	0.076861	-0.961786	3.300045
H	-1.391202	-7.709756	-1.921080	C	0.005258	0.365417	3.737617
H	1.306481	-6.809673	1.312266	C	-0.476456	0.681782	5.018723
H	0.170891	-8.472533	-0.146767	C	-0.868005	-0.360362	5.859429
H	-3.898860	1.778391	1.061074	C	-0.798019	-1.689778	5.435962
H	-2.269766	1.921089	-2.911515	C	-0.329704	-1.986342	4.153974
H	3.749628	0.396777	1.521390	H	0.444538	-1.174291	2.301780
H	5.296821	0.256168	-2.483255	H	-1.236687	-0.124458	6.855394
C	-6.031366	-0.746793	-2.230033	H	-1.109719	-2.488561	6.103026
C	-6.665251	-0.567098	-3.471688	H	-0.278589	-3.016355	3.813492
C	-6.408544	-1.849029	-1.442793	C	-0.570048	2.141446	5.391673
C	-7.646294	-1.455717	-3.910456	H	-1.534928	2.551406	5.056436
H	-6.403032	0.290981	-4.084800	H	-0.537276	2.269353	6.479338
C	-7.389797	-2.737473	-1.882462	C	0.570251	2.929783	4.732869
H	-5.903084	-2.028832	-0.497631	H	0.472057	4.004048	4.896203
				H	1.531042	2.621290	5.172560

C	0.666546	2.664599	3.240449	H	0.911793	-6.270902	2.540111
N	0.401465	1.407096	2.861266	H	2.232230	-4.768770	1.145559
H	0.531609	1.138503	1.871912	H	-1.283448	-7.079785	3.355995
C	0.368614	3.729222	-1.202695	C	2.774940	-2.725078	-0.514162
C	1.636748	3.194945	-0.717459	C	3.098197	-2.466265	-1.857119
H	-0.538754	3.330055	-0.751325	C	3.780546	-2.534903	0.442168
H	1.585490	2.197544	-0.290484	C	4.375166	-2.047806	-2.214931
C	-2.455660	-1.193112	-0.820624	C	5.058570	-2.107428	0.076367
C	-2.240088	-2.558900	-0.932406	C	5.390728	-1.855303	-1.261225
C	-3.165203	-3.339999	-1.706973	H	4.581898	-1.870635	-3.266854
C	-4.328708	-2.698104	-2.244051	H	5.795781	-1.968544	0.859687
C	-4.521541	-1.310796	-2.031547	C	-3.816570	0.931059	-1.204741
C	-3.603944	-0.532713	-1.351533	C	-3.615722	1.603972	0.013222
H	-2.070880	-5.211067	-1.640740	C	-4.270327	1.688623	-2.292655
C	-2.965149	-4.717083	-2.002596	C	-3.866863	2.968234	0.125122
C	-5.262035	-3.461597	-2.997256	C	-4.520570	3.056923	-2.173328
H	-5.422183	-0.846325	-2.424497	C	-4.327305	3.733553	-0.961956
C	-5.048913	-4.798005	-3.244633	H	-3.705920	3.442513	1.089627
C	-3.880597	-5.425125	-2.750657	H	-4.863540	3.593073	-3.051583
H	-6.145576	-2.961081	-3.386570	O	0.320610	-1.575882	-1.454808
H	-5.766092	-5.369414	-3.827549	O	-1.522787	-0.431147	-0.136168
H	-3.700351	-6.474623	-2.967540	P	-0.077671	-0.096127	-0.852901
C	-1.032148	-3.164529	-0.294760	O	0.835971	0.350488	0.257533
C	-1.131091	-4.219796	0.676668	C	6.790252	-1.397144	-1.708260
C	0.226287	-2.668132	-0.606776	C	7.406864	-2.472003	-2.635872
C	-2.373236	-4.693664	1.183333	H	8.403313	-2.160835	-2.973817
C	0.073615	-4.791991	1.202328	H	6.790125	-2.642037	-3.524697
C	1.438814	-3.236139	-0.110545	H	7.508629	-3.429086	-2.111563
C	-2.421678	-5.695679	2.128100	C	6.680950	-0.061188	-2.481167
H	-3.293282	-4.245754	0.826490	H	6.241208	0.723135	-1.854157
C	-0.011662	-5.837567	2.162893	H	6.057456	-0.155939	-3.375977
C	1.328657	-4.296615	0.768779	H	7.674537	0.275708	-2.802161
C	-1.231397	-6.284413	2.617482	C	-4.594627	5.239053	-0.787492
H	-3.383487	-6.033574	2.504357	C	-5.663869	5.448440	0.311811

H	-5.941146	-1.763101	-1.110438	C	-5.319617	2.822997	0.605940
C	-5.111096	-5.532675	-2.354948	H	-4.278675	2.461747	2.467368
C	-3.777438	-5.966676	-2.167923	H	-6.222272	2.781186	-1.357256
H	-6.497070	-3.915909	-2.104804	O	-0.076138	-1.519900	-1.445666
H	-5.834743	-6.191446	-2.827246	O	-1.746758	-0.760230	0.306460
H	-3.479912	-6.954605	-2.509186	P	-0.602350	-0.143926	-0.702129
C	-0.869298	-3.364613	-0.160307	O	0.443212	0.485372	0.171357
C	-0.586532	-4.468748	0.715873	C	6.061286	0.029376	-2.757912
C	0.195347	-2.638626	-0.677817	C	6.615166	-0.726223	-3.989706
C	-1.597211	-5.180402	1.420449	H	7.439566	-0.162790	-4.444215
C	0.778795	-4.848759	0.930490	H	5.848405	-0.872280	-4.757867
C	1.562773	-3.003842	-0.481805	H	6.994707	-1.714506	-3.705402
C	-1.278957	-6.226521	2.259040	C	5.550661	1.422940	-3.196821
H	-2.632381	-4.882986	1.300646	H	5.158111	1.982970	-2.340188
C	1.071850	-5.944617	1.788461	H	4.753195	1.344760	-3.943865
C	1.814298	-4.115668	0.300373	H	6.367092	2.005448	-3.641917
C	0.067454	-6.623575	2.439087	C	-5.775939	4.237596	1.005141
H	-2.069891	-6.748864	2.790561	C	-6.655117	4.156083	2.276074
H	2.112388	-6.228239	1.928732	H	-6.983128	5.158187	2.579803
H	2.841408	-4.438489	0.447950	H	-6.113016	3.712598	3.117905
H	0.304334	-7.455199	3.097140	H	-7.547599	3.546040	2.095564
C	2.684819	-2.222239	-1.065158	C	-4.536053	5.116478	1.298298
C	2.670090	-1.753331	-2.390654	H	-4.845426	6.128267	1.589638
C	3.828512	-1.956499	-0.299536	H	-3.894134	5.197500	0.413554
C	3.751817	-1.049362	-2.910634	H	-3.932033	4.704576	2.113912
C	4.908825	-1.247632	-0.828257	O	-1.225522	0.672596	-1.816822
C	4.898513	-0.770351	-2.145064	S	3.314958	3.267445	0.409585
H	3.697848	-0.713637	-3.943043	O	-0.231783	2.831161	-2.476154
H	5.763748	-1.062926	-0.186651	H	1.572238	1.743156	-2.110094
C	-4.423446	0.196151	-0.066998	H	0.392370	2.713611	-0.236086
C	-4.102260	0.778348	1.170964	C	0.525147	4.829085	-0.805149
C	-5.198391	0.951733	-0.955792	C	1.019389	5.797795	-1.697962
C	-4.544780	2.056382	1.494585	C	-0.186946	5.248162	0.334410
C	-5.635165	2.236308	-0.626098	C	0.804928	7.150288	-1.453430

H	1.571106	5.493345	-2.581381	H	-1.967250	1.328104	6.837928
C	-0.399754	6.601640	0.576948	C	-1.340445	2.545975	5.154560
H	-0.567863	4.501548	1.025543	H	-1.977873	3.408811	5.352997
C	0.095983	7.554223	-0.317470	H	-0.361753	2.752143	5.614227
H	1.190794	7.892288	-2.146323	C	-1.104658	2.441073	3.658380
H	-0.950278	6.914401	1.459205	N	-0.675996	1.245894	3.224433
H	-0.068424	8.611767	-0.129905	H	-0.382815	1.148647	2.240054
H	3.863818	-2.282103	0.736218	C	-2.070841	3.053751	-0.691691
H	1.807450	-1.945376	-3.018768	C	-0.776580	3.595459	-0.288494
H	-3.505172	0.223020	1.886296	H	-2.373456	2.111279	-0.238457
H	-5.442475	0.540653	-1.931547	H	-0.068041	2.861193	0.081143
C	7.218131	0.237137	-1.762092	C	-1.269284	-2.340573	-0.701453
H	6.896053	0.800007	-0.878521	C	-0.309702	-3.342640	-0.727375
H	7.644853	-0.715279	-1.427027	C	-0.586702	-4.531146	-1.492556
H	8.021139	0.808200	-2.241903	C	-1.887016	-4.692165	-2.072853
C	-6.597513	4.923995	-0.102958	C	-2.846449	-3.656106	-1.937011
H	-6.020389	5.037194	-1.027734	C	-2.556575	-2.466322	-1.303705
H	-7.512142	4.367185	-0.336639	H	1.382901	-5.428659	-1.344134
H	-6.896455	5.926086	0.225646	C	0.379175	-5.547966	-1.734055
(R)-5-TS1-R E= -3994.43108856				C	-2.186171	-5.872476	-2.805797
H	-0.880869	1.902277	-1.893273	H	-3.830204	-3.798957	-2.375551
C	0.213105	-0.993210	3.552437	C	-1.235249	-6.848034	-2.997126
C	-0.506910	0.101165	4.044184	C	0.063857	-6.672347	-2.465719
C	-1.094974	0.066064	5.319501	H	-3.182588	-5.981021	-3.227681
C	-0.918822	-1.074755	6.103177	H	-1.472926	-7.742773	-3.565866
C	-0.190400	-2.168321	5.628643	H	0.823948	-7.428954	-2.640998
C	0.367837	-2.127111	4.349019	C	0.990837	-3.156739	-0.016729
H	0.630835	-0.949216	2.552943	C	1.478682	-4.117980	0.937043
H	-1.364800	-1.106498	7.094862	C	1.773064	-2.036065	-0.273410
H	-0.064400	-3.048429	6.252811	C	0.684714	-5.191199	1.430250
H	0.924981	-2.976682	3.965613	C	2.807680	-3.972283	1.452746
C	-1.921516	1.254823	5.745709	C	3.111224	-1.888981	0.200961
H	-2.957240	1.130083	5.395122	C	1.186354	-6.082674	2.353826
				H	-0.335917	-5.296223	1.081201

C	3.302067	-4.920472	2.389587	H	2.495156	-0.560665	-3.507346
C	3.603566	-2.877556	1.027902	H	3.120842	-1.863674	-4.537316
C	2.512343	-5.957022	2.832332	H	4.048459	-0.369297	-4.345659
H	0.555341	-6.887319	2.721548	C	3.872324	0.252986	2.172462
H	4.317166	-4.800828	2.760765	H	3.124237	-0.536726	2.280068
H	4.627162	-2.807436	1.386528	C	5.021148	-0.062648	3.151201
H	2.898588	-6.671497	3.554098	H	5.491439	-1.026451	2.924918
C	3.977068	-0.736126	-0.217075	H	4.647959	-0.100984	4.181839
C	4.466589	-0.668411	-1.545103	H	5.803509	0.704517	3.106496
C	4.356813	0.253234	0.722399	C	3.179204	1.575887	2.550360
C	5.322499	0.377549	-1.900296	H	2.350372	1.781187	1.867500
C	5.220808	1.275860	0.316752	H	3.874818	2.423392	2.525079
C	5.718610	1.362000	-0.987568	H	2.777921	1.511506	3.569122
H	5.678041	0.440311	-2.924794	C	-3.151689	-0.845951	-3.752585
H	5.537855	2.014773	1.046954	H	-2.275445	-1.474208	-3.570128
C	-3.553809	-1.345678	-1.247120	C	-2.647219	0.425983	-4.458467
C	-4.239263	-1.070951	-0.039175	H	-2.089049	0.148873	-5.360599
C	-3.821952	-0.572413	-2.404330	H	-1.979853	0.997316	-3.810695
C	-5.161949	-0.021478	-0.004349	H	-3.469720	1.078586	-4.775831
C	-4.754432	0.467206	-2.316639	C	-4.104563	-1.621934	-4.686692
C	-5.430156	0.769774	-1.128518	H	-4.999328	-1.028533	-4.912289
H	-5.711647	0.169822	0.912427	H	-4.437703	-2.565106	-4.241137
H	-4.938372	1.081968	-3.192093	H	-3.606831	-1.853661	-5.636191
O	1.282509	-1.041252	-1.102351	C	-4.057205	-1.937099	1.206757
O	-1.006074	-1.181640	0.010124	H	-3.157314	-2.542828	1.070473
P	0.060545	-0.073907	-0.579405	C	-3.848791	-1.112692	2.489032
O	0.426429	0.790692	0.596969	H	-4.746373	-0.545886	2.764390
C	4.120956	-1.710772	-2.608916	H	-3.021397	-0.406637	2.370968
H	3.432246	-2.436932	-2.169075	H	-3.609979	-1.775677	3.328651
C	5.372943	-2.496607	-3.048270	C	-5.240960	-2.913431	1.364198
H	5.860735	-2.978147	-2.193030	H	-5.346227	-3.553708	0.481274
H	6.110831	-1.843012	-3.528762	H	-6.184915	-2.371525	1.498963
H	5.100778	-3.277113	-3.769112	H	-5.094539	-3.559737	2.238284
C	3.403545	-1.083690	-3.819746	O	-0.465281	0.570145	-1.847997

S	-1.317424	3.777985	2.660286	H	7.184578	5.790862	-0.862015
O	-1.269469	2.903981	-1.886771	H	9.062947	5.341995	-2.432954
C	-0.345326	4.978546	-0.421961				
C	-1.221154	6.017514	-0.786906				
C	1.006506	5.277925	-0.168650	H	0.497481	-2.057660	-1.951784
C	-0.752064	7.322438	-0.896823	C	-0.637683	0.638241	3.620868
H	-2.266592	5.806195	-0.986759	C	0.266410	-0.333519	4.065288
C	1.471904	6.584664	-0.276788	C	0.825789	-0.266734	5.352148
H	1.681656	4.476979	0.119154	C	0.439552	0.777614	6.193010
C	0.593243	7.607908	-0.642416	C	-0.469640	1.748060	5.764798
H	-1.433722	8.119391	-1.179135	C	-1.000956	1.678889	4.474869
H	2.516191	6.806296	-0.077848	H	-1.033596	0.572465	2.613586
H	0.955162	8.628850	-0.727899	H	0.863240	0.832518	7.193469
H	-2.908468	3.728626	-0.853051	H	-0.757126	2.554582	6.433373
C	-6.397556	1.895947	-1.061705	H	-1.700243	2.434035	4.127576
C	-7.252608	2.183240	-2.140021	C	1.849085	-1.310414	5.729376
C	-6.479627	2.710364	0.081742	H	2.849896	-0.978699	5.413596
C	-8.155007	3.244561	-2.078188	H	1.891585	-1.441067	6.816414
H	-7.225002	1.552103	-3.023857	C	1.522524	-2.647470	5.050589
C	-7.383025	3.771260	0.145041	H	2.305452	-3.389250	5.214335
H	-5.813574	2.521897	0.919428	H	0.592758	-3.056666	5.474664
C	-8.224839	4.044002	-0.935179	C	1.290301	-2.495623	3.557544
H	-8.811510	3.441639	-2.921846	N	0.650880	-1.377166	3.185663
H	-7.423112	4.390417	1.037624	H	0.349652	-1.274018	2.203734
H	-8.928869	4.870388	-0.886548	C	0.365745	-3.676298	-0.704899
C	6.637979	2.458307	-1.387932	C	1.768084	-3.324845	-0.520448
C	7.701847	2.223639	-2.276372	H	0.097467	-4.724405	-0.814804
C	6.472464	3.761223	-0.886785	C	0.605901	2.422734	-0.716425
C	8.566168	3.252044	-2.650333	C	-0.523342	3.229083	-0.762019
H	7.866009	1.219269	-2.656595	C	-0.470022	4.434442	-1.548283
C	7.337292	4.790045	-1.258144	C	0.779184	4.828868	-2.128225
H	5.642557	3.971458	-0.217797	C	1.919897	4.004942	-1.951708
C	8.388758	4.540680	-2.142579	C	1.857805	2.797314	-1.288726
H	9.386004	3.043575	-3.333013	H	-2.574733	4.943090	-1.419603

(R)-5-TS1-S E= -3994.43057784

C	-1.610495	5.243763	-1.811639	C	4.956397	1.166360	0.186094
C	0.851931	6.028452	-2.887043	C	4.725727	0.428013	-2.083753
H	2.867843	4.332243	-2.370349	C	5.444676	0.403913	-0.881842
C	-0.266801	6.799756	-3.101901	H	5.519276	1.190264	1.114814
C	-1.511490	6.391415	-2.567809	H	5.077253	-0.175371	-2.914868
H	1.812017	6.317028	-3.308508	O	-1.681277	0.692872	-1.110461
H	-0.201027	7.710727	-3.690399	O	0.558376	1.235345	-0.005868
H	-2.400749	6.985709	-2.759999	P	-0.319452	-0.046113	-0.555757
C	-1.769660	2.827891	-0.043611	O	-0.564312	-0.916859	0.645987
C	-2.412480	3.698436	0.904656	C	-4.549792	0.828557	-2.635232
C	-2.345406	1.588059	-0.289479	H	-4.020371	1.675304	-2.190582
C	-1.816999	4.898995	1.382070	C	-5.910945	1.363604	-3.124419
C	-3.693451	3.326288	1.428243	H	-6.505561	1.758831	-2.292857
C	-3.637192	1.213622	0.188207	H	-6.500655	0.578284	-3.612241
C	-2.462394	5.697174	2.301584	H	-5.765544	2.170818	-3.852641
H	-0.832520	5.176734	1.023725	C	-3.693369	0.327044	-3.813946
C	-4.341247	4.181736	2.360988	H	-2.714092	-0.015491	-3.467519
C	-4.289413	2.107689	1.012531	H	-3.536649	1.135141	-4.538960
C	-3.742924	5.344486	2.790229	H	-4.180694	-0.500926	-4.342895
H	-1.981135	6.603989	2.657837	C	-4.083389	-0.995658	2.188133
H	-5.318244	3.890306	2.739355	H	-3.489323	-0.085295	2.301401
H	-5.284669	1.865277	1.375632	C	-5.294860	-0.874018	3.134137
H	-4.244890	5.986493	3.508889	H	-5.921678	-0.011735	2.879351
C	-4.290381	-0.073540	-0.223525	H	-4.960094	-0.755217	4.171837
C	-4.730580	-0.243454	-1.560200	H	-5.929481	-1.767315	3.087808
C	-4.521269	-1.098706	0.726729	C	-3.179659	-2.171301	2.605063
C	-5.384640	-1.426319	-1.914403	H	-2.306787	-2.233461	1.949786
C	-5.187520	-2.260013	0.321192	H	-3.712519	-3.129125	2.570205
C	-5.627350	-2.451308	-0.992665	H	-2.827886	-2.027051	3.633806
H	-5.699822	-1.564278	-2.944683	C	2.845648	1.162987	-3.595699
H	-5.391344	-3.032206	1.057382	H	1.840613	1.569487	-3.451544
C	3.081186	1.938512	-1.143950	C	2.674737	-0.252788	-4.175843
C	3.791905	1.932170	0.079811	H	2.068201	-0.207347	-5.088037
C	3.554100	1.176407	-2.240116	H	2.166165	-0.906954	-3.464842

H	1.197820	-2.739191	6.596228	C	-2.050027	5.217046	2.623177
C	0.244331	-3.510982	4.805215	C	-2.795521	3.411573	1.105503
H	0.541336	-4.554600	4.919478	C	-1.046380	5.992866	3.156645
H	-0.759429	-3.409918	5.245622	H	1.081088	6.419019	3.147152
C	0.104795	-3.197837	3.326087	H	-3.075276	5.324413	2.969416
N	0.140329	-1.895403	3.006725	H	-3.815863	3.568329	1.445472
H	-0.060976	-1.614704	2.034581	H	-1.270408	6.726850	3.925849
C	0.771402	-3.774315	-1.104095	C	-3.636124	1.511823	-0.298352
C	-0.635619	-3.753230	-0.720562	C	-4.065915	1.621083	-1.640573
H	1.437907	-3.103159	-0.565021	C	-4.292111	0.603605	0.569559
H	-0.966506	-2.830971	-0.253508	C	-5.128914	0.824064	-2.085941
C	1.859585	1.818861	-0.576745	C	-5.353606	-0.158914	0.072416
C	1.167223	3.021864	-0.550673	C	-5.796650	-0.075692	-1.252946
C	1.745409	4.156262	-1.223474	H	-5.440720	0.928236	-3.118939
C	3.067836	4.040547	-1.761996	H	-5.851539	-0.843759	0.752957
C	3.753378	2.802794	-1.666720	C	3.907778	0.370387	-1.093237
C	3.169766	1.677797	-1.122653	C	4.498415	-0.080656	0.111454
H	0.036709	5.482190	-1.056477	C	4.065738	-0.388286	-2.275073
C	1.054524	5.385437	-1.415068	C	5.229407	-1.271059	0.104115
C	3.662407	5.159042	-2.406556	C	4.813796	-1.574276	-2.224721
H	4.763497	2.736226	-2.061559	C	5.406799	-2.043785	-1.050932
C	2.974221	6.341308	-2.552147	H	5.684161	-1.599686	1.034203
C	1.651383	6.445844	-2.061754	H	4.930083	-2.139283	-3.141985
H	4.671663	5.054447	-2.797757	O	-0.917176	1.223382	-1.129121
H	3.435818	7.187462	-3.053660	O	1.295981	0.707268	0.030975
H	1.096947	7.370002	-2.201345	P	0.003174	-0.049272	-0.646710
C	-0.162587	3.114902	0.122752	O	-0.625597	-0.854364	0.459005
C	-0.430503	4.096089	1.141043	C	-3.450512	2.613792	-2.627240
C	-1.185431	2.243996	-0.231504	H	-2.631198	3.134528	-2.124491
C	0.584825	4.903153	1.726733	C	-4.471266	3.693344	-3.041084
C	-1.771373	4.245094	1.623999	H	-4.868016	4.220666	-2.166034
C	-2.533787	2.393011	0.212070	H	-5.320685	3.259556	-3.582241
C	0.285470	5.822078	2.709484	H	-4.000058	4.433125	-3.699810
H	1.610861	4.779405	1.400132	C	-2.849410	1.913050	-3.860823

H	-2.097861	1.175943	-3.563647	S	-0.142086	-4.428046	2.205275
H	-2.366603	2.648454	-4.515931	O	0.126002	-3.171445	-2.249768
H	-3.619326	1.401621	-4.451187	C	-1.613491	-4.800804	-0.969244
C	-3.894588	0.417501	2.034756	C	-1.259701	-6.079733	-1.436824
H	-2.987692	0.999848	2.217300	C	-2.968335	-4.511546	-0.719322
C	-4.983240	0.950959	2.987645	C	-2.239908	-7.043312	-1.650312
H	-5.200082	2.009000	2.801361	H	-0.220000	-6.321507	-1.632513
H	-4.663491	0.848772	4.031851	C	-3.946309	-5.478407	-0.932418
H	-5.922388	0.396709	2.869902	H	-3.242764	-3.525955	-0.353726
C	-3.553828	-1.048347	2.363261	C	-3.582988	-6.744503	-1.399040
H	-2.765868	-1.415597	1.700218	H	-1.959530	-8.028911	-2.010196
H	-4.427630	-1.704024	2.266602	H	-4.988618	-5.245726	-0.736145
H	-3.196824	-1.129384	3.397238	H	-4.345404	-7.500600	-1.565518
C	3.479656	0.050427	-3.618858	H	1.240738	-4.721372	-1.362121
H	2.735933	0.827680	-3.421577	C	6.226528	-3.346254	-0.986728
C	2.751502	-1.083740	-4.363844	C	5.552959	-4.328620	0.001076
H	2.253713	-0.681268	-5.254103	C	6.334678	-4.043715	-2.356364
H	1.989407	-1.543985	-3.731566	C	7.660277	-3.032450	-0.496235
H	3.442701	-1.863938	-4.704901	H	5.477049	-3.905634	1.008136
C	4.571451	0.659332	-4.523727	H	4.538936	-4.582116	-0.330184
H	5.350214	-0.080060	-4.748279	H	6.129418	-5.259668	0.070979
H	5.058253	1.519614	-4.052464	H	6.831413	-3.409074	-3.099047
H	4.140834	0.993935	-5.475511	H	6.925551	-4.961691	-2.257779
C	4.412471	0.723900	1.408247	H	5.351609	-4.324646	-2.751310
H	3.674982	1.519009	1.267767	H	8.255708	-3.952265	-0.438910
C	3.933531	-0.120809	2.602288	H	8.165415	-2.342689	-1.182146
H	4.659601	-0.897294	2.871940	H	7.660585	-2.573636	0.497959
H	2.980061	-0.608166	2.378198	C	-6.976098	-0.944283	-1.728963
H	3.788569	0.514742	3.483621	C	-7.302113	-0.730015	-3.219478
C	5.759101	1.408561	1.718207	C	-6.633604	-2.439782	-1.524800
H	6.069814	2.061631	0.894871	C	-8.237976	-0.593975	-0.904464
H	6.553496	0.668781	1.875435	H	-7.595239	0.305119	-3.428100
H	5.682719	2.018632	2.626770	H	-6.451104	-0.980137	-3.863148
O	0.390678	-0.742356	-1.940704	H	-8.139267	-1.374726	-3.511287

H	-6.435894	-2.669015	-0.471952	C	0.741428	4.864227	-1.744696
H	-7.468331	-3.071708	-1.853512	C	1.903286	4.065852	-1.591353
H	-5.745853	-2.720272	-2.103656	C	1.862501	2.805354	-1.032236
H	-9.088930	-1.207844	-1.225487	H	-2.634784	4.817881	-1.141006
H	-8.085295	-0.767353	0.165997	C	-1.669298	5.179310	-1.474653
H	-8.509946	0.459539	-1.036168	C	0.798085	6.124056	-2.400242
(R)-6-TS1-S E= -3846.82712340				H	2.854383	4.459613	-1.939814
H	0.564238	-1.991069	-2.221510	C	-0.338199	6.876643	-2.587606
C	-0.550605	0.126387	3.550297	C	-1.584652	6.388618	-2.129782
C	0.292265	-0.934233	3.903554	H	1.760674	6.475279	-2.764586
C	0.844917	-1.021977	5.192025	H	-0.284362	7.835030	-3.096724
C	0.516927	-0.038448	6.125584	H	-2.486382	6.970290	-2.301428
C	-0.329213	1.020902	5.788074	C	-1.803010	2.625330	0.084513
C	-0.856216	1.103170	4.497069	C	-2.493310	3.395354	1.084898
H	-0.943240	0.180075	2.540894	C	-2.339214	1.398351	-0.282629
H	0.936142	-0.102091	7.127377	C	-1.943592	4.565327	1.679463
H	-0.572183	1.777948	6.528333	C	-3.777357	2.948960	1.538262
H	-1.507048	1.927638	4.220247	C	-3.630879	0.950391	0.127261
C	1.798408	-2.158256	5.472597	C	-2.635305	5.266595	2.643442
H	2.820683	-1.862067	5.192694	H	-0.957782	4.898047	1.375541
H	1.822622	-2.392805	6.542589	C	-4.473352	3.706381	2.519425
C	1.395731	-3.403109	4.670130	C	-4.327849	1.754717	1.005689
H	2.129867	-4.204281	4.766132	C	-3.919028	4.843052	3.062251
H	0.438326	-3.791231	5.050241	H	-2.188380	6.151378	3.088806
C	1.187877	-3.096222	3.197605	H	-5.452006	3.359763	2.842991
N	0.622087	-1.911459	2.930540	H	-5.324454	1.455839	1.319908
H	0.338406	-1.695795	1.961125	H	-4.457678	5.409437	3.817040
C	0.294338	-3.749666	-1.187968	C	-4.235084	-0.315463	-0.405808
C	1.688878	-3.468870	-0.869277	C	-4.634548	-0.393438	-1.759660
H	0.009036	-4.767202	-1.444756	C	-4.461636	-1.421910	0.450026
C	0.603538	2.343009	-0.546850	C	-5.242069	-1.566271	-2.227840
C	-0.549266	3.117396	-0.561235	C	-5.077545	-2.563786	-0.070847
C	-0.511295	4.385500	-1.241930	C	-5.478508	-2.671191	-1.407499
				H	-5.542729	-1.599730	-3.268979

H	-5.246307	-3.401936	0.599487	H	1.955641	1.605345	-3.222455
C	3.125495	2.003507	-0.889677	C	2.985444	-0.078570	-4.022422
C	3.810796	1.994663	0.348637	H	2.381807	-0.051676	-4.937229
C	3.682346	1.330306	-1.999411	H	2.546024	-0.821354	-3.353049
C	5.039472	1.335843	0.439891	H	3.990354	-0.413293	-4.307487
C	4.920465	0.686219	-1.851852	C	3.648814	2.341409	-4.320843
C	5.628610	0.678027	-0.647150	H	4.704782	2.100599	-4.496429
H	5.559430	1.353765	1.393740	H	3.602537	3.357067	-3.914365
H	5.338283	0.189403	-2.719412	H	3.137956	2.342579	-5.291534
O	-1.631758	0.598189	-1.163726	C	3.272032	2.711669	1.586504
O	0.567076	1.091843	0.048155	H	2.290374	3.125213	1.339318
P	-0.259043	-0.147873	-0.651612	C	3.067561	1.745190	2.767866
O	-0.503730	-1.148118	0.445332	H	4.017562	1.315842	3.109112
C	-4.473350	0.771040	-2.737537	H	2.403129	0.922802	2.487105
H	-3.969335	1.589688	-2.217215	H	2.615347	2.268807	3.618437
C	-5.843972	1.312072	-3.192578	C	4.170819	3.898366	1.986741
H	-6.453215	1.621593	-2.335717	H	4.273272	4.614052	1.163182
H	-6.410955	0.556152	-3.748917	H	5.177486	3.563860	2.265115
H	-5.713635	2.180736	-3.849629	H	3.745583	4.428301	2.847798
C	-3.594722	0.396570	-3.946800	O	0.418771	-0.609672	-1.928546
H	-2.608365	0.053247	-3.621500	S	1.611366	-4.222032	2.018313
H	-3.455949	1.267944	-4.598368	O	0.758093	-3.032184	-2.363218
H	-4.054764	-0.395941	-4.549339	H	-0.448095	-3.211084	-0.603189
C	-4.062291	-1.428668	1.926463	H	1.871282	-2.498092	-0.427432
H	-3.503500	-0.511761	2.131918	C	2.837805	-4.306241	-1.174887
C	-5.300297	-1.429357	2.845519	C	2.712159	-5.661466	-1.530672
H	-5.950649	-0.569735	2.647099	C	4.120247	-3.730841	-1.101507
H	-4.997175	-1.390387	3.898929	C	3.844947	-6.420088	-1.807819
H	-5.900409	-2.336231	2.703368	H	1.731613	-6.123662	-1.580793
C	-3.127750	-2.604399	2.268765	C	5.250735	-4.491770	-1.382150
H	-2.239408	-2.584652	1.632044	H	4.218197	-2.683075	-0.829992
H	-3.625319	-3.573512	2.142748	C	5.113936	-5.837149	-1.735506
H	-2.803595	-2.534466	3.314350	H	3.741181	-7.466937	-2.077523
C	3.000231	1.315343	-3.368589	H	6.236073	-4.039130	-1.323654

C	-0.669717	3.678586	-0.151861	O	-0.464681	-0.243635	0.749319
C	-1.041652	4.752968	0.730663	C	-4.002979	2.341319	-2.548837
C	-1.555531	2.619625	-0.304780	H	-3.250523	3.042496	-2.178146
C	-0.142027	5.785707	1.116919	C	-5.207913	3.185558	-3.010660
C	-2.363839	4.770949	1.282525	H	-5.632655	3.759683	-2.179261
C	-2.887117	2.631928	0.208596	H	-6.005738	2.557797	-3.424896
C	-0.537001	6.790721	1.973369	H	-4.901570	3.892640	-3.791106
H	0.873469	5.769934	0.738528	C	-3.369634	1.581363	-3.730151
C	-2.745794	5.832445	2.147537	H	-2.488662	1.019358	-3.406490
C	-3.265062	3.722730	0.964164	H	-3.057487	2.287150	-4.509422
C	-1.855295	6.825178	2.486980	H	-4.078482	0.879532	-4.185699
H	0.172653	7.562348	2.259377	C	-3.775937	0.732551	2.364536
H	-3.756859	5.835959	2.547861	H	-2.949258	1.447518	2.386683
H	-4.280031	3.774229	1.349301	C	-4.858048	1.246997	3.335012
H	-2.156530	7.627481	3.154853	H	-5.231946	2.233371	3.037601
C	-3.863072	1.532542	-0.096083	H	-4.453333	1.330605	4.350877
C	-4.391249	1.404857	-1.404684	H	-5.716505	0.565358	3.371799
C	-4.301129	0.660519	0.930569	C	-3.210692	-0.617520	2.844454
C	-5.340064	0.408464	-1.658554	H	-2.429548	-0.968795	2.165046
C	-5.259799	-0.313989	0.626153	H	-3.988609	-1.387085	2.913000
C	-5.789170	-0.459045	-0.658651	H	-2.771991	-0.505843	3.843407
H	-5.753256	0.308014	-2.658444	C	3.301801	0.620794	-3.551460
H	-5.603720	-0.984876	1.408303	H	2.421287	1.259273	-3.436515
C	3.759239	1.466831	-1.154490	C	2.806255	-0.735681	-4.084693
C	4.461164	1.363048	0.069907	H	2.215922	-0.579404	-4.995086
C	3.990642	0.526340	-2.188677	H	2.169986	-1.242358	-3.356217
C	5.377371	0.319071	0.241075	H	3.635029	-1.403744	-4.347938
C	4.913744	-0.502861	-1.965319	C	4.234986	1.278922	-4.590402
C	5.613277	-0.627385	-0.760348	H	5.139890	0.676423	-4.737944
H	5.929008	0.237860	1.173348	H	4.549448	2.281137	-4.281628
H	5.097932	-1.233409	-2.747285	H	3.728494	1.367851	-5.559185
O	-1.172823	1.527293	-1.065661	C	4.297251	2.388000	1.191562
O	1.146957	1.536156	0.008504	H	3.428333	3.009856	0.959212
P	-0.030315	0.496868	-0.486383	C	4.027696	1.735515	2.559012

H	4.887823	1.154494	2.912779	C	-8.727292	-3.528265	-1.500389
H	3.161394	1.068963	2.510736	H	-9.464622	-4.300793	-1.710044
H	3.817823	2.504350	3.311453	C	5.625117	-5.011730	2.016376
C	5.520974	3.324354	1.255691	H	5.371283	-5.838925	2.673930
H	5.675250	3.840846	0.301575	C	4.701181	-3.940494	1.843396
H	6.435940	2.764822	1.484938	H	3.750614	-3.957226	2.371172
H	5.386259	4.083880	2.035649	C	9.447041	-0.692107	-2.727414
O	0.413147	-0.290150	-1.706171	H	9.732930	0.136078	-3.370472
S	0.726954	-3.370457	2.959769	C	10.342191	-1.787014	-2.556104
O	0.675340	-2.742051	-1.636566	H	11.297593	-1.787247	-3.073911
C	-0.612991	-4.537665	-0.082284	C	-5.704345	-5.079909	-3.008314
C	0.060482	-5.752620	-0.308820	H	-5.412652	-5.983184	-3.537557
C	-2.009117	-4.548454	0.097484	C	-4.727514	-4.081129	-2.727017
C	-0.649760	-6.947635	-0.353158	H	-3.698624	-4.235539	-3.039779
H	1.137196	-5.763155	-0.443875	C	-8.601121	-0.161774	0.134612
C	-2.717783	-5.745170	0.046448	C	-9.908564	-0.018863	0.521047
H	-2.531570	-3.612388	0.273496	C	-10.861989	-1.043893	0.256312
C	-2.037677	-6.945188	-0.177374	H	-7.885526	0.627392	0.337293
H	-0.124042	-7.882578	-0.523518	H	-10.225594	0.886360	1.032124
H	-3.795689	-5.740801	0.173877	H	-11.893744	-0.913295	0.571495
H	-2.588645	-7.881033	-0.214287	C	-7.002732	-4.898902	-2.612574
H	2.141958	-3.823397	-0.572250	H	-7.756175	-5.655502	-2.819787
C	6.582657	-1.748661	-0.552533	C	-5.073882	-2.930681	-2.065737
C	7.826850	-1.744131	-1.228968	H	-4.322277	-2.176128	-1.860890
C	6.248877	-2.820882	0.310886	C	9.999383	-2.828660	-1.736441
C	8.746792	-2.844700	-1.045628	H	10.677173	-3.666759	-1.591246
C	7.178155	-3.914547	0.488022	C	8.235188	-0.671076	-2.086838
C	8.397500	-3.898270	-0.195577	H	7.566235	0.171684	-2.220607
H	9.092332	-4.725051	-0.061363	C	5.004082	-2.886806	1.018845
C	-6.806741	-1.516266	-0.953873	H	4.297401	-2.072661	0.902939
C	-8.149784	-1.341306	-0.542740	C	6.824844	-4.995211	1.356740
C	-6.421717	-2.692922	-1.640058	H	7.536904	-5.808033	1.480736
C	-9.124417	-2.372622	-0.820867	C	-10.477748	-2.183775	-0.397579
C	-7.406184	-3.714793	-1.918305	H	-11.197991	-2.970277	-0.610992

(R)-7-TS1-S E= -4608.96757008

H	-0.221463	-1.271766	-1.992484	H	3.795783	4.262689	-2.274610
C	0.080405	0.823957	3.977776	C	1.226955	7.282790	-3.118526
C	0.543744	-0.478689	4.198032	C	-0.072179	7.158804	-2.572473
C	1.145626	-0.838376	5.415359	H	3.163579	6.379433	-3.294635
C	1.249878	0.126081	6.417879	H	1.472787	8.134229	-3.747153
C	0.780529	1.426349	6.216346	H	-0.824013	7.910897	-2.796135
C	0.202494	1.772253	4.992995	C	-1.032951	3.841181	0.112448
H	-0.359296	1.076517	3.018708	C	-1.487501	4.874502	1.004923
H	1.709021	-0.146082	7.365657	C	-1.844978	2.729111	-0.070021
H	0.869183	2.164037	7.008824	C	-0.666245	5.960273	1.418655
H	-0.158375	2.782741	4.823678	C	-2.816876	4.797196	1.533956
C	1.675667	-2.245350	5.547772	C	-3.177597	2.638283	0.433142
H	2.703824	-2.293552	5.158161	C	-1.142905	6.927210	2.276982
H	1.724825	-2.547196	6.599770	H	0.354758	6.016745	1.059297
C	0.790064	-3.220438	4.760386	C	-3.284700	5.821638	2.401314
H	1.204011	-4.229710	4.748755	C	-3.639403	3.692628	1.194296
H	-0.201592	-3.281531	5.234266	C	-2.469389	6.868312	2.765944
C	0.560559	-2.763351	3.330698	H	-0.491572	7.741015	2.584267
N	0.427668	-1.441528	3.162168	H	-4.300611	5.752916	2.783247
H	0.152523	-1.075177	2.236550	H	-4.658745	3.668867	1.570738
C	-1.092385	-2.769526	-0.940710	H	-2.835600	7.641690	3.435547
C	0.297684	-3.205998	-0.864061	C	-4.054199	1.459260	0.129020
H	-1.867420	-3.508561	-1.129705	C	-4.493386	1.222522	-1.198131
C	1.207476	2.929828	-0.537531	C	-4.475778	0.597598	1.172389
C	0.264906	3.946804	-0.619523	C	-5.319074	0.123011	-1.454339
C	0.556701	5.079906	-1.459941	C	-5.325241	-0.472599	0.865634
C	1.856461	5.187056	-2.052355	C	-5.748713	-0.738664	-0.439040
C	2.805583	4.155239	-1.840126	H	-5.646167	-0.070043	-2.472194
C	2.502622	3.012402	-1.130455	H	-5.661261	-1.128198	1.663842
H	-1.401521	6.009011	-1.365954	C	3.520041	1.918805	-0.971033
C	-0.397882	6.090256	-1.765695	C	4.232539	1.796297	0.245039
C	2.167231	6.311455	-2.864184	C	3.801705	1.046100	-2.051217
				C	5.207276	0.798725	0.363914
				C	4.790143	0.068873	-1.883761

C	5.497012	-0.076338	-0.686348	H	4.906105	1.296966	-4.616031
H	5.761875	0.700384	1.293086	H	4.265979	2.867661	-4.110799
H	5.017744	-0.606297	-2.703404	H	3.457371	1.955834	-5.397672
O	-1.387033	1.687773	-0.856093	C	4.009470	2.745272	1.421568
O	0.922408	1.804768	0.222827	H	3.154643	3.384943	1.184495
P	-0.180405	0.708784	-0.309434	C	3.665998	1.995414	2.721128
O	-0.599634	-0.100951	0.887091	H	4.495866	1.362941	3.058415
C	-4.148956	2.150910	-2.363499	H	2.785183	1.360907	2.586320
H	-3.464235	2.920807	-1.999438	H	3.447502	2.707687	3.525580
C	-5.409041	2.880956	-2.872492	C	5.225262	3.673162	1.619563
H	-5.892125	3.447424	-2.068004	H	5.433688	4.253397	0.713462
H	-6.146517	2.176403	-3.275166	H	6.128206	3.101305	1.865019
H	-5.146793	3.583513	-3.672877	H	5.041353	4.377648	2.439914
C	-3.433197	1.414705	-3.511876	O	0.320314	-0.003926	-1.551306
H	-2.518489	0.931469	-3.157162	S	0.435973	-3.890292	2.082481
H	-3.159115	2.125220	-4.301025	O	-0.551801	-2.255842	-2.187152
H	-4.075024	0.650632	-3.966399	H	-1.387894	-1.995235	-0.234685
C	-4.035639	0.761707	2.627651	H	0.988098	-2.467593	-0.477540
H	-3.294189	1.563640	2.670910	C	0.839257	-4.466252	-1.331645
C	-5.213593	1.170105	3.534429	C	0.024565	-5.507594	-1.819279
H	-5.678980	2.103236	3.196834	C	2.234134	-4.653479	-1.272975
H	-4.870696	1.315657	4.565975	C	0.597324	-6.701887	-2.240877
H	-5.992839	0.398570	3.547370	H	-1.051486	-5.379436	-1.875765
C	-3.349178	-0.510125	3.161990	C	2.801624	-5.855209	-1.684407
H	-2.512792	-0.791888	2.516396	H	2.866343	-3.861056	-0.883880
H	-4.043615	-1.356730	3.219722	C	1.984249	-6.878004	-2.172167
H	-2.959707	-0.332127	4.171433	H	-0.034361	-7.499499	-2.620535
C	3.090210	1.150190	-3.401226	H	3.876801	-5.992108	-1.621757
H	2.191124	1.756228	-3.259352	H	2.425835	-7.815956	-2.497732
C	2.627271	-0.212972	-3.947235	C	6.528193	-1.151256	-0.537444
H	2.030248	-0.063684	-4.854744	C	6.221048	-2.325298	0.191228
H	2.006097	-0.733085	-3.215217	C	7.209888	-3.373335	0.312740
H	3.471264	-0.858662	-4.217759	C	8.460397	-3.211735	-0.291381
C	3.982595	1.862196	-4.439332	H	9.201357	-4.003498	-0.199075

C	-6.625915	-1.909755	-0.746942	C	-8.520225	-0.397342	-1.367459
C	-7.945027	-1.702465	-1.223916	H	-7.926744	0.467137	-1.093091
C	-6.137084	-3.229507	-0.570891	H	-4.163692	-2.681658	0.155546
C	-8.774732	-2.838822	-1.557399	H	-7.134968	-6.518076	-0.954781
C	-6.982794	-4.356780	-0.895590	H	-10.707043	-3.483740	-2.298530
C	-8.271459	-4.131736	-1.387589	H	-11.612037	-1.195848	-2.552199
H	-8.900895	-4.983629	-1.637271	H	-10.210655	0.774026	-1.925184
C	4.945439	-2.536874	0.810951				
C	4.667609	-3.690289	1.500754				
H	3.689349	-3.827142	1.954688	(S)-1 E= -384.838385435			
C	5.649222	-4.717191	1.620430	C	0.636528	0.539994	0.074112
H	5.413056	-5.623459	2.171750	C	0.980021	1.929960	-0.293241
C	6.881139	-4.558872	1.043580	H	1.100265	2.180239	-1.347512
H	7.637446	-5.336017	1.128813	H	1.533457	2.557075	0.407055
H	4.194131	-1.758381	0.732303	O	-0.346692	1.583123	0.107665
C	7.800651	-1.002714	-1.139244	H	0.951865	0.196378	1.061554
C	8.781783	-2.057291	-1.011945	C	0.470422	-0.534481	-0.948314
C	10.062973	-1.893798	-1.626960	C	1.206427	-1.720848	-0.839349
C	10.372915	-0.757030	-2.324333	C	-0.405563	-0.369632	-2.028820
H	11.350415	-0.645890	-2.785954	C	1.083918	-2.720582	-1.805226
C	9.413850	0.289861	-2.443051	H	1.878211	-1.862047	0.004852
C	8.173893	0.171738	-1.870546	C	-0.530199	-1.370744	-2.991729
H	10.789004	-2.697176	-1.525196	H	-0.997948	0.538282	-2.090910
H	9.672733	1.191731	-2.991397	C	0.216007	-2.547309	-2.885325
H	7.453378	0.976707	-1.963935	H	1.661466	-3.636360	-1.710568
C	-6.482245	-5.684019	-0.707452	H	-1.216405	-1.235451	-3.823717
C	-5.220777	-5.904807	-0.224118	H	0.116241	-3.327257	-3.635408
H	-4.857686	-6.918443	-0.077036				
C	-4.378221	-4.799550	0.089457	(S)-2 E= -707.829268328			
H	-3.381931	-4.981271	0.485624	C	1.702463	0.013227	1.167884
C	-4.816987	-3.511719	-0.087157	C	1.726306	-0.729978	-0.120133
C	-10.101236	-2.616873	-2.044858	H	1.082459	0.904617	1.236008
C	-10.601725	-1.350257	-2.183018	H	1.755135	-0.569031	2.085368
C	-9.799444	-0.227492	-1.830562	S	3.282740	0.217335	0.267914
				H	1.166357	-0.270187	-0.931955

C	1.743428	-2.221746	-0.177308	C	-2.722522	4.096683	-2.826181
C	0.966413	-2.867811	-1.148121	H	-3.487364	2.348629	-1.872272
C	2.486553	-3.002736	0.720947	C	-0.521059	4.838223	-2.171548
C	0.918692	-4.261739	-1.214192	C	0.768194	3.540566	-0.509465
H	0.391485	-2.274298	-1.855456	C	-1.649958	5.012604	-2.937979
C	2.438388	-4.393298	0.656114	H	-3.602359	4.219262	-3.451875
H	3.124089	-2.515571	1.453634	H	0.320259	5.520968	-2.261845
C	1.653113	-5.029265	-0.310517	H	1.583820	4.251312	-0.611123
H	0.309511	-4.744438	-1.973736	H	-1.715260	5.840990	-3.637859
H	3.021906	-4.984196	1.357184	C	2.217370	2.215544	1.055098
H	1.621095	-6.114217	-0.360920	C	2.277401	2.448953	2.451184
				C	3.378403	1.807615	0.356553
				C	3.494705	2.273216	3.115013
				C	4.571786	1.652124	1.073866
				C	4.657222	1.876087	2.447678
				H	3.536390	2.457366	4.185810
				H	5.467345	1.340000	0.541758
				C	-3.309394	-2.909001	-0.030930
				C	-3.065160	-3.431916	-1.325832
				C	-3.405262	-3.788747	1.075734
				C	-2.909075	-4.812164	-1.481870
				C	-3.243526	-5.163568	0.857279
				C	-2.990657	-5.699937	-0.405231
				H	-2.726270	-5.205159	-2.478913
				H	-3.319749	-5.843104	1.703015
				O	-0.020743	0.458962	1.286710
				O	-1.194585	-1.041318	-0.387552
				P	0.086844	-1.003364	0.603681
				O	1.316755	-1.404780	-0.101497
				C	1.067597	2.922132	3.257176
				H	0.206343	2.973550	2.584837
				C	1.284515	4.344534	3.811337
				H	1.501987	5.055346	3.006119
				H	2.121500	4.376390	4.518844
(R)-C1 E= -2582.02345706							
C	-2.425690	-0.511315	0.002496				
C	-2.556175	0.863113	0.132222				
C	-3.819581	1.380040	0.590684				
C	-4.921605	0.477206	0.742034				
C	-4.732938	-0.905184	0.487973				
C	-3.501101	-1.432811	0.158953				
H	-3.190952	3.437237	0.869672				
C	-4.022029	2.745174	0.936332				
C	-6.181551	0.977424	1.169708				
H	-5.584763	-1.572563	0.585879				
C	-6.348483	2.308727	1.473079				
C	-5.250942	3.195221	1.367380				
H	-7.009766	0.279685	1.266999				
H	-7.314103	2.678552	1.806443				
H	-5.376245	4.241127	1.633790				
C	-1.405331	1.763784	-0.172471				
C	-1.518331	2.848609	-1.112254				
C	-0.176600	1.561982	0.437514				
C	-2.660499	3.045978	-1.937092				
C	-0.416801	3.753077	-1.259275				
C	0.932817	2.445194	0.313479				

H	0.388113	4.691872	4.339637	H	-5.372003	-3.311896	3.915019
C	0.701346	1.937162	4.384166	C	-2.815730	-7.201207	-0.594490
H	0.511698	0.936905	3.982896	H	-2.937690	-7.666907	0.393303
H	-0.202891	2.274291	4.905633	C	-3.895956	-7.794783	-1.518815
H	1.502485	1.859668	5.128824	H	-3.785844	-8.883424	-1.592567
C	5.977322	1.694237	3.185773	H	-3.822686	-7.384032	-2.532803
H	6.720831	1.376656	2.441831	H	-4.901878	-7.577752	-1.142939
C	6.477043	3.015312	3.801203	C	-1.403139	-7.552784	-1.099024
H	7.456442	2.876035	4.274927	H	-1.277734	-8.639757	-1.173229
H	5.785692	3.383426	4.568722	H	-0.632992	-7.165550	-0.422869
H	6.574085	3.795613	3.038283	H	-1.218367	-7.127108	-2.092367
C	5.891868	0.585527	4.252075	C	-3.020957	-2.550703	-2.574406
H	5.571509	-0.364059	3.809730	H	-3.104065	-1.506453	-2.261394
H	5.175083	0.844980	5.040401	C	-1.693724	-2.688218	-3.344215
H	6.867858	0.430168	4.727798	H	-1.558942	-3.701277	-3.741678
C	3.393187	1.544210	-1.150125	H	-0.839348	-2.457163	-2.701250
H	2.359439	1.562144	-1.507195	H	-1.676897	-1.996979	-4.195556
C	4.160796	2.654605	-1.896503	C	-4.227275	-2.836902	-3.492108
H	3.732678	3.644786	-1.702410	H	-5.174559	-2.691520	-2.960492
H	4.134557	2.479562	-2.978914	H	-4.209869	-3.867532	-3.865984
H	5.212714	2.683788	-1.587259	H	-4.217125	-2.166282	-4.359973
C	3.961235	0.156563	-1.504642	O	-0.282912	-1.875666	1.906254
H	3.394205	-0.633626	-1.006528	H	0.189121	-2.724731	1.871059
H	5.017603	0.063547	-1.225391				
H	3.895308	-0.004761	-2.587773				
C	-3.709005	-3.312544	2.498558	TS1-R E= -3768.21045413			
H	-3.645086	-2.221241	2.514011	H	0.286981	2.038152	-2.312366
C	-2.697241	-3.832433	3.537375	C	-0.232407	-0.090548	3.535327
H	-2.935936	-3.427479	4.527981	C	-0.278090	1.278146	3.825303
H	-1.680202	-3.519054	3.286263	C	-0.749100	1.741404	5.064951
H	-2.711615	-4.925418	3.618188	C	-1.147732	0.803665	6.018016
C	-5.143447	-3.699781	2.914922	C	-1.097587	-0.565726	5.744935
H	-5.267229	-4.789136	2.940674	C	-0.646002	-1.008870	4.499524
H	-5.888482	-3.300905	2.217809	H	0.111530	-0.417750	2.560147
				H	-1.508027	1.153151	6.983103

H	-1.413050	-1.280919	6.499339	C	1.075067	-4.272750	1.852074
H	-0.613856	-2.070606	4.272379	C	2.131159	-2.631456	0.370142
C	-0.833041	3.234804	5.268454	C	-1.215245	-5.460632	2.965665
H	-1.797534	3.606027	4.890170	H	-2.344944	-4.301282	1.573041
H	-0.796710	3.487411	6.333992	C	1.186396	-5.221476	2.904902
C	0.306990	3.939628	4.520371	C	2.221619	-3.629243	1.319168
H	0.208099	5.025622	4.556019	C	0.067835	-5.807268	3.452063
H	1.268473	3.686444	4.992742	H	-2.099365	-5.905846	3.414013
C	0.407069	3.501439	3.070084	H	2.177512	-5.463881	3.281088
N	0.126976	2.210575	2.837853	H	3.200415	-3.917189	1.693655
H	0.283757	1.828860	1.892588	H	0.165045	-6.524624	4.262342
C	0.082870	3.877741	-1.434564	C	3.359359	-1.941311	-0.147309
C	1.427219	3.566094	-0.963427	C	3.800751	-2.182560	-1.472936
H	-0.743065	3.422767	-0.890564	C	4.107478	-1.084666	0.695064
H	1.511858	2.635706	-0.410324	C	4.967823	-1.559633	-1.924536
C	-2.112700	-1.462943	-0.574147	C	5.272631	-0.491260	0.189642
C	-1.605521	-2.750572	-0.461363	C	5.722255	-0.707859	-1.112829
C	-2.327662	-3.826591	-1.089325	H	5.301001	-1.755460	-2.940657
C	-3.606784	-3.552817	-1.672891	H	5.854137	0.160032	0.838907
C	-4.106009	-2.225615	-1.664678	C	-3.922455	0.231721	-1.227178
C	-3.376562	-1.166523	-1.165649	C	-4.502029	0.812553	-0.074059
H	-0.833779	-5.373405	-0.800676	C	-3.913876	0.946749	-2.448599
C	-1.818956	-5.151588	-1.193318	C	-5.062382	2.090743	-0.165177
C	-4.343692	-4.609419	-2.273478	C	-4.491615	2.222729	-2.482520
H	-5.088510	-2.037863	-2.089228	C	-5.069701	2.816262	-1.359559
C	-3.832028	-5.885033	-2.333880	H	-5.512729	2.527119	0.722954
C	-2.549412	-6.150533	-1.799374	H	-4.493373	2.774789	-3.419142
H	-5.318258	-4.383514	-2.699897	O	0.730647	-1.315750	-1.077689
H	-4.400966	-6.683395	-2.802393	O	-1.405178	-0.410950	-0.011377
H	-2.132356	-7.151383	-1.872262	P	0.005005	0.104271	-0.680188
C	-0.318793	-2.998797	0.254449	O	0.731129	0.850391	0.407143
C	-0.219467	-3.950145	1.329502	C	3.078118	-3.139884	-2.421583
C	0.829069	-2.311600	-0.119144	H	2.183340	-3.513786	-1.917076
C	-1.355263	-4.561318	1.930573	C	3.953426	-4.368562	-2.742142

H	4.249592	-4.894838	-1.827529	H	-5.118864	0.657602	-4.965932
H	4.869199	-4.082491	-3.273279	H	-5.062785	-0.920974	-4.169283
H	3.405318	-5.073768	-3.378779	H	-4.025383	-0.601112	-5.570585
C	2.610420	-2.438843	-3.711245	C	-5.686461	4.206567	-1.446734
H	1.955704	-1.593280	-3.481544	H	-5.562937	4.548364	-2.483723
H	2.053046	-3.141069	-4.343141	C	-7.197615	4.186548	-1.146754
H	3.458409	-2.067683	-4.299626	H	-7.632004	5.185485	-1.275703
C	6.998598	-0.046717	-1.617305	H	-7.394941	3.868749	-0.115982
H	7.380553	0.580717	-0.799546	H	-7.723930	3.495974	-1.814802
C	8.088272	-1.085319	-1.946139	C	-4.958541	5.216969	-0.539645
H	9.018581	-0.589723	-2.249593	H	-5.378915	6.222611	-0.662839
H	7.776578	-1.740761	-2.768117	H	-3.889478	5.262612	-0.775749
H	8.305420	-1.718794	-1.079100	H	-5.053415	4.943650	0.517938
C	6.735124	0.875792	-2.822631	C	-4.578632	0.071141	1.260120
H	5.991371	1.643435	-2.581354	H	-4.012122	-0.859622	1.165397
H	6.359609	0.309813	-3.683191	C	-3.939186	0.869595	2.410364
H	7.658871	1.378944	-3.133903	H	-4.485959	1.798220	2.614828
C	3.711914	-0.780951	2.140546	H	-2.903016	1.129035	2.174645
H	2.722999	-1.210885	2.320500	H	-3.936974	0.276931	3.332715
C	4.689416	-1.435064	3.138040	C	-6.032236	-0.319363	1.594328
H	4.748260	-2.519841	2.994030	H	-6.468662	-0.937539	0.801641
H	4.369034	-1.246438	4.169968	H	-6.666707	0.567409	1.712591
H	5.703059	-1.032140	3.022851	H	-6.073089	-0.888069	2.531498
C	3.593811	0.730764	2.409044	O	-0.241928	0.790141	-2.011891
H	2.882286	1.187776	1.716233	S	0.907897	4.577171	1.877210
H	4.558831	1.242643	2.310332	O	0.618628	3.049092	-2.492896
H	3.235242	0.904049	3.430967	C	2.634002	4.335086	-1.221472
C	-3.331298	0.364833	-3.737869	C	2.614323	5.614939	-1.805660
H	-2.696692	-0.483369	-3.465207	C	3.868873	3.764625	-0.857648
C	-2.439811	1.359732	-4.503677	C	3.802811	6.305052	-2.020467
H	-1.962413	0.852801	-5.350718	H	1.671868	6.070912	-2.091466
H	-1.650830	1.755704	-3.860975	C	5.055678	4.459789	-1.070988
H	-3.015244	2.199566	-4.911796	H	3.886345	2.776981	-0.405136
C	-4.451082	-0.158020	-4.661861	C	5.023671	5.729497	-1.653917

H	3.780267	7.293024	-2.470907	C	1.475687	2.916163	-1.069557
H	6.003247	4.014047	-0.783561	H	-3.240449	4.345849	-1.155137
H	5.949526	6.273046	-1.821170	C	-2.330787	4.821155	-1.502346
H	-0.141577	4.882109	-1.787470	C	-0.009647	6.057141	-2.462550
TS1-S E= -3768.20792842				H	2.243846	4.671154	-2.003581
H	0.768844	-2.010740	-2.257400	C	-1.233069	6.658719	-2.647184
C	-0.529829	-0.100015	3.573699	C	-2.404221	6.023602	-2.171303
C	0.522437	-0.967294	3.890052	H	0.898304	6.521988	-2.839631
C	1.113858	-0.954193	5.164052	H	-1.304518	7.610062	-3.167214
C	0.610328	-0.074555	6.122972	H	-3.373328	6.485545	-2.339845
C	-0.446747	0.788407	5.823474	C	-2.128618	2.282531	0.078391
C	-1.009393	0.777649	4.545029	C	-2.904996	2.966620	1.077988
H	-0.947619	-0.115491	2.573145	C	-2.505018	0.993261	-0.273869
H	1.058509	-0.062763	7.114120	C	-2.507336	4.204327	1.656498
H	-0.824550	1.467240	6.582798	C	-4.116425	2.361882	1.547028
H	-1.823487	1.452776	4.297202	C	-3.724345	0.385943	0.151087
C	2.293700	-1.865481	5.401223	C	-3.276823	4.819539	2.620113
H	3.221446	-1.354955	5.101560	H	-1.575846	4.659450	1.340163
H	2.396851	-2.102425	6.465975	C	-4.897137	3.032147	2.528047
C	2.142875	-3.157391	4.586800	C	-4.512241	1.101455	1.029535
H	3.033429	-3.784393	4.649198	C	-4.490894	4.236909	3.054970
H	1.302135	-3.746307	4.984391	H	-2.945518	5.759545	3.053204
C	1.831356	-2.885686	3.125537	H	-5.819590	2.564165	2.863872
N	1.022288	-1.843180	2.892926	H	-5.459287	0.679310	1.355406
H	0.671064	-1.681954	1.935479	H	-5.092394	4.736232	3.809658
C	0.864668	-3.742969	-1.170634	C	-4.163350	-0.952591	-0.367291
C	2.218781	-3.232573	-0.998548	C	-4.572036	-1.086017	-1.718383
H	0.724663	-4.802883	-1.369390	C	-4.221514	-2.072445	0.495885
C	0.288821	2.303385	-0.569203	C	-5.025568	-2.328402	-2.170921
C	-0.952752	2.925025	-0.581079	C	-4.692864	-3.290884	-0.010965
C	-1.080495	4.181163	-1.273245	C	-5.097399	-3.447128	-1.336102
C	0.097951	4.808250	-1.792936	H	-5.339435	-2.420226	-3.207830
C	1.352836	4.165174	-1.641550	H	-4.743460	-4.151724	0.652091
				C	2.827636	2.274147	-0.933393

C	3.506639	2.338182	0.307384	H	-5.750039	-1.360917	2.718237
C	3.456639	1.677396	-2.050959	H	-4.688779	-2.065292	3.953760
C	4.802585	1.820941	0.400830	H	-5.508002	-3.111226	2.780885
C	4.755931	1.171958	-1.899797	C	-2.727895	-3.076125	2.299994
C	5.451081	1.235915	-0.690241	H	-1.859591	-2.966768	1.644809
H	5.323677	1.888721	1.352556	H	-3.117253	-4.096174	2.198452
H	5.250586	0.726926	-2.760221	H	-2.392866	-2.953357	3.337206
O	-1.706574	0.281815	-1.153410	C	2.787556	1.604340	-3.424395
O	0.416029	1.065077	0.039452	H	1.719797	1.797136	-3.286395
P	-0.247386	-0.278285	-0.642710	C	2.908339	0.218054	-4.082578
O	-0.356529	-1.289379	0.466261	H	2.322685	0.195583	-5.009132
C	-4.575961	0.086109	-2.700770	H	2.522778	-0.562560	-3.423423
H	-4.184535	0.967965	-2.186640	H	3.944471	-0.024528	-4.348334
C	-6.009332	0.435192	-3.149781	C	3.346624	2.689880	-4.367702
H	-6.651412	0.658605	-2.290155	H	4.420978	2.546094	-4.537475
H	-6.470639	-0.390617	-3.704350	H	3.206972	3.695564	-3.957580
H	-6.001193	1.313457	-3.806816	H	2.843556	2.649444	-5.341587
C	-3.660335	-0.172775	-3.912607	C	6.883109	0.724229	-0.586651
H	-2.635180	-0.376431	-3.590071	H	7.111832	0.212930	-1.532685
H	-3.644084	0.704853	-4.570557	C	7.881584	1.890247	-0.442717
H	-4.009635	-1.025151	-4.508153	H	8.914219	1.520390	-0.423966
C	-5.599943	-4.792615	-1.843159	H	7.706304	2.444112	0.487395
H	-5.554652	-5.492272	-0.997031	H	7.786426	2.597164	-1.274150
C	-7.068430	-4.722300	-2.303631	C	7.070583	-0.298069	0.549594
H	-7.427361	-5.713251	-2.607584	H	8.095816	-0.687853	0.551510
H	-7.184690	-4.049053	-3.161290	H	6.383644	-1.145563	0.446761
H	-7.717489	-4.354898	-1.501143	H	6.890187	0.155483	1.531116
C	-4.699591	-5.359596	-2.957448	C	2.889297	2.991327	1.543567
H	-3.660805	-5.446469	-2.620239	H	1.855027	3.256744	1.308390
H	-4.708675	-4.714320	-3.843882	C	2.842345	2.029409	2.744842
H	-5.044148	-6.354255	-3.265967	H	3.848171	1.753361	3.084285
C	-3.794201	-2.016660	1.962867	H	2.305504	1.111697	2.487407
H	-3.337386	-1.040367	2.145817	H	2.324426	2.497530	3.590193
C	-5.006670	-2.143925	2.906912	C	3.618836	4.300569	1.904502

H	3.598722	5.008277	1.067981	H	0.510611	7.546454	-3.444127
H	4.669263	4.116022	2.160060	H	-1.670115	7.081383	-2.323484
H	3.143475	4.781047	2.768464	C	-1.226276	2.981075	0.515227
O	0.479788	-0.656538	-1.920073	C	-1.645837	3.943040	1.498507
S	2.442380	-3.889369	1.918755	C	-1.956406	1.808771	0.372781
O	1.098073	-3.013363	-2.406670	C	-0.874142	5.086756	1.847853
H	0.099887	-3.301745	-0.535100	C	-2.880235	3.729385	2.190250
H	2.283289	-2.222926	-0.614057	C	-3.198491	1.587264	1.037649
C	3.456371	-3.893628	-1.378616	C	-1.316506	5.979395	2.799563
C	3.523292	-5.271960	-1.652519	H	0.082428	5.247806	1.364594
C	4.627290	-3.116653	-1.465069	C	-3.317973	4.678230	3.153720
C	4.735023	-5.856894	-2.005796	C	-3.638422	2.567085	1.905405
H	2.631624	-5.885919	-1.578544	C	-2.556563	5.784076	3.453036
C	5.836584	-3.704953	-1.822337	H	-0.703887	6.840063	3.054361
H	4.576310	-2.050576	-1.259638	H	-4.264052	4.503474	3.660579
C	5.891452	-5.075216	-2.092321	H	-4.595681	2.436155	2.402889
H	4.781270	-6.922280	-2.211111	H	-2.896426	6.499906	4.196478
H	6.734848	-3.098399	-1.888952	C	-4.073055	0.390733	0.793930
H	6.836074	-5.535938	-2.368003	C	-4.895895	0.354088	-0.358533
				C	-4.183593	-0.625505	1.772284
				C	-5.828515	-0.680730	-0.495178
				C	-5.131207	-1.639542	1.580461
				C	-5.974103	-1.683554	0.468815
				H	-6.476460	-0.686325	-1.368649
				H	-5.231226	-2.414300	2.337115
				C	3.426821	1.592394	-0.920978
				C	4.207801	1.547507	0.259848
				C	3.828616	0.852284	-2.059726
				C	5.381212	0.785164	0.270305
				C	5.019694	0.115883	-1.996242
				C	5.819143	0.075275	-0.851714
				H	5.983799	0.768843	1.174935
				H	5.344681	-0.434683	-2.876170
				O	-1.497506	0.841239	-0.517805
TS2-R E= -3768.22513512							
C	1.014272	2.295212	-0.332876				
C	-0.022539	3.217868	-0.330377				
C	0.086143	4.385737	-1.162186				
C	1.319410	4.632865	-1.844681				
C	2.381595	3.705042	-1.709017				
C	2.253375	2.526296	-1.001167				
H	-1.940840	5.109406	-0.891904				
C	-0.986087	5.298377	-1.368536				
C	1.452368	5.793722	-2.654071				
H	3.327666	3.925089	-2.195630				
C	0.401325	6.666265	-2.816499				
C	-0.832721	6.404917	-2.174906				
H	2.401071	5.970232	-3.155583				

O	0.873389	1.134708	0.418202	H	2.048402	1.279313	-3.161290
P	-0.171661	-0.036093	-0.092413	C	2.796455	-0.565582	-3.924014
O	-0.417009	-0.977812	1.044842	H	2.125595	-0.515299	-4.789729
C	-4.840878	1.442086	-1.432008	H	2.335637	-1.216336	-3.177555
H	-4.054985	2.150452	-1.156857	H	3.728805	-1.034942	-4.261545
C	-6.158992	2.239014	-1.493790	C	3.717866	1.724906	-4.439403
H	-6.397593	2.684305	-0.521379	H	4.714219	1.336276	-4.684211
H	-7.002571	1.601671	-1.784503	H	3.838463	2.760897	-4.106816
H	-6.083513	3.048526	-2.229987	H	3.125088	1.734063	-5.362227
C	-4.466362	0.877213	-2.814940	C	7.149575	-0.668468	-0.863372
H	-3.501256	0.361693	-2.779433	H	7.182216	-1.254299	-1.792690
H	-4.391162	1.687886	-3.549845	C	8.331504	0.321703	-0.903077
H	-5.220998	0.170333	-3.181594	H	9.286361	-0.213944	-0.972075
C	-7.052657	-2.755224	0.362852	H	8.356377	0.938737	0.003225
H	-6.856517	-3.486497	1.159138	H	8.254538	0.996036	-1.763017
C	-8.449548	-2.155803	0.623644	C	7.302770	-1.653334	0.308413
H	-9.217763	-2.938829	0.610776	H	8.245122	-2.207787	0.221959
H	-8.709678	-1.417309	-0.144441	H	6.481878	-2.377366	0.334417
H	-8.489229	-1.652918	1.596169	H	7.313190	-1.135219	1.274249
C	-7.026096	-3.516896	-0.973829	C	3.845906	2.347789	1.511485
H	-6.043646	-3.961802	-1.161096	H	2.918609	2.891591	1.312853
H	-7.261314	-2.856188	-1.817150	C	3.579881	1.434853	2.722814
H	-7.772973	-4.320004	-0.970201	H	4.464664	0.844599	2.989360
C	-3.351871	-0.626053	3.056338	H	2.758573	0.743207	2.511993
H	-2.562296	0.122623	2.947064	H	3.302004	2.035026	3.597928
C	-4.216827	-0.227335	4.270247	C	4.920998	3.405103	1.832887
H	-4.682456	0.754486	4.131735	H	5.080563	4.077944	0.982716
H	-3.605717	-0.186219	5.180120	H	5.884471	2.942186	2.077185
H	-5.020304	-0.955058	4.438105	H	4.615878	4.011733	2.694221
C	-2.650445	-1.971682	3.316663	O	0.342396	-0.634063	-1.407967
H	-1.972806	-2.217559	2.496440	C	-2.698975	-2.788746	-1.683259
H	-3.365200	-2.792563	3.450635	C	-1.656833	-3.696497	-1.490711
H	-2.052430	-1.906006	4.233715	C	-1.561295	-4.868137	-2.261385
C	3.033370	0.851414	-3.367381	C	-2.519076	-5.103653	-3.246332

C	-3.564115	-4.199945	-3.454929				
C	-3.650568	-3.048367	-2.670726				
H	-2.765909	-1.891118	-1.076652				
H	-2.445003	-6.003238	-3.853239				
H	-4.303327	-4.393206	-4.227017				
H	-4.456279	-2.338548	-2.825025				
C	-0.398403	-5.787218	-1.969609				
H	-0.619372	-6.426331	-1.101386				
H	-0.203894	-6.454501	-2.815763				
C	0.843133	-4.929465	-1.687192				
H	1.721087	-5.537388	-1.456406				
H	1.072106	-4.330233	-2.573973				
C	0.569583	-3.968154	-0.534354				
S	1.263802	-4.316797	1.095489				
N	-0.696683	-3.492589	-0.466255				
H	-0.857151	-2.742997	0.218433				
C	2.940964	-3.619805	0.753892				
C	2.662208	-2.324650	-0.020923				
H	2.271616	-1.556181	0.651280				
H	3.580662	-1.957489	-0.491395				
O	1.713021	-2.619343	-1.046654				
H	1.055939	-1.697870	-1.234865				
H	3.480200	-4.319453	0.107184				
C	3.705645	-3.427946	2.044015				
C	4.907788	-4.115886	2.252638				
C	3.231120	-2.568372	3.047608				
C	5.634288	-3.940003	3.431857				
H	5.277176	-4.794287	1.486954				
C	3.956872	-2.393763	4.225370				
H	2.288047	-2.046096	2.910751				
C	5.160692	-3.076392	4.420190				
H	6.565963	-4.479883	3.577203				
H	3.578581	-1.725350	4.993757				
H	5.722941	-2.938821	5.339825				
				TS2-S E= -3768.22276445			
				C	-0.373564	2.588361	0.212130
				C	0.835428	3.234268	0.429480
				C	0.876343	4.335874	1.351965
				C	-0.354288	4.830505	1.889218
				C	-1.569595	4.200656	1.523648
				C	-1.612445	3.071557	0.729268
				H	3.032637	4.559570	1.418577
				C	2.087761	4.944021	1.784888
				C	-0.334231	5.931968	2.787501
				H	-2.500993	4.612600	1.902213
				C	0.854214	6.508485	3.171848
				C	2.076052	5.997770	2.672374
				H	-1.280107	6.300776	3.177358
				H	0.859417	7.344687	3.865633
				H	3.015315	6.438314	2.995789
				C	2.058756	2.782517	-0.290660
				C	2.805820	3.691179	-1.118423
				C	2.482007	1.463568	-0.192397
				C	2.362225	5.007691	-1.428268
				C	4.037969	3.245849	-1.693133
				C	3.713895	1.005431	-0.745462
				C	3.111841	5.840350	-2.230037
				H	1.412895	5.352604	-1.036070
				C	4.797974	4.135179	-2.500659
				C	4.470266	1.918471	-1.453901
				C	4.349422	5.408600	-2.763798
				H	2.745988	6.837713	-2.458850
				H	5.737372	3.781381	-2.918919
				H	5.427880	1.603308	-1.859260
				H	4.933702	6.078377	-3.388811
				C	4.264537	-0.379119	-0.551980
				C	4.928013	-0.702944	0.656393

C	4.261770	-1.301932	-1.624960	C	6.142147	-4.984881	0.992407
C	5.610272	-1.921948	0.750800	H	5.075656	-5.228145	1.032624
C	4.955992	-2.509361	-1.472365	H	6.407292	-4.475892	1.927346
C	5.652310	-2.835533	-0.307306	H	6.707949	-5.923907	0.960425
H	6.145388	-2.149481	1.669801	C	3.572665	-1.007535	-2.958656
H	4.971882	-3.215001	-2.299785	H	2.928156	-0.135228	-2.818433
C	-2.942485	2.450642	0.414126	C	4.605368	-0.664149	-4.052361
C	-3.504416	2.595230	-0.878871	H	5.226528	0.192530	-3.770293
C	-3.694522	1.825495	1.439592	H	4.099129	-0.418093	-4.993757
C	-4.804688	2.133032	-1.111663	H	5.275390	-1.511637	-4.243372
C	-4.997148	1.393531	1.152301	C	2.661053	-2.155834	-3.428092
C	-5.579822	1.543457	-0.108323	H	1.887454	-2.363459	-2.685996
H	-5.232444	2.266060	-2.102079	H	3.222753	-3.076660	-3.625151
H	-5.583670	0.932559	1.944192	H	2.159407	-1.871980	-4.360880
O	1.709286	0.568218	0.543443	C	-3.154194	1.620060	2.856903
O	-0.392537	1.474431	-0.617095	H	-2.090905	1.874012	2.852607
P	0.281879	0.060827	-0.097280	C	-3.258405	0.155522	3.324456
O	0.445749	-0.837926	-1.282516	H	-2.795108	0.046145	4.312292
C	4.969734	0.259346	1.843956	H	-2.741845	-0.516588	2.635245
H	4.370212	1.137849	1.590256	H	-4.301354	-0.173056	3.414195
C	6.402639	0.758458	2.115770	C	-3.857544	2.549898	3.867013
H	6.828204	1.241033	1.228723	H	-4.930287	2.328940	3.927877
H	7.069114	-0.064725	2.399681	H	-3.752676	3.604635	3.591354
H	6.406370	1.487945	2.934868	H	-3.431552	2.419104	4.869124
C	4.344681	-0.356347	3.110001	C	-7.026761	1.128999	-0.349059
H	3.310293	-0.664421	2.926616	H	-7.348504	0.557888	0.532792
H	4.341381	0.374902	3.927418	C	-7.941260	2.366231	-0.456044
H	4.908090	-1.232309	3.454334	H	-8.990303	2.065587	-0.566658
C	6.473434	-4.117882	-0.234790	H	-7.673594	2.978636	-1.325589
H	6.224542	-4.707156	-1.128077	H	-7.858513	2.998521	0.434767
C	7.983131	-3.808466	-0.294230	C	-7.199265	0.214686	-1.574866
H	8.569826	-4.735319	-0.304970	H	-8.247075	-0.091431	-1.678096
H	8.298630	-3.221470	0.576925	H	-6.592348	-0.692433	-1.485647
H	8.234479	-3.233426	-1.192207	H	-6.914361	0.725332	-2.502500

C	1.464921	2.049219	-0.516763	H	3.618946	2.740112	0.909557
C	-0.073863	5.189128	-1.867355	C	5.701469	2.888318	1.338059
C	2.086089	4.117316	-2.287355	H	5.976737	3.326401	0.371894
C	2.711202	2.005717	-1.207778	H	6.547425	2.281405	1.681795
C	0.225391	6.157299	-2.800871	H	5.566341	3.705935	2.056611
H	-1.031128	5.209936	-1.359734	C	3.992204	1.482527	2.592802
C	2.372861	5.141920	-3.229993	H	3.045258	0.940601	2.514834
C	2.999778	3.059004	-2.051890	H	3.868165	2.292228	3.322695
C	1.465553	6.144832	-3.482221	H	4.742485	0.787680	2.987655
H	-0.500400	6.936138	-3.018610	C	6.834886	-2.073042	-0.422929
H	3.322241	5.108564	-3.759225	H	6.742957	-2.786428	-1.253940
H	3.957795	3.075871	-2.564015	C	8.235995	-1.437432	-0.516393
H	1.691969	6.918990	-4.210194	H	9.016513	-2.204789	-0.444085
C	3.721933	0.916950	-0.986267	H	8.398453	-0.717853	0.294993
C	4.540891	0.958040	0.167399	H	8.366695	-0.905019	-1.464953
C	3.913078	-0.098705	-1.952678	C	6.678635	-2.866751	0.887170
C	5.526030	-0.020286	0.335151	H	5.692095	-3.337763	0.955146
C	4.920404	-1.048318	-1.736626	H	6.789905	-2.218836	1.764232
C	5.736830	-1.032798	-0.604076	H	7.440785	-3.652731	0.955245
H	6.150984	0.017023	1.223949	C	3.085522	-0.168146	-3.237328
H	5.081387	-1.826997	-2.478370	H	2.174238	0.416154	-3.078508
C	-3.789886	1.080945	0.914248	C	3.848833	0.452200	-4.426363
C	-4.579738	0.961922	-0.254589	H	4.109092	1.498944	-4.241209
C	-4.020746	0.220937	2.013963	H	3.239843	0.412786	-5.338076
C	-5.571174	-0.022420	-0.306018	H	4.780636	-0.093478	-4.619919
C	-5.033428	-0.741315	1.909718	C	2.641294	-1.597700	-3.595758
C	-5.816637	-0.886968	0.764338	H	2.148066	-2.081382	-2.749311
H	-6.175990	-0.107523	-1.205646	H	3.483527	-2.225867	-3.908963
H	-5.217916	-1.403767	2.751760	H	1.932217	-1.568227	-4.431695
O	1.156807	0.999588	0.351123	C	-3.235197	0.328167	3.321969
O	-1.263270	0.992553	-0.470958	H	-2.348570	0.940412	3.131010
P	-0.044414	-0.019322	-0.081152	C	-2.738433	-1.032240	3.844133
O	0.288054	-0.844882	-1.286090	H	-2.098507	-0.881399	4.721836
C	4.410202	2.054070	1.225346	H	-2.154539	-1.564489	3.089734

H	-3.565716	-1.680823	4.156008	H	-5.063026	-3.491716	-4.285681
C	-4.070416	1.036098	4.409634	H	-3.516355	-1.552498	-4.523795
H	-4.974579	0.460940	4.644116	C	-2.169558	-5.642728	-1.253818
H	-4.387195	2.036475	4.096175	H	-2.517888	-5.397717	-0.242220
H	-3.489131	1.139367	5.334113	H	-2.638058	-6.590879	-1.537521
C	-6.902599	-1.952947	0.696712	C	-0.646621	-5.805951	-1.220350
H	-6.900793	-2.475581	1.663101	H	-0.323018	-6.446706	-0.398505
C	-8.302984	-1.339318	0.508027	H	-0.286244	-6.261856	-2.156165
H	-9.073566	-2.119824	0.523752	C	0.055345	-4.482375	-1.087209
H	-8.382007	-0.813709	-0.451239	N	-0.440803	-3.432472	-1.721440
H	-8.529900	-0.619309	1.302017	H	-0.012638	-2.492463	-1.599558
C	-6.607807	-3.001075	-0.393238	C	1.934988	-3.639029	0.229825
H	-7.367163	-3.792964	-0.384090	H	1.760593	-2.603719	-0.071978
H	-5.626225	-3.462879	-0.242316	C	1.364422	-3.964735	1.620343
H	-6.608513	-2.547945	-1.391769	H	1.470238	-5.049785	1.736162
C	-4.423665	1.908287	-1.445280	S	-0.444578	-3.640483	1.597002
H	-3.588533	2.583270	-1.238654	H	-0.412285	-1.890754	1.299701
C	-4.082530	1.157842	-2.745303	C	2.201585	-3.321965	2.722186
H	-4.890171	0.478601	-3.043409	C	3.370375	-3.987540	3.126928
H	-3.170890	0.565974	-2.620818	C	1.873131	-2.113607	3.347296
H	-3.924419	1.868325	-3.566211	C	4.193219	-3.461893	4.123120
C	-5.675969	2.790019	-1.623373	H	3.630467	-4.938851	2.665737
H	-5.885657	3.366623	-0.715359	C	2.694152	-1.587710	4.347828
H	-6.563563	2.185976	-1.846384	H	0.968422	-1.588585	3.065459
H	-5.535521	3.496608	-2.450704	C	3.855460	-2.255383	4.739261
O	-0.389607	-0.749100	1.238830	H	5.087655	-4.000649	4.425433
C	-2.040336	-2.368919	-3.195122	H	2.416921	-0.652522	4.826906
C	-1.702953	-3.448885	-2.374453	H	4.485799	-1.845417	5.524101
C	-2.569233	-4.541090	-2.209072	H	3.001562	-3.863124	0.154012
C	-3.776057	-4.537453	-2.909424	O	1.322519	-4.564163	-0.712233
C	-4.120899	-3.472732	-3.745550				
C	-3.253307	-2.387689	-3.882078	TS3-S E= -3768.23019491			
H	-1.356891	-1.530494	-3.283909	C	-2.240219	1.703964	0.407630
H	-4.453927	-5.379907	-2.794778	C	-1.652785	2.952438	0.556813

C	-2.201805	3.851931	1.537481	H	5.631418	1.328754	1.379384
C	-3.418265	3.491608	2.200735	H	5.283170	0.312057	-2.757569
C	-4.029188	2.247802	1.902719	C	-4.139395	0.014522	0.794420
C	-3.455893	1.326968	1.049258	C	-4.847461	-0.186368	-0.415345
H	-0.631142	5.346117	1.452436	C	-4.153822	-0.986500	1.794620
C	-1.574387	5.073382	1.910769	C	-5.564603	-1.373598	-0.592929
C	-3.984020	4.378436	3.156764	C	-4.891812	-2.154390	1.563354
H	-4.973307	2.003999	2.381914	C	-5.607601	-2.370572	0.385553
C	-3.361870	5.562525	3.478205	H	-6.115291	-1.516982	-1.519583
C	-2.137532	5.902789	2.855961	H	-4.911867	-2.924015	2.331277
H	-4.914410	4.092372	3.641596	O	0.649831	1.347876	0.431970
H	-3.798775	6.229292	4.216504	O	-1.671290	0.794437	-0.481694
H	-1.632764	6.825270	3.129972	P	-0.238537	0.094278	-0.139412
C	-0.471139	3.339248	-0.267798	O	0.316591	-0.474721	-1.412351
C	-0.476150	4.532524	-1.071737	C	3.389493	2.755144	1.678748
C	0.666697	2.545078	-0.276276	H	2.433244	3.240200	1.465577
C	-1.641827	5.319104	-1.287679	C	4.370469	3.870493	2.094193
C	0.736852	4.936764	-1.716415	H	4.512863	4.595097	1.284535
C	1.888794	2.932929	-0.899185	H	5.355124	3.465850	2.356802
C	-1.599388	6.454901	-2.066357	H	3.987549	4.408606	2.969692
H	-2.579079	5.009014	-0.840896	C	3.145569	1.770878	2.838327
C	0.752421	6.124928	-2.496779	H	2.383881	1.033150	2.566932
C	1.898270	4.136482	-1.575481	H	2.791947	2.308911	3.726202
C	-0.389020	6.873325	-2.668353	H	4.061946	1.236775	3.117083
H	-2.506231	7.032646	-2.223311	C	6.986541	0.062684	-0.662082
H	1.685725	6.422946	-2.968674	H	7.062618	-0.544366	-1.575233
H	2.821888	4.474813	-2.037487	C	8.104251	1.124536	-0.723143
H	-0.367877	7.775456	-3.273535	H	9.091563	0.648691	-0.768180
C	3.141185	2.110110	-0.810260	H	8.079910	1.767770	0.164859
C	3.861067	2.046216	0.408498	H	7.993180	1.767142	-1.603456
C	3.654546	1.467682	-1.963400	C	7.198015	-0.877856	0.536932
C	5.078010	1.356181	0.444555	H	6.426851	-1.653584	0.591373
C	4.879405	0.793406	-1.869239	H	7.185643	-0.332353	1.487610
C	5.615351	0.729340	-0.683897	H	8.171906	-1.375710	0.460379

C	2.944210	1.503310	-3.318241	H	-3.261333	-0.009704	-2.686634
H	1.963023	1.963441	-3.174290	H	-4.278533	1.121391	-3.603008
C	3.721821	2.369432	-4.330198	C	-6.314717	1.405890	-1.741091
H	3.871162	3.389233	-3.958351	H	-6.723554	1.825587	-0.815063
H	3.178330	2.431489	-5.280820	H	-6.998035	0.618021	-2.079761
H	4.711911	1.945727	-4.537789	H	-6.314414	2.195959	-2.502073
C	2.691488	0.096538	-3.892199	O	-0.392408	-0.826574	1.083011
H	2.070466	-0.489383	-3.210095	C	-1.365125	-2.946157	-3.029330
H	3.625073	-0.448618	-4.076349	C	-0.512719	-3.752765	-2.268301
H	2.162270	0.173230	-4.849961	C	-0.819938	-5.097952	-2.009251
C	-3.416604	-0.834534	3.126145	C	-1.989225	-5.625063	-2.559910
H	-2.737456	0.018497	3.039132	C	-2.842653	-4.835926	-3.334373
C	-2.550740	-2.060200	3.471398	C	-2.531400	-3.493519	-3.559968
H	-1.968692	-1.861596	4.379136	H	-1.110342	-1.903641	-3.191834
H	-1.848925	-2.286300	2.665579	H	-2.235026	-6.667856	-2.372890
H	-3.158608	-2.952418	3.663409	H	-3.746470	-5.266854	-3.754832
C	-4.400366	-0.536761	4.276729	H	-3.194273	-2.867866	-4.150084
H	-5.107277	-1.364322	4.413991	C	0.096105	-5.897904	-1.109505
H	-4.985377	0.369949	4.088254	H	-0.243535	-5.811067	-0.069395
H	-3.857910	-0.399182	5.220115	H	0.061267	-6.961169	-1.369567
C	-6.427729	-3.641040	0.199449	C	1.539457	-5.391962	-1.200193
H	-6.204227	-4.295581	1.053128	H	2.164880	-5.802828	-0.406271
C	-7.939714	-3.342246	0.231718	H	1.987253	-5.683673	-2.163176
H	-8.521761	-4.268642	0.150902	C	1.615275	-3.891262	-1.132853
H	-8.230473	-2.689952	-0.600630	N	0.687734	-3.180603	-1.770609
H	-8.223715	-2.839962	1.163030	H	0.686625	-2.144443	-1.706554
C	-6.046934	-4.407857	-1.079917	C	3.002681	-2.167711	-0.181219
H	-6.604271	-5.350661	-1.142567	H	2.374073	-1.392238	-0.621841
H	-4.976472	-4.637182	-1.103613	C	2.665325	-2.379203	1.307505
H	-6.281736	-3.825401	-1.979024	S	1.053542	-3.281380	1.435743
C	-4.887569	0.864752	-1.524718	H	0.165841	-1.888598	1.166683
H	-4.271841	1.713645	-1.214748	H	4.049735	-1.903508	-0.332481
C	-4.289256	0.332539	-2.840880	O	2.832305	-3.416155	-0.896838
H	-4.875044	-0.505481	-3.238209	H	2.490519	-1.376513	1.713552

C	3.759119	-3.036611	2.128206	H	2.700226	-1.931530	-0.795943
C	4.583925	-4.052539	1.622475	C	0.124058	2.371328	-0.375444
C	3.955956	-2.618182	3.452450	C	-1.144867	2.928252	-0.279145
C	5.576932	-4.628141	2.418806	C	-1.362246	4.240459	-0.829799
H	4.450260	-4.397981	0.602492	C	-0.238521	4.978295	-1.323975
C	4.943710	-3.194544	4.249984	C	1.048462	4.384504	-1.296623
H	3.321499	-1.835580	3.861737	C	1.254897	3.089968	-0.866245
C	5.760840	-4.203444	3.735096	H	-3.520984	4.280241	-0.615991
H	6.206747	-5.412510	2.006429	C	-2.650160	4.835501	-0.943306
H	5.077257	-2.852977	5.273226	C	-0.433360	6.283559	-1.851817
H	6.532994	-4.653003	4.353717	H	1.896570	4.964869	-1.650398
TS4-R E= -3768.22254126				C	-1.690422	6.837635	-1.924682
C	-0.309507	-0.270739	3.652596	C	-2.808897	6.096140	-1.476496
C	0.722008	-1.209359	3.753809	H	0.434661	6.831273	-2.211316
C	1.437611	-1.377418	4.949416	H	-1.828888	7.833452	-2.336773
C	1.081007	-0.600840	6.052988	H	-3.805205	6.522323	-1.558668
C	0.048003	0.335705	5.968477	C	-2.263770	2.157811	0.339953
C	-0.640482	0.502667	4.764747	C	-3.040062	2.689878	1.428119
H	-0.830164	-0.149356	2.708433	C	-2.588337	0.897005	-0.144002
H	1.624935	-0.728442	6.986287	C	-2.681058	3.874301	2.130201
H	-0.214798	0.932491	6.837195	C	-4.209472	1.981242	1.855491
H	-1.439485	1.234131	4.684928	C	-3.764294	0.187705	0.245352
C	2.585032	-2.360359	4.953199	C	-3.450188	4.344728	3.172684
H	3.499760	-1.860352	4.600504	H	-1.779997	4.403793	1.842553
H	2.794592	-2.713980	5.968333	C	-4.992249	2.504236	2.920555
C	2.277393	-3.549837	4.033868	C	-4.560100	0.765967	1.213380
H	3.143958	-4.199334	3.890762	C	-4.625734	3.662378	3.567197
H	1.474846	-4.163998	4.467943	H	-3.149390	5.247250	3.698050
C	1.793860	-3.106737	2.664669	H	-5.883833	1.960302	3.223730
N	1.064688	-1.983539	2.612955	H	-5.476608	0.264923	1.513670
H	0.614030	-1.702590	1.719560	H	-5.228498	4.048654	4.384629
C	2.634881	-3.007017	-0.968638	C	-4.156960	-1.111895	-0.394360
C	1.509800	-3.636733	-0.276794	C	-4.600735	-1.129626	-1.740639
				C	-4.143559	-2.312407	0.354813

C	-5.014141	-2.340843	-2.302818	H	-3.537159	-5.314491	-3.126341
C	-4.576676	-3.495443	-0.258423	H	-4.670809	-4.512201	-4.222758
C	-5.012086	-3.538560	-1.582299	H	-4.902788	-6.219446	-3.813190
H	-5.355803	-2.345523	-3.335049	C	-3.675989	-2.380934	1.809066
H	-4.570968	-4.418945	0.316463	H	-3.258004	-1.406862	2.076372
C	2.636742	2.501862	-0.893595	C	-4.849993	-2.661173	2.768341
C	3.393247	2.427737	0.300731	H	-5.635698	-1.902709	2.677417
C	3.216419	2.100168	-2.119900	H	-4.504102	-2.667302	3.809456
C	4.713875	1.972139	0.242291	H	-5.307932	-3.636254	2.562311
C	4.543139	1.647864	-2.119593	C	-2.552034	-3.415152	2.008304
C	5.314137	1.580983	-0.958170	H	-1.717784	-3.198280	1.336531
H	5.294711	1.937280	1.160532	H	-2.897491	-4.438633	1.819523
H	4.996859	1.350861	-3.062596	H	-2.185650	-3.376123	3.041953
O	-1.781412	0.325450	-1.113429	C	2.466329	2.180160	-3.450200
O	0.333177	1.089972	0.106766	H	1.411834	2.369745	-3.230960
P	-0.290855	-0.223099	-0.678258	C	2.521932	0.864844	-4.248846
O	-0.383192	-1.298880	0.380150	H	1.922909	0.959473	-5.162756
C	-4.688899	0.133806	-2.596990	H	2.110836	0.042695	-3.658893
H	-4.316318	0.975299	-2.007023	H	3.544133	0.610404	-4.554969
C	-6.151475	0.459889	-2.961028	C	2.985546	3.354331	-4.305661
H	-6.769526	0.570096	-2.062582	H	4.042113	3.215698	-4.566325
H	-6.598327	-0.329031	-3.577697	H	2.897552	4.310352	-3.777789
H	-6.205465	1.397043	-3.528552	H	2.416300	3.429877	-5.240151
C	-3.808010	0.041983	-3.857617	C	6.770375	1.135494	-1.014336
H	-2.764894	-0.149935	-3.590238	H	6.963015	0.794222	-2.041156
H	-3.850652	0.983243	-4.419178	C	7.726626	2.312192	-0.735584
H	-4.144660	-0.758013	-4.528155	H	8.772308	1.997543	-0.840763
C	-5.470138	-4.848436	-2.210750	H	7.593440	2.696045	0.283056
H	-5.355606	-5.629871	-1.446632	H	7.547083	3.140613	-1.429596
C	-6.958976	-4.805841	-2.605047	C	7.066314	-0.046235	-0.072824
H	-7.282921	-5.775753	-3.002057	H	8.108406	-0.371628	-0.179525
H	-7.144013	-4.050963	-3.378545	H	6.419373	-0.902517	-0.291114
H	-7.589683	-4.561112	-1.743230	H	6.914057	0.230631	0.977203
C	-4.592424	-5.246706	-3.412455	C	2.832233	2.885864	1.646319

H	1.761454	3.070025	1.524025	C	-0.399245	0.640751	4.829393
C	2.978435	1.812728	2.739871	H	0.184956	0.426553	2.752905
H	4.030202	1.617365	2.982417	H	-1.075275	3.605746	6.353846
H	2.520141	0.870773	2.423758	H	-0.987653	1.171586	6.837793
H	2.481818	2.136589	3.661977	H	-0.368540	-0.426789	5.027543
C	3.471857	4.217991	2.086572	C	-0.583536	4.856595	3.928328
H	3.312148	5.000080	1.335840	H	-1.581450	5.072808	3.517539
H	4.553737	4.110858	2.232000	H	-0.465602	5.492929	4.811867
H	3.037604	4.561502	3.033673	C	0.479307	5.208139	2.879623
O	0.442979	-0.502498	-1.965937	H	0.349983	6.214660	2.475686
H	1.413530	-4.713195	-0.293170	H	1.481814	5.160473	3.329200
H	0.636117	-3.034481	-0.055317	C	0.476565	4.234611	1.714457
O	2.067855	-3.822963	1.667624	N	0.190096	2.953644	1.994651
S	1.565264	-3.242891	-2.504419	H	0.305037	2.224837	1.264938
H	0.920420	-1.991661	-2.349938	C	2.083268	3.055861	-1.344758
C	3.979855	-3.674871	-1.054107	C	0.798989	3.741886	-1.240746
C	4.291815	-4.834041	-0.334095	C	-2.280155	-1.482900	-0.357037
C	4.956977	-3.103771	-1.884141	C	-1.833293	-2.778407	-0.130950
C	5.556146	-5.417404	-0.453507	C	-2.606395	-3.870703	-0.663037
H	3.565729	-5.263222	0.347101	C	-3.874653	-3.591594	-1.267367
C	6.216908	-3.685990	-2.000209	C	-4.319315	-2.248482	-1.361572
H	4.719195	-2.205007	-2.447913	C	-3.542445	-1.184971	-0.951982
C	6.519089	-4.849913	-1.286806	H	-1.181457	-5.451468	-0.242173
H	5.786157	-6.316007	0.112620	C	-2.156732	-5.220909	-0.654104
H	6.961845	-3.234127	-2.649246	C	-4.658428	-4.661587	-1.778056
H	7.500891	-5.306418	-1.378062	H	-5.298643	-2.053521	-1.790496
				C	-4.202666	-5.958814	-1.731572
				C	-2.931570	-6.234372	-1.174981
				H	-5.623845	-4.429953	-2.221934
				H	-4.807056	-6.768057	-2.132190
				H	-2.559005	-7.255187	-1.162691
				C	-0.563029	-3.022529	0.615039
				C	-0.518030	-3.874934	1.773499
				C	0.618618	-2.429126	0.190266
TS4-S E= -3768.22149008							
H	0.688631	1.548881	-2.697029				
C	-0.083004	1.107876	3.553824				
C	-0.123877	2.482521	3.298522				
C	-0.493616	3.395232	4.299407				
C	-0.795212	2.904580	5.570824				
C	-0.748654	1.535657	5.842705				

C	-1.685215	-4.381784	2.410160	C	3.605610	-4.933058	-2.168392
C	0.755087	-4.207159	2.340345	H	3.859215	-5.376452	-1.198726
C	1.899593	-2.767769	0.721187	H	4.541677	-4.770511	-2.715741
C	-1.595764	-5.192909	3.520568	H	3.012531	-5.663477	-2.732172
H	-2.659062	-4.112203	2.018110	C	2.404718	-3.031801	-3.356632
C	0.813811	-5.061962	3.474467	H	1.803934	-2.127183	-3.226050
C	1.935020	-3.671365	1.763511	H	1.807194	-3.760583	-3.917771
C	-0.334784	-5.549706	4.054311	H	3.278852	-2.780277	-3.969337
H	-2.503337	-5.559253	3.992925	C	6.945843	-0.749143	-1.467736
H	1.789692	-5.313364	3.883458	H	7.353711	-0.040432	-0.732780
H	2.896384	-3.971077	2.172825	C	7.963022	-1.898541	-1.609423
H	-0.277715	-6.197061	4.925183	H	8.934551	-1.517933	-1.947850
C	3.167025	-2.207445	0.144339	H	7.621444	-2.640094	-2.341340
C	3.597144	-2.616993	-1.143433	H	8.111142	-2.415939	-0.655163
C	3.966112	-1.315459	0.898001	C	6.783387	0.008158	-2.799233
C	4.806598	-2.126116	-1.643703	H	6.096609	0.855336	-2.696214
C	5.172482	-0.858882	0.347620	H	6.388545	-0.646253	-3.585087
C	5.614851	-1.246632	-0.917580	H	7.750795	0.393236	-3.144234
H	5.132303	-2.450889	-2.628787	C	3.582131	-0.833312	2.297629
H	5.795023	-0.184064	0.931706	H	2.573371	-1.194743	2.514241
C	-4.046635	0.222575	-1.094194	C	4.523326	-1.417770	3.370229
C	-4.579246	0.892854	0.033122	H	4.525348	-2.513456	3.351303
C	-4.054207	0.855702	-2.359245	H	4.212394	-1.096137	4.371767
C	-5.104332	2.179173	-0.126446	H	5.556749	-1.083530	3.217521
C	-4.597533	2.143073	-2.462188	C	3.534826	0.703040	2.394146
C	-5.124775	2.825650	-1.365451	H	2.837073	1.108138	1.656425
H	-5.516871	2.685601	0.743012	H	4.520096	1.155627	2.230412
H	-4.611898	2.632353	-3.433196	H	3.193491	1.007337	3.391059
O	0.579511	-1.536745	-0.865222	C	-3.525106	0.174438	-3.622052
O	-1.512897	-0.419231	0.091287	H	-2.937989	-0.694771	-3.312539
P	-0.092770	-0.046565	-0.659147	C	-2.582313	1.075830	-4.440294
O	0.682140	0.785400	0.336167	H	-2.165001	0.508668	-5.281109
C	2.816127	-3.619744	-1.993414	H	-1.753814	1.424348	-3.820034
H	1.894616	-3.875027	-1.464006	H	-3.102385	1.945187	-4.860422

C	-4.685773	-0.328318	-4.505137	H	2.602757	5.750693	-1.835693
H	-5.309243	0.507078	-4.847264	C	5.871531	5.095589	-1.182271
H	-5.334566	-1.026197	-3.964995	H	6.662450	3.167385	-0.622388
H	-4.298643	-0.844201	-5.392468	H	4.788367	6.874205	-1.744868
C	-5.702952	4.226013	-1.525477	H	6.834640	5.596825	-1.139723
H	-5.603524	4.495988	-2.585866	O	0.770003	4.665829	0.572228
C	-7.202945	4.274801	-1.177069	S	1.475675	2.662662	-3.095934
H	-7.610675	5.277128	-1.356809				
H	-7.374888	4.029750	-0.122202		TS5-R E= -3060.57191219		
H	-7.772323	3.560556	-1.781855	H	1.881062	1.432159	-2.455826
C	-4.914660	5.268632	-0.709819	C	-0.104198	-0.392611	3.132109
H	-5.311696	6.276910	-0.880464	C	1.077384	0.246566	3.524531
H	-3.854398	5.267105	-0.986560	C	1.256210	0.694077	4.844114
H	-4.979384	5.062309	0.365322	C	0.235015	0.468940	5.767664
C	-4.643025	0.241508	1.414349	C	-0.946972	-0.173531	5.390206
H	-4.127455	-0.721585	1.361676	C	-1.115144	-0.597633	4.070006
C	-3.922314	1.077939	2.486840	H	-0.219455	-0.714722	2.103155
H	-4.405861	2.050939	2.636784	H	0.367392	0.806551	6.793313
H	-2.879399	1.254263	2.207675	H	-1.731909	-0.338928	6.122820
H	-3.929823	0.554464	3.450412	H	-2.033049	-1.091401	3.763846
C	-6.100459	-0.052698	1.822306	C	2.535909	1.427170	5.167325
H	-6.595346	-0.694912	1.084982	H	2.417569	2.498416	4.943798
H	-6.686990	0.870168	1.907152	H	2.768612	1.354843	6.235540
H	-6.133815	-0.561243	2.793792	C	3.696588	0.864134	4.334863
O	-0.317754	0.488897	-2.052841	H	4.611242	1.444368	4.465675
H	2.099173	2.121911	-0.784584	H	3.915594	-0.164597	4.659374
H	-0.086585	3.153067	-1.044558	C	3.363835	0.794304	2.854669
H	0.664868	4.734644	-1.641854	N	2.096167	0.468681	2.565392
C	3.380017	3.804870	-1.291215	H	1.831105	0.310022	1.580012
C	4.537644	3.092057	-0.947369	C	3.453855	2.217713	-1.408101
C	3.484764	5.172422	-1.577268	C	3.801626	0.808079	-1.265014
C	5.775197	3.733036	-0.893087	H	2.689506	2.602288	-0.734769
H	4.466560	2.030929	-0.721258	H	3.028608	0.188498	-0.819567
C	4.722830	5.812556	-1.523052	C	-2.319122	1.239167	-0.625519

C	-3.152862	0.144495	-0.805048	C	2.664495	-4.600393	-2.174842
C	-4.421604	0.344510	-1.450204	H	1.970497	-3.846399	-4.074060
C	-4.821510	1.678833	-1.786983	H	3.078741	-5.222253	-0.149429
C	-3.952538	2.760656	-1.501137	C	-1.807454	3.738979	-0.696856
C	-2.701493	2.576266	-0.944360	C	-1.665779	4.732448	-1.679677
H	-4.985069	-1.744041	-1.602453	C	-1.128228	3.904843	0.522693
C	-5.287582	-0.724596	-1.812159	C	-0.877172	5.860173	-1.451749
C	-6.078357	1.893111	-2.415871	C	-0.341481	5.033328	0.750109
H	-4.285979	3.768970	-1.732282	C	-0.212468	6.016177	-0.234416
C	-6.901080	0.837195	-2.733432	H	-0.776695	6.612445	-2.229874
C	-6.492130	-0.484623	-2.436978	H	0.168370	5.147278	1.703421
H	-6.371070	2.913178	-2.653532	O	-0.731640	-0.894521	-1.698230
H	-7.856107	1.013021	-3.220882	O	-1.061318	1.034541	-0.080460
H	-7.131712	-1.319803	-2.709636	P	0.115432	0.329786	-0.992818
C	-2.689051	-1.208786	-0.374579	O	1.148364	-0.175809	-0.022875
C	-3.419693	-2.001091	0.576807	O	0.535433	1.234109	-2.134519
C	-1.488500	-1.703143	-0.864678	S	4.550281	1.051317	1.688475
C	-4.578690	-1.528119	1.253555	O	2.926366	1.632059	-2.620237
C	-2.937385	-3.311580	0.901144	C	5.025706	0.169925	-1.721290
C	-0.992532	-3.006015	-0.558275	C	6.143586	0.894377	-2.174662
C	-5.241474	-2.318688	2.167623	C	5.083232	-1.236511	-1.691716
H	-4.935655	-0.525307	1.049817	C	7.290488	0.225288	-2.588811
C	-3.655774	-4.108402	1.834185	H	6.117105	1.979020	-2.201914
C	-1.743266	-3.784116	0.301954	C	6.233291	-1.901907	-2.105496
C	-4.785924	-3.627696	2.454518	H	4.221766	-1.798140	-1.341279
H	-6.120995	-1.931560	2.675028	C	7.337094	-1.172380	-2.554714
H	-3.283900	-5.105502	2.058131	H	8.150562	0.790321	-2.936090
H	-1.408159	-4.791289	0.535690	H	6.269164	-2.986958	-2.078422
H	-5.322489	-4.243763	3.170866	H	8.235790	-1.691178	-2.877195
C	0.282069	-3.520966	-1.126257	H	4.236277	2.943285	-1.621135
C	0.582433	-3.404203	-2.494375	H	3.579753	-5.022293	-2.582491
C	1.200982	-4.181992	-0.294774	H	-0.112301	-2.895333	-3.153389
C	1.760541	-3.940545	-3.011860	H	0.996303	-4.255645	0.769564
C	2.380880	-4.717289	-0.812472	H	-1.223402	3.150295	1.295779

H	0.402831	6.893960	-0.054655	C	5.566420	0.419610	1.298607
H	-2.161223	4.604913	-2.638046	C	6.283655	3.040598	0.622422
TS5-S E= -3060.57044857				H	4.331404	4.430957	-0.592371
H	-1.688921	2.216279	1.948529	C	7.186394	2.226911	1.267127
C	-0.461631	-2.660709	-1.939396	C	6.815525	0.906801	1.616757
C	-1.855933	-2.764028	-2.000665	H	6.546947	4.063488	0.363496
C	-2.478660	-3.649756	-2.896008	H	8.176167	2.597237	1.519811
C	-1.675026	-4.450743	-3.707708	H	7.520168	0.272650	2.148062
C	-0.281722	-4.368368	-3.645554	C	2.911162	-0.667381	0.444659
C	0.321113	-3.467893	-2.764461	C	3.633100	-1.730177	-0.203059
H	-0.009145	-1.949583	-1.256727	C	1.806854	-0.994839	1.216567
H	-2.149160	-5.143396	-4.399673	C	4.677762	-1.502452	-1.141487
H	0.328092	-5.001024	-4.284312	C	3.258086	-3.086418	0.070673
H	1.403235	-3.393129	-2.710533	C	1.418084	-2.337610	1.506265
C	-3.987329	-3.648913	-2.950656	C	5.334729	-2.552768	-1.745081
H	-4.332790	-2.880301	-3.658546	H	4.949334	-0.483881	-1.391903
H	-4.365516	-4.607991	-3.321586	C	3.968845	-4.147742	-0.554791
C	-4.569978	-3.353906	-1.561829	C	2.172296	-3.348962	0.942550
H	-5.654250	-3.237363	-1.591012	C	4.988451	-3.891112	-1.442419
H	-4.350929	-4.194744	-0.885984	H	6.124014	-2.350424	-2.464036
C	-3.956154	-2.116691	-0.931118	H	3.679693	-5.170543	-0.324700
N	-2.649147	-1.937936	-1.166220	H	1.922718	-4.383327	1.163291
H	-2.151228	-1.185987	-0.669746	H	5.520340	-4.710162	-1.918764
C	-3.331727	0.999259	2.299327	C	0.245992	-2.657929	2.364199
C	-3.700397	1.474395	0.971010	C	0.016684	-2.001005	3.585857
H	-4.092818	0.945291	3.075012	C	-0.644705	-3.672624	1.974766
C	2.376770	1.683288	-0.220585	C	-1.065969	-2.354986	4.390704
C	3.296184	0.765293	0.272283	C	-1.728211	-4.023960	2.779899
C	4.614708	1.226789	0.615174	C	-1.943196	-3.366943	3.992336
C	4.982309	2.572792	0.293521	H	-1.219634	-1.841947	5.336719
C	4.034647	3.418020	-0.333456	H	-2.409255	-4.806169	2.454800
C	2.735353	3.018716	-0.579847	C	1.796697	3.955613	-1.260165
H	5.294691	-0.589534	1.586041	C	2.202555	4.578389	-2.452545
				C	0.538624	4.279536	-0.726953

C	1.376921	5.499600	-3.097521	C	-2.458725	0.856251	0.168964
C	-0.282708	5.204443	-1.372405	C	-3.746175	1.295279	0.641267
C	0.129397	5.816812	-2.558146	C	-4.804474	0.336701	0.752402
H	1.707767	5.964697	-4.022698	C	-4.551543	-1.022443	0.436275
H	-1.249180	5.452008	-0.940096	C	-3.294851	-1.479285	0.096359
O	1.051198	0.035441	1.750845	H	-3.215748	3.367111	1.002989
O	1.079585	1.269511	-0.481742	C	-4.013657	2.634810	1.038646
P	0.052100	0.860383	0.734147	C	-6.087532	0.759544	1.194307
O	-1.015852	-0.003509	0.132025	H	-5.375049	-1.729027	0.484479
O	-0.365925	2.083053	1.535944	C	-6.317723	2.068435	1.549692
S	-4.882484	-1.092655	0.030674	C	-5.263090	3.009155	1.482925
O	-2.720398	2.309476	2.250291	H	-6.881908	0.020034	1.261086
H	-2.625612	0.171442	2.331443	H	-7.300238	2.378710	1.894410
H	-2.967154	1.260935	0.202159	H	-5.438028	4.036614	1.790188
C	-4.871940	2.265341	0.624504	C	-1.360740	1.826000	-0.118528
C	-5.924943	2.500329	1.527189	C	-1.547924	2.925938	-1.028963
C	-4.944446	2.813045	-0.669719	C	-0.116487	1.681841	0.476784
C	-7.021127	3.264938	1.141192	C	-2.705461	3.072174	-1.843077
H	-5.886774	2.087380	2.530020	C	-0.509236	3.904637	-1.155267
C	-6.043137	3.575448	-1.054027	C	0.930541	2.641906	0.372963
H	-4.134536	2.628823	-1.370153	C	-2.841859	4.141588	-2.701009
C	-7.082561	3.802984	-0.148255	H	-3.484874	2.320987	-1.795403
H	-7.830420	3.441535	1.843605	C	-0.689973	5.006878	-2.034574
H	-6.090306	3.991386	-2.056092	C	0.691022	3.747852	-0.416593
H	-7.941548	4.397864	-0.446250	C	-1.832747	5.129243	-2.790538
H	-2.787658	-3.638561	4.620219	H	-3.731897	4.223963	-3.318876
H	0.692520	-1.216113	3.906704	H	0.104224	5.745962	-2.107890
H	-0.498124	-4.169614	1.019928	H	1.459007	4.512335	-0.500157
H	0.212975	3.818128	0.198947	H	-1.956873	5.971905	-3.465040
H	-0.515765	6.535359	-3.057344	C	2.233222	2.477516	1.099037
H	3.167161	4.322659	-2.882991	C	2.287697	2.644548	2.505016
				C	3.417120	2.197947	0.376539
				C	3.520861	2.530142	3.152628
				C	4.625574	2.098184	1.078503
V E= -3060.43164707							
C	-2.259745	-0.505361	-0.004551				

C	4.705206	2.257986	2.461438	H	7.040350	0.831724	4.624645
H	3.556466	2.663209	4.231048	C	3.439415	1.998503	-1.139742
H	5.538193	1.883408	0.526906	H	2.407874	2.023478	-1.501372
C	-3.057302	-2.933146	-0.196625	C	4.201530	3.137817	-1.845559
C	-2.875894	-3.360625	-1.535227	H	3.765600	4.116899	-1.615579
C	-3.072928	-3.885710	0.851245	H	4.175134	3.001763	-2.933597
C	-2.719908	-4.725257	-1.796669	H	5.253701	3.164834	-1.537545
C	-2.922438	-5.240529	0.528062	C	4.014503	0.624519	-1.534456
C	-2.744229	-5.685723	-0.781973	H	3.438405	-0.176404	-1.062541
H	-2.583961	-5.045951	-2.826632	H	5.065558	0.522268	-1.238866
H	-2.939961	-5.976452	1.328135	H	3.963260	0.495429	-2.622955
O	0.113440	0.582126	1.304190	C	-3.263008	-3.498803	2.319404
O	-0.996542	-0.959095	-0.384498	H	-3.082978	-2.423420	2.408907
P	0.240158	-0.902163	0.667605	C	-2.266002	-4.202347	3.261165
O	1.501174	-1.242854	-0.044823	H	-2.338776	-3.770037	4.266104
C	1.054094	2.985996	3.340979	H	-1.233784	-4.095157	2.919103
H	0.183289	2.996453	2.679495	H	-2.481044	-5.273841	3.354935
C	1.166633	4.398303	3.950005	C	-4.705916	-3.779190	2.789076
H	1.316081	5.155364	3.171788	H	-4.939102	-4.848392	2.712935
H	2.008678	4.468178	4.648850	H	-5.445221	-3.236035	2.191501
H	0.253328	4.652278	4.501833	H	-4.833988	-3.481072	3.836919
C	0.780889	1.931323	4.430475	C	-2.577561	-7.169694	-1.082829
H	0.661840	0.936164	3.991692	H	-2.661190	-7.703182	-0.125933
H	-0.139014	2.177170	4.974985	C	-3.690718	-7.701652	-2.005370
H	1.595693	1.887384	5.162982	H	-3.584020	-8.782586	-2.157743
C	6.040049	2.134958	3.184973	H	-3.654998	-7.222131	-2.990861
H	6.804891	1.944123	2.419467	H	-4.681866	-7.512948	-1.578577
C	6.427485	3.439638	3.906863	C	-1.185054	-7.482546	-1.663363
H	7.416198	3.345385	4.372203	H	-1.059771	-8.561947	-1.812841
H	5.709770	3.685269	4.698596	H	-0.391232	-7.135182	-0.991950
H	6.456835	4.284294	3.209666	H	-1.037297	-6.992033	-2.632764
C	6.053612	0.940464	4.158089	C	-2.880934	-2.389732	-2.716070
H	5.814614	0.005605	3.639556	H	-2.992140	-1.374623	-2.325134
H	5.318076	1.073632	4.960302	C	-1.556683	-2.428342	-3.502806

H	-1.389501	-3.409278	-3.963696	C	1.519497	0.583338	5.726426
H	-0.706811	-2.208928	-2.849563	C	0.529521	1.562124	5.607333
H	-1.570691	-1.683234	-4.307605	C	-0.336992	1.550985	4.512487
C	-4.086313	-2.643107	-3.643841	H	-0.881807	0.533430	2.677450
H	-5.032148	-2.567995	-3.095388	H	2.201846	0.598735	6.572854
H	-4.042198	-3.640710	-4.096765	H	0.440571	2.334211	6.366044
H	-4.105444	-1.908047	-4.457769	H	-1.098994	2.317012	4.405407
O	-0.113999	-1.771975	1.928025	C	2.747237	-1.459689	4.788598
H	0.460066	-2.609775	2.011982	H	3.614104	-1.096140	4.217387
C	4.098992	-3.648367	-1.534340	H	3.097009	-1.639200	5.809902
C	3.469765	-4.461512	-0.586611	C	2.250815	-2.773170	4.170948
C	3.752131	-5.836378	-0.514545	H	3.059498	-3.487246	3.999011
C	4.691712	-6.371402	-1.396637	H	1.523461	-3.258834	4.838483
C	5.329971	-5.568316	-2.344659	C	1.543080	-2.535799	2.862947
C	5.025868	-4.207392	-2.413374	N	0.865214	-1.432357	2.673862
H	3.861691	-2.589100	-1.575645	H	0.293724	-1.233516	1.779827
H	4.919539	-7.433701	-1.342775	C	1.989894	-3.432161	-0.429478
H	6.057636	-6.002980	-3.023836	C	0.972587	-3.616264	0.697327
H	5.514420	-3.573619	-3.148075	H	2.298413	-2.384124	-0.471928
C	2.983081	-6.664628	0.488824	C	0.448015	2.439978	-0.639308
H	2.031704	-6.991214	0.041076	C	-0.691389	3.233776	-0.593014
H	3.534071	-7.575614	0.746142	C	-0.699738	4.471206	-1.327747
C	2.685457	-5.848060	1.754323	C	0.507731	4.907579	-1.962400
H	2.000695	-6.364409	2.430891	C	1.666328	4.093928	-1.883580
H	3.616433	-5.662195	2.309504	C	1.659385	2.860298	-1.266521
C	2.084734	-4.492474	1.431764	H	-2.798888	4.945194	-1.051915
N	2.521883	-3.898443	0.297438	C	-1.863189	5.275408	-1.487268
H	2.192830	-2.940040	0.114155	C	0.521456	6.138007	-2.673482
O	1.264329	-3.957806	2.199356	H	2.585046	4.451665	-2.340900
				C	-0.616729	6.902315	-2.788072
				C	-1.822298	6.455390	-2.197672
(R)-5-CP-R E= -3994.46576769				H	1.451147	6.456402	-3.139310
C	-0.228086	0.555103	3.542184	H	-0.597037	7.837664	-3.340650
C	0.760104	-0.421854	3.682523	H	-2.727886	7.045421	-2.310747
C	1.653837	-0.417258	4.763417				

C	-1.890620	2.782664	0.173293	O	-0.705921	-0.894016	0.676118
C	-2.481701	3.594491	1.203300	C	-4.843767	0.917468	-2.335213
C	-2.467848	1.550661	-0.108365	H	-4.271912	1.733670	-1.886156
C	-1.868854	4.776155	1.706473	C	-6.236661	1.485998	-2.673917
C	-3.724456	3.180232	1.783878	H	-6.753753	1.834291	-1.772429
C	-3.724937	1.137822	0.428880	H	-6.873476	0.733407	-3.153997
C	-2.463548	5.517228	2.704939	H	-6.145588	2.333608	-3.364031
H	-0.912974	5.086541	1.300341	C	-4.091231	0.487848	-3.609100
C	-4.321140	3.977600	2.798314	H	-3.087588	0.127655	-3.365965
C	-4.332765	1.978082	1.339608	H	-3.994066	1.338186	-4.295086
C	-3.708317	5.123554	3.251682	H	-4.622428	-0.308901	-4.143590
H	-1.970837	6.411738	3.076660	C	-4.001051	-1.191137	2.314376
H	-5.270976	3.655380	3.218815	H	-3.380280	-0.297495	2.420755
H	-5.302650	1.704822	1.746991	C	-5.127477	-1.102280	3.362859
H	-4.171553	5.721429	4.031879	H	-5.750783	-0.214046	3.210879
C	-4.399877	-0.128311	-0.011044	H	-4.708702	-1.053023	4.375781
C	-4.943318	-0.218204	-1.316447	H	-5.785311	-1.978404	3.315359
C	-4.557124	-1.210067	0.889902	C	-3.090308	-2.401745	2.594657
C	-5.629174	-1.377735	-1.687548	H	-2.286186	-2.446898	1.855675
C	-5.258743	-2.345161	0.471030	H	-3.645222	-3.347034	2.566876
C	-5.804672	-2.455274	-0.812171	H	-2.644486	-2.312841	3.593990
H	-6.025000	-1.454076	-2.696162	C	2.459637	1.177048	-3.606373
H	-5.407323	-3.161530	1.172189	H	1.440790	1.482254	-3.350690
C	2.913772	2.035004	-1.218539	C	2.361323	-0.239624	-4.197914
C	3.745682	2.104334	-0.076808	H	1.656600	-0.237078	-5.037686
C	3.300034	1.247864	-2.330417	H	1.993692	-0.949210	-3.454571
C	4.947732	1.391041	-0.066145	H	3.323695	-0.595637	-4.585670
C	4.508903	0.546014	-2.267865	C	2.999559	2.159416	-4.667695
C	5.350961	0.601755	-1.149654	H	4.025398	1.897579	-4.956130
H	5.607042	1.479706	0.792926	H	3.008790	3.191985	-4.303357
H	4.795458	-0.081571	-3.105454	H	2.377619	2.125831	-5.570433
O	-1.844608	0.712029	-1.012233	C	3.399532	2.979119	1.127495
O	0.445361	1.226282	0.023324	H	2.378700	3.348376	0.994641
P	-0.447397	-0.047723	-0.565627	C	3.419558	2.187864	2.447326

H	4.427321	1.831240	2.694108	H	-8.515065	-6.867864	-2.324014
H	2.753494	1.321663	2.387358	C	6.635518	-0.145538	-1.115407
H	3.080351	2.818078	3.277899	C	7.424624	-0.286162	-2.270727
C	4.323024	4.210953	1.204839	C	7.102596	-0.730695	0.075117
H	4.257979	4.811901	0.291095	C	8.630149	-0.985866	-2.238226
H	5.371064	3.915332	1.335315	H	7.099075	0.178417	-3.196893
H	4.045443	4.849693	2.052478	C	8.310717	-1.428179	0.110414
O	0.152121	-0.651170	-1.790297	H	6.501525	-0.652854	0.976961
H	0.566040	-4.627207	0.704289	C	9.080499	-1.560465	-1.047544
H	0.166219	-2.886299	0.627052	H	9.224089	-1.074654	-3.144168
O	1.646186	-3.521555	2.018223	H	8.648813	-1.871852	1.043671
S	1.085816	-3.781185	-2.016892	H	10.021822	-2.102780	-1.021841
H	0.478610	-2.562068	-2.070237				
C	3.215779	-4.313474	-0.307771	(R)-5-TS4-R E= -3994.44419331			
C	3.111448	-5.703856	-0.156259	C	-0.298207	0.371251	3.722482
C	4.490682	-3.736409	-0.357016	C	0.428138	-0.802947	3.944402
C	4.255540	-6.494774	-0.051837	C	1.069362	-1.040024	5.170234
H	2.132690	-6.176818	-0.133045	C	0.950283	-0.083162	6.179401
C	5.637553	-4.525829	-0.253368	C	0.223972	1.092152	5.973326
H	4.589604	-2.661845	-0.490422	C	-0.394429	1.318509	4.741468
C	5.522655	-5.908030	-0.097949	H	-0.766863	0.535609	2.757704
H	4.156864	-7.571348	0.060699	H	1.438470	-0.260800	7.135110
H	6.615651	-4.054782	-0.298899	H	0.143511	1.826185	6.769963
H	6.413195	-6.526032	-0.018916	H	-0.955957	2.231807	4.566921
C	-6.549711	-3.670994	-1.229236	C	1.890122	-2.301395	5.306495
C	-7.697399	-3.574270	-2.035043	H	2.910070	-2.120359	4.934773
C	-6.129300	-4.951099	-0.828860	H	1.988906	-2.592207	6.357778
C	-8.398773	-4.714258	-2.426227	C	1.258223	-3.444753	4.501023
H	-8.054597	-2.593437	-2.336406	H	1.903935	-4.324278	4.449773
C	-6.830670	-6.091758	-1.218393	H	0.313343	-3.757230	4.969127
H	-5.228591	-5.051544	-0.229694	C	0.923707	-3.027497	3.080024
C	-7.969078	-5.979041	-2.019192	N	0.538944	-1.755227	2.896767
H	-9.287658	-4.613193	-3.043780	H	0.175309	-1.459384	1.970074
H	-6.480677	-7.071724	-0.903868	C	1.927716	-3.297500	-0.415563

C	0.644254	-3.688184	0.164699	C	-4.548911	-1.166635	0.588939
H	2.152119	-2.238276	-0.287652	C	-5.535474	-1.084587	-2.028323
C	0.587353	2.459380	-0.454373	C	-5.258952	-2.243884	0.048948
C	-0.530165	3.278999	-0.359236	C	-5.761866	-2.229693	-1.256424
C	-0.485072	4.578853	-0.975992	H	-5.896889	-1.064992	-3.052504
C	0.750643	5.035150	-1.538121	H	-5.448127	-3.114308	0.670506
C	1.880558	4.179677	-1.516878	C	3.041534	2.018599	-1.073219
C	1.822412	2.893324	-1.021456	C	3.819200	1.821282	0.092541
H	-2.577770	5.088639	-0.711653	C	3.464769	1.464964	-2.306106
C	-1.621061	5.429015	-1.089549	C	5.009657	1.094535	0.001247
C	0.818525	6.325395	-2.130364	C	4.663756	0.744533	-2.344897
H	2.816858	4.544219	-1.931364	C	5.459848	0.552669	-1.209071
C	-0.294014	7.131427	-2.200530	H	5.628640	0.983520	0.887132
C	-1.527576	6.667925	-1.685479	H	4.981854	0.306150	-3.286173
H	1.769136	6.656800	-2.541649	O	-1.723022	0.831291	-1.034273
H	-0.232894	8.113346	-2.661706	O	0.541414	1.193145	0.101883
H	-2.413042	7.292789	-1.765875	P	-0.378341	-0.004941	-0.575916
C	-1.765085	2.794614	0.324862	O	-0.678582	-0.949814	0.564753
C	-2.374463	3.529092	1.401207	C	-4.676762	1.238798	-2.445618
C	-2.364094	1.610575	-0.085856	H	-4.108862	1.999542	-1.903720
C	-1.747134	4.637633	2.035837	C	-6.041889	1.866819	-2.791603
C	-3.652637	3.106722	1.891035	H	-6.592408	2.145512	-1.885837
C	-3.652613	1.190810	0.362453	H	-6.670527	1.174985	-3.364865
C	-2.361173	5.303530	3.074910	H	-5.903618	2.770095	-3.398199
H	-0.764752	4.950623	1.700899	C	-3.879637	0.901210	-3.720160
C	-4.268826	3.828874	2.948868	H	-2.895060	0.496987	-3.468184
C	-4.275822	1.969117	1.316645	H	-3.735364	1.803773	-4.326568
C	-3.640593	4.905887	3.531378	H	-4.405005	0.165895	-4.341507
H	-1.856931	6.141318	3.549148	C	-4.042975	-1.281221	2.027445
H	-5.244754	3.501805	3.299808	H	-3.379456	-0.433957	2.219678
H	-5.269736	1.693007	1.658565	C	-5.202153	-1.209673	3.041531
H	-4.117629	5.445107	4.345214	H	-5.774215	-0.281206	2.937103
C	-4.340052	-0.014841	-0.208973	H	-4.818825	-1.257271	4.068252
C	-4.840247	0.022342	-1.534018	H	-5.900738	-2.044239	2.905087

C	-3.208300	-2.556150	2.251186	H	2.189117	-5.846563	0.662834
H	-2.381584	-2.598549	1.537808	C	5.526353	-4.431304	-0.712103
H	-3.810323	-3.466405	2.145022	H	4.406055	-2.662015	-1.204523
H	-2.790502	-2.556204	3.265747	C	5.481156	-5.717263	-0.167264
C	2.676978	1.644659	-3.605115	H	4.233040	-7.216218	0.752947
H	1.706682	2.080905	-3.352512	H	6.462789	-4.020857	-1.077832
C	2.390315	0.309310	-4.316099	H	6.384183	-6.319495	-0.114413
H	1.780291	0.488846	-5.209737	C	-6.512604	-3.389584	-1.802616
H	1.836065	-0.361714	-3.656307	C	-7.624880	-3.201741	-2.641422
H	3.309966	-0.190222	-4.643759	C	-6.132700	-4.707453	-1.494512
C	3.396129	2.623981	-4.555557	C	-8.330678	-4.290088	-3.153174
H	4.379150	2.237504	-4.852047	H	-7.952009	-2.191923	-2.873119
H	3.552428	3.602523	-4.087849	C	-6.838552	-5.796578	-2.004522
H	2.806741	2.774940	-5.467980	H	-5.259947	-4.876641	-0.869915
C	3.435376	2.429801	1.440671	C	-7.941341	-5.593296	-2.836741
H	2.440732	2.872756	1.342603	H	-9.192167	-4.119113	-3.793729
C	3.345839	1.368702	2.552291	H	-6.520316	-6.806563	-1.758706
H	4.321446	0.911962	2.759046	H	-8.491266	-6.441685	-3.235268
H	2.647579	0.573613	2.274203	C	6.748560	-0.183948	-1.288598
H	2.987549	1.820668	3.484465	C	7.579170	-0.067295	-2.417395
C	4.399630	3.567061	1.832765	C	7.180319	-1.010275	-0.235964
H	4.418503	4.351094	1.067514	C	8.791559	-0.751683	-2.493151
H	5.424461	3.197053	1.957179	H	7.280993	0.587029	-3.231573
H	4.090373	4.023802	2.780860	C	8.395426	-1.692441	-0.308696
O	0.244285	-0.531261	-1.843179	H	6.546288	-1.136652	0.637003
H	0.356192	-4.728803	0.184174	C	9.206890	-1.567799	-1.438614
H	-0.120145	-2.928341	0.280193	H	9.418234	-0.638451	-3.374015
O	0.988112	-3.886264	2.165470	H	8.705204	-2.327015	0.517904
S	0.991876	-3.456134	-2.052099	H	10.153543	-2.098354	-1.495471
H	0.552213	-2.113242	-2.044181				
C	3.146535	-4.165737	-0.303956				
C	3.111636	-5.450813	0.251844	(R)-6-CP-R E= -3846.86114415			
C	4.366478	-3.661778	-0.778631	H	-0.367560	2.424484	-2.209949
C	4.273653	-6.221752	0.316784	C	-0.211832	-0.285744	3.345789
				C	-0.674121	1.017505	3.551386

C	-1.402786	1.368188	4.698538	H	-2.822235	-7.433389	-2.997937
C	-1.645517	0.382909	5.654745	H	-0.517609	-7.459919	-2.040306
C	-1.182473	-0.922482	5.468390	C	0.392042	-3.085772	0.216597
C	-0.471710	-1.255613	4.313467	C	0.654270	-4.013403	1.284779
H	0.326700	-0.524939	2.436551	C	1.388407	-2.180864	-0.128441
H	-2.206010	0.640158	6.550232	C	-0.349676	-4.848472	1.851256
H	-1.380780	-1.677605	6.223511	C	1.974508	-4.078266	1.838485
H	-0.120668	-2.270910	4.156554	C	2.719581	-2.251246	0.384770
C	-1.914663	2.783990	4.805306	C	-0.057856	-5.713543	2.884036
H	-2.886296	2.871031	4.297390	H	-1.361372	-4.791098	1.466454
H	-2.076903	3.066138	5.850462	C	2.247201	-4.995975	2.889308
C	-0.911518	3.747474	4.159401	C	2.983470	-3.218252	1.333243
H	-1.293411	4.770915	4.129369	C	1.255706	-5.799959	3.403999
H	0.019845	3.765176	4.745033	H	-0.844884	-6.334713	3.303397
C	-0.537283	3.289420	2.763601	H	3.258024	-5.040758	3.288112
N	-0.421265	2.002028	2.545930	H	3.992897	-3.313978	1.724963
H	-0.064325	1.600561	1.621651	H	1.475140	-6.493019	4.211637
C	-0.953596	3.753819	-0.920068	C	3.808003	-1.346794	-0.113549
C	0.298794	3.944872	-0.027067	C	4.306841	-1.496927	-1.427435
H	-1.616047	3.010859	-0.449606	C	4.384966	-0.375133	0.741336
H	0.779095	2.976348	0.128273	C	5.361509	-0.679859	-1.856092
C	-1.660847	-1.918134	-0.604689	C	5.439215	0.407747	0.261817
C	-0.906638	-3.081923	-0.519768	C	5.952014	0.282183	-1.034752
C	-1.389551	-4.264736	-1.182218	H	5.727693	-0.816169	-2.867145
C	-2.691965	-4.239897	-1.777064	H	5.873945	1.145008	0.931227
C	-3.453742	-3.044505	-1.732113	C	-3.810474	-0.634681	-1.168202
C	-2.961317	-1.874667	-1.191722	C	-4.570840	-0.337120	-0.012934
H	0.383015	-5.484367	-0.904334	C	-3.907675	0.200688	-2.303684
C	-0.622106	-5.456660	-1.308432	C	-5.407713	0.781931	-0.019524
C	-3.192821	-5.406362	-2.415991	C	-4.762277	1.312020	-2.253749
H	-4.455230	-3.050948	-2.153870	C	-5.523928	1.630441	-1.127059
C	-2.432371	-6.549876	-2.499864	H	-5.992420	0.992166	0.872085
C	-1.128787	-6.565836	-1.950155	H	-4.821487	1.944109	-3.130902
H	-4.188284	-5.370456	-2.852471	O	1.116035	-1.214893	-1.076665

O	-1.173210	-0.764239	-0.015853	H	-3.741329	-1.961336	1.103019
P	0.109799	0.037030	-0.698155	C	-4.210203	-0.430896	2.508857
O	0.682870	0.835940	0.463803	H	-4.999203	0.289463	2.757037
C	3.773910	-2.550410	-2.398852	H	-3.270941	0.118080	2.390646
H	2.946181	-3.075971	-1.915498	H	-4.101319	-1.108215	3.364311
C	4.847631	-3.611603	-2.714551	C	-5.856927	-2.008338	1.390007
H	5.213368	-4.091772	-1.799608	H	-6.057168	-2.625990	0.507453
H	5.710972	-3.171821	-3.228134	H	-6.709412	-1.331166	1.522869
H	4.434613	-4.391132	-3.366440	H	-5.812790	-2.669269	2.264770
C	3.214784	-1.921868	-3.689646	O	-0.244995	0.706005	-1.985292
H	2.427219	-1.198040	-3.461981	S	-0.231873	4.586200	1.668018
H	2.789175	-2.700304	-4.334665	O	-0.571282	3.392475	-2.213770
H	3.997599	-1.410919	-4.263236	C	1.305409	4.947452	-0.547749
C	3.905615	-0.139558	2.174758	C	0.925842	6.246295	-0.915643
H	3.016616	-0.754304	2.338913	C	2.651763	4.577201	-0.662120
C	4.965143	-0.576211	3.206090	C	1.873197	7.155331	-1.385746
H	5.236357	-1.630736	3.082425	H	-0.115569	6.550158	-0.846085
H	4.589286	-0.440410	4.227913	C	3.598787	5.483933	-1.139298
H	5.884400	0.013682	3.107193	H	2.955394	3.569848	-0.388847
C	3.483564	1.322972	2.411334	C	3.212485	6.776241	-1.499290
H	2.713367	1.612608	1.691392	H	1.563731	8.157389	-1.670262
H	4.329081	2.014502	2.316638	H	4.637318	5.178019	-1.231142
H	3.077233	1.439246	3.424601	H	3.949425	7.483120	-1.871002
C	-3.140138	-0.088718	-3.594632	H	-1.510954	4.696282	-0.982091
H	-2.262350	-0.685860	-3.330859	C	-6.459001	2.853142	-1.064868
C	-2.620761	1.178179	-4.298339	C	-5.997129	3.794465	0.073280
H	-1.921054	0.893901	-5.092643	C	-6.463864	3.660172	-2.377454
H	-2.095126	1.841339	-3.608191	C	-7.907114	2.385700	-0.784496
H	-3.432150	1.744598	-4.773225	H	-6.010893	3.291852	1.046393
C	-4.001910	-0.911319	-4.576249	H	-4.975538	4.149673	-0.106131
H	-4.907172	-0.357836	-4.856375	H	-6.655561	4.669957	0.139150
H	-4.313787	-1.868271	-4.146394	H	-6.809007	3.057014	-3.224764
H	-3.439219	-1.122258	-5.494014	H	-7.142897	4.515561	-2.281907
C	-4.539152	-1.224177	1.231605	H	-5.469504	4.051229	-2.620325

H	-8.583907	3.247651	-0.727916	C	1.499841	-3.135946	2.745419
H	-8.265075	1.724449	-1.581928	N	0.859728	-1.960076	2.694484
H	-7.984276	1.838787	0.161185	H	0.435102	-1.640969	1.801098
C	7.116841	1.178400	-1.494612	C	2.291488	-3.189212	-0.919341
C	7.540429	0.894662	-2.948659	C	1.123212	-3.672571	-0.182165
C	6.692864	2.664176	-1.401342	H	2.478324	-2.123159	-0.780054
C	8.343367	0.939954	-0.581792	C	0.338935	2.445238	-0.396079
H	7.887073	-0.136887	-3.078515	C	-0.869841	3.129141	-0.374478
H	6.720487	1.071490	-3.653780	C	-0.933909	4.427778	-0.993216
H	8.366920	1.558112	-3.228670	C	0.275809	5.026031	-1.472758
H	6.417181	2.943340	-0.378659	C	1.494936	4.310326	-1.365306
H	7.516464	3.317452	-1.716110	C	1.553613	3.023792	-0.870970
H	5.831592	2.864463	-2.049341	H	-3.084524	4.688985	-0.874121
H	9.180066	1.579381	-0.890090	C	-2.150811	5.139627	-1.188943
H	8.120744	1.163458	0.466877	C	0.232681	6.316015	-2.067723
H	8.674755	-0.103418	-0.637205	H	2.409479	4.786734	-1.708874
(R)-6-TS4-R E= -3846.84173783				C	-0.959065	6.986189	-2.219826
C	-0.381649	-0.150518	3.736629	C	-2.162318	6.381370	-1.786307
C	0.577635	-1.162968	3.836070	H	1.164052	6.756911	-2.415336
C	1.279756	-1.385364	5.030668	H	-0.981567	7.968821	-2.683045
C	0.981418	-0.587375	6.136201	H	-3.107173	6.898373	-1.931105
C	0.019195	0.421906	6.054481	C	-2.078827	2.508368	0.243105
C	-0.654860	0.641935	4.851133	C	-2.827621	3.173919	1.275729
H	-0.890184	0.011308	2.791716	C	-2.513822	1.260088	-0.183656
H	1.515299	-0.756234	7.068721	C	-2.373459	4.356293	1.924307
H	-0.199371	1.034108	6.924722	C	-4.071704	2.606962	1.703499
H	-1.398256	1.430113	4.774071	C	-3.762459	0.690023	0.207325
C	2.352348	-2.449289	5.031144	C	-3.120191	4.956835	2.914734
H	3.299848	-2.017107	4.675475	H	-1.417719	4.780455	1.638815
H	2.538701	-2.817482	6.045602	C	-4.827429	3.262052	2.713712
C	1.955911	-3.612945	4.112766	C	-4.522256	1.396077	1.117884
H	2.772870	-4.323050	3.965430	C	-4.366680	4.414496	3.308133
H	1.113506	-4.168569	4.550194	H	-2.746144	5.854118	3.400538
				H	-5.775318	2.823738	3.017326

H	-5.490562	1.002921	1.416437	C	-5.157609	-1.880773	2.856893
H	-4.949951	4.902534	4.084258	H	-5.852889	-1.046429	2.710838
C	-4.264281	-0.600099	-0.372221	H	-4.828466	-1.868651	3.903338
C	-4.679344	-0.656660	-1.721857	H	-5.718232	-2.809066	2.692999
C	-4.385037	-1.754172	0.441113	C	-2.943432	-2.918956	2.188459
C	-5.204023	-1.854108	-2.226885	H	-2.084549	-2.837838	1.517393
C	-4.923658	-2.918531	-0.113838	H	-3.396132	-3.909552	2.060489
C	-5.341904	-3.003903	-1.447075	H	-2.583101	-2.852582	3.222769
H	-5.518826	-1.871185	-3.264231	C	2.770302	1.890604	-3.363586
H	-5.014659	-3.793849	0.523289	H	1.735856	2.206122	-3.200783
C	2.867055	2.297952	-0.817190	C	2.707910	0.543679	-4.107376
C	3.566869	2.194682	0.408998	H	2.161544	0.664667	-5.050727
C	3.450790	1.786685	-1.997474	H	2.181331	-0.200000	-3.505202
C	4.829104	1.596722	0.421860	H	3.705883	0.162323	-4.356954
C	4.721127	1.194461	-1.925727	C	3.453611	2.960525	-4.240166
C	5.438506	1.088204	-0.732507	H	4.496778	2.692831	-4.449404
H	5.360255	1.540357	1.367852	H	3.455361	3.941954	-3.753312
H	5.156260	0.818610	-2.844445	H	2.933788	3.059869	-5.200907
O	-1.746414	0.562105	-1.100504	C	3.011269	2.769646	1.711762
O	0.400850	1.173003	0.148796	H	1.970477	3.056966	1.539383
P	-0.322103	-0.102891	-0.610352	C	3.005486	1.739397	2.854985
O	-0.533889	-1.134272	0.474977	H	4.021597	1.454105	3.153719
C	-4.617157	0.551714	-2.656593	H	2.469298	0.832922	2.558683
H	-4.173823	1.387282	-2.108451	H	2.506422	2.152289	3.739378
C	-6.028112	1.001451	-3.086565	C	3.771125	4.048007	2.118697
H	-6.653789	1.231798	-2.216683	H	3.717579	4.807222	1.330345
H	-6.538894	0.224873	-3.668284	H	4.830824	3.837174	2.307467
H	-5.968999	1.900723	-3.711820	H	3.345293	4.477285	3.034158
C	-3.719092	0.289404	-3.880850	O	0.410179	-0.487219	-1.872183
H	-2.706854	0.015835	-3.569377	H	0.908190	-4.731834	-0.167936
H	-3.653815	1.190233	-4.503482	H	0.326077	-2.973079	0.043728
H	-4.116859	-0.517482	-4.508470	O	1.712333	-3.873707	1.748855
C	-3.947524	-1.785278	1.906491	S	1.160538	-3.342942	-2.421253
H	-3.430840	-0.846582	2.124146	H	0.667659	-2.024339	-2.275811

C	2.751894	2.566920	-1.303007	C	4.519865	1.397958	0.051215
H	-0.929701	5.841323	-1.419169	C	3.915762	0.472493	-2.140143
C	0.067415	5.854999	-1.843390	C	5.490511	0.398088	0.182140
C	2.615583	5.901477	-3.002364	C	4.898648	-0.509452	-1.960083
H	4.112999	3.742129	-2.447157	C	5.695254	-0.562166	-0.812321
C	1.744434	6.944071	-3.219339	H	6.113552	0.366793	1.071825
C	0.453414	6.909769	-2.641600	H	5.050655	-1.258998	-2.730216
H	3.603976	5.902917	-3.455955	O	-1.255212	1.545245	-1.001136
H	2.038142	7.784522	-3.842181	O	1.089320	1.450152	0.037990
H	-0.244109	7.720488	-2.834388	P	-0.121553	0.451917	-0.505737
C	-0.684974	3.628120	0.014871	O	-0.589453	-0.253497	0.758102
C	-1.010721	4.661145	0.962136	C	-4.070969	2.479527	-2.384920
C	-1.596931	2.597721	-0.175684	H	-3.292372	3.140010	-1.994408
C	-0.077943	5.651289	1.380697	C	-5.254317	3.379945	-2.793831
C	-2.318683	4.678659	1.547087	H	-5.650435	3.931951	-1.933697
C	-2.916920	2.614495	0.369776	H	-6.076563	2.795122	-3.222728
C	-0.427829	6.616079	2.301017	H	-4.935366	4.108870	-3.548669
H	0.926456	5.634308	0.973432	C	-3.476593	1.751385	-3.605847
C	-2.654206	5.699388	2.477953	H	-2.610444	1.148440	-3.318412
C	-3.251559	3.670154	1.193011	H	-3.152050	2.480378	-4.358219
C	-1.732249	6.651441	2.849204	H	-4.213142	1.092486	-4.081120
H	0.305935	7.356231	2.608911	C	-3.834054	0.640287	2.446919
H	-3.655698	5.704814	2.901924	H	-2.994327	1.338815	2.492949
H	-4.256874	3.724892	1.602687	C	-4.889819	1.117739	3.463748
H	-1.998771	7.423030	3.566321	H	-5.249225	2.125778	3.227745
C	-3.927672	1.558635	0.028378	H	-4.468495	1.137390	4.476493
C	-4.475131	1.506477	-1.277422	H	-5.760634	0.451290	3.477074
C	-4.382011	0.654436	1.019460	C	-3.283938	-0.744040	2.839454
C	-5.458898	0.553654	-1.562404	H	-2.524096	-1.063732	2.121285
C	-5.375469	-0.274203	0.685437	H	-4.073033	-1.504069	2.876532
C	-5.925141	-0.343345	-0.597218	H	-2.826435	-0.697704	3.836239
H	-5.886225	0.511567	-2.560366	C	3.109147	0.491271	-3.439321
H	-5.731589	-0.969177	1.440829	H	2.172303	1.019740	-3.240356
C	3.729748	1.439046	-1.121899	C	2.731054	-0.913003	-3.944237

H	2.007810	-0.823045	-4.762799	C	6.494082	-2.749189	0.159974
H	2.276176	-1.520498	-3.159012	C	9.001010	-2.504214	-1.154046
H	3.600112	-1.452936	-4.340614	C	7.513332	-3.762986	0.315010
C	3.867865	1.255314	-4.545408	C	8.736451	-3.613834	-0.345448
H	4.826057	0.768301	-4.766612	H	9.500410	-4.380004	-0.228528
H	4.075388	2.291659	-4.260909	C	-6.982840	-1.349150	-0.928133
H	3.278121	1.272010	-5.470013	C	-8.312262	-1.149911	-0.484768
C	4.387991	2.444402	1.157553	C	-6.650664	-2.498039	-1.685486
H	3.468302	3.009394	0.981327	C	-9.328155	-2.128071	-0.804318
C	4.263084	1.816596	2.557083	C	-7.676931	-3.464865	-2.006619
H	5.179839	1.295660	2.857914	C	-8.983948	-3.255315	-1.556411
H	3.436386	1.099851	2.590426	H	-9.752330	-3.987080	-1.798403
H	4.065945	2.593001	3.305507	C	6.038557	-5.046719	1.772702
C	5.557033	3.448485	1.105644	H	5.846680	-5.918650	2.392523
H	5.601409	3.953316	0.134316	C	5.026884	-4.055630	1.614753
H	6.518176	2.944737	1.264679	H	4.068517	-4.186271	2.111529
H	5.445165	4.215371	1.882273	C	9.520198	-0.244675	-2.760889
O	0.277193	-0.327661	-1.715724	H	9.734833	0.622746	-3.379436
S	0.684339	-3.708107	2.437982	C	10.509096	-1.259218	-2.610058
O	0.892696	-2.963516	-1.566186	H	11.465261	-1.157768	-3.116431
C	-0.725778	-4.572230	0.290226	C	-6.043333	-4.824625	-3.201902
C	-0.130201	-5.824573	0.081133	H	-5.793155	-5.705272	-3.787491
C	-2.112901	-4.447844	0.139475	C	-5.024838	-3.882158	-2.876847
C	-0.907243	-6.928496	-0.268400	H	-4.006143	-4.056721	-3.211372
H	0.946201	-5.939701	0.179096	C	-8.710951	0.004759	0.264897
C	-2.890467	-5.549471	-0.219793	C	-10.006353	0.171571	0.681283
H	-2.584293	-3.479829	0.289767	C	-11.000216	-0.802492	0.376043
C	-2.288960	-6.793454	-0.420193	H	-7.965021	0.756429	0.498576
H	-0.431771	-7.892114	-0.430210	H	-10.282640	1.057454	1.247105
H	-3.961765	-5.430361	-0.351758	H	-12.021758	-0.653706	0.715599
H	-2.893125	-7.652689	-0.698896	C	-7.328431	-4.619718	-2.775689
H	2.024522	-3.917208	-0.179717	H	-8.112668	-5.334545	-3.014548
C	6.745428	-1.617841	-0.651966	C	-5.318143	-2.760832	-2.143506
C	7.990251	-1.482177	-1.311704	H	-4.533648	-2.051379	-1.904156

C 10.253814 -2.353544 -1.827891
H 11.002500 -3.132387 -1.702550
C 8.305936 -0.351770 -2.133781
H 7.560950 0.426876 -2.254447
C 5.246844 -2.948115 0.836873
H 4.468833 -2.202183 0.716939
C 7.243334 -4.901155 1.138743
H 8.021048 -5.653755 1.246844
C -10.667167 -1.915946 -0.347730
H -11.418485 -2.663071 -0.593208

(R)-7-TS4-R E= -4608.98148470

C 0.552317 0.363419 4.104703
C 1.064655 -0.925194 3.929027
C 1.919132 -1.504864 4.880125
C 2.232006 -0.773962 6.026855
C 1.720098 0.511137 6.220949
C 0.885894 1.078056 5.255584
H -0.089695 0.790524 3.340876
H 2.888569 -1.216834 6.772290
H 1.974174 1.065990 7.119490
H 0.488737 2.079315 5.395231
C 2.471289 -2.879005 4.583362
H 3.368291 -2.792673 3.952101
H 2.780103 -3.384969 5.504054
C 1.421345 -3.718552 3.844155
H 1.822251 -4.671995 3.493255
H 0.576637 -3.942480 4.512106
C 0.852403 -2.982200 2.644591
N 0.723502 -1.652263 2.756328
H 0.286262 -1.104647 1.991519
C 0.555475 -3.303006 -1.120832
C -0.441856 -3.066133 -0.080841
H 1.335988 -2.542039 -1.147377

C 1.160476 2.954220 -0.670676
C 0.203933 3.952451 -0.794138
C 0.465068 5.038729 -1.702216
C 1.752101 5.127800 -2.324939
C 2.724355 4.129519 -2.060178
C 2.451633 3.030162 -1.273966
H -1.502782 5.946357 -1.616640
C -0.509515 6.017524 -2.043961
C 2.029181 6.205502 -3.209047
H 3.709118 4.230872 -2.508677
C 1.069598 7.147438 -3.500255
C -0.215840 7.040685 -2.919038
H 3.015597 6.261936 -3.663457
H 1.290296 7.963018 -4.183422
H -0.981901 7.769715 -3.169221
C -1.070070 3.874232 -0.019476
C -1.495559 4.944669 0.843076
C -1.877304 2.748325 -0.118111
C -0.668897 6.056632 1.166673
C -2.797694 4.879929 1.436975
C -3.187114 2.675322 0.442687
C -1.116205 7.058142 2.000696
H 0.333544 6.105640 0.757634
C -3.236048 5.938507 2.278130
C -3.623582 3.755508 1.181593
C -2.417184 7.009040 2.554840
H -0.460916 7.891828 2.238458
H -4.232098 5.877896 2.710533
H -4.627100 3.741536 1.598668
H -2.760573 7.809062 3.204978
C -4.088173 1.498606 0.202031
C -4.677270 1.314144 -1.072748
C -4.398965 0.608987 1.259096
C -5.563972 0.248401 -1.262646

C	-5.300918	-0.435165	1.020514	H	-3.898987	-1.363059	3.288033
C	-5.892151	-0.634722	-0.229838	H	-2.653138	-0.411847	4.105438
H	-6.024539	0.104029	-2.236178	C	3.144653	1.019453	-3.388166
H	-5.550176	-1.120200	1.826017	H	2.251584	1.648018	-3.331958
C	3.492981	1.979484	-1.017284	C	2.676128	-0.373492	-3.845288
C	4.185171	1.977200	0.216842	H	2.148465	-0.290719	-4.803028
C	3.801941	1.015190	-2.007284	H	1.985308	-0.799760	-3.114525
C	5.149815	0.991031	0.452367	H	3.514938	-1.063891	-3.995972
C	4.779563	0.052677	-1.725331	C	4.093602	1.634596	-4.438284
C	5.452692	0.015280	-0.500577	H	5.007849	1.036480	-4.538307
H	5.682136	0.978141	1.399706	H	4.392369	2.653294	-4.168474
H	5.027642	-0.692825	-2.475137	H	3.607287	1.673802	-5.420653
O	-1.443975	1.673965	-0.874101	C	3.950649	3.041058	1.288337
O	0.893783	1.864975	0.144801	H	3.129239	3.682272	0.956595
P	-0.199124	0.732441	-0.342041	C	3.529964	2.431628	2.637238
O	-0.576423	-0.038836	0.901143	H	4.320576	1.805401	3.067376
C	-4.414543	2.256964	-2.247111	H	2.632746	1.816412	2.525751
H	-3.697369	3.015515	-1.922672	H	3.309771	3.225613	3.361206
C	-5.697603	3.004252	-2.662956	C	5.189674	3.945429	1.446317
H	-6.119131	3.566790	-1.822083	H	5.457515	4.420722	0.495723
H	-6.468998	2.312917	-3.022049	H	6.060658	3.375765	1.791907
H	-5.481755	3.712327	-3.472206	H	4.996114	4.737910	2.179643
C	-3.783253	1.523410	-3.445730	O	0.284139	-0.015332	-1.563670
H	-2.843019	1.044932	-3.156044	H	-1.192765	-3.816753	0.123257
H	-3.569960	2.232828	-4.254526	H	-0.622244	-2.053623	0.262536
H	-4.453133	0.754228	-3.848346	O	0.513186	-3.647919	1.632476
C	-3.793815	0.742216	2.656839	S	-0.819565	-2.703915	-2.271069
H	-2.992620	1.484893	2.604290	H	-0.459432	-1.348715	-2.083163
C	-4.835905	1.246864	3.675036	C	1.059253	-4.683126	-1.434738
H	-5.256378	2.214022	3.377821	C	0.668018	-5.814155	-0.708018
H	-4.380269	1.366373	4.665696	C	1.961405	-4.835479	-2.498499
H	-5.668350	0.539381	3.772718	C	1.161210	-7.075683	-1.049850
C	-3.153885	-0.571858	3.142712	H	0.008743	-5.713278	0.146927
H	-2.409095	-0.919796	2.422507	C	2.452816	-6.093310	-2.837476

H	2.270840	-3.961123	-3.065861	C	-5.106228	-3.063257	-1.680525
C	2.049939	-7.219982	-2.114838	C	-4.732252	-4.187750	-2.369972
H	0.851661	-7.944817	-0.475784	H	-4.388416	-2.267434	-1.514548
H	3.150936	-6.194597	-3.663637	H	-3.717559	-4.274001	-2.749319
H	2.432511	-8.202335	-2.377937	C	-5.659516	-5.246097	-2.593732
C	-6.851469	-1.761607	-0.454501	H	-7.652547	-5.953798	-2.271324
C	-8.172699	-1.675534	0.046879	H	-5.345877	-6.128576	-3.145103
C	-6.436064	-2.911820	-1.167766	H	10.005020	1.709498	-1.362746
C	-8.655466	-0.527898	0.756728	H	11.684102	-0.070747	-0.868713
C	-9.093617	-2.769261	-0.169100	C	6.596283	-4.635952	0.931014
C	-7.368665	-3.995392	-1.385409	C	5.265446	-4.909719	1.099757
C	-9.940483	-0.471805	1.230953	H	7.347960	-5.398390	1.122712
H	-7.982264	0.307497	0.913853	H	4.944949	-5.896701	1.422626
C	-10.424915	-2.670448	0.345030	C	4.672411	-2.649649	0.433693
C	-8.668155	-3.895848	-0.879348	C	4.290664	-3.900126	0.849282
C	-10.839403	-1.558196	1.027402	H	3.925428	-1.884709	0.249430
H	-11.103921	-3.503450	0.177583	H	3.236542	-4.131582	0.975952
H	-9.365852	-4.714926	-1.043046				
C	6.471609	-1.044768	-0.215765	(R)-C2 E= -1874.38440659			
C	7.848336	-0.771628	-0.392628	H	1.229811	-3.574454	-0.848892
C	6.052506	-2.321148	0.228448	C	1.516685	0.045992	0.254183
C	8.326957	0.499024	-0.850206	C	0.702049	1.093204	-0.144272
C	8.824962	-1.801407	-0.116134	C	1.285228	2.154790	-0.919462
C	7.036535	-3.346524	0.494452	C	2.698615	2.140155	-1.155372
C	9.666904	0.737327	-1.013950	C	3.479735	1.069455	-0.655080
H	7.604484	1.277850	-1.068378	C	2.922837	0.004478	0.026974
C	10.213398	-1.509663	-0.299183	H	-0.555997	3.207621	-1.371737
C	8.393409	-3.058766	0.317746	C	0.519511	3.201314	-1.503768
C	10.626009	-0.278446	-0.733570	C	3.291534	3.190486	-1.908285
H	10.936618	-2.293362	-0.085481	H	4.553221	1.086676	-0.823111
H	9.131253	-3.832671	0.520478	C	2.523775	4.200392	-2.440026
H	-11.854075	-1.496318	1.411610	C	1.122366	4.194877	-2.244059
H	-10.281703	0.411057	1.765118	H	4.367059	3.170919	-2.067033
C	-6.937358	-5.150066	-2.111520	H	2.986750	4.994053	-3.019776

H	0.514224	4.979448	-2.685893	P	0.017597	-2.081188	0.097032
C	-0.753300	1.064576	0.188278	O	-0.622588	-3.063169	0.987317
C	-1.384810	2.119851	0.933188	O	0.939029	-2.676800	-1.081853
C	-1.523452	-0.023770	-0.190936	H	-6.004888	-4.198084	-1.680845
C	-0.664556	3.205823	1.503122	H	-2.876748	-1.350343	-2.441196
C	-2.799143	2.057178	1.153865	H	-4.795332	-1.459552	1.404576
C	-2.932652	-0.104330	0.003175	H	2.951081	-1.262097	2.467903
C	-1.311618	4.190190	2.217805	H	6.111004	-4.045630	1.607278
H	0.411476	3.249157	1.381732	H	4.787890	-1.293090	-1.419507
C	-3.438439	3.098752	1.880605				
C	-3.535268	0.953426	0.657576				
C	-2.714242	4.146408	2.400276	(R)-C3 E= -2336.49015629			
H	-0.737893	5.005347	2.650198	H	0.954219	-2.276195	-1.108559
H	-4.514127	3.042252	2.028820	C	1.536809	1.338133	-0.054505
H	-4.612079	0.938955	0.802457	C	0.671663	2.398169	-0.270463
H	-3.212502	4.932805	2.960346	C	1.095835	3.458106	-1.145161
C	-3.741545	-1.261272	-0.465223	C	2.428452	3.425715	-1.671397
C	-3.610458	-1.777217	-1.765638	C	3.282254	2.342987	-1.347230
C	-4.702069	-1.829486	0.387408	C	2.865861	1.281206	-0.566446
C	-4.422805	-2.824063	-2.198606	H	-0.781947	4.541906	-1.195278
C	-5.511878	-2.878771	-0.046174	C	0.241409	4.520305	-1.550850
C	-5.376333	-3.378889	-1.342029	C	2.866551	4.473180	-2.527279
H	-4.311368	-3.205679	-3.210115	H	4.298176	2.349576	-1.732920
H	-6.242026	-3.310892	0.632930	C	2.020186	5.497811	-2.882041
C	3.769609	-1.133948	0.474047	C	0.691301	5.511069	-2.396229
C	4.721583	-1.677378	-0.405447	H	3.884797	4.439852	-2.907278
C	3.677227	-1.666984	1.771577	H	2.363757	6.289139	-3.542403
C	5.559597	-2.716812	-0.001498	H	0.016546	6.308082	-2.696317
C	4.516348	-2.705462	2.174167	C	-0.682842	2.385144	0.358432
C	5.460533	-3.234557	1.291100	C	-1.129811	3.441135	1.226140
H	6.284705	-3.125966	-0.700170	C	-1.529459	1.309097	0.143195
H	4.432843	-3.100029	3.183252	C	-0.293541	4.516474	1.635205
O	-0.891871	-1.101508	-0.821746	C	-2.465452	3.390150	1.742491
O	0.938051	-1.030279	0.929341	C	-2.866465	1.240817	0.631601
				C	-0.763307	5.501534	2.476340

H	0.732050	4.551826	1.286971	C	-7.293786	-3.145261	-1.669320
C	-2.924273	4.431996	2.594390	C	-6.730418	-4.166235	0.441363
C	-3.303123	2.298368	1.407408	C	-8.189235	-4.181261	-1.932145
C	-2.095050	5.469035	2.953569	H	-7.188223	-2.332853	-2.383023
H	-0.102280	6.308583	2.780168	C	-7.626289	-5.202068	0.179398
H	-3.944427	4.384386	2.967547	H	-6.143820	-4.181936	1.355689
H	-4.324662	2.294449	1.777766	C	-8.360082	-5.214703	-1.008627
H	-2.454320	6.255792	3.611047	H	-8.760720	-4.176306	-2.856730
C	-3.769506	0.098336	0.336390	H	-7.744064	-6.006100	0.901278
C	-3.915860	-0.420195	-0.961120	H	-9.057769	-6.022349	-1.213051
C	-4.549382	-0.462945	1.360158	C	6.538331	-3.123061	0.404834
C	-4.812332	-1.452038	-1.220310	C	7.775116	-3.180289	-0.261033
C	-5.443218	-1.497243	1.098805	C	6.222874	-4.154349	1.306618
C	-5.595835	-2.014540	-0.197883	C	8.664047	-4.230151	-0.033998
H	-4.889601	-1.845224	-2.230103	H	8.051745	-2.380354	-0.942290
H	-6.043962	-1.898415	1.910133	C	7.111755	-5.204186	1.534504
C	3.773613	0.134941	-0.301612	H	5.261926	-4.145043	1.813491
C	3.926495	-0.421291	0.980205	C	8.336578	-5.247196	0.865185
C	4.545321	-0.403165	-1.345275	H	9.618269	-4.248752	-0.554076
C	4.818450	-1.465766	1.204126	H	6.842699	-5.994501	2.230412
C	5.435025	-1.449670	-1.118943	H	9.029300	-6.065300	1.042850
C	5.592541	-2.004978	0.161902				
H	4.937691	-1.851323	2.212667				
H	5.990551	-1.865230	-1.955007	(R)-C4 E= -2188.88958457			
O	-1.058811	0.230506	-0.613838	H	-1.031192	-2.620355	1.058960
O	1.095241	0.263111	0.719279	C	-1.534087	0.983636	0.018347
P	0.008940	-0.769233	0.088030	C	-0.672620	2.037879	0.273698
O	-0.446040	-1.753230	1.083751	C	-1.121612	3.090668	1.144446
O	0.658402	-1.362932	-1.260394	C	-2.471610	3.059101	1.624065
H	-4.441671	-0.093169	2.375972	C	-3.318282	1.983502	1.259692
H	-3.323906	-0.012300	-1.773407	C	-2.879744	0.926751	0.484307
H	3.355278	-0.022751	1.811277	H	0.758532	4.164305	1.271417
H	4.421696	-0.015562	-2.352705	C	-0.276742	4.144298	1.590834
C	-6.548164	-3.118297	-0.477882	C	-2.934388	4.099832	2.475115
				H	-4.346853	1.990687	1.610187

C	-2.096177	5.116546	2.869859	H	-4.856283	-2.173788	-2.386194
C	-0.751069	5.128242	2.430798	H	-6.082746	-2.182183	1.737318
H	-3.965306	4.067352	2.819401	O	1.041450	-0.139652	0.650142
H	-2.458845	5.902660	3.526290	O	-1.069876	-0.085161	-0.751234
H	-0.083451	5.918577	2.762904	P	-0.010497	-1.126922	-0.090752
C	0.701602	2.026696	-0.310381	O	0.467079	-2.110898	-1.076038
C	1.178724	3.091003	-1.151277	C	6.578085	-3.527892	0.713597
C	1.538920	0.946492	-0.078934	C	7.566397	-3.047414	1.803184
C	0.357235	4.170705	-1.578695	H	8.260218	-3.853830	2.071197
C	2.531457	3.044475	-1.620985	H	7.047258	-2.737104	2.716090
C	2.892375	0.882267	-0.520311	H	8.156678	-2.194640	1.448385
C	0.856083	5.163689	-2.393325	C	5.776663	-4.739394	1.247426
H	-0.680020	4.202753	-1.266436	H	5.069533	-5.103885	0.493727
C	3.019920	4.094603	-2.445819	H	5.204611	-4.485218	2.145882
C	3.356361	1.948873	-1.267426	H	6.455180	-5.562171	1.504942
C	2.203837	5.135428	-2.823691	C	-6.591508	-3.478463	-0.704119
H	0.206088	5.973802	-2.712495	C	-7.588436	-2.997343	-1.785602
H	4.052497	4.050102	-2.783593	H	-8.288314	-3.801721	-2.043363
H	4.390563	1.948139	-1.600736	H	-7.077281	-2.693050	-2.704892
H	2.585958	5.928466	-3.460474	H	-8.171195	-2.140694	-1.427977
C	3.785454	-0.263650	-0.208073	C	-5.799679	-4.693997	-1.243108
C	3.885150	-0.805371	1.084676	H	-6.483901	-5.513134	-1.496445
C	4.606896	-0.807144	-1.204238	H	-5.090758	-5.064224	-0.493486
C	4.776910	-1.837035	1.357548	H	-5.231242	-4.443371	-2.144742
C	5.496989	-1.844565	-0.923128	O	-0.705238	-1.721909	1.235035
C	5.607594	-2.385640	0.364243	H	4.533548	-0.430397	-2.220797
H	4.825237	-2.219520	2.373512	H	3.267865	-0.409274	1.884094
H	6.101888	-2.234003	-1.734424	H	-3.294744	-0.362974	-1.920094
C	-3.783499	-0.213100	0.179057	H	-4.506326	-0.378900	2.201429
C	-3.901228	-0.757052	-1.111983	C	7.397517	-3.993346	-0.504961
C	-4.591513	-0.758069	1.186572	H	6.755804	-4.378551	-1.305480
C	-4.795699	-1.790465	-1.371318	H	8.010587	-3.183545	-0.917007
C	-5.486141	-1.795683	0.918316	H	8.075189	-4.801495	-0.206905
C	-5.614281	-2.338119	-0.367257	C	-7.401255	-3.937795	0.523235

H	-6.754221	-4.324121	1.319135	H	4.376612	2.342037	-1.685212
H	-8.007426	-3.124778	0.939024	H	2.512166	6.304760	-3.527067
H	-8.084590	-4.744014	0.233373	C	3.785440	0.083891	-0.315671
(R)-C5 E= -2808.24370205				C	4.310146	-0.066250	0.990467
H	-0.824080	-2.388926	1.023417	C	4.141200	-0.835046	-1.333124
C	-1.540774	1.333328	0.079686	C	5.181135	-1.127281	1.252077
C	-0.663098	2.392060	0.256052	C	5.021690	-1.875436	-1.019504
C	-1.087963	3.488755	1.087071	C	5.553896	-2.045382	0.263420
C	-2.439125	3.512528	1.562812	H	5.565446	-1.258500	2.259647
C	-3.308413	2.435889	1.252998	H	5.321457	-2.564559	-1.803243
C	-2.883651	1.323710	0.555702	C	-3.797500	0.160242	0.306687
H	0.817679	4.520597	1.178466	C	-4.269773	-0.102737	-1.002904
C	-0.219372	4.540290	1.491460	C	-4.212113	-0.663325	1.384694
C	-2.880258	4.602151	2.362164	C	-5.126735	-1.186684	-1.210381
H	-4.335304	2.479421	1.605152	C	-5.075719	-1.732138	1.121970
C	-2.019289	5.615521	2.714311	C	-5.541861	-2.020604	-0.165596
C	-0.672238	5.572403	2.284037	H	-5.511780	-1.370431	-2.209213
H	-3.912571	4.609420	2.703545	H	-5.376431	-2.379534	1.940362
H	-2.365196	6.439466	3.332168	O	1.076178	0.199029	0.566039
H	0.014510	6.358595	2.585459	O	-1.133839	0.234380	-0.678418
C	0.687170	2.368443	-0.379908	P	-0.000069	-0.786792	-0.132326
C	1.147582	3.439144	-1.225400	O	0.428320	-1.720381	-1.188617
C	1.536628	1.290831	-0.180629	C	3.979085	0.901914	2.126418
C	0.308587	4.504151	-1.656267	H	3.274109	1.647247	1.746721
C	2.501928	3.417501	-1.692369	C	5.232303	1.671208	2.589900
C	2.886543	1.244160	-0.628980	H	5.695270	2.213718	1.757869
C	0.792171	5.506270	-2.468794	H	5.987245	0.994882	3.008099
H	-0.730509	4.517331	-1.349324	H	4.969642	2.398818	3.367446
C	2.974952	4.477413	-2.513076	C	3.293291	0.192847	3.310192
C	3.344065	2.329719	-1.347115	H	2.382640	-0.319571	2.985424
C	2.142016	5.504286	-2.892615	H	3.019752	0.922078	4.082509
H	0.127883	6.303223	-2.791571	H	3.954517	-0.548149	3.774684
H	4.008792	4.450507	-2.848621	C	3.626708	-0.719846	-2.769110
				H	2.821323	0.020500	-2.780304

C	4.735942	-0.214286	-3.714391	C	-7.176846	-5.027659	-1.813647
H	5.137961	0.752037	-3.389372	H	-5.534846	-3.722327	-2.287964
H	4.347067	-0.094568	-4.732873	C	-8.174682	-5.351102	-0.891828
H	5.572538	-0.922350	-3.756138	H	-9.091302	-4.822319	0.988006
C	3.024239	-2.037251	-3.293433	H	-7.054701	-5.621711	-2.715643
H	2.213705	-2.378141	-2.644839	H	-8.838425	-6.191688	-1.075336
H	3.777235	-2.830895	-3.368831	C	6.483572	-3.164093	0.566396
H	2.614764	-1.881690	-4.299108	C	7.577841	-2.982128	1.429693
C	-3.775767	-0.424054	2.832611	C	6.293586	-4.435598	-0.001993
H	-2.977835	0.323306	2.828901	C	8.449474	-4.032521	1.715210
C	-3.202387	-1.683109	3.509933	H	7.759454	-2.001168	1.860103
H	-2.860111	-1.438801	4.522450	C	7.165447	-5.486266	0.281897
H	-2.345430	-2.073563	2.954433	H	5.439141	-4.605893	-0.650979
H	-3.947462	-2.481702	3.600554	C	8.247706	-5.289886	1.142234
C	-4.940606	0.144248	3.670384	H	9.293425	-3.865606	2.379709
H	-5.766804	-0.573993	3.736594	H	6.993231	-6.462874	-0.163252
H	-5.341305	1.066350	3.235309	H	8.927103	-6.108519	1.364106
H	-4.607788	0.367522	4.691291				
C	-3.934568	0.795580	-2.193840		(R)-C6 E= -2660.64249695		
H	-3.210012	1.545278	-1.864712	H	-0.871125	-2.634605	1.072559
C	-3.285055	0.018689	-3.354458	C	-1.547314	1.050112	0.039570
H	-3.970940	-0.723033	-3.780788	C	-0.684169	2.115608	0.244699
H	-2.381061	-0.501094	-3.023797	C	-1.151569	3.216335	1.046785
H	-3.006903	0.708421	-4.160352	C	-2.523265	3.237083	1.459492
C	-5.184581	1.563843	-2.669706	C	-3.372806	2.154019	1.118117
H	-5.617676	2.159300	-1.858025	C	-2.911207	1.037192	0.451988
H	-5.961228	0.880234	-3.032441	H	0.744084	4.256056	1.218552
H	-4.926609	2.243469	-3.490937	C	-0.306532	4.274302	1.482962
O	-0.571767	-1.468700	1.209573	C	-3.005050	4.330565	2.229545
C	-6.451147	-3.168827	-0.415276	H	-4.415305	2.195874	1.421659
C	-7.460853	-3.506386	0.502514	C	-2.165160	5.349995	2.613856
C	-6.324809	-3.949350	-1.577467	C	-0.799417	5.309721	2.246808
C	-8.312529	-4.585274	0.267702	H	-4.051972	4.335704	2.523235
H	-7.594265	-2.900619	1.394555	H	-2.542512	6.176644	3.209332

H	-0.130457	6.100731	2.574508	P	0.014246	-1.061030	-0.076207
C	0.690858	2.097092	-0.335792	O	0.482491	-2.015594	-1.096266
C	1.174682	3.164353	-1.172522	C	3.905646	0.648161	2.296829
C	1.540178	1.027443	-0.096029	H	3.207435	1.388182	1.894404
C	0.344454	4.218755	-1.644669	C	5.138883	1.427502	2.795829
C	2.545816	3.149486	-1.587718	H	5.623291	1.969910	1.976032
C	2.905826	0.985984	-0.494944	H	5.885573	0.758056	3.239181
C	0.850942	5.217896	-2.446829	H	4.848046	2.156447	3.562210
H	-0.705874	4.225619	-1.378459	C	3.188478	-0.061497	3.461584
C	3.041729	4.206504	-2.398590	H	2.291564	-0.580719	3.110253
C	3.381624	2.070006	-1.203720	H	2.886252	0.667799	4.223143
C	2.216121	5.223561	-2.818358	H	3.839916	-0.796755	3.948741
H	0.193227	6.006469	-2.802079	C	3.741594	-0.978121	-2.603715
H	4.087736	4.184788	-2.694513	H	2.942564	-0.232242	-2.650097
H	4.425547	2.086268	-1.504876	C	4.885041	-0.488653	-3.516124
H	2.604087	6.021805	-3.444971	H	5.282673	0.477854	-3.185975
C	3.800339	-0.167659	-0.147177	H	4.532017	-0.375648	-4.548413
C	4.276177	-0.320283	1.173316	H	5.717819	-1.202609	-3.523247
C	4.206734	-1.082552	-1.149804	C	3.147344	-2.296259	-3.135869
C	5.147253	-1.377961	1.467001	H	2.313111	-2.625710	-2.511766
C	5.083268	-2.113515	-0.800197	H	3.896544	-3.096081	-3.176920
C	5.571355	-2.291787	0.500037	H	2.773691	-2.148449	-4.156677
H	5.502433	-1.474670	2.486826	C	-3.928422	-0.684400	2.700677
H	5.391455	-2.805977	-1.577860	H	-3.148794	0.081164	2.736553
C	-3.806062	-0.134015	0.171974	C	-3.364669	-1.924821	3.419697
C	-4.210513	-0.420418	-1.155986	H	-3.093891	-1.668848	4.450925
C	-4.274933	-0.945274	1.232120	H	-2.463433	-2.292059	2.921063
C	-5.051652	-1.510717	-1.387976	H	-4.091668	-2.743712	3.465854
C	-5.123015	-2.023615	0.938104	C	-5.151944	-0.137242	3.465435
C	-5.525165	-2.337477	-0.361179	H	-5.967330	-0.870479	3.483314
H	-5.354096	-1.714552	-2.411266	H	-5.542231	0.776187	3.003076
H	-5.476444	-2.629392	1.764360	H	-4.886033	0.094731	4.503952
O	1.060201	-0.060144	0.644821	C	-3.811420	0.455986	-2.343961
O	-1.099156	-0.054235	-0.686896	H	-3.110447	1.216458	-1.988928

C	-3.773746	0.907107	0.447398	H	-4.212180	0.686421	4.888839
C	-4.330086	0.751143	-0.845072	H	-5.445679	-0.161568	3.940416
C	-4.092811	-0.012407	1.476679	C	-2.883300	-1.204411	3.385958
C	-5.195858	-0.321695	-1.083329	H	-2.085388	-1.516811	2.707772
C	-4.969149	-1.065513	1.186624	H	-3.611983	-2.018977	3.473647
C	-5.526433	-1.239870	-0.082511	H	-2.447024	-1.049487	4.380408
H	-5.628496	-0.451030	-2.071653	C	3.696792	0.447776	-2.920332
H	-5.224019	-1.776893	1.966773	H	2.883871	1.178546	-2.890554
C	3.782923	1.018952	-0.393286	C	3.139012	-0.812626	-3.608016
C	4.292652	0.757338	0.902258	H	2.763452	-0.557194	-4.605748
C	4.164707	0.197091	-1.484515	H	2.307706	-1.238811	-3.039802
C	5.155043	-0.329029	1.084944	H	3.901880	-1.588974	-3.734997
C	5.033608	-0.875205	-1.246785	C	4.835802	1.049889	-3.770270
C	5.532388	-1.161418	0.027347	H	5.674992	0.349224	-3.857138
H	5.552197	-0.534338	2.075022	H	5.223618	1.975928	-3.332038
H	5.332385	-1.513064	-2.073605	H	4.481768	1.277026	-4.783131
O	-1.107552	1.059878	-0.549826	C	3.983238	1.648260	2.105465
O	1.136376	1.062401	0.632798	H	3.254826	2.402486	1.795352
P	-0.006413	0.055597	0.078416	C	3.353607	0.863903	3.272154
O	-0.401165	-0.924604	1.105455	H	4.042723	0.112850	3.675919
C	-4.048517	1.727768	-1.986787	H	2.439113	0.353720	2.955421
H	-3.334456	2.475531	-1.629657	H	3.097260	1.547526	4.090376
C	-5.324555	2.490438	-2.396595	C	5.245091	2.408230	2.563131
H	-5.755073	3.029718	-1.545087	H	5.664419	3.009195	1.748185
H	-6.092272	1.810281	-2.783735	H	6.025935	1.718884	2.905168
H	-5.098410	3.220743	-3.182966	H	5.005494	3.081736	3.394799
C	-3.404740	1.030253	-3.200416	O	0.531318	-0.567439	-1.305831
H	-2.478454	0.522488	-2.914762	C	6.442878	-2.328188	0.250752
H	-3.166144	1.766113	-3.977959	C	7.793734	-2.262751	-0.166877
H	-4.078561	0.287884	-3.643876	C	5.946624	-3.497898	0.875572
C	-3.536662	0.102616	2.896924	C	8.662248	-3.400282	0.039684
H	-2.752007	0.864830	2.892236	C	6.826630	-4.626545	1.082021
C	-4.629094	0.568172	3.881397	C	8.156227	-4.548072	0.656952
H	-5.065166	1.527750	3.580517	H	8.813785	-5.401363	0.811193

C	-6.448050	-2.385310	-0.366904	H	3.908912	-2.793394	1.154466
C	-7.847945	-2.181594	-0.377662	C	6.313903	-5.803543	1.712996
C	-5.913202	-3.669225	-0.627440	H	6.989882	-6.642080	1.863605
C	-8.730385	-3.291599	-0.660275	C	-10.143876	-3.071922	-0.667473
C	-6.805141	-4.772502	-0.906450	H	-10.794571	-3.916009	-0.884297
C	-8.186130	-4.553762	-0.916603				
H	-8.853894	-5.386554	-1.128625				
C	5.007884	-5.878237	2.116912				
H	4.631705	-6.778342	2.595520				
C	4.133667	-4.773112	1.907126				
H	3.097415	-4.842620	2.226975				
C	9.670604	-1.061966	-1.172433				
H	10.073867	-0.163872	-1.632856				
C	10.517980	-2.190958	-0.979847				
H	11.555573	-2.145728	-1.299494				
C	-4.897688	-6.268746	-1.164321				
H	-4.490667	-7.256041	-1.365742				
C	-4.014653	-5.183407	-0.895592				
H	-2.941564	-5.355244	-0.895836				
C	-8.443630	-0.907155	-0.104657				
C	-9.804077	-0.739537	-0.119273				
C	-10.669113	-1.834668	-0.406619				
H	-7.795166	-0.067039	0.118727				
H	-10.231236	0.237170	0.092411				
H	-11.745081	-1.682436	-0.414503				
C	-6.251596	-6.064980	-1.169762				
H	-6.935308	-6.885244	-1.376158				
C	-4.503863	-3.929063	-0.637751				
H	-3.820810	-3.111575	-0.434400				
C	10.024851	-3.323167	-0.388815				
H	10.663305	-4.189229	-0.230436				
C	8.357733	-1.096260	-0.779396				
H	7.725407	-0.227595	-0.925904				
C	4.585944	-3.626590	1.306873				
				TS1-R-cyclohexyl-anthryl E= -4612.13924318			
				H	0.240162	-1.896573	-1.463692
				C	0.225967	1.820704	3.613827
				C	0.827718	0.677431	4.150783
				C	1.537100	0.728582	5.361281
				C	1.609722	1.946680	6.037548
				C	1.005227	3.094059	5.517693
				C	0.319848	3.029558	4.302396
				H	-0.291983	1.752817	2.663616
				H	2.152325	1.996124	6.978921
				H	1.073551	4.034044	6.057879
				H	-0.142776	3.918863	3.884558
				C	2.217184	-0.534000	5.831768
				H	3.220569	-0.602711	5.385572
				H	2.357294	-0.521965	6.918123
				C	1.395927	-1.763877	5.422610
				H	1.917247	-2.695385	5.648274
				H	0.448599	-1.778810	5.983048
				C	1.027388	-1.745807	3.950235
				N	0.748482	-0.546860	3.434622
				H	0.395583	-0.475067	2.463390
				C	1.158365	-3.196921	-0.237975
				C	-0.118467	-3.177379	0.477010
				H	1.847305	-2.378512	-0.033500
				H	-0.473515	-2.187305	0.750908
				C	1.587084	2.558291	-0.827249
				C	0.736368	3.647641	-0.957555
				C	1.101823	4.696206	-1.874112

C	2.387533	4.646766	-2.503920	H	-5.565079	-0.850462	1.391836
C	3.247334	3.548684	-2.246366	C	3.798732	1.330434	-1.224408
C	2.867303	2.487258	-1.452101	C	4.581422	1.289095	-0.047379
H	-0.759954	5.806617	-1.786391	C	3.935141	0.317558	-2.205446
C	0.233941	5.770824	-2.216464	C	5.488608	0.237704	0.129135
C	2.772992	5.687085	-3.392243	C	4.856719	-0.712490	-1.981912
H	4.231203	3.539839	-2.707719	C	5.639991	-0.772388	-0.824404
C	1.917369	6.724707	-3.681904	H	6.100794	0.203150	1.026296
C	0.630252	6.755057	-3.095640	H	4.973876	-1.495003	-2.725406
H	3.757516	5.637423	-3.851471	O	-1.110266	1.530567	-1.020506
H	2.219988	7.510719	-4.368262	O	1.226597	1.522723	0.019328
H	-0.056128	7.559729	-3.345189	P	-0.001153	0.496369	-0.376790
C	-0.545338	3.700401	-0.193544	O	-0.458412	-0.095487	0.933769
C	-0.878491	4.811061	0.658425	C	-3.937695	2.501274	-2.531865
C	-1.461353	2.662491	-0.304593	H	-3.183280	3.195883	-2.152626
C	0.053198	5.830442	1.000877	C	-5.134289	3.355427	-2.996659
C	-2.192874	4.881150	1.225216	H	-5.560925	3.927454	-2.164829
C	-2.790788	2.733897	0.210098	H	-5.933421	2.735614	-3.420160
C	-0.302371	6.869460	1.833736	H	-4.818217	4.064973	-3.770945
H	1.061711	5.776642	0.607335	C	-3.301535	1.743137	-3.713058
C	-2.533269	5.975727	2.065922	H	-2.425772	1.174846	-3.385915
C	-3.129653	3.853919	0.940503	H	-2.981137	2.449961	-4.488049
C	-1.611262	6.952651	2.365615	H	-4.011689	1.046552	-4.174745
H	0.431031	7.630265	2.086993	C	-3.748350	0.872310	2.372783
H	-3.538350	6.018813	2.478889	H	-2.902562	1.564648	2.395288
H	-4.140920	3.950032	1.327048	C	-4.835157	1.437480	3.310039
H	-1.881287	7.780952	3.014890	H	-5.178129	2.425273	2.981883
C	-3.801179	1.664265	-0.088181	H	-4.448517	1.535312	4.331772
C	-4.337086	1.559642	-1.395548	H	-5.710905	0.778008	3.345162
C	-4.252925	0.791943	0.931744	C	-3.230330	-0.479947	2.895786
C	-5.300262	0.580062	-1.657188	H	-2.440172	-0.861506	2.244218
C	-5.216810	-0.174041	0.616635	H	-4.027946	-1.229252	2.961633
C	-5.750131	-0.302152	-0.669897	H	-2.814300	-0.356320	3.903247
H	-5.721517	0.501404	-2.655574	C	3.142524	0.335927	-3.513733

H	2.270128	0.979174	-3.365598	H	-4.425426	-4.809434	-0.226406
C	2.609477	-1.047797	-3.926697	H	-3.664968	-5.181136	1.320486
H	1.953617	-0.942724	-4.798854	H	-1.228930	-7.723755	-0.166246
H	2.027073	-1.502871	-3.122939	H	-1.701215	-6.971977	1.353581
H	3.415921	-1.734764	-4.210080	H	-3.693775	-7.217713	-0.100818
C	3.987946	0.934486	-4.658008	H	-2.890232	-6.351524	-1.406846
H	4.885123	0.329187	-4.837973	C	-6.769109	-1.352031	-0.979495
H	4.313785	1.955293	-4.433721	C	-6.437985	-2.427491	-1.842098
H	3.408641	0.962717	-5.588973	C	-8.064205	-1.274624	-0.408876
C	4.501841	2.374219	1.025786	C	-5.143770	-2.570089	-2.442959
H	3.691026	3.057690	0.758464	C	-7.424714	-3.445022	-2.129728
C	4.162836	1.795777	2.411835	C	-9.035650	-2.307670	-0.692153
H	4.952197	1.128097	2.777767	C	-8.476974	-0.188462	0.430705
H	3.226090	1.231568	2.378256	C	-4.856966	-3.616992	-3.281909
H	4.044828	2.602982	3.144309	H	-4.382312	-1.829502	-2.227065
C	5.798720	3.206386	1.071549	C	-7.082803	-4.521652	-3.007763
H	6.008939	3.665817	0.099107	C	-8.690569	-3.361839	-1.542599
H	6.662248	2.586639	1.341180	C	-10.336712	-2.223560	-0.103232
H	5.715570	4.007729	1.815890	H	-7.773555	0.611514	0.631584
O	0.388614	-0.418293	-1.515208	C	-9.736407	-0.141635	0.970344
S	0.933173	-3.198396	3.089206	C	-5.839049	-4.606808	-3.573737
O	0.265973	-2.932133	-1.344638	H	-3.869709	-3.693803	-3.729784
H	1.665609	-4.150553	-0.365233	H	-7.839775	-5.274108	-3.216783
C	-1.068686	-4.328955	0.602206	H	-9.426956	-4.133850	-1.757238
C	-2.452482	-3.959209	0.007423	C	-10.680032	-1.175879	0.708216
C	-0.560838	-5.673360	0.052068	H	-11.051461	-3.013721	-0.321549
H	-1.214207	-4.434531	1.688583	H	-10.022952	0.695961	1.600798
C	-3.472909	-5.081830	0.241747	H	-5.594521	-5.427862	-4.242278
H	-2.334114	-3.783797	-1.068784	H	-11.672638	-1.123484	1.147396
H	-2.809080	-3.018904	0.445418	C	6.613301	-1.890851	-0.617653
C	-1.596800	-6.788624	0.273927	C	7.833577	-1.907334	-1.335279
H	-0.360758	-5.566938	-1.022760	C	6.308699	-2.934908	0.288862
H	0.386800	-5.947637	0.532926	C	8.207913	-0.864359	-2.244114
C	-2.968710	-6.421800	-0.312117	C	8.761814	-2.999834	-1.146317

C	7.245551	-4.021374	0.470949	C	-0.891627	3.384484	4.726903
C	5.087497	-2.976959	1.038234	H	-1.950079	3.096445	4.817055
C	9.397852	-0.904366	-2.923587	H	-0.830642	4.457133	4.916396
H	7.529960	-0.030181	-2.386495	C	-0.483893	3.109975	3.290616
C	9.991009	-3.004029	-1.878081	N	-0.152473	1.845854	3.015166
C	8.442605	-4.025401	-0.251293	H	0.072881	1.573744	2.042086
C	6.922550	-5.073323	1.385261	C	-0.984272	3.786309	-1.074189
H	4.374159	-2.168973	0.916524	C	0.346732	3.814093	-0.467759
C	4.814496	-4.003450	1.905831	H	-1.689336	3.053613	-0.683187
C	10.302808	-1.989854	-2.743420	H	0.682394	2.865456	-0.056683
H	9.658394	-0.099269	-3.605577	C	-1.856183	-1.782635	-0.601700
H	10.676176	-3.835155	-1.727414	C	-1.165061	-2.986346	-0.580122
H	9.143465	-4.846314	-0.112339	C	-1.739473	-4.115616	-1.264244
C	5.744923	-5.068125	2.083683	C	-3.057359	-3.994084	-1.812841
H	7.638967	-5.881843	1.512167	C	-3.741514	-2.755594	-1.715974
H	3.881261	-4.004074	2.463299	C	-3.161085	-1.635498	-1.158586
H	11.240708	-2.005285	-3.292112	H	-0.034777	-5.445724	-1.090596
H	5.513448	-5.874086	2.775062	C	-1.049396	-5.345037	-1.457135
				C	-3.648606	-5.107663	-2.468870
				H	-4.748123	-2.684949	-2.118984
				C	-2.961498	-6.290432	-2.615597
				C	-1.643004	-6.400530	-2.114759
				H	-4.654366	-4.998896	-2.867893
				H	-3.420528	-7.132703	-3.125930
				H	-1.089333	-7.325047	-2.255031
				C	0.161804	-3.081652	0.098801
				C	0.427108	-4.066717	1.114183
				C	1.185571	-2.208645	-0.248472
				C	-0.589816	-4.876862	1.692900
				C	1.766192	-4.216107	1.602081
				C	2.533256	-2.362585	0.195383
				C	-0.293964	-5.798281	2.674597
				H	-1.614360	-4.754249	1.360920
				C	2.041266	-5.190421	2.599754
TS1-R-cyclohexyl-iPr E= -3771.45761032							
H	-0.209598	2.250849	-2.122062				
C	-0.070755	-0.528988	3.537416				
C	-0.101153	0.799693	3.975015				
C	-0.057508	1.115706	5.342628				
C	0.004185	0.071028	6.265319				
C	0.032253	-1.259992	5.842268				
C	-0.002550	-1.556676	4.477795				
H	-0.106908	-0.744586	2.475579				
H	0.033066	0.305940	7.326992				
H	0.079612	-2.060520	6.575033				
H	0.017143	-2.588206	4.138501				
C	-0.053342	2.575577	5.726236				
H	-0.442693	2.713977	6.740781				
H	0.977968	2.959523	5.729828				

C	2.792506	-3.382323	1.087608	H	2.377992	-2.707059	-4.520684
C	1.036098	-5.968685	3.127164	H	3.630773	-1.458957	-4.474580
H	-1.090766	-6.397924	3.106430	C	6.949884	0.925246	-1.802737
H	3.065259	-5.298192	2.949607	H	7.290298	1.546068	-0.962327
H	3.812300	-3.541666	1.427874	C	8.144220	0.060801	-2.249384
H	1.257718	-6.704882	3.894980	H	8.984533	0.692452	-2.562372
C	3.637885	-1.488072	-0.322535	H	7.876390	-0.580820	-3.097212
C	4.074940	-1.628305	-1.663922	H	8.488351	-0.588052	-1.436468
C	4.281265	-0.561289	0.531052	C	6.507356	1.878194	-2.929717
C	5.136920	-0.840709	-2.117200	H	5.685663	2.524529	-2.600762
C	5.347160	0.194722	0.024601	H	6.159944	1.321447	-3.808085
C	5.791806	0.077646	-1.291801	H	7.340312	2.517376	-3.247434
H	5.466835	-0.955976	-3.146764	C	3.867755	-0.346236	1.987203
H	5.847137	0.903702	0.680641	H	2.942141	-0.900552	2.163829
C	-3.896643	-0.326265	-1.125857	C	4.930550	-0.893415	2.961300
C	-4.505686	0.110240	0.075240	H	5.121871	-1.959361	2.793634
C	-4.028457	0.446352	-2.304594	H	4.601191	-0.767569	3.999996
C	-5.233445	1.304568	0.074260	H	5.884779	-0.364973	2.845577
C	-4.770225	1.633961	-2.248106	C	3.562627	1.132525	2.292018
C	-5.380174	2.084649	-1.076454	H	4.455829	1.762668	2.204991
H	-5.707029	1.629060	0.997627	H	3.188295	1.234147	3.318108
H	-4.880904	2.229304	-3.151307	H	2.798571	1.511411	1.608021
O	0.920430	-1.181676	-1.138342	C	-3.424417	0.016418	-3.642796
O	-1.296091	-0.679285	0.021694	H	-2.681460	-0.760219	-3.440527
P	0.001903	0.090401	-0.645056	C	-2.690937	1.156555	-4.372848
O	0.625661	0.860975	0.490734	H	-3.380322	1.937957	-4.714809
C	3.459562	-2.639982	-2.631078	H	-2.184784	0.760500	-5.261257
H	2.639223	-3.150357	-2.119345	H	-1.935131	1.612599	-3.730326
C	4.479617	-3.727455	-3.024827	C	-4.504819	-0.589289	-4.563554
H	4.008835	-4.478014	-3.671613	H	-4.062129	-0.918501	-5.511640
H	4.874784	-4.240096	-2.140398	H	-5.281379	0.150720	-4.793613
H	5.330244	-3.303507	-3.571744	H	-4.996293	-1.452528	-4.102772
C	2.859823	-1.960729	-3.877288	C	-6.189270	3.375488	-1.067984
H	2.108320	-1.218383	-3.593144	H	-6.121675	3.804224	-2.077437

C	-7.679994	3.112414	-0.779275	H	4.057254	5.706534	-0.357580
H	-7.821594	2.691264	0.223288	H	1.551110	8.159981	-1.871541
H	-8.103332	2.404850	-1.500576	H	2.187014	7.592081	-0.331736
H	-8.256402	4.043979	-0.834496	H	3.979677	7.525494	-2.045179
C	-5.614811	4.414210	-0.086334	H	2.973796	6.540339	-3.104487
H	-4.563655	4.631020	-0.307316				
H	-5.668847	4.057763	0.949091	TS1-R-cyclohexyl-Ph E= -3997.67380844			
H	-6.176559	5.354462	-0.144074	H	-0.090710	-2.136185	-1.890769
C	-4.437094	-0.707186	1.364618	C	0.455361	0.847745	3.598948
H	-3.743905	-1.537813	1.204992	C	0.791265	-0.452389	3.992682
C	-3.891510	0.109392	2.550132	C	1.456663	-0.696283	5.204778
H	-3.777318	-0.530714	3.433053	C	1.758615	0.389110	6.027698
H	-4.563498	0.932018	2.823202	C	1.421824	1.691810	5.650867
H	-2.912112	0.534701	2.311162	C	0.775911	1.918066	4.433155
C	-5.809143	-1.325353	1.700663	H	-0.036778	1.005600	2.645700
H	-6.170817	-1.954780	0.879785	H	2.269324	0.210062	6.971196
H	-6.562542	-0.549392	1.882808	H	1.665876	2.524839	6.303975
H	-5.742439	-1.946599	2.602362	H	0.519936	2.927954	4.125785
O	-0.379362	0.809072	-1.919765	C	1.842159	-2.121461	5.518466
S	-0.514894	4.359895	2.154109	H	2.819862	-2.348363	5.067331
O	-0.195453	3.297294	-2.182173	H	1.953153	-2.268772	6.598286
H	-1.455540	4.734857	-1.322711	C	0.791106	-3.090791	4.960974
C	1.354404	4.913852	-0.617584	H	1.096181	-4.132227	5.074334
C	2.634561	4.386214	-1.318011	H	-0.153417	-2.968161	5.512758
C	0.836448	6.198309	-1.288201	C	0.478701	-2.822497	3.499654
H	1.639627	5.155732	0.417492	N	0.482479	-1.538355	3.131475
C	3.719165	5.471770	-1.377650	H	0.183104	-1.279152	2.174940
H	2.367142	4.066985	-2.332570	C	0.467249	-3.745398	-0.813508
H	3.007618	3.498640	-0.792387	C	-0.815477	-3.524064	-0.146922
C	1.934700	7.272413	-1.353470	H	1.304219	-3.131540	-0.483308
H	0.498043	5.959864	-2.305884	H	-0.961139	-2.520218	0.243843
H	-0.030794	6.588552	-0.740416	C	1.888872	1.976468	-0.758289
C	3.201335	6.752241	-2.049569	C	1.196415	3.179726	-0.788080
H	4.594012	5.085107	-1.915385	C	1.718703	4.248899	-1.599044

C	2.997896	4.083248	-2.222219	H	-5.627784	-0.636204	1.302488
C	3.694716	2.857863	-2.067104	C	3.912773	0.494003	-1.275713
C	3.157807	1.787866	-1.382124	C	4.628704	0.196425	-0.092407
H	0.021070	5.588259	-1.423376	C	3.959127	-0.398627	-2.374539
C	1.010045	5.457912	-1.846436	C	5.381118	-0.980075	-0.031277
C	3.537669	5.138862	-3.005962	C	4.728190	-1.561961	-2.263557
H	4.675445	2.756144	-2.524099	C	5.447780	-1.876152	-1.104411
C	2.835327	6.305116	-3.203781	H	5.961331	-1.190283	0.862693
C	1.552252	6.455550	-2.627181	H	4.750747	-2.260332	-3.094468
H	4.515376	4.998064	-3.460777	O	-0.913071	1.347440	-1.065564
H	3.254465	7.102419	-3.811355	O	1.375936	0.923933	-0.017420
H	0.984849	7.364919	-2.806192	P	0.035672	0.113675	-0.527738
C	-0.082179	3.334633	-0.032263	O	-0.528987	-0.545136	0.706456
C	-0.283435	4.399949	0.913502	C	-3.560109	2.624001	-2.485594
C	-1.123315	2.439169	-0.241184	H	-2.710481	3.183632	-2.085907
C	0.766689	5.253205	1.353812	C	-4.628015	3.661875	-2.886595
C	-1.588420	4.594064	1.472433	H	-4.952844	4.251620	-2.021786
C	-2.437188	2.627363	0.283792	H	-5.516008	3.181055	-3.313955
C	0.532124	6.257238	2.268497	H	-4.227751	4.352634	-3.638734
H	1.767922	5.098589	0.968435	C	-3.049903	1.844442	-3.712483
C	-1.801514	5.652138	2.397664	H	-2.268763	1.134207	-3.426094
C	-2.642480	3.719897	1.101321	H	-2.628988	2.535975	-4.452371
C	-0.766576	6.470495	2.788870	H	-3.857956	1.288818	-4.203705
H	1.353399	6.889685	2.594727	C	-3.637110	0.808445	2.358644
H	-2.801083	5.793257	2.802097	H	-2.715844	1.393740	2.418293
H	-3.637526	3.908473	1.495655	C	-4.657071	1.449458	3.321646
H	-0.940166	7.271439	3.502279	H	-4.879839	2.486069	3.044782
C	-3.562389	1.700171	-0.070558	H	-4.270398	1.448185	4.348077
C	-4.081866	1.695187	-1.388989	H	-5.604596	0.896916	3.320080
C	-4.134739	0.856591	0.913442	C	-3.286909	-0.620639	2.813419
C	-5.148079	0.845969	-1.695802	H	-2.552557	-1.067226	2.138205
C	-5.204139	0.028306	0.555043	H	-4.170334	-1.269404	2.849583
C	-5.725792	-0.001244	-0.743120	H	-2.857058	-0.596886	3.822324
H	-5.564488	0.866071	-2.698803	C	3.222718	-0.120960	-3.686494

H	2.469672	0.647852	-3.490774	H	-5.288912	-4.110445	-1.321936
C	2.472721	-1.348852	-4.234270	H	-4.776738	-4.730233	0.243296
H	1.875953	-1.057114	-5.106643	H	-2.819026	-7.664629	-1.222729
H	1.793484	-1.760229	-3.485007	H	-3.259380	-6.907563	0.304193
H	3.158147	-2.139850	-4.561774	H	-5.109116	-6.626478	-1.324359
C	4.192864	0.424815	-4.755280	H	-4.012337	-5.892968	-2.491587
H	4.975005	-0.309941	-4.983555	C	-6.853991	-0.900609	-1.097861
H	4.687064	1.344425	-4.425185	C	-6.899013	-1.544512	-2.347330
H	3.655755	0.645225	-5.685885	C	-7.906325	-1.135167	-0.195885
C	4.657194	1.149449	1.101979	C	-7.955968	-2.391559	-2.681566
H	3.902174	1.923472	0.938110	H	-6.086516	-1.393906	-3.052748
C	4.296542	0.448400	2.423857	C	-8.962709	-1.982589	-0.528664
H	5.047019	-0.299037	2.708390	H	-7.906774	-0.627929	0.764934
H	3.326792	-0.052300	2.347098	C	-8.992899	-2.615359	-1.773128
H	4.234907	1.179563	3.238251	H	-7.965658	-2.882013	-3.651627
C	6.020637	1.862219	1.204565	H	-9.768880	-2.141727	0.182962
H	6.248592	2.414821	0.286174	H	-9.816517	-3.274864	-2.033077
H	6.832652	1.144418	1.372293	C	6.258329	-3.118457	-1.016991
H	6.022555	2.573953	2.039347	C	6.982864	-3.589786	-2.125704
O	0.325464	-0.720816	-1.754660	C	6.324420	-3.857124	0.177259
S	0.099750	-4.107496	2.470385	C	7.743848	-4.755432	-2.044100
O	-0.282217	-3.162599	-1.904471	H	6.967915	-3.021514	-3.051561
H	0.757618	-4.767668	-1.045696	C	7.086595	-5.021957	0.260705
C	-1.999958	-4.438648	-0.192261	H	5.752088	-3.526130	1.039416
C	-3.207697	-3.734535	-0.866634	C	7.800106	-5.477277	-0.849968
C	-1.746664	-5.827938	-0.803171	H	8.301749	-5.095214	-2.913001
H	-2.268320	-4.571246	0.867281	H	7.115759	-5.579862	1.193253
C	-4.464141	-4.615258	-0.805153	H	8.393821	-6.385219	-0.785632
H	-2.945943	-3.526189	-1.911277				
H	-3.395362	-2.767121	-0.385365				
C	-3.015187	-6.695673	-0.747175	TS1-R-cyclohexyl-tBu E= -3850.06666655			
H	-1.432008	-5.709567	-1.849410	H	-0.311866	2.217766	-2.032938
H	-0.928260	-6.332031	-0.273267	C	-0.042430	-0.670456	3.580562
C	-4.211668	-6.001823	-1.415265	C	-0.126286	0.648105	4.041360
				C	-0.086235	0.942455	5.413894

C	0.026260	-0.114257	6.317896	H	-0.786008	-7.379361	-2.396603
C	0.108152	-1.435447	5.871608	C	0.268311	-3.144579	0.063550
C	0.076324	-1.710109	4.502471	C	0.580718	-4.138997	1.055731
H	-0.076317	-0.869193	2.515320	C	1.251084	-2.220540	-0.268860
H	0.052753	0.103450	7.383291	C	-0.397751	-5.004650	1.620019
H	0.194916	-2.245561	6.590102	C	1.927303	-4.240344	1.535219
H	0.138105	-2.733901	4.145287	C	2.606887	-2.327098	0.163550
C	-0.140107	2.394473	5.823045	C	-0.058093	-5.932361	2.581381
H	-0.530041	2.498878	6.841422	H	-1.428037	-4.919347	1.293924
H	0.874708	2.820096	5.829439	C	2.248504	-5.222124	2.511597
C	-1.015317	3.186345	4.841827	C	2.914343	-3.353356	1.032931
H	-2.061073	2.855082	4.932049	C	1.280027	-6.053769	3.026114
H	-0.995842	4.257132	5.049708	H	-0.826143	-6.575085	3.003219
C	-0.605223	2.952694	3.399000	H	3.277679	-5.292737	2.855666
N	-0.227163	1.707246	3.100004	H	3.942153	-3.476948	1.363931
H	-0.001254	1.459759	2.120578	H	1.536483	-6.795229	3.777861
C	-1.120873	3.719954	-0.962813	C	3.671447	-1.399949	-0.345215
C	0.204623	3.756648	-0.344797	C	4.099447	-1.491035	-1.693421
H	-1.816864	2.968762	-0.591050	C	4.292815	-0.470636	0.518460
H	0.552225	2.805011	0.049047	C	5.127979	-0.656494	-2.135298
C	-1.809725	-1.923695	-0.599750	C	5.328714	0.335135	0.021694
C	-1.063347	-3.093914	-0.610137	C	5.768822	0.268075	-1.300924
C	-1.585161	-4.231067	-1.322424	H	5.444797	-0.741741	-3.171026
C	-2.907951	-4.157065	-1.867556	H	5.796581	1.035398	0.704158
C	-3.650317	-2.955888	-1.735484	C	-3.925790	-0.558373	-1.065532
C	-3.123168	-1.825091	-1.147370	C	-4.553936	-0.199340	0.150723
H	0.180584	-5.483263	-1.183023	C	-4.106188	0.252104	-2.209227
C	-0.838132	-5.421214	-1.546932	C	-5.341826	0.953433	0.193845
C	-3.446746	-5.279490	-2.553040	C	-4.911034	1.397152	-2.109256
H	-4.661168	-2.923618	-2.132946	C	-5.542092	1.775807	-0.922097
C	-2.704828	-6.424346	-2.730588	H	-5.823443	1.210496	1.133362
C	-1.382163	-6.485739	-2.232274	H	-5.043231	2.002339	-2.998233
H	-4.456909	-5.207767	-2.949337	O	0.934635	-1.185211	-1.132078
H	-3.124197	-7.273525	-3.263132	O	-1.297826	-0.811099	0.048525

P	-0.036898	0.031340	-0.600775	H	-3.547126	1.868976	-4.559782
O	0.560263	0.796364	0.553038	H	-2.300144	0.774613	-5.161067
C	3.510026	-2.498481	-2.681275	H	-2.079392	1.575736	-3.598528
H	2.715453	-3.052609	-2.174378	C	-4.540412	-0.719436	-4.505155
C	4.563773	-3.536414	-3.117292	H	-4.085588	-0.993117	-5.465115
H	4.111414	-4.288102	-3.775833	H	-5.353484	-0.011205	-4.707693
H	4.991764	-4.055362	-2.252027	H	-4.986973	-1.621503	-4.073785
H	5.389198	-3.067334	-3.666229	C	-6.432743	3.027304	-0.805886
C	2.869752	-1.808091	-3.900971	C	-7.864427	2.604416	-0.398040
H	2.095295	-1.101992	-3.587544	H	-7.875547	2.074880	0.560390
H	2.407245	-2.553656	-4.559269	H	-8.305572	1.941171	-1.150959
H	3.614167	-1.261948	-4.493101	H	-8.510768	3.485761	-0.300308
C	6.903731	1.148367	-1.856070	C	-5.854958	3.975070	0.271888
C	8.048135	0.247287	-2.378624	H	-4.841757	4.299213	0.006930
H	8.863861	0.860001	-2.782484	H	-5.802356	3.493137	1.253446
H	7.708825	-0.422637	-3.175467	H	-6.482281	4.869692	0.371424
H	8.456077	-0.373225	-1.572404	C	-4.436691	-1.054194	1.412172
C	6.362725	2.012171	-3.020323	H	-3.725082	-1.860304	1.212293
H	5.553437	2.667676	-2.677348	C	-3.886391	-0.256963	2.608793
H	5.967750	1.397008	-3.835452	H	-3.741431	-0.916197	3.473019
H	7.160623	2.642415	-3.432833	H	-4.571051	0.543674	2.914450
C	3.887324	-0.298729	1.982878	H	-2.921467	0.195917	2.362045
H	2.991574	-0.899846	2.160354	C	-5.782600	-1.721160	1.759551
C	4.985287	-0.809899	2.937182	H	-6.147183	-2.332960	0.926693
H	5.222619	-1.863645	2.751760	H	-6.552779	-0.974079	1.986425
H	4.662633	-0.713836	3.981137	H	-5.676327	-2.369766	2.637859
H	5.913492	-0.237358	2.819494	O	-0.454608	0.768705	-1.853196
C	3.513832	1.158600	2.314168	S	-0.691116	4.219754	2.284303
H	4.373328	1.833720	2.224287	O	-0.317152	3.264808	-2.074454
H	3.148991	1.227227	3.346442	H	-1.604953	4.665754	-1.196868
H	2.722203	1.508239	1.645999	C	1.197504	4.873273	-0.465470
C	-3.488086	-0.093691	-3.565542	C	2.494580	4.370428	-1.152670
H	-2.704709	-0.837892	-3.395910	C	0.671448	6.158000	-1.129134
C	-2.817519	1.109270	-4.254057	H	1.462554	5.106269	0.577112

C	3.565172	5.470757	-1.187814	C	1.970689	-1.142474	5.790014
H	2.245200	4.057498	-2.173790	H	2.992089	-1.268881	5.400802
H	2.872768	3.482936	-0.630762	H	2.037883	-1.228170	6.880008
C	1.756559	7.246735	-1.170310	C	1.074740	-2.255802	5.230744
H	0.348267	5.925401	-2.153033	H	1.498853	-3.245867	5.405289
H	-0.207217	6.531569	-0.587984	H	0.095963	-2.230481	5.733793
C	3.038842	6.750040	-1.854985	C	0.801954	-2.087624	3.747183
H	4.452234	5.100913	-1.717387	N	0.670288	-0.830751	3.317319
H	3.886453	5.700728	-0.161209	H	0.381912	-0.654208	2.338878
H	1.367834	8.134196	-1.684721	C	1.179647	-3.142026	-0.584978
H	1.991847	7.559762	-0.142467	C	-0.126476	-3.156233	0.069732
H	3.806314	7.533807	-1.833668	H	1.885790	-2.368555	-0.288101
H	2.827665	6.544667	-2.914570	H	-0.487564	-2.196837	0.426142
C	7.491536	2.094489	-0.791444	C	1.937578	2.546545	-0.658586
H	6.737643	2.786294	-0.398379	C	1.176215	3.705327	-0.729412
H	7.920662	1.542334	0.052453	C	1.655012	4.789135	-1.547776
H	8.293377	2.696140	-1.234825	C	2.957726	4.689083	-2.135126
C	-6.526089	3.810012	-2.129684	C	3.722866	3.511782	-1.936157
H	-5.544309	4.163057	-2.465619	C	3.232875	2.424573	-1.243501
H	-6.963627	3.205180	-2.931972	H	-0.122806	6.027298	-1.439658
H	-7.165367	4.689986	-1.993487	C	0.882536	5.948932	-1.836032
				C	3.453667	5.760103	-2.926871
				H	4.720189	3.461471	-2.364668
				C	2.688410	6.878158	-3.165331
				C	1.384482	6.962520	-2.623077
				H	4.449431	5.669822	-3.354528
				H	3.074695	7.687537	-3.778649
				H	0.769063	7.832937	-2.834068
				C	-0.128097	3.797691	-0.008278
				C	-0.413392	4.866174	0.912295
				C	-1.111585	2.841350	-0.225501
				C	0.576351	5.783521	1.363227
				C	-1.741007	4.995289	1.435863
				C	-2.449362	2.969368	0.255602
TS1-R-n-hexyl-anthryl E= -4613.33394631							
H	0.341853	-1.690472	-1.706430				
C	0.355611	1.555164	3.658957				
C	0.812486	0.321520	4.135031				
C	1.438136	0.211197	5.387144				
C	1.571050	1.360599	6.166662				
C	1.109002	2.597003	5.708434				
C	0.508148	2.692432	4.451096				
H	-0.098276	1.611559	2.675864				
H	2.048262	1.284938	7.141163				
H	1.222266	3.481246	6.329152				
H	0.157074	3.651203	4.080994				

C	0.264108	6.785789	2.256299	H	-4.239644	4.593878	-3.724592
H	1.594033	5.678352	1.005252	C	-2.885895	2.175083	-3.742136
C	-2.034826	6.052294	2.340052	H	-2.062059	1.529171	-3.424450
C	-2.736097	4.060137	1.050143	H	-2.494616	2.894652	-4.471485
C	-1.056613	6.932507	2.743241	H	-3.630257	1.555904	-4.256981
H	1.040673	7.467759	2.591988	C	-3.605172	1.085228	2.298373
H	-3.050199	6.143090	2.718670	H	-2.722439	1.724303	2.386345
H	-3.750802	4.200934	1.413187	C	-4.691488	1.665842	3.226648
H	-1.291912	7.731995	3.440378	H	-4.963714	2.688329	2.940896
C	-3.513425	1.982663	-0.128201	H	-4.338467	1.686926	4.264897
C	-3.996662	1.956515	-1.460008	H	-5.605003	1.059647	3.195770
C	-4.058891	1.103071	0.838586	C	-3.186346	-0.321257	2.765401
C	-5.000011	1.043049	-1.799848	H	-2.407791	-0.723595	2.112274
C	-5.064582	0.210698	0.447789	H	-4.031395	-1.019942	2.774533
C	-5.542800	0.157442	-0.864223	H	-2.790316	-0.272974	3.787195
H	-5.376770	1.019379	-2.818628	C	3.478481	0.477422	-3.504085
H	-5.483824	-0.473167	1.180229	H	2.676256	1.205058	-3.350669
C	4.060374	1.180348	-1.087957	C	2.823747	-0.798957	-4.062780
C	4.765130	0.955999	0.117893	H	2.246014	-0.553394	-4.961604
C	4.178024	0.262409	-2.160685	H	2.140320	-1.241918	-3.335605
C	5.571391	-0.182397	0.232181	H	3.567238	-1.551523	-4.351980
C	4.996100	-0.862049	-1.995622	C	4.459563	1.061722	-4.542775
C	5.697680	-1.105108	-0.810154	H	5.286300	0.365759	-4.732043
H	6.124126	-0.356032	1.151343	H	4.892555	2.009958	-4.207428
H	5.093521	-1.573648	-2.809772	H	3.947355	1.242775	-5.495567
O	-0.819176	1.744667	-1.018472	C	4.716888	1.940340	1.285873
O	1.467177	1.478510	0.088244	H	3.956227	2.694123	1.063934
P	0.189392	0.581060	-0.438182	C	4.305553	1.263896	2.606065
O	-0.350595	-0.101413	0.793009	H	5.048254	0.527632	2.936260
C	-3.498836	2.918063	-2.539420	H	3.343411	0.754283	2.498358
H	-2.708430	3.537787	-2.107779	H	4.203955	2.011119	3.401798
C	-4.621210	3.875367	-2.988975	C	6.059656	2.683223	1.436133
H	-5.026001	4.439362	-2.140857	H	6.324000	3.214530	0.514848
H	-5.451364	3.331078	-3.454366	H	6.876011	1.988231	1.666443

H	6.004726	3.418087	2.248643	C	4.891160	-3.375826	0.871679
O	0.557451	-0.248688	-1.649032	C	9.484383	-1.446470	-2.838454
S	0.620964	-3.449455	2.762190	H	7.696640	-0.434433	-2.272297
O	0.310308	-2.741043	-1.671260	C	9.846247	-3.663473	-1.941028
H	1.658182	-4.098240	-0.792386	C	8.167213	-4.643374	-0.423064
C	-6.596957	-0.830468	-1.252640	C	6.512819	-5.655695	1.101159
C	-6.251326	-1.956660	-2.039144	H	4.261102	-2.496421	0.795562
C	-7.933727	-0.648153	-0.822969	C	4.498820	-4.432088	1.653678
C	-4.913570	-2.200518	-2.494682	C	10.275940	-2.625289	-2.723239
C	-7.268390	-2.921857	-2.393601	H	9.838815	-0.623041	-3.452877
C	-8.940595	-1.623095	-1.178407	H	10.444423	-4.566035	-1.838998
C	-8.348646	0.488447	-0.054817	H	8.783674	-5.535549	-0.331571
C	-4.608424	-3.300673	-3.255212	C	5.321377	-5.589750	1.772477
H	-4.135851	-1.491817	-2.232799	H	7.147521	-6.535205	1.182688
C	-6.906159	-4.056033	-3.187439	H	3.553302	-4.385736	2.188170
C	-8.581505	-2.731464	-1.951576	H	11.221732	-2.692515	-3.254156
C	-10.286674	-1.427948	-0.735347	H	4.996595	-6.417791	2.396949
H	-7.610347	1.239362	0.203537	C	-1.017043	-4.360097	0.042950
C	-9.650517	0.640230	0.346785	C	-2.484005	-4.058651	0.374166
C	-5.617042	-4.242506	-3.609974	C	-3.375034	-5.304769	0.305712
H	-3.587400	-3.456201	-3.593399	H	-2.535916	-3.618477	1.378981
H	-7.684048	-4.769360	-3.449937	H	-2.864856	-3.300680	-0.322480
H	-9.343035	-3.460971	-2.220329	H	-3.336037	-5.721936	-0.711456
C	-10.634905	-0.332170	0.007921	H	-2.971586	-6.081756	0.972526
H	-11.030681	-2.173219	-1.007088	C	-4.835867	-5.020072	0.678517
H	-9.939218	1.513058	0.926408	H	-5.224483	-4.221015	0.032322
H	-5.357534	-5.106698	-4.215567	H	-4.877701	-4.632255	1.707353
H	-11.661566	-0.195865	0.336979	C	-5.746361	-6.249154	0.561407
C	6.557247	-2.321882	-0.666539	H	-5.713457	-6.621747	-0.472182
C	7.789360	-2.404333	-1.359866	H	-5.351078	-7.058506	1.192348
C	6.131956	-3.394911	0.154192	H	-0.610690	-5.097276	0.749832
C	8.286523	-1.339530	-2.180331	H	-0.926066	-4.819969	-0.950016
C	8.604584	-3.592064	-1.234242	C	-7.199815	-5.958609	0.951230
C	6.957422	-4.576131	0.274202	H	-7.826783	-6.852684	0.853417

H	-7.270041	-5.615077	1.990883	H	1.448979	5.180344	-1.182149
H	-7.629471	-5.175703	0.314692	C	2.351719	4.823570	-1.663611
TS1-R-n-hexyl-iPr E= -3772.64965077				C	4.660985	3.928254	-2.968349
H	-0.461707	-2.276488	-2.028950	H	5.142900	1.303282	-2.672200
C	0.652599	0.399854	3.526686	C	4.287809	5.249001	-3.064171
C	0.765203	-0.949636	3.877456	C	3.112566	5.693497	-2.414065
C	1.402351	-1.341425	5.065730	H	5.549586	3.566033	-3.480095
C	1.899164	-0.349810	5.911883	H	4.882565	5.946713	-3.647301
C	1.781775	1.002302	5.580010	H	2.802586	6.730447	-2.511969
C	1.164559	1.373636	4.383274	C	0.796527	2.943600	0.079856
H	0.180006	0.668763	2.588603	C	0.922873	3.951759	1.098791
H	2.388648	-0.643141	6.837900	C	-0.454568	2.377060	-0.130359
H	2.175028	1.760842	6.250821	C	2.178698	4.458667	1.535742
H	1.079661	2.421404	4.110915	C	-0.261395	4.441850	1.739633
C	1.548517	-2.820417	5.329085	C	-1.652237	2.882199	0.459535
H	2.464917	-3.193123	4.847189	C	2.255541	5.412118	2.528005
H	1.654088	-3.019060	6.401166	H	3.087371	4.074066	1.087157
C	0.338956	-3.581242	4.770018	C	-0.148941	5.439377	2.746294
H	0.467120	-4.662227	4.844888	C	-1.524878	3.919701	1.360379
H	-0.560826	-3.320569	5.347983	C	1.081485	5.918566	3.134790
C	0.048096	-3.215250	3.325907	H	3.227721	5.775506	2.850057
N	0.255112	-1.938720	2.994983	H	-1.058899	5.808361	3.213661
H	-0.022665	-1.602545	2.055440	H	-2.419644	4.342508	1.809840
C	-0.017789	-3.946442	-0.987872	H	1.155138	6.676231	3.910160
C	-1.287029	-3.669178	-0.318659	C	-3.007664	2.363941	0.075168
H	0.858084	-3.394889	-0.648733	C	-3.536405	2.668859	-1.204380
H	-1.389292	-2.672402	0.100322	C	-3.789710	1.634357	1.000806
C	2.309989	1.168583	-0.818276	C	-4.828511	2.241853	-1.523870
C	1.961294	2.510247	-0.747585	C	-5.079518	1.234179	0.626546
C	2.720757	3.456481	-1.522414	C	-5.622214	1.524169	-0.624754
C	3.887520	3.001729	-2.217878	H	-5.228984	2.486459	-2.504645
C	4.239306	1.628834	-2.164134	H	-5.684103	0.676627	1.338661
C	3.461707	0.693918	-1.513114	C	3.852188	-0.756704	-1.511524
				C	4.502865	-1.304483	-0.380111

C	3.626387	-1.560729	-2.654343	H	1.188582	-2.297783	-3.784826
C	4.916812	-2.640051	-0.414144	H	2.399206	-2.880900	-4.948254
C	4.063488	-2.891993	-2.633667	C	4.009520	-0.640429	-4.982674
C	4.708441	-3.454417	-1.530858	H	4.590816	-1.520069	-5.286164
H	5.424860	-3.052050	0.454497	H	4.713865	0.111486	-4.612841
H	3.898817	-3.513799	-3.510128	H	3.522096	-0.234249	-5.877492
O	-0.573880	1.322854	-1.020936	C	4.812765	-0.469437	0.861884
O	1.557756	0.244929	-0.110372	H	4.312516	0.497219	0.756084
P	0.036921	-0.147981	-0.609421	C	4.273251	-1.111757	2.152455
O	-0.633572	-0.744272	0.603211	H	4.775405	-2.060676	2.377492
C	-2.765520	3.482805	-2.244109	H	3.199466	-1.304760	2.070555
H	-1.780823	3.721864	-1.833932	H	4.432486	-0.443158	3.006699
C	-3.462666	4.827722	-2.532513	C	6.323956	-0.183871	0.972105
H	-3.587937	5.414264	-1.615127	H	6.694352	0.333148	0.079729
H	-4.456225	4.681294	-2.972454	H	6.898168	-1.111774	1.082218
H	-2.870363	5.422374	-3.238681	H	6.535324	0.447713	1.843820
C	-2.530925	2.685356	-3.541291	O	0.067228	-0.928571	-1.905170
H	-1.999015	1.752255	-3.333583	S	-0.556597	-4.386341	2.267830
H	-1.929442	3.273570	-4.245142	O	-0.737432	-3.292043	-2.056735
H	-3.476119	2.438778	-4.039988	H	0.203820	-4.982791	-1.241075
C	-3.292852	1.264804	2.398569	C	-2.483631	-4.555725	-0.455567
H	-2.239567	1.549420	2.470066	C	-3.762237	-3.794832	-0.849692
C	-4.055136	2.040472	3.491681	C	-4.988883	-4.713084	-0.921676
H	-3.967558	3.124139	3.353086	H	-3.942453	-2.992362	-0.121471
H	-3.660892	1.792959	4.484958	H	-3.599933	-3.308001	-1.819012
H	-5.123392	1.792132	3.484080	C	-6.276073	-3.970825	-1.303746
C	-3.363025	-0.252102	2.657009	H	-4.802187	-5.515525	-1.650677
H	-2.797084	-0.794666	1.895164	H	-5.130283	-5.209598	0.049854
H	-4.396285	-0.619090	2.656322	H	-6.462279	-3.169138	-0.573887
H	-2.931939	-0.486444	3.638297	H	-6.133870	-3.471901	-2.273729
C	2.956976	-1.017723	-3.918581	C	-7.508029	-4.882595	-1.379499
H	2.414460	-0.108520	-3.643723	H	-7.645582	-5.386376	-0.412090
C	1.926051	-1.985511	-4.526939	H	-7.323979	-5.679664	-2.113928
H	1.390797	-1.488288	-5.344385	C	-8.791105	-4.131670	-1.751176

H	-9.650871	-4.809516	-1.802472	H	1.416478	-0.648510	2.527830
H	-9.022811	-3.354397	-1.012544	H	-0.076013	-2.164463	7.013082
H	-8.694194	-3.640953	-2.727486	H	2.073194	-2.993895	6.085040
H	-2.640873	-5.041932	0.516342	H	2.818179	-2.245730	3.827048
H	-2.267153	-5.354219	-1.175590	C	-1.877260	-0.439813	5.794219
C	-7.037246	1.087036	-0.981004	H	-2.674332	-1.100735	5.421683
C	-7.075240	0.197196	-2.237214	H	-1.935200	-0.463887	6.887886
C	-7.981037	2.295972	-1.133312	C	-2.123907	0.986690	5.286494
H	-6.734996	0.742892	-3.125244	H	-3.129813	1.336211	5.523539
H	-6.431949	-0.681528	-2.119085	H	-1.416965	1.677390	5.771096
H	-8.096925	-0.150422	-2.432999	C	-1.895179	1.111390	3.791017
H	-9.007765	1.965515	-1.333353	N	-0.883941	0.392257	3.295447
H	-7.989809	2.907987	-0.224615	H	-0.600586	0.519707	2.308038
H	-7.668941	2.938984	-1.965059	C	-3.128195	1.455584	-0.355172
C	5.175082	-4.904825	-1.558768	C	-2.287147	2.523096	0.183302
C	4.488329	-5.753724	-0.472174	H	-2.888474	0.434684	-0.060907
C	6.708447	-5.014522	-1.454849	H	-1.272592	2.230318	0.438834
H	4.752676	-5.404476	0.532978	C	0.253982	-2.726370	-0.802543
H	3.397259	-5.707393	-0.563056	C	1.581593	-3.119859	-0.893581
H	4.792731	-6.804559	-0.550213	C	1.903552	-4.245174	-1.733016
H	7.029114	-6.060714	-1.530970	C	0.834769	-4.996726	-2.321470
H	7.200070	-4.447142	-2.252646	C	-0.506117	-4.580383	-2.119134
H	7.070183	-4.623649	-0.496308	C	-0.821363	-3.439964	-1.411084
H	-7.408955	0.484485	-0.140428	H	4.062919	-4.053350	-1.647006
H	4.881718	-5.318792	-2.533366	C	3.237369	-4.633427	-2.041705
TS1-R-n-hexyl-Ph E= -3998.86681623				C	1.134637	-6.126990	-3.129295
H	-1.605927	1.265973	-1.666173	H	-1.304673	-5.165141	-2.567712
C	1.111992	-0.979538	3.514191	C	2.436775	-6.489977	-3.384888
C	-0.088734	-0.507869	4.054814	C	3.495593	-5.722931	-2.845049
C	-0.536411	-0.938746	5.314191	H	0.309088	-6.691037	-3.557007
C	0.259501	-1.830467	6.033772	H	2.654188	-7.351173	-4.010661
C	1.466945	-2.299265	5.510642	H	4.524192	-5.991370	-3.070515
C	1.887080	-1.877559	4.247266	C	2.644683	-2.353540	-0.177137
				C	3.573707	-2.996562	0.714047

C	2.768022	-0.982484	-0.372625	H	4.312854	-0.446467	-2.308684
C	3.423968	-4.343477	1.147868	C	5.996509	0.482694	-3.228139
C	4.678407	-2.242388	1.227786	H	6.693674	0.265562	-2.410820
C	3.882437	-0.221729	0.093844	H	6.302587	1.431903	-3.683663
C	4.328860	-4.917722	2.014228	H	6.106414	-0.301552	-3.987007
H	2.573479	-4.917843	0.799276	C	3.555437	0.783577	-3.879608
C	5.605010	-2.870044	2.104865	H	2.522609	0.784479	-3.519386
C	4.823343	-0.880139	0.859078	H	3.654534	-0.006099	-4.634450
C	5.438873	-4.180674	2.491201	H	3.747272	1.741743	-4.377703
H	4.185727	-5.945185	2.337719	C	3.619634	1.939627	2.175649
H	6.444664	-2.286539	2.475196	H	3.378249	0.876899	2.258675
H	5.695231	-0.335206	1.211706	C	4.810154	2.214140	3.115813
H	6.150132	-4.647509	3.167079	H	5.693468	1.631843	2.829209
C	4.063575	1.222725	-0.272093	H	4.551463	1.952875	4.149168
C	4.382159	1.575114	-1.607527	H	5.094362	3.273293	3.100573
C	3.977847	2.231655	0.718297	C	2.370184	2.718199	2.630050
C	4.606863	2.918309	-1.919939	H	1.521396	2.492479	1.978839
C	4.218355	3.560644	0.353861	H	2.539313	3.801610	2.621038
C	4.533232	3.931892	-0.957365	H	2.104292	2.434737	3.656061
H	4.881666	3.182604	-2.937119	C	-2.207191	-2.195476	-3.756975
H	4.128441	4.336903	1.108382	H	-1.132464	-2.338288	-3.614855
C	-2.239438	-2.963974	-1.287943	C	-2.393430	-0.793874	-4.366385
C	-2.936857	-3.130169	-0.066935	H	-1.803544	-0.712125	-5.287070
C	-2.887100	-2.364027	-2.396627	H	-2.053782	-0.018848	-3.676916
C	-4.255776	-2.677751	0.029798	H	-3.438242	-0.593925	-4.633008
C	-4.209851	-1.931053	-2.249091	C	-2.700012	-3.271674	-4.747515
C	-4.912595	-2.066773	-1.046079	H	-3.776506	-3.168830	-4.932508
H	-4.803299	-2.833102	0.954607	H	-2.525078	-4.285200	-4.371204
H	-4.700687	-1.444968	-3.086639	H	-2.182785	-3.173615	-5.709683
O	1.819165	-0.318618	-1.130874	C	-2.316260	-3.865443	1.120395
O	-0.065349	-1.630350	-0.019062	H	-1.235983	-3.916174	0.960286
P	0.302336	-0.106241	-0.531494	C	-2.534816	-3.143573	2.461301
O	0.260202	0.739287	0.716459	H	-3.590382	-3.138690	2.758856
C	4.541270	0.539694	-2.721140	H	-2.189334	-2.106502	2.408382

H	-1.973136	-3.647922	3.256140	H	-4.361567	3.935033	-1.141072
C	-2.834939	-5.316876	1.184611	H	-4.746331	3.858129	0.579099
H	-2.615310	-5.857515	0.257262	C	-5.791119	6.228954	-0.446804
H	-3.920931	-5.340823	1.336300	H	-4.051296	6.258412	0.839131
H	-2.365041	-5.859556	2.014117	H	-3.672958	6.337540	-0.876427
O	-0.525510	0.288400	-1.734107	H	-6.072692	5.827764	-1.431648
S	-2.863249	2.154854	2.881606	H	-6.452065	5.736881	0.282153
O	-2.437213	1.895918	-1.547939	C	-6.050565	7.741094	-0.422981
H	-4.198786	1.629130	-0.434728	H	-5.392160	8.233277	-1.152840
C	-2.629834	3.982745	0.150851	H	-5.766665	8.140961	0.560904
C	4.782636	5.352122	-1.314815	C	-7.508369	8.106841	-0.721649
C	4.338932	5.879035	-2.540187	H	-7.661984	9.191686	-0.694860
C	5.469319	6.208905	-0.437064	H	-7.811182	7.751941	-1.714525
C	4.573570	7.212174	-2.875627	H	-8.188238	7.655727	0.011739
H	3.783480	5.242331	-3.223164	H	-1.957028	4.451127	-0.581244
C	5.703015	7.542526	-0.770693	H	-2.331571	4.395042	1.122639
H	5.844221	5.816714	0.504263				
C	5.256535	8.050875	-1.992293				
H	4.214115	7.598537	-3.826012	TS1-R-<i>n</i>-hexyl-tBu E= -3851.25955242			
H	6.243276	8.183331	-0.078430	H	-2.059395	0.573953	-1.802925
H	5.439135	9.089884	-2.253332	C	1.125704	-0.215712	3.535032
C	-6.309269	-1.576738	-0.914331	C	-0.175616	-0.148830	4.044007
C	-7.225000	-1.703267	-1.973409	C	-0.474150	-0.607487	5.337062
C	-6.752075	-0.967459	0.273135	C	0.565052	-1.109449	6.121024
C	-8.533426	-1.237114	-1.850956	C	1.871180	-1.170929	5.629014
H	-6.912473	-2.193764	-2.891028	C	2.147203	-0.729606	4.333030
C	-8.061048	-0.501895	0.396840	H	1.319780	0.121847	2.523238
H	-6.056181	-0.838847	1.097823	H	0.344710	-1.461446	7.126386
C	-8.958169	-0.634093	-0.665013	H	2.667389	-1.565779	6.253645
H	-9.225328	-1.353394	-2.681210	H	3.157026	-0.783928	3.937311
H	-8.377673	-0.027901	1.322430	C	-1.915928	-0.568934	5.781252
H	-9.978091	-0.271492	-0.569313	H	-2.425786	-1.491189	5.464441
C	-4.088091	4.338900	-0.157490	H	-1.988449	-0.529633	6.873623
C	-4.334909	5.853445	-0.143359	C	-2.629157	0.641149	5.163750
				H	-3.699349	0.635805	5.376023

H	-2.218320	1.568758	5.590847	H	6.075781	-3.504188	2.560146
C	-2.421760	0.725756	3.662251	H	6.587933	0.767147	2.523365
N	-1.216573	0.356542	3.220137	H	5.121602	2.165880	1.158423
H	-0.975302	0.490413	2.222706	H	7.294493	-1.466291	3.330254
C	-3.597427	0.357589	-0.507941	C	3.020170	2.828327	-0.404672
C	-3.160756	1.674819	-0.051329	C	3.180189	3.218548	-1.758430
H	-3.047687	-0.506221	-0.136312	C	2.505707	3.757022	0.527429
H	-2.113425	1.742471	0.228910	C	2.820160	4.513480	-2.136820
C	1.224962	-2.379214	-0.723755	C	2.164490	5.045846	0.090415
C	2.595717	-2.176951	-0.804941	C	2.306328	5.454882	-1.235905
C	3.376958	-3.097781	-1.588990	H	2.953000	4.797466	-3.176980
C	2.737236	-4.259945	-2.129814	H	1.771729	5.740936	0.823885
C	1.345769	-4.446997	-1.929295	C	-0.917043	-3.717866	-1.134511
C	0.564666	-3.517775	-1.274422	C	-1.459512	-4.145656	0.100780
H	5.249603	-2.003717	-1.526165	C	-1.773222	-3.526168	-2.242925
C	4.754265	-2.897690	-1.886016	C	-2.835861	-4.364588	0.199356
C	3.500292	-5.193716	-2.882082	C	-3.146891	-3.767084	-2.088417
H	0.879788	-5.343209	-2.329940	C	-3.710182	-4.184301	-0.880359
C	4.837046	-4.981410	-3.128328	H	-3.234804	-4.698556	1.153171
C	5.462383	-3.812242	-2.635033	H	-3.786085	-3.621882	-2.951160
H	2.998613	-6.075408	-3.273981	O	1.645753	0.446821	-1.185544
H	5.408784	-5.698200	-3.711341	O	0.459885	-1.479027	-0.000033
H	6.511164	-3.629775	-2.853489	P	0.170885	0.032260	-0.588506
C	3.226436	-1.004166	-0.129072	O	-0.233659	0.850934	0.611652
C	4.319444	-1.158889	0.793822	C	3.774380	2.293575	-2.821692
C	2.769623	0.281407	-0.393341	H	3.975612	1.323192	-2.360324
C	4.739191	-2.424034	1.291837	C	5.126612	2.828748	-3.334898
C	4.994821	0.011270	1.271261	H	5.837289	2.967094	-2.512112
C	3.452754	1.460026	0.034536	H	5.011481	3.794256	-3.841769
C	5.781521	-2.526703	2.187565	H	5.568642	2.126863	-4.052637
H	4.217336	-3.317263	0.968328	C	2.796291	2.044372	-3.985836
C	6.078886	-0.130494	2.180211	H	1.855030	1.622909	-3.621380
C	4.565157	1.290557	0.833566	H	3.232645	1.338747	-4.703426
C	6.468677	-1.371392	2.630473	H	2.571049	2.970117	-4.529082

C	2.293095	3.424240	2.004863	C	-3.956067	2.938529	-0.185774
H	2.521787	2.365232	2.150100	C	-5.445882	2.785083	-0.509528
C	3.248498	4.227401	2.909869	C	-6.164372	4.138347	-0.599177
H	4.297627	4.050067	2.646512	H	-5.559676	2.249403	-1.461279
H	3.109858	3.945643	3.960891	H	-5.926896	2.169916	0.263300
H	3.065937	5.305623	2.826395	C	-7.659674	4.009006	-0.916132
C	0.828567	3.626804	2.437539	H	-6.039248	4.679207	0.350270
H	0.160416	3.030360	1.810539	H	-5.680494	4.756703	-1.369567
H	0.524598	4.678185	2.370368	H	-7.784849	3.470765	-1.867366
H	0.697585	3.312248	3.480442	H	-8.140987	3.385550	-0.147991
C	-1.255849	-3.099876	-3.618170	C	-8.385360	5.358652	-0.998527
H	-0.237841	-2.721154	-3.490556	H	-7.905398	5.981370	-1.766845
C	-2.076214	-1.961169	-4.252488	H	-8.257697	5.896001	-0.048035
H	-1.593110	-1.630847	-5.179770	C	-9.879180	5.221857	-1.311193
H	-2.140420	-1.102643	-3.581016	H	-10.368325	6.201314	-1.361872
H	-3.092882	-2.279507	-4.513386	H	-10.038759	4.719528	-2.273272
C	-1.193443	-4.305003	-4.580045	H	-10.392794	4.632457	-0.541555
H	-2.193687	-4.722230	-4.750821	H	-3.457530	3.548588	-0.952180
H	-0.562672	-5.108716	-4.185679	H	-3.823667	3.488724	0.753968
H	-0.785917	-4.001174	-5.552109	C	1.931124	6.865862	-1.725640
C	-0.581933	-4.428254	1.319829	C	1.363997	7.748993	-0.597593
H	0.436388	-4.104512	1.087868	C	3.188626	7.564171	-2.296114
C	-1.029536	-3.638334	2.562549	C	0.858245	6.757731	-2.835352
H	-2.023171	-3.949574	2.907878	H	0.453127	7.320945	-0.163372
H	-1.062404	-2.566225	2.347991	H	2.090164	7.896978	0.209945
H	-0.327256	-3.797377	3.389380	H	1.107676	8.737624	-0.995796
C	-0.516517	-5.940271	1.614975	H	3.619610	7.004555	-3.132817
H	-0.140484	-6.496280	0.748790	H	2.938089	8.568940	-2.659048
H	-1.506354	-6.341533	1.864156	H	3.963300	7.663812	-1.527024
H	0.149951	-6.139795	2.463157	H	0.582768	7.755072	-3.200390
O	-0.734819	-0.010691	-1.800207	H	1.214530	6.175624	-3.691543
S	-3.661146	1.313087	2.676041	H	-0.048030	6.271425	-2.456318
O	-3.055504	0.912976	-1.728497	C	-5.217098	-4.452010	-0.705468
H	-4.665350	0.172345	-0.600813	C	-5.783441	-3.519357	0.391530

C	-6.014202	-4.205872	-2.000734
C	-5.434421	-5.924905	-0.283091
H	-5.284540	-3.671306	1.354188
H	-5.656152	-2.466098	0.114077
H	-6.855213	-3.703776	0.536698
H	-5.684837	-4.863564	-2.813083
H	-7.077329	-4.405932	-1.824127
H	-5.925818	-3.168971	-2.344900
H	-6.503654	-6.130872	-0.147919
H	-5.049863	-6.610724	-1.046678
H	-4.928531	-6.157676	0.659683

TS1-S-cyclohexyl-anthryl E= -4612.13935299

H	-0.236351	-1.798420	-1.351540
C	-0.399629	1.923919	3.681447
C	0.252097	0.821759	4.246229
C	0.871594	0.908375	5.503268
C	0.804262	2.117654	6.195878
C	0.149131	3.223566	5.648162
C	-0.445977	3.124804	4.388344
H	-0.847576	1.830448	2.698290
H	1.276434	2.193000	7.172806
H	0.107680	4.157401	6.201582
H	-0.948198	3.981838	3.948911
C	1.611305	-0.306821	6.007852
H	2.646177	-0.293038	5.634130
H	1.673184	-0.301300	7.101525
C	0.916654	-1.588593	5.528738
H	1.488956	-2.481642	5.784023
H	-0.065036	-1.681277	6.017857
C	0.655539	-1.575093	4.033244
N	0.316914	-0.393984	3.513338
H	0.011010	-0.334709	2.525075
C	-0.791263	-3.005892	0.180378

C	0.660316	-3.064169	0.335623
H	-1.351656	-3.931767	0.280414
C	0.992206	2.828089	-0.860592
C	0.029041	3.810092	-1.057804
C	0.304707	4.853899	-2.011701
C	1.606975	4.926782	-2.604150
C	2.576085	3.944879	-2.276940
C	2.291307	2.880128	-1.448457
H	-1.674748	5.741857	-2.032096
C	-0.668933	5.804029	-2.429861
C	1.899933	5.965180	-3.529360
H	3.567429	4.025844	-2.715110
C	0.941151	6.882818	-3.891330
C	-0.359631	6.788168	-3.343440
H	2.898203	6.009498	-3.958482
H	1.173961	7.667920	-4.605412
H	-1.125849	7.494920	-3.650513
C	-1.279546	3.749576	-0.340098
C	-1.780535	4.852545	0.436683
C	-2.061028	2.606137	-0.426309
C	-0.993217	5.992262	0.760355
C	-3.119766	4.791330	0.944097
C	-3.405415	2.530620	0.048221
C	-1.509562	7.023524	1.515070
H	0.033474	6.038126	0.415523
C	-3.628358	5.881154	1.701920
C	-3.911325	3.639691	0.693120
C	-2.844438	6.977159	1.982277
H	-0.884118	7.878913	1.755969
H	-4.650470	5.824434	2.068920
H	-4.939441	3.629067	1.045393
H	-3.242674	7.800560	2.568790
C	-4.221121	1.292751	-0.182392
C	-4.607408	0.945201	-1.501215

C	-4.591784	0.462172	0.904023	C	-3.572631	-0.373970	3.093525
C	-5.312461	-0.243941	-1.710514	H	-2.682942	-0.698585	2.548103
C	-5.302834	-0.715346	0.640330	H	-4.240968	-1.234236	3.216494
C	-5.651444	-1.097903	-0.657199	H	-3.264665	-0.053426	4.096206
H	-5.601397	-0.522520	-2.720122	C	2.904199	0.762107	-3.469288
H	-5.576215	-1.368463	1.464171	H	2.014704	1.395923	-3.412009
C	3.330978	1.835355	-1.159469	C	2.418418	-0.655434	-3.822170
C	4.054662	1.882184	0.055161	H	1.840986	-0.626667	-4.754025
C	3.618767	0.834403	-2.119001	H	1.771806	-1.047063	-3.034087
C	5.049501	0.926307	0.290542	H	3.252329	-1.350112	-3.979202
C	4.622987	-0.099533	-1.836021	C	3.805356	1.316275	-4.592780
C	5.347116	-0.074577	-0.639188	H	4.716254	0.713814	-4.697755
H	5.616761	0.962344	1.216708	H	4.111109	2.349788	-4.396031
H	4.853766	-0.870470	-2.565319	H	3.277253	1.297080	-5.553846
O	-1.550057	1.496041	-1.075652	C	3.815892	2.964176	1.107068
O	0.734994	1.788199	0.017656	H	2.971928	3.577107	0.778138
P	-0.373704	0.619800	-0.330108	C	3.433229	2.367219	2.473760
O	-0.818727	0.074282	1.002424	H	4.251396	1.774783	2.901047
C	-4.322928	1.838857	-2.708624	H	2.554215	1.722462	2.382487
H	-3.715119	2.683861	-2.374342	H	3.193621	3.164525	3.187170
C	-5.632114	2.426236	-3.274894	C	5.033194	3.902253	1.228662
H	-6.180356	2.987648	-2.509718	H	5.274357	4.365391	0.265165
H	-6.295599	1.637829	-3.649788	H	5.923743	3.361861	1.571197
H	-5.417329	3.106392	-4.108126	H	4.830548	4.703494	1.949847
C	-3.522969	1.109938	-3.805242	O	0.132730	-0.337511	-1.386513
H	-2.579882	0.722341	-3.409281	S	0.748943	-3.016317	3.151426
H	-3.292765	1.800468	-4.625651	O	-0.381734	-2.817592	-1.202116
H	-4.088864	0.272328	-4.229842	H	-1.286979	-2.137859	0.609269
C	-4.258830	0.792763	2.359391	H	1.153223	-2.100488	0.395886
H	-3.553921	1.628306	2.364806	C	1.529096	-4.268640	0.149804
C	-5.522040	1.243662	3.121650	C	0.781331	-5.611809	0.100806
H	-5.993588	2.112156	2.647589	C	2.464357	-4.093058	-1.077466
H	-5.273207	1.514514	4.155052	H	2.186514	-4.265822	1.033004
H	-6.268559	0.440794	3.154900	C	1.765760	-6.785739	-0.031147

H	0.097744	-5.611660	-0.759585	H	5.668009	-4.917957	3.297149
H	0.167892	-5.736637	1.001923	C	-6.334518	-2.404044	-0.914578
C	3.438495	-5.274743	-1.194684	C	-7.714811	-2.556247	-0.645317
H	1.843471	-4.022721	-1.978415	C	-5.584263	-3.492220	-1.422756
H	3.017575	-3.150316	-0.992083	C	-8.525158	-1.483363	-0.149963
C	2.694302	-6.617564	-1.243006	C	-8.355373	-3.829958	-0.886528
H	1.207718	-7.727358	-0.103654	C	-6.236104	-4.759881	-1.664479
H	2.371481	-6.850996	0.884456	C	-4.180824	-3.400075	-1.700622
H	4.056575	-5.148391	-2.092074	C	-9.861373	-1.658000	0.101174
H	4.125215	-5.264244	-0.336748	H	-8.060602	-0.518595	0.022111
H	3.411074	-7.447126	-1.286225	C	-9.751794	-3.969215	-0.608612
H	2.098035	-6.669508	-2.165981	C	-7.600548	-4.894454	-1.388938
C	6.410072	-1.091907	-0.368181	C	-5.466041	-5.851086	-2.177851
C	7.624054	-1.058683	-1.097768	H	-3.673386	-2.458257	-1.523897
C	6.198069	-2.095779	0.609132	C	-3.477835	-4.470238	-2.192180
C	7.913220	-0.046370	-2.070514	C	-10.485691	-2.918314	-0.127134
C	8.635983	-2.062208	-0.853129	H	-10.454781	-0.827819	0.475122
C	7.220464	-3.090328	0.848358	H	-10.219061	-4.934093	-0.791834
C	4.989454	-2.188893	1.375154	H	-8.086980	-5.850913	-1.570470
C	9.097520	-0.038270	-2.761029	C	-4.128298	-5.714440	-2.436798
H	7.175385	0.726790	-2.252893	H	-5.971859	-6.796847	-2.358538
C	9.855712	-2.019718	-1.599413	H	-2.416217	-4.362886	-2.399139
C	8.406889	-3.048976	0.110271	H	-11.545956	-3.038328	0.078813
C	6.992595	-4.102098	1.834131	H	-3.557850	-6.552112	-2.829384
H	4.209621	-1.453801	1.208938				
C	4.809590	-3.173854	2.313737		TS1-S-cyclohexyl-iPr E= -3771.45532489		
C	10.082568	-1.040779	-2.529181	H	1.154971	-1.884361	-2.122182
H	9.291860	0.742915	-3.491149	C	-0.781063	-0.058521	3.546561
H	10.603373	-2.785621	-1.406437	C	-0.082894	-1.206839	3.936244
H	9.171549	-3.801727	0.291864	C	-0.116542	-1.662699	5.263920
C	5.825551	-4.145466	2.549105	C	-0.852647	-0.934399	6.199146
H	7.774067	-4.839427	2.003422	C	-1.551304	0.215900	5.824564
H	3.884508	-3.213143	2.883496	C	-1.516323	0.649109	4.497175
H	11.014224	-1.019625	-3.088158	H	-0.742273	0.267119	2.513401

H	-0.880672	-1.276954	7.231120	C	-4.311843	2.159770	1.372633
H	-2.119627	0.770032	6.566170	C	-3.720999	0.289283	-0.096313
H	-2.057811	1.540928	4.195072	C	-3.668879	4.579337	2.649528
C	0.625121	-2.936891	5.586747	H	-1.873256	4.570796	1.493429
H	0.893056	-2.975672	6.648185	C	-5.193512	2.735284	2.327535
H	-0.022046	-3.805403	5.392579	C	-4.607221	0.917509	0.754451
C	1.887839	-3.044491	4.720912	C	-4.883753	3.920529	2.954606
H	2.600653	-2.256440	5.007757	H	-3.414705	5.504187	3.160448
H	2.394638	-4.001514	4.854347	H	-6.115611	2.209490	2.563800
C	1.584861	-2.845986	3.246514	H	-5.555978	0.437411	0.978900
N	0.650865	-1.937223	2.962425	H	-5.562197	4.346536	3.688710
H	0.417910	-1.723548	1.975430	C	-4.059076	-1.032748	-0.721567
C	1.209505	-3.573203	-1.005950	C	-4.364816	-1.099926	-2.104488
C	2.486132	-2.995425	-0.591685	C	-4.130990	-2.203286	0.070058
H	1.180259	-4.641886	-1.204580	C	-4.731484	-2.329522	-2.659234
C	0.235142	2.419001	-0.400559	C	-4.511044	-3.406632	-0.538959
C	-1.030247	2.986356	-0.470859	C	-4.812525	-3.498423	-1.897177
C	-1.169505	4.273041	-1.101823	H	-4.968361	-2.372099	-3.719528
C	0.011455	4.979591	-1.499248	H	-4.570587	-4.307193	0.068097
C	1.280883	4.380431	-1.299517	C	2.790300	2.507795	-0.624373
C	1.422718	3.106182	-0.790243	C	3.389889	2.470139	0.657781
H	-3.338026	4.336319	-1.134507	C	3.513832	2.056439	-1.753108
C	-2.429568	4.870300	-1.386742	C	4.699561	1.996712	0.782345
C	-0.107650	6.259971	-2.104530	C	4.824609	1.593242	-1.570341
H	2.169937	4.939668	-1.578853	C	5.441069	1.557922	-0.318367
C	-1.342041	6.818153	-2.343829	H	5.158246	1.984489	1.768086
C	-2.512439	6.105697	-1.991566	H	5.390379	1.259686	-2.437410
H	0.801564	6.784429	-2.388964	O	-1.602610	0.343622	-1.235336
H	-1.421660	7.794511	-2.813911	O	0.376206	1.159996	0.159999
H	-3.488034	6.534060	-2.205303	P	-0.169069	-0.186545	-0.624749
C	-2.217364	2.253582	0.060880	O	-0.342202	-1.228554	0.448666
C	-3.098506	2.842528	1.034175	C	-4.351719	0.129512	-3.013282
C	-2.501594	0.970664	-0.388948	H	-4.026859	0.990147	-2.422715
C	-2.802843	4.057955	1.712383	C	-5.767157	0.456924	-3.530624

H	-6.467008	0.609465	-2.701063	H	4.645919	3.075454	-4.116052
H	-6.164483	-0.350312	-4.157460	H	3.417018	4.202713	-3.525441
H	-5.751593	1.371503	-4.135990	H	3.120704	3.263067	-4.999965
C	-3.353815	-0.021401	-4.177263	C	6.883913	1.090054	-0.171367
H	-2.344429	-0.214610	-3.802671	H	7.207310	0.725055	-1.156148
H	-3.326926	0.897313	-4.776087	C	7.815388	2.255957	0.215367
H	-3.635649	-0.843237	-4.846564	H	8.858892	1.921200	0.264051
C	-5.218851	-4.829129	-2.517315	H	7.548421	2.665165	1.197147
H	-5.187676	-5.580474	-1.716019	H	7.751152	3.070981	-0.513802
C	-6.661284	-4.793268	-3.057564	C	7.026997	-0.077214	0.822771
H	-6.955103	-5.776375	-3.445362	H	8.065303	-0.428595	0.859053
H	-6.762008	-4.069244	-3.874866	H	6.390725	-0.922709	0.538068
H	-7.370569	-4.509549	-2.272226	H	6.744207	0.223484	1.838472
C	-4.230904	-5.280402	-3.609715	C	2.673303	2.975155	1.909577
H	-3.209786	-5.342950	-3.217714	H	1.645155	3.227418	1.636250
H	-4.220869	-4.579189	-4.452577	C	2.594456	1.899085	3.007989
H	-4.509183	-6.266865	-4.000394	H	3.588009	1.628639	3.385422
C	-3.818115	-2.214963	1.566600	H	2.115834	0.991129	2.628708
H	-3.394319	-1.243146	1.832976	H	2.005469	2.263282	3.858156
C	-5.096281	-2.411930	2.406760	C	3.325412	4.266982	2.441874
H	-5.842294	-1.637255	2.196463	H	3.329633	5.051718	1.677043
H	-4.861520	-2.374656	3.477616	H	4.364059	4.094131	2.748497
H	-5.562505	-3.382957	2.199179	H	2.777072	4.644222	3.313827
C	-2.761419	-3.273253	1.934017	O	0.684842	-0.501035	-1.833257
H	-1.848009	-3.117481	1.354116	S	2.453650	-3.723755	2.090272
H	-3.120594	-4.293484	1.753899	O	1.557656	-2.843266	-2.209794
H	-2.510476	-3.196217	2.998999	H	0.323879	-3.189926	-0.503809
C	2.934630	2.088342	-3.168466	H	2.434234	-1.974411	-0.230576
H	1.862770	2.289764	-3.087967	C	3.844948	-3.559908	-0.884269
C	3.077941	0.743288	-3.903890	C	3.847707	-5.017198	-1.378032
H	2.583324	0.799610	-4.881162	C	4.637026	-2.636790	-1.847858
H	2.606659	-0.059387	-3.332496	H	4.369876	-3.523118	0.082552
H	4.127798	0.482468	-4.084981	C	5.282516	-5.525819	-1.593168
C	3.565572	3.225644	-3.998107	H	3.294749	-5.075665	-2.325728

H	3.327736	-5.660788	-0.657385	C	1.769413	-3.224607	0.012056
C	6.067220	-3.158423	-2.053269	H	0.194862	-4.694841	-0.380560
H	4.108328	-2.603130	-2.807431	C	0.559962	2.493287	-0.734897
H	4.652602	-1.611532	-1.458060	C	-0.588783	3.266692	-0.836941
C	6.073463	-4.614366	-2.543232	C	-0.543197	4.453621	-1.651863
H	5.255321	-6.551272	-1.981696	C	0.712901	4.868677	-2.201980
H	5.796731	-5.573675	-0.622112	C	1.867737	4.077784	-1.974988
H	6.592000	-2.512784	-2.768439	C	1.816601	2.884493	-1.285713
H	6.620938	-3.090175	-1.105249	H	-2.664539	4.906153	-1.606487
H	7.104091	-4.976886	-2.644307	C	-1.695867	5.224204	-1.972923
H	5.624459	-4.659606	-3.546170	C	0.778210	6.051506	-2.987298
				H	2.817828	4.415076	-2.380993
				C	-0.353054	6.786467	-3.256731
				C	-1.603106	6.355830	-2.753682
				H	1.743458	6.355782	-3.385283
				H	-0.292602	7.684763	-3.864955
				H	-2.501541	6.919803	-2.989645
				C	-1.848995	2.846262	-0.154957
				C	-2.556582	3.722278	0.740932
				C	-2.377974	1.583166	-0.389331
				C	-2.015393	4.950919	1.211891
				C	-3.849192	3.328533	1.217854
				C	-3.678998	1.184794	0.043348
				C	-2.722321	5.754062	2.080629
				H	-1.024003	5.247484	0.889330
				C	-4.560972	4.189351	2.097398
				C	-4.392421	2.082913	0.810704
				C	-4.013802	5.378829	2.521542
				H	-2.281899	6.682973	2.432839
				H	-5.545805	3.880484	2.439839
				H	-5.396045	1.822267	1.136334
				H	-4.564508	6.025062	3.199569
				C	-4.274847	-0.134592	-0.351533
				C	-4.622436	-0.375997	-1.704683
TS1-S-cyclohexyl-Ph E= -3997.67215499							
H	0.634912	-2.143135	-1.699904				
C	-0.804805	0.866798	3.605093				
C	0.062582	-0.098194	4.128904				
C	0.567010	0.010420	5.434873				
C	0.164325	1.094543	6.215410				
C	-0.708873	2.059949	5.708204				
C	-1.186745	1.946389	4.400679				
H	-1.157792	0.765875	2.584955				
H	0.544912	1.184011	7.230456				
H	-1.010843	2.897624	6.330433				
H	-1.857921	2.697230	3.993964				
C	1.550504	-1.036259	5.899146				
H	2.571304	-0.738521	5.615570				
H	1.541884	-1.124248	6.991037				
C	1.222821	-2.392806	5.261246				
H	1.979753	-3.144177	5.490674				
H	0.265196	-2.764292	5.656968				
C	1.060036	-2.293155	3.755091				
N	0.467124	-1.184220	3.307017				
H	0.209884	-1.108247	2.306336				
C	0.409937	-3.629674	-0.339439				

C	-4.543744	-1.122671	0.628148	C	-3.267574	-2.078642	2.613209
C	-5.222305	-1.591007	-2.045251	H	-2.360004	-2.131641	2.006062
C	-5.152498	-2.319016	0.234454	H	-3.762582	-3.056600	2.586490
C	-5.499439	-2.580562	-1.094934	H	-2.976508	-1.884710	3.652930
H	-5.516374	-1.761249	-3.076968	C	2.889868	1.274351	-3.568160
H	-5.334377	-3.086154	0.981543	H	1.894120	1.713951	-3.462070
C	3.050485	2.048499	-1.108243	C	2.687697	-0.150742	-4.114924
C	3.729395	2.047146	0.133343	H	2.133661	-0.109171	-5.060494
C	3.562358	1.297467	-2.194378	H	2.111337	-0.753715	-3.409968
C	4.898149	1.292833	0.268591	H	3.640507	-0.654497	-4.319173
C	4.739121	0.563540	-2.009841	C	3.677056	2.134130	-4.578682
C	5.423141	0.539205	-0.788175	H	4.685381	1.731589	-4.736703
H	5.435858	1.318039	1.212213	H	3.784176	3.168911	-4.235123
H	5.121290	-0.031258	-2.833905	H	3.166543	2.150566	-5.549269
O	-1.653515	0.683933	-1.152390	C	3.256556	2.882989	1.322027
O	0.525864	1.327993	0.011134	H	2.303938	3.347508	1.053108
P	-0.302313	-0.000805	-0.506788	C	2.999988	2.020914	2.571535
O	-0.591971	-0.798978	0.738026	H	3.923337	1.558536	2.941574
C	-4.419998	0.660503	-2.810302	H	2.281970	1.225354	2.352283
H	-3.921556	1.531882	-2.378170	H	2.588729	2.634234	3.381952
C	-5.771514	1.153316	-3.366303	C	4.244823	4.026391	1.626594
H	-6.399975	1.570092	-2.570941	H	4.386807	4.670375	0.751389
H	-6.332427	0.340428	-3.842529	H	5.228342	3.639033	1.918542
H	-5.613127	1.934744	-4.119515	H	3.872157	4.648074	2.449882
C	-3.511694	0.133307	-3.937324	O	0.393976	-0.669627	-1.670424
H	-2.541930	-0.181351	-3.541224	S	1.570405	-3.569088	2.770543
H	-3.338561	0.918780	-4.683117	O	0.869041	-3.155815	-1.630172
H	-3.965987	-0.719263	-4.456598	H	-0.392456	-3.031707	0.087167
C	-4.188436	-0.952863	2.105792	H	1.892495	-2.168688	0.225436
H	-3.634306	-0.017531	2.217141	C	3.013325	-4.041429	-0.169531
C	-5.453760	-0.845407	2.980634	C	2.773647	-5.536620	-0.440632
H	-6.098178	-0.018639	2.660219	C	3.940885	-3.415143	-1.245115
H	-5.182113	-0.676626	4.029846	H	3.543406	-3.944834	0.790279
H	-6.050132	-1.764773	2.933859	C	4.105201	-6.298304	-0.547091

H	2.215498	-5.645818	-1.380885			
H	2.157053	-5.972085	0.355851			
C	5.265703	-4.186692	-1.340694			
H	3.418004	-3.441858	-2.208283			
H	4.129238	-2.360467	-1.012771			
C	5.031190	-5.681176	-1.605966			
H	3.908801	-7.352733	-0.777325			
H	4.607913	-6.280546	0.431033			
H	5.885349	-3.748063	-2.132076			
H	5.828481	-4.060947	-0.404850			
H	5.988001	-6.217745	-1.629340			
H	4.576743	-5.805698	-2.599870			
C	6.665155	-0.259464	-0.618767			
C	7.607871	-0.364364	-1.656523			
C	6.931708	-0.935456	0.585217			
C	8.770918	-1.117626	-1.498195			
H	7.437840	0.171777	-2.585954			
C	8.095758	-1.687395	0.745489			
H	6.208378	-0.885950	1.394497			
C	9.020963	-1.783173	-0.296219			
H	9.488351	-1.175918	-2.312744			
H	8.276911	-2.204257	1.684550			
H	9.927903	-2.368704	-0.171935			
C	-6.141489	-3.862212	-1.484792			
C	-5.809828	-4.498806	-2.693378			
C	-7.098488	-4.473748	-0.656416			
C	-6.412859	-5.701362	-3.060742			
H	-5.053977	-4.057041	-3.336752			
C	-7.701052	-5.676948	-1.022111			
H	-7.389589	-3.986344	0.269954			
C	-7.361501	-6.296696	-2.226583			
H	-6.134332	-6.178393	-3.996967			
H	-8.444462	-6.126485	-0.368648			
H	-7.831632	-7.233893	-2.512315			
				TS1-S-cyclohexyl-tBu E= -3850.06512782		
H	0.860296	-2.088523	-1.954253			
C	-0.800463	0.360187	3.575062			
C	-0.230878	-0.828090	4.045722			
C	-0.289286	-1.173913	5.405489			
C	-0.917928	-0.295762	6.288872			
C	-1.487862	0.895453	5.833016			
C	-1.430458	1.218948	4.475430			
H	-0.742798	0.600177	2.519536			
H	-0.963614	-0.552315	7.344914			
H	-1.973575	1.566923	6.535345			
H	-1.871432	2.142099	4.110715			
C	0.310518	-2.495931	5.819112			
H	0.594743	-2.482744	6.876937			
H	-0.434345	-3.297513	5.702545			
C	1.534429	-2.812539	4.949375			
H	2.336314	-2.089733	5.163687			
H	1.934066	-3.807225	5.152823			
C	1.225192	-2.696128	3.467721			
N	0.395049	-1.710437	3.123546			
H	0.172347	-1.543537	2.124959			
C	0.706194	-3.682103	-0.716388			
C	2.055209	-3.251324	-0.356870			
H	0.532885	-4.749150	-0.833708			
C	0.498085	2.426070	-0.491063			
C	-0.696452	3.129439	-0.580322			
C	-0.694495	4.398838	-1.259770			
C	0.555339	4.954578	-1.684227			
C	1.750644	4.224960	-1.464515			
C	1.752211	2.962314	-0.908326			
H	-2.842586	4.701707	-1.292339			
C	-1.881760	5.122238	-1.564262			
C	0.576336	6.218546	-2.334109			

H	2.694771	4.671108	-1.766194	C	5.601898	1.015275	-0.411490
C	-0.589408	6.902523	-2.590242	H	5.361718	1.527525	1.663333
C	-1.830002	6.337663	-2.211454	H	5.474580	0.672413	-2.529178
H	1.536680	6.628348	-2.638184	O	-1.570969	0.540302	-1.226583
H	-0.562266	7.865006	-3.093730	O	0.505194	1.183742	0.120369
H	-2.753004	6.864403	-2.438504	P	-0.215184	-0.128692	-0.576243
C	-1.955912	2.561162	-0.015160	O	-0.520732	-1.063861	0.563765
C	-2.757263	3.289114	0.932838	C	-4.321943	0.556048	-2.999815
C	-2.389881	1.302441	-0.409732	H	-3.895650	1.399733	-2.450745
C	-2.317257	4.487624	1.561515	C	-5.690743	1.022222	-3.535424
C	-4.041122	2.768596	1.297870	H	-6.365997	1.294111	-2.716080
C	-3.678187	0.779770	-0.087509	H	-6.180755	0.238102	-4.124873
C	-3.112915	5.146068	2.474553	H	-5.570321	1.899402	-4.183020
H	-1.334153	4.877673	1.323888	C	-3.352200	0.235775	-4.153368
C	-4.846311	3.483907	2.225457	H	-2.369515	-0.051450	-3.768016
C	-4.481906	1.543736	0.733657	H	-3.224476	1.115568	-4.795845
C	-4.396784	4.649404	2.803193	H	-3.726982	-0.580615	-4.782841
H	-2.749627	6.054435	2.947700	C	-5.752715	-4.243441	-2.344168
H	-5.823488	3.081081	2.481380	C	-7.146318	-3.964840	-2.956317
H	-5.479037	1.187570	0.978350	H	-7.553696	-4.875886	-3.412605
H	-5.018329	5.183017	3.517067	H	-7.102736	-3.193641	-3.732382
C	-4.167146	-0.521020	-0.653355	H	-7.850264	-3.625118	-2.187771
C	-4.476167	-0.618941	-2.033259	C	-4.796159	-4.736774	-3.455984
C	-4.375029	-1.639254	0.184987	H	-3.802395	-4.955414	-3.048435
C	-4.978382	-1.822874	-2.531452	H	-4.673489	-3.992406	-4.249457
C	-4.887394	-2.821501	-0.370341	H	-5.185344	-5.654054	-3.915503
C	-5.195823	-2.947620	-1.725398	C	-4.070990	-1.621474	1.684025
H	-5.214138	-1.878388	-3.590655	H	-3.544048	-0.691449	1.913151
H	-5.042032	-3.665480	0.291997	C	-5.366688	-1.642712	2.519690
C	3.046838	2.223273	-0.728214	H	-6.022280	-0.800632	2.270884
C	3.651081	2.156281	0.550357	H	-5.135492	-1.587560	3.590554
C	3.712757	1.666674	-1.842389	H	-5.934849	-2.564706	2.346044
C	4.906103	1.556740	0.677401	C	-3.136910	-2.771294	2.105553
C	4.974058	1.078709	-1.657541	H	-2.207165	-2.736649	1.531945

H	-3.600770	-3.754280	1.960611	H	-0.112068	-3.148256	-0.237952
H	-2.888234	-2.679381	3.169970	H	2.147925	-2.207835	-0.078302
C	3.127754	1.706896	-3.255385	C	3.320786	-4.015422	-0.608671
H	2.096179	2.062391	-3.182100	C	3.121256	-5.500383	-0.958227
C	3.070078	0.315490	-3.913291	C	4.203762	-3.301547	-1.667263
H	2.594741	0.388515	-4.899124	H	3.869755	-3.955385	0.343734
H	2.479941	-0.372195	-3.302975	C	4.471423	-6.213184	-1.138093
H	4.069703	-0.110228	-4.063537	H	2.544203	-5.576333	-1.890383
C	3.898954	2.700118	-4.148301	H	2.537555	-5.997252	-0.173218
H	4.945787	2.395277	-4.268987	C	5.547587	-4.026402	-1.837781
H	3.895497	3.710462	-3.724306	H	3.659804	-3.288330	-2.618827
H	3.447539	2.750151	-5.146657	H	4.363085	-2.255178	-1.378523
C	7.004561	0.412394	-0.205183	C	5.350732	-5.510118	-2.182776
C	7.956460	1.509014	0.331332	H	4.300872	-7.258515	-1.423485
H	8.962140	1.099685	0.489655	H	4.998792	-6.235281	-0.173212
H	7.607970	1.918311	1.285218	H	6.134462	-3.528011	-2.619588
H	8.035209	2.339944	-0.379092	H	6.129733	-3.941659	-0.908319
C	6.932737	-0.743145	0.820668	H	6.322126	-6.014117	-2.260843
H	7.930021	-1.168674	0.989000	H	4.874110	-5.590540	-3.170599
H	6.278186	-1.545903	0.461304	C	-5.902768	-5.374307	-1.308690
H	6.545905	-0.407621	1.788394	H	-4.942249	-5.637384	-0.851032
C	2.999296	2.759852	1.794115	H	-6.600781	-5.105238	-0.507687
H	1.996843	3.101319	1.522164	H	-6.293411	-6.273820	-1.798436
C	2.829686	1.724135	2.920743	C	7.606052	-0.142291	-1.510618
H	3.797028	1.371717	3.298894	H	6.991564	-0.944442	-1.935345
H	2.265638	0.855403	2.567457	H	7.720314	0.638532	-2.270884
H	2.283947	2.162440	3.764670	H	8.600609	-0.558078	-1.311758
C	3.776579	3.996662	2.287038				
H	3.848882	4.757057	1.501295				
H	4.796831	3.732771	2.590780	TS1-S-n-hexyl-anthryl E= -4613.33476277			
H	3.275983	4.448365	3.152444	H	0.630907	-1.885376	-0.886926
O	0.585083	-0.635306	-1.755702	C	-0.521882	2.265758	3.565816
S	1.963362	-3.757266	2.376376	C	-0.096360	1.208330	4.377140
O	1.127000	-3.096597	-1.975018	C	0.313555	1.427142	5.702460
				C	0.264398	2.726897	6.206733

C	-0.169351	3.790256	5.411170	C	-2.077088	4.491912	0.417309
C	-0.556593	3.557677	4.089602	C	-2.217607	2.220060	-0.418266
H	-0.810627	2.068901	2.538818	C	-1.359154	5.683751	0.715954
H	0.573677	2.906287	7.234049	C	-3.393262	4.343439	0.963073
H	-0.202091	4.795455	5.821738	C	-3.550994	2.069336	0.068499
H	-0.888272	4.378822	3.461271	C	-1.921665	6.680101	1.485352
C	0.820536	0.242154	6.488746	H	-0.348649	5.798119	0.340322
H	1.899124	0.112795	6.312431	C	-3.952399	5.398223	1.734415
H	0.697184	0.405667	7.564845	C	-4.114283	3.145235	0.722681
C	0.081757	-1.034282	6.064200	C	-3.236475	6.545067	1.991645
H	0.502690	-1.924156	6.534274	H	-1.348901	7.576885	1.705995
H	-0.972556	-0.968998	6.374051	H	-4.957444	5.273805	2.130441
C	0.081503	-1.220189	4.558240	H	-5.136690	3.070973	1.083531
N	-0.048299	-0.102415	3.835597	H	-3.671955	7.341209	2.589110
H	-0.207443	-0.176381	2.817312	C	-4.337875	0.816236	-0.183612
C	0.069486	-3.282102	0.508344	C	-4.766201	0.514522	-1.500800
C	1.196451	-2.748000	1.267077	C	-4.697600	-0.036214	0.888034
H	-0.061580	-4.363462	0.483593	C	-5.536709	-0.632574	-1.717043
C	0.776136	2.678666	-1.028737	C	-5.476817	-1.168500	0.618550
C	-0.263213	3.590698	-1.155928	C	-5.902898	-1.487245	-0.673177
C	-0.125296	4.654979	-2.117958	H	-5.871861	-0.867222	-2.723569
C	1.127991	4.818948	-2.792732	H	-5.757082	-1.828878	1.434373
C	2.168295	3.883219	-2.566220	C	3.074749	1.740539	-1.650091
C	2.007192	2.790374	-1.740571	C	3.869359	1.612136	-0.486751
H	-2.157336	5.409476	-2.007135	C	3.305435	0.891887	-2.762099
C	-1.184186	5.540998	-2.464064	C	4.870234	0.634196	-0.451662
C	1.294114	5.885024	-3.718097	C	4.332176	-0.055477	-2.683928
H	3.106336	4.008802	-3.101007	C	5.120021	-0.211135	-1.539762
C	0.257113	6.741927	-4.005000	H	5.480873	0.529091	0.441052
C	-0.997955	6.553338	-3.380338	H	4.523327	-0.700539	-3.536591
H	2.257517	5.997465	-4.209777	O	-1.642887	1.124669	-1.043128
H	0.392496	7.549047	-4.719632	O	0.663811	1.653928	-0.106459
H	-1.827368	7.209616	-3.629876	P	-0.366391	0.385511	-0.311343
C	-1.521608	3.422600	-0.370296	O	-0.668751	-0.108056	1.077616

C	-4.462669	1.413894	-2.699434	H	3.236186	2.460387	2.844937
H	-3.838953	2.244014	-2.358098	H	4.224252	1.098249	2.296100
C	-5.754097	2.033044	-3.271676	C	4.940584	3.442254	0.893992
H	-6.297396	2.598620	-2.506044	H	5.843028	2.854437	1.100895
H	-6.431041	1.263684	-3.661234	H	4.793876	4.134916	1.731662
H	-5.516871	2.716634	-4.095904	H	5.127493	4.035480	-0.008455
C	-3.669784	0.671947	-3.792819	O	0.152330	-0.601502	-1.337823
H	-3.426823	1.356864	-4.614268	S	0.182801	-2.764192	3.886282
H	-4.246906	-0.158997	-4.215565	O	0.952568	-2.838304	-0.550812
H	-2.733525	0.271422	-3.392896	H	-0.863745	-2.725651	0.565320
C	-4.275490	0.221889	2.334297	H	1.171577	-1.678484	1.429546
H	-3.568179	1.055754	2.337537	C	2.412127	-3.554197	1.605900
C	-5.481844	0.629440	3.204253	C	3.629386	-2.707393	1.996558
H	-5.982559	1.520709	2.809048	C	4.856778	-3.562843	2.333844
H	-5.160176	0.848507	4.229702	H	3.872121	-2.027419	1.169887
H	-6.226250	-0.174585	3.250974	H	3.365618	-2.079377	2.858679
C	-3.545926	-0.986785	2.949252	C	6.095839	-2.728433	2.683414
H	-2.674644	-1.260697	2.348425	H	4.615443	-4.231056	3.174211
H	-4.199292	-1.862967	3.032919	H	5.090347	-4.212271	1.478698
H	-3.199593	-0.740686	3.960434	H	6.328912	-2.061182	1.841342
C	2.484623	0.954858	-4.051709	H	5.869195	-2.076081	3.540337
H	1.674649	1.673682	-3.905734	C	7.331194	-3.579587	3.005666
C	1.823090	-0.397179	-4.383325	H	7.546506	-4.234872	2.150195
H	1.200165	-0.297281	-5.280756	H	7.103842	-4.244000	3.851833
H	1.186727	-0.726686	-3.557331	C	8.572826	-2.741712	3.329119
H	2.566628	-1.177724	-4.586078	H	9.434508	-3.377641	3.563637
C	3.337911	1.456230	-5.234232	H	8.849614	-2.104321	2.480642
H	3.772825	2.441425	-5.029671	H	8.397327	-2.088068	4.192821
H	2.725398	1.537666	-6.140247	H	2.649126	-4.184193	0.739538
H	4.163993	0.768198	-5.450843	H	2.146712	-4.240514	2.421166
C	3.704773	2.536287	0.719195	C	-6.728306	-2.709047	-0.930095
H	2.851835	3.193396	0.528371	C	-6.136152	-3.849345	-1.524526
C	3.398347	1.762584	2.014779	C	-8.098708	-2.723570	-0.575420
H	2.493206	1.159018	1.900334	C	-4.751760	-3.896622	-1.892431

C	-1.211411	2.854439	0.655766	C	-5.195998	-2.702401	-2.748806
C	-1.464042	4.272076	0.619983	H	-5.536071	-0.943694	-3.934228
C	-0.371871	5.161916	0.360308	H	-4.744184	-4.224063	-1.315083
C	0.911016	4.626604	0.083352	C	2.499599	2.758385	-0.384589
C	1.142494	3.268807	0.003808	C	3.352512	2.183695	0.585392
H	-3.607451	4.187847	0.946662	C	2.955738	2.918284	-1.717294
C	-2.756586	4.841272	0.796203	C	4.643218	1.794268	0.207330
C	-0.597182	6.565311	0.350224	C	4.259934	2.522767	-2.036067
H	1.731385	5.313724	-0.107159	C	5.124346	1.961482	-1.093061
C	-1.855821	7.082211	0.552351	H	5.304949	1.364283	0.956716
C	-2.946253	6.205715	0.762299	H	4.608303	2.661434	-3.056053
H	0.247917	7.223517	0.162552	O	-1.865566	0.665773	-0.997841
H	-2.017931	8.156454	0.535239	O	0.298892	1.037506	0.301986
H	-3.945959	6.611594	0.891899	P	-0.357282	0.030930	-0.825057
C	-2.293237	1.889577	1.013156	O	-0.352701	-1.333236	-0.187797
C	-3.026228	1.994526	2.247134	C	-4.787275	1.078849	-2.365392
C	-2.638963	0.871602	0.132483	H	-4.385574	1.644008	-1.520282
C	-2.632364	2.854746	3.310148	C	-6.246156	1.541939	-2.553586
C	-4.182866	1.171326	2.439430	H	-6.722453	1.037738	-3.402806
C	-3.813420	0.073568	0.279883	H	-6.283307	2.621561	-2.743679
C	-3.355803	2.915185	4.482242	H	-6.848071	1.332524	-1.661871
H	-1.740996	3.460840	3.194843	C	-3.928440	1.433348	-3.594726
C	-4.918832	1.273243	3.651258	H	-4.296139	0.936068	-4.500606
C	-4.569967	0.266280	1.417776	H	-2.886269	1.139348	-3.440653
C	-4.518748	2.126826	4.653920	H	-3.956456	2.514585	-3.777423
H	-3.028924	3.574134	5.282203	C	-3.760809	-2.893559	0.790205
H	-5.800666	0.649198	3.775514	H	-3.302904	-2.096289	1.382061
H	-5.483306	-0.307567	1.549585	C	-4.924560	-3.475348	1.617757
H	-5.085369	2.190633	5.578829	H	-5.685016	-2.716995	1.835975
C	-4.249229	-0.895578	-0.779984	H	-4.557508	-3.870999	2.572798
C	-4.718252	-0.411031	-2.027837	H	-5.420912	-4.295155	1.084282
C	-4.255450	-2.286862	-0.522889	C	-2.673023	-3.959297	0.560315
C	-5.175630	-1.324489	-2.981882	H	-1.835302	-3.541001	-0.004281
C	-4.734272	-3.154641	-1.513499	H	-3.058122	-4.828583	0.014596

C	-0.698091	-0.011160	3.624523	H	1.107035	7.082487	-1.780951
C	0.019619	-1.180475	3.898675	H	-1.000902	8.381723	-1.677984
C	0.483160	-1.462648	5.193861	H	-3.093298	7.278847	-0.879737
C	0.188940	-0.560222	6.216312	C	-2.055023	2.607886	0.590135
C	-0.537556	0.604979	5.958845	C	-2.715363	3.162228	1.742518
C	-0.974357	0.879957	4.661028	C	-2.562888	1.433502	0.047418
H	-1.022050	0.190976	2.609481	C	-2.170344	4.232489	2.505817
H	0.537738	-0.772958	7.224408	C	-3.957390	2.592051	2.172417
H	-0.758159	1.295547	6.767853	C	-3.819442	0.874427	0.430623
H	-1.531852	1.787517	4.449588	C	-2.830119	4.727330	3.610433
C	1.307436	-2.712137	5.390166	H	-1.214354	4.653252	2.215869
H	2.367675	-2.492947	5.192932	C	-4.623174	3.139866	3.302674
H	1.247805	-3.060892	6.426884	C	-4.497388	1.487611	1.464247
C	0.833600	-3.817860	4.437244	C	-4.075993	4.186646	4.009053
H	1.481396	-4.694763	4.476692	H	-2.388170	5.539590	4.181255
H	-0.176456	-4.145669	4.727162	H	-5.571182	2.702890	3.607384
C	0.737006	-3.334390	3.001990	H	-5.469112	1.103108	1.762341
N	0.308801	-2.079205	2.838493	H	-4.590637	4.591870	4.875927
H	0.074670	-1.745026	1.887795	C	-4.416552	-0.294188	-0.297369
C	0.532448	-3.455274	-1.498473	C	-4.890809	-0.127676	-1.622483
C	1.705080	-3.135406	-0.689929	C	-4.562352	-1.546391	0.348158
H	0.493834	-4.438431	-1.966705	C	-5.491864	-1.210524	-2.269206
C	0.298122	2.569548	-0.259729	C	-5.179364	-2.595747	-0.341279
C	-0.877117	3.274950	-0.038878	C	-5.650022	-2.456315	-1.651127
C	-0.946824	4.644186	-0.481491	H	-5.881143	-1.072562	-3.273897
C	0.237480	5.266347	-0.993965	H	-5.269674	-3.562707	0.144821
C	1.426638	4.504516	-1.117025	C	2.726841	2.369495	-1.045037
C	1.475864	3.162283	-0.803390	C	3.556368	1.995890	0.038638
H	-3.066225	4.948678	-0.130887	C	3.103770	2.039270	-2.370679
C	-2.146306	5.410132	-0.469012	C	4.746008	1.308910	-0.221661
C	0.193949	6.626017	-1.406048	C	4.303533	1.351302	-2.577847
H	2.317552	4.990607	-1.506099	C	5.142648	0.976164	-1.522807
C	-0.977486	7.345114	-1.353322	H	5.377765	1.011530	0.610862
C	-2.160756	6.721113	-0.893254	H	4.611081	1.125850	-3.594805

O	-1.872673	0.809492	-0.978358	C	3.215559	2.347762	1.486175
O	0.375722	1.247817	0.143368	H	2.235022	2.831836	1.496354
P	-0.451204	0.052920	-0.635025	C	3.109827	1.097287	2.378507
O	-0.592338	-1.053819	0.375588	H	2.371879	0.396229	1.977435
C	-4.821393	1.206988	-2.365605	H	2.795687	1.376767	3.391151
H	-4.311736	1.931882	-1.725500	H	4.071049	0.575323	2.461052
C	-6.231693	1.769589	-2.635300	C	4.223236	3.360366	2.066202
H	-6.798371	1.884517	-1.704222	H	5.235658	2.940618	2.106434
H	-6.808405	1.112950	-3.297325	H	3.938748	3.643954	3.086843
H	-6.165335	2.752862	-3.116803	H	4.264304	4.271507	1.458745
C	-4.004156	1.101804	-3.667372	O	0.154555	-0.260777	-1.986262
H	-3.928644	2.084922	-4.147765	S	1.101891	-4.378775	1.726265
H	-4.474784	0.419250	-4.385353	O	1.217713	-2.502451	-2.346542
H	-2.991465	0.741631	-3.464029	H	-0.426485	-3.103879	-1.123637
C	-4.070215	-1.808057	1.772161	H	1.623803	-2.237014	-0.092935
H	-3.487704	-0.940796	2.094743	C	3.019114	-3.842266	-0.840998
C	-5.250243	-1.965975	2.752342	C	4.181456	-3.169879	-0.100044
H	-5.901999	-1.084987	2.747757	C	5.502817	-3.930723	-0.265834
H	-4.883921	-2.110718	3.776072	H	4.298575	-2.140000	-0.462770
H	-5.868003	-2.834026	2.491703	H	3.926454	-3.104441	0.966074
C	-3.133049	-3.027470	1.850672	C	6.655548	-3.325421	0.545239
H	-2.281886	-2.904013	1.175776	H	5.358233	-4.979223	0.035600
H	-3.647876	-3.960379	1.593124	H	5.779762	-3.950640	-1.329982
H	-2.748939	-3.137780	2.872238	H	6.797624	-2.277163	0.248718
C	2.272833	2.433441	-3.593327	H	6.379483	-3.312187	1.610536
H	1.319454	2.834038	-3.238994	C	7.980637	-4.079979	0.376064
C	1.940743	1.230737	-4.496792	H	8.262197	-4.075482	-0.686111
H	1.308596	1.556892	-5.331715	H	7.838202	-5.134732	0.652708
H	1.397447	0.467173	-3.934997	C	9.121757	-3.482571	1.205966
H	2.842354	0.778493	-4.927747	H	10.054761	-4.040864	1.065415
C	2.971995	3.546929	-4.399659	H	9.308181	-2.440257	0.920692
H	3.167380	4.431594	-3.783057	H	8.883723	-3.496818	2.277035
H	2.348610	3.856069	-5.247471	H	3.231844	-3.910297	-1.915973
H	3.933911	3.203505	-4.799360	H	2.893463	-4.876759	-0.493447

C	-6.296104	-3.589774	-2.361764	H	2.696775	-1.600319	3.999060
C	-6.076285	-3.802080	-3.733926	C	-1.687000	0.950233	5.860861
C	-7.145055	-4.481204	-1.683056	H	-2.561401	0.312032	5.663097
C	-6.683215	-4.864676	-4.402597	H	-1.667075	1.128340	6.941525
C	-7.751290	-5.545042	-2.350377	C	-1.851383	2.280300	5.113235
C	-7.523789	-5.741845	-3.714059	H	-2.804693	2.759949	5.339668
H	-7.996716	-6.570149	-4.234866	H	-1.055356	2.975924	5.419963
C	6.419172	0.260084	-1.780759	C	-1.724121	2.110349	3.610340
C	7.579931	0.561140	-1.046698	N	-0.816138	1.221423	3.200833
C	6.504181	-0.731406	-2.774558	H	-0.580452	1.156059	2.194406
C	8.781155	-0.102718	-1.297494	C	-1.945544	3.070769	-0.661030
C	7.704569	-1.396236	-3.025702	C	-2.886746	2.153624	-0.025308
C	8.849463	-1.085202	-2.288300	H	-2.278273	4.087333	-0.859207
H	9.786102	-1.598969	-2.486900	C	0.513525	-2.548662	-0.642650
H	-8.410168	-6.216231	-1.805320	C	1.877300	-2.785494	-0.747970
H	-6.491807	-5.012424	-5.462423	C	2.315801	-3.928155	-1.506441
H	-5.403501	-3.141330	-4.273479	C	1.335139	-4.850464	-1.996265
H	-7.349954	-4.322058	-0.627982	C	-0.039951	-4.594780	-1.762188
H	5.615000	-0.992306	-3.341845	C	-0.478637	-3.451077	-1.128064
H	7.744743	-2.160425	-3.797762	H	4.435861	-3.467651	-1.507396
H	7.544905	1.343326	-0.293523	C	3.679921	-4.174164	-1.828980
H	9.668902	0.158019	-0.726877	C	1.753143	-5.995305	-2.727402
TS1-S-n-hexyl-tBu E= -3851.25724677				H	-0.770822	-5.317202	-2.115787
H	-1.560075	1.419002	-1.806091	C	3.083511	-6.214829	-3.000401
C	1.077523	-0.262450	3.554166	C	4.051841	-5.284184	-2.555924
C	-0.041650	0.403308	4.066243	H	0.993926	-6.689072	-3.080844
C	-0.430138	0.248282	5.406687	H	3.391006	-7.089538	-3.566898
C	0.341407	-0.570095	6.232012	H	5.100007	-5.442316	-2.795320
C	1.467004	-1.233010	5.736404	C	2.857929	-1.847833	-0.124100
C	1.828921	-1.081799	4.395852	C	3.866480	-2.306324	0.794060
H	1.338124	-0.140475	2.508690	C	2.821976	-0.493969	-0.433793
H	0.052161	-0.691893	7.273452	C	3.877355	-3.620571	1.339455
H	2.055673	-1.866471	6.393834	C	4.886684	-1.392939	1.216681
				C	3.851052	0.423147	-0.061516

C	4.853802	-4.014373	2.228961	H	6.024609	0.229204	-4.161819
H	3.094040	-4.314812	1.057587	C	3.367242	1.022166	-4.102112
C	5.891501	-1.837174	2.118761	H	2.344651	0.935458	-3.723540
C	4.871896	-0.059692	0.731373	H	3.552062	0.184065	-4.785164
C	5.880239	-3.120310	2.616474	H	3.440270	1.946812	-4.687499
H	4.833500	-5.020830	2.638335	C	3.386413	2.722127	1.826233
H	6.664768	-1.134057	2.419212	H	3.235852	1.653952	2.004446
H	5.683847	0.605816	1.012539	C	4.582286	3.170565	2.690284
H	6.649392	-3.445893	3.311489	H	5.498911	2.633708	2.420698
C	3.860791	1.840216	-0.555936	H	4.380641	2.985728	3.752581
C	4.120645	2.107023	-1.923847	H	4.780507	4.242432	2.568526
C	3.669227	2.918348	0.336468	C	2.095623	3.433523	2.273823
C	4.178476	3.433534	-2.355916	H	1.245440	3.098728	1.673559
C	3.743297	4.230962	-0.153460	H	2.175858	4.523487	2.186232
C	3.993842	4.522728	-1.494682	H	1.887013	3.203750	3.326162
H	4.383054	3.619828	-3.406520	C	-2.188682	-2.556492	-3.419776
H	3.595436	5.042256	0.549822	H	-1.100011	-2.496769	-3.334030
C	-1.946813	-3.203016	-0.933376	C	-2.657860	-1.224419	-4.033592
C	-2.539995	-3.433890	0.330824	H	-2.150224	-1.058387	-4.991449
C	-2.755913	-2.803120	-2.020360	H	-2.416509	-0.387857	-3.374610
C	-3.919604	-3.267093	0.473579	H	-3.736428	-1.218047	-4.232922
C	-4.136750	-2.654636	-1.820571	C	-2.522459	-3.728754	-4.365639
C	-4.749516	-2.879593	-0.586150	H	-3.607120	-3.837412	-4.489660
H	-4.360764	-3.458488	1.447913	H	-2.135873	-4.680392	-3.984990
H	-4.741219	-2.355943	-2.668851	H	-2.086415	-3.558979	-5.357691
O	1.788958	-0.011137	-1.218970	C	-1.729302	-3.900268	1.540016
O	0.079657	-1.428006	0.046089	H	-0.673342	-3.914604	1.256202
P	0.271731	0.080268	-0.589307	C	-1.859269	-2.936014	2.733400
O	0.174228	1.019626	0.584492	H	-2.886543	-2.899746	3.116233
C	4.385152	1.000547	-2.945533	H	-1.565402	-1.922194	2.445997
H	4.276516	0.035824	-2.443143	H	-1.209699	-3.255636	3.556911
C	5.831932	1.063163	-3.475787	C	-2.104871	-5.339922	1.943798
H	6.558102	1.005067	-2.656945	H	-1.959397	-6.035683	1.109763
H	6.020772	1.994362	-4.023256	H	-3.154105	-5.408209	2.255564

H	-1.484334	-5.678989	2.782465	C	-6.524248	-1.681447	0.747431
O	-0.628779	0.302455	-1.785197	C	-6.856107	-4.091678	0.079530
S	-2.662566	3.060716	2.573758	H	-6.052967	-1.963241	1.694758
O	-2.268026	2.198162	-1.771062	H	-6.128142	-0.700989	0.456933
H	-0.912245	2.998952	-0.328113	H	-7.600666	-1.571595	0.929015
H	-2.450407	1.234398	0.345362	H	-7.936567	-4.004802	0.250280
C	-4.381627	2.243038	-0.104240	H	-6.693611	-4.854093	-0.690875
C	-4.959396	3.558179	-0.637455	H	-6.398941	-4.452469	1.006969
C	-6.492922	3.539864	-0.691328	C	4.077611	5.960366	-2.040721
H	-4.628287	4.389902	-0.000494	C	3.010949	6.156340	-3.144598
H	-4.562333	3.746893	-1.643236	C	5.483735	6.201823	-2.640150
C	-7.093059	4.841747	-1.237892	H	3.152397	5.459007	-3.976685
H	-6.824200	2.696778	-1.315414	H	2.002113	5.998727	-2.745929
H	-6.890779	3.349546	0.316221	H	3.062088	7.174911	-3.549362
H	-6.759193	5.685518	-0.615845	H	5.557551	7.218131	-3.047147
H	-6.694242	5.030130	-2.245668	H	6.260129	6.084667	-1.875241
C	-8.626375	4.831081	-1.294259	H	5.705924	5.500357	-3.451003
H	-9.024192	4.645068	-0.286470	C	3.835448	7.020236	-0.948904
H	-8.959818	3.986325	-1.913685	H	2.840304	6.923128	-0.500017
C	-9.217655	6.132984	-1.845395	H	4.579961	6.956825	-0.147109
H	-10.312576	6.094489	-1.873646	H	3.905195	8.023220	-1.385598
H	-8.930237	6.992243	-1.226858	C	-7.009763	-2.274902	-1.630481
H	-8.864486	6.327439	-2.865589	H	-6.651382	-1.302124	-1.986890
H	-4.764974	2.037470	0.902791	H	-6.902657	-2.996995	-2.447808
H	-4.715737	1.398283	-0.723221	H	-8.080272	-2.175241	-1.416529
C	-6.265975	-2.730398	-0.360321				

11.M062X Geometries for All the Optimized Compounds and Transition States

M-(R)-3-TS1-R E= -3522.40452989

H	-0.356897	2.544212	-1.179780	C	-1.394995	-3.089634	-0.669165
C	0.607067	-2.102711	2.791622	C	-1.276081	-4.315902	0.064350
C	1.651607	-1.299209	3.250680	C	-0.248100	-2.381128	-0.965879
C	2.362811	-1.616633	4.413243	C	-2.402550	-5.039806	0.542879
C	2.024223	-2.779163	5.099400	C	0.023661	-4.806369	0.375052
C	0.990108	-3.599071	4.649364	C	1.059976	-2.844224	-0.642617
C	0.278661	-3.255113	3.501086	C	-2.240201	-6.198200	1.262182
H	0.061651	-1.816086	1.895654	H	-3.399974	-4.659897	0.348113
H	2.574632	-3.037799	6.000352	C	0.159053	-6.017448	1.105589
H	0.736874	-4.501147	5.197340	C	1.165042	-4.057077	-0.002308
H	-0.534169	-3.884528	3.150258	C	-0.946554	-6.702329	1.539284
C	3.421517	-0.649738	4.873567	H	-3.113375	-6.731708	1.625448
H	2.958029	0.129512	5.493579	H	1.160295	-6.378308	1.326625
H	4.165021	-1.156787	5.494863	H	2.148439	-4.450202	0.244410
C	4.101070	0.002973	3.670391	H	-0.835769	-7.623650	2.102806
H	4.797255	0.785678	3.972902	C	2.269623	-2.037998	-0.938430
H	4.673150	-0.752664	3.110886	C	2.456565	-1.408328	-2.175345
C	3.098354	0.573233	2.694754	C	3.283842	-1.931085	0.021627
N	1.980094	-0.121023	2.539162	C	3.625513	-0.706150	-2.442117
H	1.324969	0.151051	1.789837	C	4.449330	-1.221977	-0.245231
C	0.662027	3.281858	0.400421	C	4.642971	-0.597938	-1.483616
C	1.853887	2.765565	-0.270497	H	3.743111	-0.219237	-3.406752
H	0.118801	2.558492	1.004959	H	5.229212	-1.167312	0.509811
H	1.821768	1.710934	-0.528699	C	-4.589760	0.766458	-0.485153
C	-3.030530	-1.236479	-0.646630	C	-4.362489	1.169871	0.836576
C	-2.712968	-2.515246	-1.059333	C	-5.184748	1.678111	-1.364433
C	-3.637216	-3.220611	-1.897417	C	-4.736549	2.437630	1.264614
C	-4.885239	-2.609035	-2.205950	C	-5.553799	2.946876	-0.935572
C	-5.172317	-1.312688	-1.712614	C	-5.342659	3.347755	0.388839
C	-4.269371	-0.605173	-0.953648	H	-4.584421	2.713344	2.304549
H	-2.388609	-4.954993	-2.275233	H	-5.987017	3.645042	-1.646161
C	-3.351350	-4.492446	-2.464950	O	-0.377654	-1.152386	-1.583056
C	-5.820961	-3.300530	-3.020955	O	-2.119842	-0.543177	0.122560
H	-6.138053	-0.870401	-1.945163	P	-0.789768	0.089485	-0.596379
C	-5.525489	-4.536119	-3.535058	O	0.216962	0.270750	0.491040
C	-4.270317	-5.130374	-3.260916	O	-1.131403	1.247970	-1.487019
H	-6.772755	-2.821245	-3.234850	S	3.439932	1.970002	1.814459
H	-6.243925	-5.056073	-4.161215	O	0.190934	3.380112	-0.951666
H	-4.030190	-6.098484	-3.690117	C	2.910228	3.589327	-0.834327
				C	3.024495	4.960921	-0.560950

C	3.855833	2.964233	-1.658001	C	0.347785	-3.299886	3.515551
C	4.069873	5.688081	-1.112973	H	0.108846	-1.840018	1.932522
H	2.299128	5.458813	0.074376	H	2.828410	-3.249593	5.840741
C	4.906972	3.691685	-2.199891	H	0.849559	-4.590279	5.165301
H	3.759390	1.900589	-1.854109	H	-0.524960	-3.875596	3.220132
C	5.010775	5.055148	-1.928536	C	3.737844	-0.909957	4.672257
H	4.157230	6.749775	-0.905998	H	3.371485	-0.117195	5.338163
H	5.642517	3.194502	-2.826017	H	4.494686	-1.472336	5.226078
H	5.829897	5.629274	-2.351348	C	4.361675	-0.276101	3.430021
H	0.726191	4.263547	0.864850	H	5.125594	0.457704	3.688062
H	3.151349	-2.407008	0.990558	H	4.842011	-1.054097	2.816446
H	1.686155	-1.476697	-2.936062	C	3.323070	0.371273	2.545451
H	-3.913693	0.477048	1.540570	N	2.163392	-0.263822	2.450187
H	-5.337517	1.396050	-2.402450	H	1.470629	0.056915	1.755761
C	5.883069	0.166510	-1.770023	C	2.231619	1.850104	-1.244490
C	6.438418	0.176594	-3.056428	C	1.921849	2.756286	-0.143685
C	6.515162	0.907893	-0.762575	H	3.157867	2.007527	-1.794153
C	7.598718	0.898111	-3.325327	C	-2.954731	-1.320607	-0.609968
H	5.972291	-0.405959	-3.846356	C	-2.589379	-2.612739	-0.930833
C	7.676258	1.627186	-1.030836	C	-3.484137	-3.405819	-1.723810
H	6.074384	0.947128	0.230439	C	-4.752084	-2.865032	-2.077235
C	8.223737	1.624232	-2.312487	C	-5.092643	-1.552483	-1.665750
H	8.020213	0.883779	-4.326170	C	-4.221057	-0.763952	-0.951646
H	8.146720	2.201247	-0.238088	H	-2.167483	-5.112453	-1.988298
H	9.129846	2.184596	-2.522325	C	-3.146015	-4.699404	-2.207789
C	-5.762758	4.694843	0.849999	C	-5.654870	-3.643224	-2.850658
C	-6.934157	5.280799	0.352637	H	-6.075870	-1.165881	-1.923110
C	-5.008269	5.406550	1.791395	C	-5.308947	-4.897635	-3.282225
C	-7.339418	6.540693	0.781987	C	-4.034276	-5.422870	-2.964376
H	-7.544679	4.732730	-0.359587	H	-6.622693	-3.215587	-3.100044
C	-5.414347	6.666248	2.222727	H	-6.001905	-5.484402	-3.877236
H	-4.084288	4.979469	2.171356	H	-3.752267	-6.406153	-3.328451
C	-6.581054	7.238534	1.719696	C	-1.249606	-3.123792	-0.527129
H	-8.254770	6.973489	0.389331	C	-1.073676	-4.316842	0.249136
H	-4.813006	7.205749	2.948578	C	-0.127979	-2.412985	-0.899155
H	-6.897624	8.220917	2.056715	C	-2.165745	-5.028636	0.816311
				C	0.246190	-4.785253	0.505533
				C	1.199332	-2.865981	-0.654208
				C	-1.953993	-6.155052	1.573264
				H	-3.175307	-4.663366	0.658036
				C	0.431620	-5.964227	1.275306
				C	1.358900	-4.048521	0.026654
				C	-0.642397	-6.638269	1.797581
				H	-2.800562	-6.678522	2.007179
M-(R)-3-TS1-S E= -3522.40381627							
H	0.274427	2.058953	-1.731437				
C	0.696226	-2.164868	2.788202				
C	1.818867	-1.431181	3.173655				
C	2.591103	-1.803652	4.280317				
C	2.231673	-2.949712	4.983090				
C	1.117960	-3.699392	4.606233				

H	1.446629	-6.309297	1.455029
H	2.360019	-4.426894	0.220232
H	-0.491244	-7.534694	2.391212
C	2.362560	-2.061228	-1.100808
C	2.459267	-1.588518	-2.416221
C	3.396982	-1.767746	-0.207019
C	3.555114	-0.835978	-2.818585
C	4.483306	-0.994845	-0.605596
C	4.576538	-0.511355	-1.915772
H	3.599353	-0.458881	-3.836735
H	5.274217	-0.772519	0.105910
C	-4.602152	0.612989	-0.547649
C	-4.389776	1.079567	0.755753
C	-5.239600	1.460410	-1.460270
C	-4.810783	2.348241	1.131816
C	-5.657974	2.731175	-1.082588
C	-5.453548	3.196834	0.221181
H	-4.621221	2.692705	2.144609
H	-6.165577	3.363054	-1.806094
O	-0.292449	-1.200683	-1.533587
O	-2.080830	-0.537287	0.113528
P	-0.721416	0.058363	-0.571779
O	0.250165	0.249418	0.546500
O	-0.993661	1.199846	-1.508769
S	3.665753	1.788034	1.699321
O	1.148721	2.583252	-1.845035
H	2.021188	0.796487	-1.061550
H	1.097859	2.445589	0.491630
C	2.443867	4.110298	-0.016139
C	3.588382	4.528047	-0.710619
C	1.785371	5.001491	0.841803
C	4.056919	5.825657	-0.552510
H	4.115800	3.841333	-1.366054
C	2.255843	6.299517	0.994056
H	0.905600	4.666373	1.384416
C	3.390707	6.710856	0.295730
H	4.943209	6.147822	-1.089597
H	1.741973	6.988872	1.656107
H	3.761328	7.724410	0.415351
H	3.337562	-2.138084	0.813873
H	1.664492	-1.804344	-3.123450
H	-3.895528	0.442046	1.481131
H	-5.400908	1.121697	-2.479959
C	5.698278	0.369120	-2.325858

C	6.262376	0.273199	-3.604252
C	6.196288	1.335843	-1.441208
C	7.299632	1.118124	-3.987010
H	5.897145	-0.481834	-4.295104
C	7.232125	2.183194	-1.826615
H	5.752346	1.435014	-0.452628
C	7.787786	2.076646	-3.100214
H	7.731989	1.023189	-4.978624
H	7.601607	2.930682	-1.130593
H	8.597094	2.735306	-3.400324
C	-5.908390	4.549699	0.629748
C	-6.422194	4.773226	1.913875
C	-5.838626	5.630226	-0.259066
C	-6.854202	6.039119	2.297895
H	-6.504921	3.942219	2.608970
C	-6.271470	6.896231	0.124416
H	-5.419343	5.481213	-1.250261
C	-6.780976	7.105925	1.404436
H	-7.257570	6.189695	3.294925
H	-6.202164	7.722742	-0.576722
H	-7.118454	8.093545	1.703863

M-(R)-4-TS1-R E= -3374.79928976

H	-1.763587	1.193811	-2.355397
C	1.191449	-0.807338	2.710006
C	-0.176938	-0.969706	2.928308
C	-0.670746	-2.005075	3.728390
C	0.237056	-2.881261	4.317723
C	1.606559	-2.729688	4.114281
C	2.080513	-1.692094	3.312981
H	1.542033	0.003001	2.075124
H	-0.138822	-3.687544	4.942437
H	2.305639	-3.419231	4.577363
H	3.148363	-1.569760	3.159306
C	-2.163486	-2.114966	3.887642
H	-2.581713	-2.698510	3.055655
H	-2.414281	-2.647496	4.809301
C	-2.787324	-0.720146	3.902778
H	-3.877228	-0.761039	3.917896
H	-2.465785	-0.179394	4.804495
C	-2.340638	0.114205	2.723977
N	-1.089964	-0.070096	2.321476
H	-0.713096	0.519214	1.559693
C	-3.285790	0.885318	-1.155498

C	-2.825118	2.096433	-0.482939	C	-3.644652	-2.376007	0.285188
H	-2.758639	-0.034375	-0.895747	C	-4.092532	-2.503065	-2.060086
H	-1.772802	2.114947	-0.209021	C	-4.583766	-2.370152	-0.758734
C	0.643302	-2.166988	-0.960214	H	-3.985396	-2.266219	1.312575
C	1.991765	-2.407658	-1.120058	H	-4.770368	-2.486451	-2.906637
C	2.395753	-3.483052	-1.977370	O	1.904678	0.341343	-1.466906
C	1.394155	-4.302808	-2.572053	O	0.244245	-1.079067	-0.215930
C	0.023791	-4.037583	-2.317453	P	0.365372	0.394516	-0.926082
C	-0.372122	-2.983677	-1.529520	O	0.165517	1.364610	0.197472
H	4.529425	-3.105408	-1.877552	C	3.089887	6.560621	-0.688920
C	3.757039	-3.744299	-2.292612	C	4.158515	7.093894	-1.657046
C	1.782737	-5.374297	-3.419861	H	4.022530	8.170713	-1.811233
H	-0.725205	-4.692537	-2.756419	H	4.098880	6.605839	-2.635132
C	3.105635	-5.613308	-3.689516	H	5.164931	6.930133	-1.256188
C	4.100681	-4.780271	-3.125337	C	1.695056	6.807491	-1.287232
H	1.005469	-5.995938	-3.856887	H	0.912751	6.429396	-0.619482
H	3.392924	-6.432727	-4.341027	H	1.578714	6.312986	-2.257129
H	5.146034	-4.959850	-3.357519	H	1.531752	7.881579	-1.434545
C	2.966466	-1.513543	-0.433160	C	-6.078913	-2.273539	-0.440365
C	3.938000	-2.015057	0.493075	C	-6.492613	-3.535548	0.336111
C	2.879696	-0.148852	-0.624345	H	-7.563988	-3.504454	0.566208
C	3.996503	-3.382307	0.878935	H	-5.945694	-3.619495	1.281420
C	4.837101	-1.099594	1.109834	H	-6.293397	-4.438074	-0.252026
C	3.754102	0.786048	0.000559	C	-6.368489	-1.038683	0.426506
C	4.914958	-3.814271	1.803367	H	-7.434544	-1.003029	0.679308
H	3.288567	-4.084777	0.452462	H	-6.117845	-0.113415	-0.104554
C	5.793116	-1.581333	2.045151	H	-5.803708	-1.049063	1.363467
C	4.727467	0.285978	0.834271	O	-0.470269	0.457957	-2.173119
C	5.833727	-2.908724	2.386757	S	-3.371675	1.261116	2.042392
H	4.934061	-4.860238	2.094108	O	-2.718882	1.566449	-2.284168
H	6.479873	-0.869341	2.495580	C	-3.572374	3.342287	-0.396987
H	5.425255	0.969496	1.311990	C	-4.950032	3.411087	-0.647119
H	6.559733	-3.267677	3.109684	C	-2.869992	4.501148	-0.036267
C	3.589497	2.248809	-0.191714	C	-5.610262	4.628371	-0.543487
C	3.392481	2.821746	-1.455550	H	-5.504007	2.518214	-0.920263
C	3.637783	3.099903	0.913900	C	-3.534046	5.716258	0.065724
C	3.247601	4.195084	-1.591957	H	-1.803738	4.433537	0.163829
C	3.490106	4.478222	0.769518	C	-4.903739	5.778817	-0.189066
C	3.287125	5.056804	-0.485323	H	-6.676647	4.683104	-0.736817
H	3.096570	4.605134	-2.587104	H	-2.987488	6.611743	0.342840
H	3.522078	5.095743	1.660639	H	-5.425085	6.727932	-0.108544
C	-1.807320	-2.709546	-1.262696	H	-4.356291	0.735692	-1.277932
C	-2.285569	-2.536789	0.045236	H	3.766173	2.677100	1.907027
C	-2.729433	-2.670509	-2.308814	H	3.356103	2.187613	-2.335185

H	-1.585021	-2.552218	0.876935
H	-2.377320	-2.768995	-3.332192
C	3.197936	7.339874	0.625010
H	2.431274	7.030193	1.343817
H	4.180568	7.211240	1.092375
H	3.058326	8.408531	0.429265
C	-6.933690	-2.180066	-1.707645
H	-6.668087	-1.304238	-2.310661
H	-6.833488	-3.072892	-2.334196
H	-7.988946	-2.087362	-1.429277

M-(R)-4-TS1-S E= -3374.79823285

H	0.195388	2.399553	-1.730924
C	0.767581	-1.982202	2.642015
C	2.022675	-1.410710	2.855688
C	2.890876	-1.900729	3.838281
C	2.486180	-2.999224	4.591321
C	1.239710	-3.588889	4.383033
C	0.380085	-3.073728	3.414443
H	0.110384	-1.570759	1.879478
H	3.156970	-3.390919	5.351850
H	0.940287	-4.447048	4.976576
H	-0.592474	-3.528339	3.245655
C	4.193955	-1.175420	4.049551
H	4.041464	-0.349416	4.757125
H	4.940284	-1.843052	4.489139
C	4.708013	-0.614932	2.723828
H	5.595600	0.003477	2.860668
H	4.980023	-1.442169	2.049643
C	3.649187	0.178726	1.996786
N	2.412350	-0.291439	2.082786
H	1.678231	0.124708	1.489155
C	2.174705	2.042405	-1.562128
C	2.123481	2.841888	-0.342190
H	3.012874	2.182219	-2.241486
C	-3.091465	-0.751631	-0.358183
C	-2.899331	-2.067957	-0.724398
C	-3.944842	-2.744922	-1.435687
C	-5.172848	-2.062549	-1.663878
C	-5.325841	-0.726718	-1.216694
C	-4.310410	-0.049268	-0.583100
H	-2.855177	-4.580349	-1.829223
C	-3.798404	-4.060113	-1.955833
C	-6.224390	-2.725642	-2.351977

H	-6.277867	-0.228630	-1.383135
C	-6.060933	-4.003358	-2.821013
C	-4.827794	-4.670197	-2.628745
H	-7.158547	-2.191964	-2.506643
H	-6.867893	-4.501404	-3.349372
H	-4.692694	-5.672480	-3.023733
C	-1.593907	-2.727024	-0.437996
C	-1.496564	-3.937811	0.323522
C	-0.431265	-2.137435	-0.892065
C	-2.614024	-4.526108	0.976759
C	-0.222057	-4.552568	0.476460
C	0.854256	-2.735266	-0.748537
C	-2.469924	-5.670837	1.721676
H	-3.586508	-4.051743	0.894879
C	-0.108472	-5.747248	1.236804
C	0.922869	-3.941312	-0.090462
C	-1.206255	-6.297367	1.847108
H	-3.333233	-6.099600	2.221518
H	0.872702	-6.203542	1.339820
H	1.884421	-4.435923	0.022951
H	-1.110995	-7.205519	2.434440
C	2.084394	-2.083838	-1.264309
C	2.144613	-1.501675	-2.538229
C	3.249779	-2.091583	-0.492965
C	3.332946	-0.959697	-3.013078
C	4.435952	-1.541719	-0.973952
C	4.507530	-0.967337	-2.245639
H	3.341791	-0.525014	-4.009893
H	5.313254	-1.563491	-0.335552
C	-4.488359	1.363031	-0.160555
C	-4.112354	1.809621	1.113656
C	-5.089820	2.279005	-1.025010
C	-4.341763	3.123270	1.497294
C	-5.314805	3.597812	-0.633860
C	-4.947450	4.049974	0.635442
H	-4.042491	3.432728	2.495369
H	-5.776951	4.273841	-1.345177
O	-0.516406	-0.910065	-1.515512
O	-2.072307	-0.087836	0.291249
P	-0.748194	0.387398	-0.537877
O	0.343304	0.513770	0.474008
C	5.795382	-0.362671	-2.810477
C	6.155411	-1.066199	-4.129150
H	7.080580	-0.645297	-4.539685

H	5.370005	-0.945858	-4.881886
H	6.309800	-2.139005	-3.969123
C	5.579237	1.135749	-3.076915
H	5.332548	1.659504	-2.145642
H	4.769311	1.304555	-3.795307
H	6.491813	1.582925	-3.488273
C	-5.166813	5.489911	1.104572
C	-6.037057	5.488982	2.372092
H	-6.201986	6.516649	2.716506
H	-5.562428	4.935076	3.188431
H	-7.013773	5.033124	2.175812
C	-3.806079	6.129605	1.425884
H	-3.945255	7.163967	1.761974
H	-3.161424	6.140215	0.540327
H	-3.282810	5.586111	2.219349
O	-1.032662	1.537124	-1.461722
S	4.051100	1.543429	1.096351
O	1.076341	2.902181	-1.905732
H	1.907715	0.992713	-1.439956
H	1.397379	2.505742	0.391703
C	2.755946	4.141499	-0.170142
C	3.718086	4.625710	-1.068009
C	2.395274	4.910855	0.944926
C	4.305274	5.865171	-0.849843
H	4.004730	4.039904	-1.936127
C	2.986696	6.148530	1.160848
H	1.656008	4.522828	1.640154
C	3.941282	6.625094	0.262681
H	5.047980	6.241183	-1.545813
H	2.706673	6.740552	2.025901
H	4.405153	7.592585	0.429316
H	3.224931	-2.527206	0.504029
H	1.258325	-1.485344	-3.164338
H	-3.647492	1.119458	1.810228
H	-5.370230	1.962966	-2.026221
C	6.975309	-0.513381	-1.845885
H	6.792314	0.004344	-0.897872
H	7.188969	-1.566243	-1.630541
H	7.872815	-0.076224	-2.296611
C	-5.863798	6.344180	0.041997
H	-5.270919	6.412042	-0.876655
H	-6.851735	5.945102	-0.213778
H	-6.003105	7.360813	0.425082

M-(R)-5-TS1-R E= -3994.07167563

H	-1.382197	1.596749	-1.874469
C	0.606478	-1.478137	3.006308
C	-0.217081	-0.519025	3.595816
C	-0.794248	-0.729857	4.853765
C	-0.511476	-1.915071	5.525690
C	0.322665	-2.875943	4.957038
C	0.877435	-2.656548	3.697884
H	1.018829	-1.299256	2.016581
H	-0.954381	-2.082620	6.504224
H	0.538790	-3.794220	5.493908
H	1.527294	-3.402748	3.251923
C	-1.722995	0.327719	5.384888
H	-2.735355	0.156998	4.991833
H	-1.786019	0.275705	6.475331
C	-1.235642	1.707850	4.949929
H	-1.929470	2.496824	5.240520
H	-0.266327	1.925363	5.422034
C	-1.003649	1.773335	3.458691
N	-0.503118	0.679336	2.895626
H	-0.197653	0.723808	1.906774
C	-2.438090	2.178118	-0.297248
C	-1.354423	3.134589	-0.095357
H	-2.269377	1.165670	0.078403
H	-0.354299	2.710710	-0.053568
C	-0.820712	-2.462365	-0.792936
C	0.209915	-3.371241	-0.920426
C	-0.026704	-4.560865	-1.686148
C	-1.339102	-4.813562	-2.176512
C	-2.370992	-3.863678	-1.952819
C	-2.128358	-2.677170	-1.307444
H	2.015749	-5.292262	-1.670549
C	1.001474	-5.490489	-2.001144
C	-1.592774	-6.000530	-2.913459
H	-3.368221	-4.080156	-2.327057
C	-0.584431	-6.890222	-3.182010
C	0.729013	-6.622324	-2.728935
H	-2.603096	-6.179964	-3.272165
H	-0.786916	-7.792147	-3.751265
H	1.530597	-7.315795	-2.964453
C	1.520751	-3.066048	-0.283184
C	2.148405	-3.956988	0.649576
C	2.125708	-1.849287	-0.530848
C	1.537099	-5.160827	1.096393

C	3.411212	-3.595866	1.200674	H	5.442688	-0.458137	2.781857
C	3.376721	-1.460380	0.022434	H	4.470929	0.162952	4.130330
C	2.162327	-5.970847	2.011987	H	5.443108	1.273112	3.146602
H	0.554947	-5.427778	0.722021	C	2.731652	1.725207	2.705700
C	4.039051	-4.461978	2.135969	H	1.918548	1.940040	2.006498
C	4.006475	-2.356222	0.851125	H	3.305333	2.644820	2.869017
C	3.432680	-5.626187	2.532753	H	2.298360	1.435386	3.670956
H	1.673663	-6.880945	2.346577	C	-2.972947	-1.033646	-3.631455
H	5.005154	-4.170994	2.540483	H	-2.022634	-1.565298	-3.523084
H	4.972744	-2.103157	1.280730	C	-2.683898	0.269196	-4.381865
H	3.916050	-6.278868	3.253182	H	-2.165861	0.040015	-5.319266
C	3.958370	-0.116154	-0.278902	H	-2.046288	0.935114	-3.798311
C	4.386410	0.191638	-1.586371	H	-3.603371	0.804419	-4.642465
C	4.083351	0.843239	0.749186	C	-3.924247	-1.899347	-4.470227
C	4.954018	1.440387	-1.838046	H	-4.887320	-1.390307	-4.597688
C	4.662732	2.077090	0.451981	H	-4.120096	-2.869025	-4.003391
C	5.104255	2.396860	-0.832387	H	-3.501548	-2.078549	-5.465016
H	5.267989	1.684563	-2.850220	C	-3.378890	-2.282289	1.319846
H	4.788459	2.807692	1.247187	H	-2.347438	-2.622053	1.183527
C	-3.172336	-1.619174	-1.139181	C	-3.427339	-1.532700	2.653237
C	-3.752575	-1.410585	0.129941	H	-4.456273	-1.318943	2.964574
C	-3.552908	-0.823409	-2.238882	H	-2.882540	-0.583101	2.591431
C	-4.728278	-0.425041	0.273025	H	-2.964059	-2.140669	3.438059
C	-4.525220	0.162183	-2.045678	C	-4.279374	-3.523073	1.365888
C	-5.125978	0.372208	-0.803661	H	-4.200340	-4.105612	0.441883
H	-5.204223	-0.277591	1.238498	H	-5.327864	-3.228911	1.493578
H	-4.805700	0.802894	-2.877131	H	-4.000810	-4.170363	2.204685
O	1.509510	-0.961719	-1.389150	O	-0.459143	0.429841	-2.001294
O	-0.609173	-1.302656	-0.076473	S	-1.311365	3.192959	2.604764
P	0.255807	-0.107214	-0.792080	O	-2.035148	2.365397	-1.659800
O	0.649553	0.796666	0.334386	C	-1.498319	4.581199	-0.200346
C	4.279764	-0.794715	-2.740478	C	-2.752533	5.206568	-0.246872
H	3.766995	-1.693660	-2.387408	C	-0.331251	5.357030	-0.237903
C	5.673440	-1.223431	-3.215214	C	-2.830634	6.589688	-0.341329
H	6.251240	-1.665591	-2.396433	H	-3.665391	4.619559	-0.214917
H	6.237699	-0.367617	-3.603623	C	-0.414730	6.740638	-0.327342
H	5.592968	-1.965341	-4.017321	H	0.635746	4.862975	-0.189547
C	3.458883	-0.221772	-3.900111	C	-1.664668	7.355761	-0.381316
H	2.470028	0.100651	-3.561134	H	-3.801138	7.073457	-0.383185
H	3.324591	-0.981494	-4.677953	H	0.490503	7.338190	-0.355380
H	3.963000	0.636446	-4.359145	H	-1.732489	8.437112	-0.453509
C	3.618487	0.592333	2.176461	H	-3.460053	2.512365	-0.132429
H	3.015668	-0.319093	2.182691	C	-6.138425	1.443855	-0.623359
C	4.814161	0.375574	3.111553	C	-7.084831	1.709959	-1.621037

C	-6.161379	2.220045	0.544084	H	-0.050807	-4.657366	-0.975856
C	-8.026822	2.721186	-1.457503	C	0.579204	2.334464	-0.932687
H	-7.093723	1.104049	-2.522746	C	-0.481337	3.213491	-1.000822
C	-7.101270	3.235137	0.706077	C	-0.322037	4.412395	-1.770046
H	-5.425208	2.038352	1.323821	C	0.953523	4.707435	-2.329513
C	-8.038050	3.488385	-0.293831	C	2.037175	3.812700	-2.119611
H	-8.758858	2.905132	-2.238235	C	1.870713	2.628902	-1.445272
H	-7.098492	3.830879	1.614055	H	-2.378892	5.082902	-1.620393
H	-8.773314	4.277007	-0.166641	C	-1.394357	5.312201	-2.015985
C	5.709301	3.722097	-1.121095	C	1.125646	5.899854	-3.080671
C	6.781621	3.842867	-2.014167	H	3.020208	4.083461	-2.497869
C	5.219319	4.881360	-0.505717	C	0.075285	6.756742	-3.288989
C	7.348149	5.085321	-2.283545	C	-1.199662	6.451690	-2.756427
H	7.189110	2.951459	-2.483424	H	2.107956	6.113117	-3.494462
C	5.785915	6.123855	-0.774015	H	0.215112	7.664509	-3.867883
H	4.372481	4.808787	0.171550	H	-2.032531	7.123519	-2.940593
C	6.852765	6.230968	-1.664114	C	-1.727756	2.888680	-0.256172
H	8.183823	5.156970	-2.973512	C	-2.255524	3.755104	0.756689
H	5.387244	7.012160	-0.292751	C	-2.340943	1.671040	-0.461689
H	7.295250	7.200442	-1.872591	C	-1.605804	4.955529	1.155023
				C	-3.444175	3.368570	1.439161
				C	-3.522109	1.257809	0.214134
				C	-2.129624	5.741472	2.151592
				H	-0.674177	5.239864	0.677904
				C	-3.968981	4.211052	2.455967
				C	-4.063676	2.129465	1.127754
				C	-3.330282	5.374098	2.804444
				H	-1.612984	6.649569	2.447180
				H	-4.880698	3.905140	2.962739
				H	-4.977550	1.859081	1.650961
				H	-3.734976	6.008324	3.587131
				C	-4.139819	-0.073055	-0.074869
				C	-4.712013	-0.317734	-1.340471
				C	-4.171551	-1.074433	0.919430
				C	-5.329499	-1.545018	-1.580333
				C	-4.804212	-2.285333	0.635096
				C	-5.390983	-2.541273	-0.604982
				H	-5.760267	-1.737939	-2.560098
				H	-4.862118	-3.046008	1.409872
				C	3.014214	1.708940	-1.157026
				C	3.599726	1.735368	0.126061
				C	3.498897	0.833044	-2.145086
				C	4.712216	0.933552	0.373619
				C	4.616436	0.046636	-1.854347
M-(R)-5-TS1-S E= -3994.06874784							
H	0.375201	-2.113383	-2.261597				
C	-0.506999	1.191691	2.945472				
C	0.289989	0.170404	3.464903				
C	0.888357	0.283825	4.725323				
C	0.652901	1.434478	5.471663				
C	-0.149800	2.458701	4.971311				
C	-0.723770	2.337227	3.706811				
H	-0.943130	1.086213	1.955745				
H	1.110873	1.528441	6.453142				
H	-0.326451	3.350108	5.565164				
H	-1.346975	3.133844	3.310641				
C	1.800099	-0.829299	5.167000				
H	2.810836	-0.648480	4.774334				
H	1.877656	-0.858193	6.257433				
C	1.285619	-2.168125	4.640238				
H	1.973375	-2.984333	4.861949				
H	0.321260	-2.406949	5.112530				
C	1.026323	-2.123981	3.152345				
N	0.537808	-0.982832	2.680789				
H	0.188115	-0.959783	1.705277				
C	0.157176	-3.591480	-0.927073				
C	1.500588	-3.174851	-0.533841				

C	-0.218047	-1.215464	3.007764	C	-1.050332	-5.931752	2.250091
C	-0.403360	0.059531	3.543669	H	-2.208385	-4.762040	0.897316
C	-0.958004	0.241027	4.815813	C	1.319749	-5.498587	2.338363
C	-1.299405	-0.884710	5.559465	C	2.296785	-3.716625	0.938539
C	-1.104848	-2.165635	5.044899	C	0.232079	-6.206569	2.781978
C	-0.569538	-2.327945	3.768354	H	-1.913729	-6.477084	2.619161
H	0.190602	-1.324708	2.006392	H	2.308541	-5.682482	2.750716
H	-1.728403	-0.750943	6.549285	H	3.268537	-3.936257	1.373775
H	-1.373932	-3.035034	5.636403	H	0.348854	-6.967947	3.546912
H	-0.420591	-3.323410	3.361499	C	3.326617	-1.809473	-0.335182
C	-1.201272	1.652510	5.275089	C	3.833501	-1.844081	-1.645997
H	-2.171280	1.997545	4.889373	C	3.913587	-0.947065	0.618096
H	-1.250336	1.703421	6.366358	C	4.927192	-1.038101	-1.980154
C	-0.095806	2.567576	4.753362	C	5.005409	-0.168378	0.236518
H	-0.290252	3.614831	4.985776	C	5.534565	-0.190315	-1.057370
H	0.863679	2.297366	5.218564	H	5.305756	-1.088795	-2.996186
C	0.102920	2.418947	3.262901	H	5.456598	0.485867	0.979038
N	-0.056076	1.195346	2.771051	C	-3.663822	0.296021	-1.076561
H	0.201253	1.018914	1.783588	C	-4.057114	0.761361	0.196097
C	-0.483491	3.588214	-0.779687	C	-3.621409	1.181236	-2.166731
C	0.917487	3.494456	-0.376251	C	-4.441095	2.092231	0.337398
H	-1.150066	2.817294	-0.386781	C	-4.008443	2.514381	-1.972031
H	1.275885	2.487484	-0.178434	C	-4.426799	2.994059	-0.732531
C	-1.988422	-1.560049	-0.763188	H	-4.758531	2.442024	1.315643
C	-1.537272	-2.862358	-0.841145	H	-3.970385	3.187171	-2.821814
C	-2.347535	-3.817150	-1.539662	O	0.757824	-1.437673	-1.437224
C	-3.632561	-3.418864	-2.006234	O	-1.218764	-0.616391	-0.117644
C	-4.067536	-2.079532	-1.820377	P	0.124612	-0.050700	-0.860684
C	-3.257513	-1.134374	-1.242696	O	0.950414	0.527264	0.247696
H	-0.920371	-5.448768	-1.492795	C	3.263701	-2.756215	-2.722753
C	-1.913084	-5.143572	-1.807421	H	2.379093	-3.259975	-2.323963
C	-4.455187	-4.363651	-2.674754	C	4.274480	-3.846850	-3.097319
H	-5.062230	-1.802376	-2.159644	H	4.558343	-4.438342	-2.220197
C	-4.017147	-5.643404	-2.899104	H	5.187132	-3.411095	-3.520080
C	-2.725598	-6.030557	-2.469437	H	3.848405	-4.525625	-3.844431
H	-5.436257	-4.043676	-3.016246	C	2.823372	-1.967069	-3.959808
H	-4.650916	-6.357158	-3.416312	H	2.113736	-1.179408	-3.689310
H	-2.371842	-7.037206	-2.670764	H	2.338325	-2.634378	-4.680823
C	-0.233061	-3.211238	-0.210760	H	3.679234	-1.502535	-4.462747
C	-0.105015	-4.237794	0.783274	C	3.412452	-0.835805	2.051270
C	0.883774	-2.460789	-0.518733	H	2.429368	-1.310616	2.105052
C	-1.215820	-4.974348	1.279411	C	4.351209	-1.572461	3.015114
C	1.179581	-4.493862	1.343543	H	4.461369	-2.629027	2.751108
C	2.172337	-2.682919	0.043129	H	3.970561	-1.514500	4.041162

H	5.350236	-1.119943	2.998283	H	-4.169368	4.541836	1.579441
C	3.239364	0.617819	2.506518	H	-2.956761	5.036486	0.389868
H	2.625736	1.180980	1.797927	H	-4.314124	6.112058	0.778945
H	4.203928	1.126362	2.616689	H	-5.313697	4.943956	-2.583573
H	2.747034	0.640899	3.486707	H	-5.001150	6.334695	-1.536496
C	-3.184601	0.728196	-3.553057	H	-3.652314	5.330847	-2.092994
H	-2.543608	-0.150848	-3.429082	H	-6.679276	5.491236	0.083275
C	-2.370791	1.787441	-4.302779	H	-6.972099	4.030407	-0.883281
H	-1.897059	1.335667	-5.180598	H	-6.516090	3.888619	0.823432
H	-1.585958	2.212013	-3.672156	C	6.730430	0.701129	-1.404223
H	-3.005345	2.606310	-4.661349	C	7.164990	0.544244	-2.864190
C	-4.400580	0.329361	-4.400702	C	6.352998	2.174034	-1.170035
H	-5.074978	1.185742	-4.522005	C	7.920020	0.333573	-0.502353
H	-4.971067	-0.484029	-3.943324	H	7.473765	-0.483277	-3.086253
H	-4.082931	0.003974	-5.397740	H	6.362099	0.820096	-3.556645
C	-4.107255	-0.173545	1.396008	H	8.019144	1.200079	-3.064758
H	-3.354402	-0.954936	1.251172	H	6.079091	2.358110	-0.125093
C	-3.770758	0.524693	2.715963	H	7.201514	2.824480	-1.414828
H	-4.580809	1.185136	3.046848	H	5.506180	2.462811	-1.803035
H	-2.857356	1.122497	2.618985	H	8.784700	0.964213	-0.740464
H	-3.610108	-0.221315	3.501963	H	7.683218	0.474588	0.557285
C	-5.478826	-0.854450	1.480369	H	8.210178	-0.712871	-0.648222
H	-5.700074	-1.417888	0.567819				
H	-6.268250	-0.105735	1.616111				
H	-5.515373	-1.547585	2.328187				
O	-0.218741	0.764296	-2.076428	M-(R)-6-TS1-S E= -3846.45961110			
S	0.578836	3.738046	2.329752	H	0.494993	-2.213909	-2.259826
O	0.100135	3.257679	-2.047793	C	-0.690129	0.905466	3.005089
C	1.898805	4.563737	-0.470325	C	0.105423	-0.119889	3.517825
C	1.535803	5.911862	-0.590944	C	0.669270	-0.037553	4.795771
C	3.254301	4.205483	-0.422983	C	0.401171	1.088749	5.568133
C	2.521731	6.886591	-0.673101	C	-0.402094	2.116527	5.075569
H	0.488675	6.197947	-0.613448	C	-0.942496	2.024638	3.793824
C	4.236486	5.183065	-0.511849	H	-1.095499	0.821951	1.999820
H	3.523022	3.156562	-0.319069	H	0.832457	1.160665	6.563465
C	3.868678	6.522696	-0.637571	H	-0.605894	2.988043	5.689864
H	2.243304	7.931468	-0.764296	H	-1.566563	2.824208	3.405495
H	5.285343	4.903755	-0.482809	C	1.577449	-1.158047	5.226530
H	4.635047	7.288981	-0.706379	H	2.593801	-0.965151	4.854794
H	-0.951151	4.570177	-0.807992	H	1.636302	-1.213942	6.317012
C	-4.863543	4.443658	-0.501363	C	1.075327	-2.484804	4.657432
C	-4.026074	5.064980	0.628737	H	1.758667	-3.305881	4.875197
C	-4.694826	5.305994	-1.755446	H	0.100630	-2.735065	5.101843
C	-6.346166	4.461720	-0.094230	C	0.852007	-2.403021	3.165443
				N	0.384839	-1.248664	2.709685
				H	0.079330	-1.190858	1.719190

C	0.091401	-3.718683	-1.000334	C	4.848453	1.025666	0.454579
C	1.423103	-3.376856	-0.504126	C	4.773664	0.254232	-1.802603
H	-0.156481	-4.772692	-1.101955	C	5.433915	0.281046	-0.574702
C	0.590982	2.273993	-0.766286	H	5.328593	1.051807	1.429910
C	-0.504165	3.113275	-0.825255	H	5.179465	-0.334755	-2.618315
C	-0.367035	4.363666	-1.513660	O	-1.644779	0.688218	-1.456270
C	0.914554	4.746282	-2.000742	O	0.478568	1.048659	-0.145561
C	2.022669	3.877540	-1.817182	P	-0.372046	-0.149314	-0.873628
C	1.881937	2.644412	-1.230236	O	-0.779331	-1.065482	0.237986
H	-2.457471	4.934291	-1.421955	C	-4.423646	0.431689	-2.776012
C	-1.467845	5.230501	-1.754112	H	-3.962855	1.332432	-2.361758
C	1.064416	5.992225	-2.665880	C	-5.845546	0.809885	-3.208070
H	3.004428	4.203562	-2.152602	H	-6.439035	1.154422	-2.354423
C	-0.012926	6.816785	-2.864786	H	-6.363367	-0.045892	-3.656213
C	-1.294324	6.422703	-2.412164	H	-5.817565	1.612987	-3.952941
H	2.052290	6.273753	-3.021323	C	-3.584092	-0.004162	-3.981986
H	0.110510	7.765929	-3.377088	H	-2.575481	-0.294680	-3.673727
H	-2.149125	7.067296	-2.593314	H	-3.500971	0.816868	-4.702667
C	-1.780938	2.684723	-0.189997	H	-4.045538	-0.853358	-4.499019
C	-2.439106	3.456192	0.824898	C	-3.606403	-1.300815	2.005252
C	-2.312921	1.457743	-0.524943	H	-3.024378	-0.377760	2.071179
C	-1.901850	4.664084	1.348937	C	-4.792045	-1.187400	2.972116
C	-3.658553	2.964762	1.373268	H	-5.451260	-0.351642	2.717504
C	-3.519614	0.937822	0.020331	H	-4.435987	-1.040154	3.998112
C	-2.555109	5.353530	2.341250	H	-5.394105	-2.103827	2.951629
H	-0.954197	5.032099	0.970867	C	-2.688990	-2.448284	2.444224
C	-4.316199	3.707218	2.389926	H	-1.881336	-2.601404	1.723438
C	-4.181980	1.720946	0.933079	H	-3.241266	-3.388585	2.555743
C	-3.780792	4.876888	2.865061	H	-2.244824	-2.214515	3.419941
H	-2.123619	6.269343	2.733633	C	2.922797	0.888081	-3.396480
H	-5.247808	3.318541	2.792778	H	1.877634	1.189286	-3.271848
H	-5.120456	1.372517	1.356522	C	2.920154	-0.536246	-3.961443
H	-4.286927	5.432694	3.648259	H	2.254353	-0.588787	-4.829416
C	-4.023799	-0.411181	-0.380511	H	2.566631	-1.257790	-3.219641
C	-4.452868	-0.643075	-1.699005	H	3.918324	-0.841930	-4.295809
C	-4.083572	-1.457587	0.567787	C	3.586997	1.847686	-4.391363
C	-4.955815	-1.901938	-2.044835	H	4.648294	1.599789	-4.514691
C	-4.599790	-2.690845	0.174405	H	3.520477	2.887263	-4.055085
C	-5.045237	-2.944427	-1.126113	H	3.106187	1.776195	-5.373484
H	-5.287242	-2.053439	-3.067318	C	3.087707	2.522869	1.446878
H	-4.649160	-3.487968	0.912281	H	2.052519	2.783752	1.206638
C	3.061968	1.754507	-0.996542	C	3.047027	1.686194	2.729804
C	3.670072	1.746443	0.275008	H	4.049866	1.523690	3.141390
C	3.591860	0.970109	-2.032559	H	2.592124	0.707834	2.541245

H	2.452720	2.197966	3.495320
C	3.858581	3.829073	1.666270
H	3.833725	4.458198	0.769905
H	4.908716	3.621129	1.903622
H	3.427487	4.398638	2.497127
O	0.352401	-0.692299	-2.072788
S	1.133441	-3.741233	2.177469
O	0.670502	-3.221055	-2.222268
H	-0.729270	-3.112923	-0.621101
H	1.585680	-2.326317	-0.281790
C	2.584589	-4.253362	-0.581468
C	2.450162	-5.647612	-0.641570
C	3.862648	-3.676124	-0.577264
C	3.581074	-6.451483	-0.702619
H	1.466006	-6.104983	-0.623956
C	4.990355	-4.485150	-0.642169
H	3.959792	-2.593029	-0.528738
C	4.849265	-5.871262	-0.704860
H	3.474859	-7.530582	-0.743814
H	5.980439	-4.039515	-0.637029
H	5.731867	-6.502025	-0.749301
C	6.759468	-0.445428	-0.328372
C	6.646830	-1.348106	0.910900
C	7.169641	-1.312251	-1.522890
C	7.859033	0.601456	-0.084026
H	6.437346	-0.772622	1.817963
H	5.847150	-2.087765	0.794256
H	7.588924	-1.885868	1.070208
H	7.354294	-0.708762	-2.418227
H	8.095295	-1.849195	-1.287806
H	6.400470	-2.054435	-1.767044
H	8.822125	0.108409	0.093578
H	7.966748	1.262924	-0.950794
H	7.629474	1.221998	0.788638
C	-5.586362	-4.330813	-1.485252
C	-6.043007	-4.414199	-2.944368
C	-4.481006	-5.376794	-1.263279
C	-6.786261	-4.662821	-0.583336
H	-6.847049	-3.701049	-3.157580
H	-5.217844	-4.220835	-3.638457
H	-6.424715	-5.419895	-3.151515
H	-4.148969	-5.397110	-0.220005
H	-4.848839	-6.377347	-1.519950
H	-3.609858	-5.159848	-1.891851

H	-7.182606	-5.654607	-0.830997
H	-6.507954	-4.668489	0.475530
H	-7.589338	-3.929856	-0.718330

M-(R)-7-TS1-R E= -4608.54088692

H	0.073866	-1.625632	-1.714403
C	0.042104	2.381591	3.016231
C	0.472873	1.231478	3.678181
C	1.115548	1.299122	4.918667
C	1.298743	2.548322	5.504117
C	0.862092	3.706755	4.862851
C	0.238745	3.621699	3.619045
H	-0.431687	2.295891	2.041245
H	1.794859	2.610645	6.469434
H	1.009725	4.674599	5.331668
H	-0.100192	4.522141	3.115385
C	1.617203	0.009969	5.510213
H	2.604140	-0.223405	5.085214
H	1.743773	0.101583	6.592534
C	0.646821	-1.124005	5.184659
H	1.025157	-2.091587	5.515990
H	-0.313406	-0.952948	5.693057
C	0.335906	-1.193720	3.707744
N	0.286845	-0.031833	3.066156
H	-0.028735	-0.020895	2.079841
C	0.757066	-2.777564	-0.257515
C	-0.617922	-2.815058	0.232171
H	1.332057	-1.891347	0.015726
H	-1.080288	-1.843798	0.387566
C	1.620015	2.646768	-0.875965
C	0.919315	3.821564	-1.060868
C	1.492148	4.825113	-1.910067
C	2.803076	4.626013	-2.427709
C	3.501537	3.424623	-2.132100
C	2.923287	2.420036	-1.397160
H	-0.224479	6.150628	-1.928414
C	0.790976	6.004478	-2.281450
C	3.386088	5.624871	-3.251829
H	4.513658	3.303353	-2.509592
C	2.693188	6.763774	-3.573796
C	1.376254	6.946744	-3.090203
H	4.390982	5.460580	-3.632177
H	3.144994	7.519042	-4.209425
H	0.820764	7.837558	-3.367005

C	-0.411215	3.982178	-0.410624	H	-3.738183	1.017053	-4.374104
C	-0.728627	5.074972	0.462387	C	-3.539344	1.280523	2.234607
C	-1.362235	3.000873	-0.593711	H	-2.713669	1.997251	2.232511
C	0.221930	6.065439	0.831640	C	-4.699772	1.885830	3.035229
C	-2.034577	5.144100	1.028114	H	-5.059869	2.820824	2.593899
C	-2.667878	3.038372	-0.027561	H	-4.390870	2.090530	4.066484
C	-0.117201	7.081858	1.690643	H	-5.544725	1.187155	3.067606
H	1.231819	6.003243	0.440957	C	-3.036979	0.008590	2.927644
C	-2.357118	6.214511	1.905025	H	-2.295431	-0.506910	2.310553
C	-2.985027	4.125808	0.747818	H	-3.854973	-0.687902	3.144623
C	-1.423292	7.165353	2.229001	H	-2.571163	0.268725	3.886000
H	0.625989	7.824154	1.965892	C	3.089664	0.272659	-3.448661
H	-3.359539	6.256022	2.323248	H	2.283277	1.008657	-3.368316
H	-3.975969	4.205767	1.187275	C	2.472949	-1.029486	-3.969110
H	-1.678484	7.976641	2.903699	H	1.867069	-0.818969	-4.856738
C	-3.591980	1.888263	-0.271697	H	1.827799	-1.494735	-3.219653
C	-4.019370	1.602863	-1.585296	H	3.242578	-1.751926	-4.264254
C	-3.958820	1.037126	0.792963	C	4.126012	0.787314	-4.456918
C	-4.786370	0.460972	-1.818113	H	4.960190	0.079336	-4.538770
C	-4.730084	-0.092804	0.513087	H	4.536675	1.757945	-4.163507
C	-5.127289	-0.409704	-0.785103	H	3.674901	0.895308	-5.449570
H	-5.104697	0.224639	-2.830774	C	4.077186	2.001996	1.272909
H	-5.007994	-0.765817	1.321117	H	3.236135	2.657614	1.028765
C	3.628230	1.134884	-1.094854	C	3.777671	1.388249	2.643746
C	4.192343	0.947464	0.182623	H	4.646044	0.858511	3.051983
C	3.715800	0.121716	-2.070145	H	2.943467	0.680340	2.578364
C	4.895674	-0.228304	0.444391	H	3.503055	2.174704	3.355597
C	4.413407	-1.048431	-1.758764	C	5.343833	2.863876	1.321513
C	5.017731	-1.234175	-0.514871	H	5.525497	3.354666	0.359303
H	5.355274	-0.376256	1.418482	H	6.219376	2.248010	1.558418
H	4.491325	-1.840295	-2.499257	H	5.253800	3.639060	2.090470
O	-1.045169	1.919473	-1.388974	O	0.300269	-0.139092	-1.794925
O	1.083324	1.653101	-0.083895	S	-0.013617	-2.667015	2.968590
P	-0.152104	0.757007	-0.676019	O	0.070600	-2.635102	-1.512679
O	-0.831802	0.187689	0.531443	C	-1.451998	-3.996138	0.313002
C	-3.693350	2.500300	-2.769943	C	-0.968559	-5.283747	0.037143
H	-2.986303	3.267520	-2.443047	C	-2.801484	-3.814016	0.654022
C	-4.957989	3.220177	-3.254083	C	-1.830796	-6.369886	0.097614
H	-5.405700	3.817089	-2.452257	H	0.070860	-5.433874	-0.237868
H	-5.708937	2.500292	-3.599508	C	-3.657763	-4.904091	0.724504
H	-4.722239	3.888809	-4.089338	H	-3.166062	-2.809127	0.857098
C	-3.036427	1.722592	-3.915398	C	-3.171148	-6.180226	0.440774
H	-2.164713	1.163084	-3.562964	H	-1.461910	-7.366213	-0.123413
H	-2.707077	2.414404	-4.698318	H	-4.702299	-4.758694	0.981599

H	-3.841153	-7.034033	0.482059
H	1.351380	-3.688222	-0.220784
C	5.767723	-2.486599	-0.208629
C	6.958697	-2.781803	-0.906818
C	5.289213	-3.372468	0.781166
C	7.677687	-3.990463	-0.609336
C	6.024883	-4.571819	1.077322
C	7.197174	-4.853366	0.375697
H	7.747196	-5.764443	0.601278
C	-5.833021	-1.694629	-1.056484
C	-7.154505	-1.892196	-0.609373
C	-5.142958	-2.731781	-1.721151
C	-7.798438	-3.158827	-0.827894
C	-5.797001	-3.995234	-1.930992
C	-7.106170	-4.178172	-1.482721
H	-7.594357	-5.137502	-1.641591
C	4.378997	-5.201277	2.754835
H	4.014777	-5.886078	3.514572
C	3.633403	-4.023070	2.453528
H	2.704348	-3.826143	2.981596
C	8.665047	-2.216473	-2.555938
H	9.064995	-1.533250	-3.299022
C	9.360709	-3.429337	-2.273615
H	10.274781	-3.661090	-2.811664
C	-3.785574	-4.885794	-2.970157
H	-3.246762	-5.700116	-3.445250
C	-3.128732	-3.638402	-2.756612
H	-2.090368	-3.522662	-3.052745
C	-7.902373	-0.862610	0.052751
C	-9.180375	-1.082360	0.477376
C	-9.810182	-2.346532	0.271895
H	-7.436929	0.105419	0.207024
H	-9.729410	-0.288013	0.973891
H	-10.826871	-2.500631	0.620496
C	-5.078617	-5.055436	-2.571021
H	-5.589158	-6.003283	-2.722327
C	-3.782030	-2.599296	-2.158683
H	-3.260823	-1.661684	-1.987531
C	8.882254	-4.283871	-1.325713
H	9.406869	-5.206418	-1.090972
C	7.511437	-1.902855	-1.897500
H	7.002372	-0.970441	-2.116259
C	4.069940	-3.143670	1.504456
H	3.486470	-2.253729	1.290493

C	5.535682	-5.465316	2.083966
H	6.111238	-6.362655	2.296542
C	-9.139560	-3.348779	-0.363498
H	-9.609001	-4.314577	-0.532494

M-(R)-7-TS1-S E= -4608.53491639

H	-0.157305	-1.541285	-2.198978
C	-0.303902	1.788634	3.073091
C	0.371409	0.656948	3.531975
C	1.075832	0.665202	4.740147
C	1.084306	1.834897	5.494481
C	0.412846	2.974233	5.052146
C	-0.277619	2.950129	3.841004
H	-0.836552	1.749206	2.126441
H	1.629857	1.851437	6.434616
H	0.428503	3.878823	5.651863
H	-0.803825	3.834619	3.491942
C	1.825344	-0.585755	5.114072
H	2.813907	-0.576176	4.631794
H	1.992423	-0.630299	6.193787
C	1.045876	-1.815892	4.649116
H	1.592359	-2.741240	4.833901
H	0.092141	-1.878658	5.193526
C	0.690351	-1.725564	3.183518
N	0.378124	-0.515267	2.738244
H	-0.015846	-0.422689	1.783469
C	-0.660324	-2.928014	-0.863474
C	0.759865	-2.839342	-0.526831
H	-1.110735	-3.916859	-0.902319
C	0.896666	2.839982	-0.797342
C	-0.001185	3.886770	-0.868992
C	0.359067	5.036802	-1.647417
C	1.666040	5.112636	-2.206048
C	2.580347	4.045164	-2.000557
C	2.213495	2.905671	-1.329577
H	-1.560626	6.037846	-1.521016
C	-0.549486	6.098086	-1.909534
C	2.035343	6.253882	-2.966418
H	3.590687	4.138901	-2.391604
C	1.141906	7.270496	-3.187210
C	-0.167868	7.182884	-2.659292
H	3.040555	6.298514	-3.377636
H	1.430609	8.136607	-3.774487
H	-0.880314	7.978647	-2.854350

C	-1.303834	3.780275	-0.154883	H	-4.325793	0.235941	-4.021032
C	-1.737129	4.746107	0.813929	C	-3.823081	0.582770	2.538308
C	-2.098016	2.674301	-0.372384	H	-3.144964	1.439364	2.508305
C	-0.929741	5.841094	1.228082	C	-4.964304	0.915015	3.506254
C	-3.012243	4.577327	1.426664	H	-5.530349	1.794842	3.182429
C	-3.356108	2.463701	0.257811	H	-4.569200	1.112882	4.508931
C	-1.379619	6.730383	2.173050	H	-5.666612	0.076269	3.580741
H	0.059646	5.963489	0.800623	C	-3.015517	-0.614590	3.054963
C	-3.455495	5.522956	2.389504	H	-2.246080	-0.897239	2.330846
C	-3.803098	3.441900	1.111579	H	-3.655811	-1.485432	3.238092
C	-2.660907	6.578873	2.755588	H	-2.529847	-0.357710	4.004305
H	-0.744528	7.555779	2.479964	C	2.696045	0.808290	-3.385949
H	-4.434249	5.380974	2.840320	H	1.745000	1.331541	-3.249498
H	-4.769118	3.328400	1.597941	C	2.373090	-0.603646	-3.883813
H	-3.006004	7.292873	3.496921	H	1.653064	-0.549791	-4.706911
C	-4.110701	1.193562	0.038974	H	1.934760	-1.217876	-3.092355
C	-4.570500	0.844391	-1.248081	H	3.266389	-1.113776	-4.262473
C	-4.346498	0.329618	1.130761	C	3.521286	1.556853	-4.440384
C	-5.243318	-0.364952	-1.422359	H	4.494570	1.070361	-4.580879
C	-5.067625	-0.845576	0.915641	H	3.701573	2.596510	-4.150439
C	-5.505329	-1.221986	-0.352745	H	3.000615	1.558038	-5.404525
H	-5.583295	-0.648287	-2.415939	C	3.577898	2.777423	1.254757
H	-5.272796	-1.504960	1.755684	H	2.584490	3.203942	1.080477
C	3.179541	1.791823	-1.072278	C	3.555018	2.154698	2.653211
C	3.850620	1.750737	0.165869	H	4.557087	1.864988	2.989446
C	3.419141	0.807420	-2.049001	H	2.915107	1.266178	2.672973
C	4.808352	0.758499	0.382874	H	3.158492	2.874660	3.376941
C	4.371567	-0.179166	-1.782841	C	4.598146	3.919146	1.181766
C	5.082764	-0.211330	-0.581342	H	4.565839	4.418196	0.207307
H	5.354041	0.731014	1.322702	H	5.613763	3.534659	1.332867
H	4.573519	-0.945462	-2.527826	H	4.397984	4.667539	1.956468
O	-1.667267	1.723778	-1.272842	O	-0.020469	-0.015900	-1.969987
O	0.562007	1.697581	-0.102347	S	0.645426	-3.102783	2.211289
P	-0.545339	0.668930	-0.740181	O	-0.157310	-2.560390	-2.161257
O	-1.040751	-0.136040	0.421650	H	-1.300691	-2.173316	-0.410372
C	-4.419366	1.756222	-2.457035	H	1.143283	-1.834913	-0.365063
H	-3.813136	2.620530	-2.173615	C	1.721295	-3.915709	-0.684591
C	-5.792733	2.285804	-2.890236	C	1.334962	-5.265176	-0.660213
H	-6.290495	2.812789	-2.069036	C	3.072733	-3.580060	-0.845908
H	-6.446098	1.465889	-3.211792	C	2.293895	-6.258499	-0.799244
H	-5.688220	2.981639	-3.730054	H	0.293077	-5.535417	-0.515141
C	-3.716459	1.055715	-3.624237	C	4.028137	-4.577602	-0.994422
H	-2.748432	0.649715	-3.317057	H	3.363628	-2.532286	-0.859353
H	-3.547330	1.766119	-4.440849	C	3.637156	-5.915107	-0.969036

H	1.998632	-7.302332	-0.773061
H	5.073557	-4.312941	-1.121828
H	4.382881	-6.696734	-1.078188
C	6.111924	-1.264394	-0.346993
C	5.949012	-2.206237	0.693046
C	6.935848	-3.236705	0.876514
C	8.040603	-3.296271	0.026665
H	8.778831	-4.083133	0.166663
C	-6.210881	-2.517347	-0.566015
C	-7.519755	-2.531928	-1.096994
C	-5.563596	-3.733200	-0.247289
C	-8.177284	-3.787298	-1.338330
C	-6.244754	-4.979903	-0.470693
C	-7.526868	-4.978780	-1.019112
H	-8.031404	-5.926350	-1.196263
C	4.806057	-2.216843	1.562969
C	4.668312	-3.161536	2.538352
H	3.782035	-3.160874	3.166022
C	5.658027	-4.171455	2.723619
H	5.525986	-4.914947	3.503554
C	6.753888	-4.206692	1.914364
H	7.513025	-4.975180	2.035846
H	4.028771	-1.471127	1.425663
C	7.246690	-1.325777	-1.187343
C	8.219191	-2.366547	-0.998253
C	9.360012	-2.427618	-1.861583
C	9.544243	-1.503897	-2.846791
H	10.413465	-1.556558	-3.495134
C	8.598800	-0.450377	-3.020049
C	7.495446	-0.362523	-2.221833
H	10.078758	-3.228072	-1.706032
H	8.765829	0.294313	-3.792288
H	6.796395	0.454631	-2.360306
C	-5.592766	-6.208992	-0.131383
C	-4.336548	-6.215873	0.396486
H	-3.853531	-7.152687	0.657126
C	-3.645228	-4.984778	0.599293
H	-2.640421	-4.997786	1.013454
C	-4.229447	-3.792248	0.281022
C	-9.497264	-3.794501	-1.893066
C	-10.145366	-2.629694	-2.176862
C	-9.513001	-1.379935	-1.907214
C	-8.252772	-1.331882	-1.385309
H	-7.795874	-0.371798	-1.171668

H	-3.680280	-2.869398	0.432657
H	-6.130146	-7.137846	-0.304964
H	-9.969902	-4.756186	-2.075962
H	-11.146832	-2.645323	-2.596042
H	-10.046916	-0.457221	-2.113702

M-TS1-R E= -3767.85472783

H	-1.923137	1.286489	-1.999175
C	0.907491	-0.748665	2.988794
C	-0.183154	-0.082980	3.547713
C	-0.650442	-0.396637	4.829158
C	0.012474	-1.382319	5.554868
C	1.113803	-2.045455	5.016549
C	1.557551	-1.728896	3.734391
H	1.231671	-0.498869	1.982002
H	-0.342214	-1.629838	6.552212
H	1.624295	-2.809178	5.594809
H	2.414924	-2.243127	3.312107
C	-1.868769	0.333194	5.326449
H	-2.773859	-0.177696	4.968634
H	-1.904527	0.327367	6.419367
C	-1.858927	1.769906	4.807653
H	-2.772058	2.304730	5.069722
H	-1.014137	2.319150	5.248676
C	-1.662445	1.826521	3.310909
N	-0.845261	0.917200	2.793092
H	-0.571336	1.001799	1.797717
C	-3.136536	1.625369	-0.459737
C	-2.350388	2.844618	-0.300179
H	-2.712190	0.711539	-0.035273
H	-1.275129	2.701785	-0.229836
C	-0.159205	-2.366741	-0.690161
C	1.101990	-2.919650	-0.784131
C	1.242583	-4.174343	-1.465616
C	0.070560	-4.856213	-1.899657
C	-1.203913	-4.257761	-1.712192
C	-1.338518	-3.009807	-1.157243
H	3.411171	-4.231689	-1.466191
C	2.506744	-4.759622	-1.749460
C	0.193434	-6.115172	-2.545519
H	-2.087226	-4.800183	-2.039252
C	1.426346	-6.666295	-2.782285
C	2.594431	-5.970776	-2.389831
H	-0.713437	-6.625434	-2.859913

H	1.511938	-7.626782	-3.280981	H	2.114486	0.913303	-3.644249
H	3.570157	-6.397393	-2.601993	H	3.249147	0.132356	-4.763686
C	2.259809	-2.184205	-0.203920	H	3.321012	1.882108	-4.514846
C	3.147416	-2.777643	0.754753	C	4.153962	5.548795	-1.491652
C	2.456341	-0.858798	-0.540739	H	4.087017	6.130109	-0.563267
C	2.941402	-4.076399	1.297576	C	5.521627	5.823432	-2.124951
C	4.250876	-2.014644	1.232409	H	5.645431	6.893784	-2.322897
C	3.533758	-0.069041	-0.052406	H	5.626424	5.294570	-3.079150
C	3.802782	-4.594264	2.233352	H	6.335857	5.499746	-1.468673
H	2.078353	-4.652815	0.982780	C	3.027039	6.008716	-2.423175
C	5.134508	-2.585062	2.187843	H	2.044749	5.845119	-1.968014
C	4.427675	-0.677171	0.794262	H	3.055768	5.454300	-3.368324
C	4.920460	-3.847738	2.677551	H	3.126881	7.075105	-2.654428
H	3.621113	-5.583230	2.643082	C	3.168625	2.065478	2.003043
H	5.976134	-1.989842	2.532377	H	2.898774	1.008964	2.073651
H	5.277050	-0.112417	1.171226	C	4.372249	2.305837	2.921808
H	5.597131	-4.272099	3.412773	H	5.238279	1.705667	2.623890
C	3.665827	1.371670	-0.430325	H	4.120191	2.051759	3.957574
C	3.954486	1.733308	-1.763275	H	4.673330	3.359995	2.896999
C	3.516534	2.371696	0.552908	C	1.961623	2.876515	2.489863
C	4.109824	3.082218	-2.081065	H	1.118997	2.769014	1.801125
C	3.691652	3.708630	0.184794	H	2.203295	3.941711	2.581583
C	3.988870	4.087232	-1.120778	H	1.652334	2.524243	3.481811
H	4.337305	3.355949	-3.109740	C	-2.624474	-1.820473	-3.553901
H	3.583953	4.483167	0.941919	H	-1.553039	-2.003727	-3.424886
C	-2.657696	-2.313623	-1.034819	C	-2.772287	-0.546377	-4.390008
C	-3.283147	-2.222770	0.224059	H	-2.190992	-0.647230	-5.312886
C	-3.251447	-1.721375	-2.169421	H	-2.406494	0.331395	-3.854444
C	-4.511565	-1.564617	0.326688	H	-3.813537	-0.367486	-4.680876
C	-4.470739	-1.059204	-2.011738	C	-3.233595	-2.999834	-4.325724
C	-5.119281	-0.972174	-0.779656	H	-4.308490	-2.839841	-4.474124
H	-4.992121	-1.497488	1.298004	H	-3.108694	-3.949103	-3.797422
H	-4.932989	-0.585176	-2.875329	H	-2.766210	-3.095335	-5.312147
O	1.585938	-0.261188	-1.429234	C	-6.455886	-0.254621	-0.692327
O	-0.314541	-1.154852	-0.049968	H	-6.409197	0.591182	-1.392681
P	0.136666	0.202633	-0.847605	C	-7.584319	-1.183631	-1.159759
O	0.243691	1.247279	0.219813	H	-8.548827	-0.664082	-1.142741
C	4.140636	0.705519	-2.870335	H	-7.653708	-2.055901	-0.499354
H	3.959237	-0.290877	-2.457987	H	-7.406278	-1.545105	-2.177592
C	5.582670	0.722439	-3.392023	C	-6.769791	0.299042	0.697858
H	6.298124	0.539631	-2.583169	H	-7.667950	0.923845	0.659209
H	5.827804	1.689135	-3.846875	H	-5.947673	0.906444	1.094154
H	5.722662	-0.051671	-4.154496	H	-6.964828	-0.507581	1.413489
C	3.144121	0.923692	-4.013217	C	-2.661845	-2.867913	1.454753

H	-1.574345	-2.863616	1.328313	N	0.700697	-1.324964	2.605103
C	-2.960397	-2.111907	2.751778	H	0.370939	-1.298513	1.622288
H	-4.004083	-2.232102	3.064520	C	0.859711	-3.696823	-1.178288
H	-2.757816	-1.040438	2.639372	C	2.094801	-3.092756	-0.684245
H	-2.326675	-2.496024	3.558752	H	0.836581	-4.776664	-1.301574
C	-3.115103	-4.328696	1.570572	C	0.244069	2.198273	-0.801430
H	-2.841563	-4.902686	0.679097	C	-0.957311	2.875540	-0.844384
H	-4.204104	-4.381920	1.687333	C	-1.002823	4.135373	-1.526791
H	-2.653936	-4.808309	2.441110	C	0.208281	4.693984	-2.024266
O	-0.715021	0.429600	-2.066795	C	1.431304	3.994523	-1.842453
S	-2.397823	3.035079	2.394878	C	1.469693	2.753326	-1.257814
O	-2.770175	1.853978	-1.826248	H	-3.149856	4.414121	-1.400039
C	-2.858458	4.198704	-0.484231	C	-2.215369	4.843051	-1.747596
C	-4.229065	4.490706	-0.516500	C	0.175961	5.947261	-2.690610
C	-1.922016	5.233180	-0.615735	H	2.355826	4.461736	-2.173555
C	-4.650760	5.802768	-0.688088	C	-1.008046	6.614030	-2.876698
H	-4.963940	3.698792	-0.406997	C	-2.216490	6.048413	-2.405182
C	-2.348239	6.544004	-0.786574	H	1.111239	6.361469	-3.058353
H	-0.861851	4.995913	-0.579178	H	-1.024339	7.568916	-3.392946
C	-3.712864	6.827526	-0.823810	H	-3.154438	6.569543	-2.571358
H	-5.711560	6.030149	-0.713693	C	-2.143402	2.279114	-0.171163
H	-1.620219	7.341882	-0.890605	C	-2.849054	2.960060	0.875200
H	-4.049292	7.851432	-0.956181	C	-2.520041	0.989870	-0.482046
H	-4.213917	1.679756	-0.319125	C	-2.438291	4.223043	1.383351
				C	-3.969080	2.318709	1.477334
				C	-3.628776	0.323839	0.110866
				C	-3.122960	4.825076	2.410034
				H	-1.559198	4.703380	0.967566
				C	-4.665359	2.974649	2.528115
				C	-4.347445	1.017184	1.054351
				C	-4.255975	4.201640	2.985094
				H	-2.786203	5.784615	2.790406
				H	-5.521304	2.473966	2.973388
				H	-5.213267	0.550561	1.517505
				H	-4.789005	4.691218	3.794225
				C	-3.971346	-1.078174	-0.280087
				C	-4.416709	-1.355929	-1.589920
				C	-3.852563	-2.123579	0.659082
				C	-4.756579	-2.666002	-1.926689
				C	-4.214076	-3.417773	0.273691
				C	-4.666940	-3.712521	-1.008625
				H	-5.105452	-2.874830	-2.936522
				H	-4.130696	-4.226749	0.996929
				C	2.759491	2.036357	-1.013495
M-TS1-S E= -3767.85161187							
H	0.889129	-2.120209	-2.404908				
C	-0.706337	0.617770	2.971289				
C	0.247262	-0.282321	3.449097				
C	0.799399	-0.147972	4.727877				
C	0.359573	0.896642	5.535356				
C	-0.601411	1.797341	5.077523				
C	-1.128253	1.658997	3.794239				
H	-1.101722	0.502833	1.965524				
H	0.782554	1.006433	6.530768				
H	-0.934790	2.607312	5.718704				
H	-1.872286	2.360856	3.428869				
C	1.882812	-1.114843	5.124050				
H	2.851756	-0.740918	4.764185				
H	1.951577	-1.196641	6.212388				
C	1.610394	-2.486880	4.509081				
H	2.424562	-3.186689	4.698194				
H	0.695341	-2.914858	4.944430				
C	1.366212	-2.394784	3.020977				

C	3.327419	2.078605	0.275408	H	2.317613	-0.324250	-4.889095
C	3.407690	1.347357	-2.053770	H	2.716127	-0.970222	-3.288256
C	4.578060	1.494394	0.482079	H	3.999651	-0.357673	-4.351053
C	4.657226	0.774947	-1.799203	C	3.328532	2.261095	-4.398522
C	5.265736	0.849313	-0.546866	H	4.413175	2.145869	-4.513879
H	5.022958	1.541531	1.472443	H	3.133865	3.278097	-4.044034
H	5.172700	0.242747	-2.596738	H	2.869069	2.151498	-5.387208
O	-1.793892	0.307660	-1.437351	C	6.649953	0.261240	-0.341298
O	0.306104	0.962775	-0.195396	H	6.793147	-0.497054	-1.123048
P	-0.378690	-0.330268	-0.935055	C	7.718114	1.344885	-0.539968
O	-0.571777	-1.330795	0.161151	H	8.724263	0.924144	-0.434720
C	-4.580600	-0.275146	-2.649518	H	7.599422	2.136360	0.209260
H	-4.213738	0.672886	-2.247069	H	7.637142	1.803320	-1.530731
C	-6.061876	-0.079596	-2.994835	C	6.826598	-0.415875	1.019846
H	-6.643414	0.181902	-2.104360	H	7.789487	-0.936876	1.061168
H	-6.490332	-0.994091	-3.420932	H	6.034172	-1.145416	1.219202
H	-6.182321	0.722986	-3.730840	H	6.820914	0.318916	1.832659
C	-3.762227	-0.587248	-3.906551	C	2.618840	2.768930	1.432591
H	-2.706043	-0.732797	-3.660943	H	1.544783	2.775073	1.221101
H	-3.837963	0.239349	-4.621659	C	2.800181	2.032281	2.762807
H	-4.128383	-1.491600	-4.405653	H	3.812290	2.156481	3.164726
C	-5.024487	-5.132615	-1.404356	H	2.607076	0.960567	2.645233
H	-4.936846	-5.754531	-0.504438	H	2.097716	2.425265	3.506241
C	-6.465301	-5.236584	-1.914214	C	3.079222	4.226570	1.551645
H	-6.718757	-6.278373	-2.138816	H	2.881137	4.782325	0.628858
H	-6.598800	-4.656043	-2.834194	H	4.156595	4.272950	1.750593
H	-7.177734	-4.861709	-1.172514	H	2.558476	4.730517	2.373453
C	-4.041977	-5.670808	-2.450710	O	0.363680	-0.704452	-2.187356
H	-3.010175	-5.617482	-2.088200	S	1.871271	-3.627027	1.986631
H	-4.103194	-5.086932	-3.376408	O	1.298576	-3.059743	-2.392319
H	-4.268742	-6.714523	-2.694904	H	-0.062670	-3.286526	-0.772236
C	-3.344749	-1.910029	2.077881	H	2.034582	-2.039397	-0.423793
H	-2.909456	-0.909008	2.137632	C	3.414927	-3.697156	-0.793184
C	-4.494546	-1.991572	3.089624	C	3.580022	-5.074983	-0.996538
H	-5.280204	-1.259572	2.876555	C	4.541974	-2.870360	-0.676646
H	-4.124927	-1.809840	4.105226	C	4.856454	-5.612845	-1.092915
H	-4.953475	-2.987508	3.069720	H	2.716320	-5.728228	-1.068344
C	-2.243815	-2.906572	2.459138	C	5.816714	-3.414184	-0.773715
H	-1.448236	-2.914117	1.709027	H	4.406337	-1.803270	-0.511787
H	-2.638145	-3.923808	2.563623	C	5.973166	-4.783830	-0.984717
H	-1.809934	-2.624899	3.426698	H	4.983172	-6.679190	-1.249090
C	2.777628	1.206876	-3.430525	H	6.689133	-2.774342	-0.682835
H	1.700779	1.367916	-3.317262	H	6.969584	-5.208404	-1.061149
C	2.968209	-0.195175	-4.017652				

M-TS5-R E= -3060.35421690

H	-2.515986	-0.197905	-2.529866
C	0.865763	0.514301	2.636492
C	-0.119971	-0.433490	2.911920
C	0.095252	-1.462364	3.835313
C	1.321463	-1.522554	4.491717
C	2.313114	-0.579231	4.234530
C	2.082330	0.437078	3.308544
H	0.671727	1.296154	1.905812
H	1.493351	-2.317309	5.213069
H	3.265016	-0.634526	4.753631
H	2.853071	1.176066	3.112810
C	-1.016386	-2.454201	4.049770
H	-0.949177	-3.253792	3.298983
H	-0.923896	-2.928641	5.030677
C	-2.367097	-1.749777	3.934054
H	-3.200039	-2.451517	3.989402
H	-2.483779	-1.032986	4.759568
C	-2.479461	-0.949465	2.656583
N	-1.366210	-0.359796	2.239059
H	-1.399223	0.249137	1.404862
C	-3.576563	-1.262364	-1.268750
C	-3.959454	0.031293	-0.712107
H	-2.607064	-1.648776	-0.950346
H	-3.139564	0.703470	-0.466930
C	1.391586	-1.317734	-0.877809
C	2.618942	-0.714113	-1.053889
C	3.626674	-1.418138	-1.790726
C	3.352273	-2.741102	-2.240799
C	2.090442	-3.330219	-1.969278
C	1.104099	-2.644262	-1.302541
H	5.089136	0.183533	-1.821126
C	4.880711	-0.837562	-2.123076
C	4.348289	-3.453177	-2.961122
H	1.908579	-4.351934	-2.294512
C	5.557280	-2.873607	-3.248257
C	5.818335	-1.546518	-2.832144
H	4.125975	-4.466580	-3.285468
H	6.311796	-3.423651	-3.802044
H	6.768128	-1.082677	-3.080668
C	2.832768	0.649962	-0.494758
C	3.870135	0.923699	0.455964
C	1.957725	1.664110	-0.827607
C	4.715246	-0.090462	0.983661

C	4.016491	2.250167	0.951817
C	2.080743	2.994435	-0.334446
C	5.668705	0.207056	1.925545
H	4.585676	-1.115229	0.652855
C	5.028846	2.531824	1.909042
C	3.117373	3.260678	0.529595
C	5.839035	1.534149	2.387491
H	6.295761	-0.584448	2.324618
H	5.133351	3.552881	2.266842
H	3.250706	4.269910	0.911680
H	6.603323	1.754309	3.126462
C	1.114846	4.056083	-0.717190
C	0.753034	4.268620	-2.053410
C	0.575939	4.889211	0.269428
C	-0.119177	5.298185	-2.391481
C	-0.299087	5.917459	-0.070011
C	-0.647955	6.125714	-1.402025
H	-0.384993	5.455701	-3.432554
H	-0.713312	6.551467	0.708296
C	-0.214848	-3.262619	-1.010834
C	-0.927488	-3.916874	-2.020959
C	-0.749607	-3.233594	0.285508
C	-2.141508	-4.542329	-1.741794
C	-1.962216	-3.858463	0.562548
C	-2.660493	-4.518422	-0.449440
H	-2.681830	-5.045523	-2.538083
H	-2.367771	-3.828028	1.570562
O	0.916366	1.386157	-1.687280
O	0.389800	-0.614068	-0.248001
P	-0.368726	0.563374	-1.102941
O	-1.142838	1.324632	-0.070930
O	-1.039358	-0.002930	-2.322417
S	-3.966364	-0.775542	1.881973
O	-3.504993	-0.469109	-2.463431
C	-5.310123	0.574968	-0.705374
C	-6.440366	-0.215922	-0.955283
C	-5.463058	1.939157	-0.420212
C	-7.704526	0.357905	-0.926633
H	-6.334261	-1.274678	-1.170607
C	-6.729253	2.508373	-0.390813
H	-4.580796	2.540199	-0.216645
C	-7.848928	1.717238	-0.645364
H	-8.579961	-0.252715	-1.122709
H	-6.845091	3.564451	-0.170077

H	-8.840171	2.160074	-0.622007
H	-4.333066	-2.040031	-1.346336
H	-1.330574	6.927050	-1.668745
H	1.164264	3.629566	-2.828016
H	0.832452	4.715325	1.311115
H	-0.199753	-2.729120	1.076110
H	-3.606399	-5.005256	-0.230981
H	-0.530488	-3.923379	-3.032352

M-TS5-S E= -3060.35267755

H	-1.833657	2.505673	1.557622
C	-0.025508	-2.311879	-1.874788
C	-1.389485	-2.592674	-1.955639
C	-1.873996	-3.656474	-2.725403
C	-0.955579	-4.457694	-3.397195
C	0.411895	-4.196000	-3.320808
C	0.872898	-3.118597	-2.567063
H	0.315108	-1.467704	-1.279357
H	-1.319999	-5.290976	-3.992853
H	1.115578	-4.830017	-3.851379
H	1.936667	-2.905595	-2.507080
C	-3.366755	-3.836661	-2.815723
H	-3.759512	-3.219937	-3.635308
H	-3.617059	-4.876064	-3.045727
C	-4.031528	-3.415750	-1.505281
H	-5.119081	-3.434413	-1.578266
H	-3.740031	-4.109228	-0.701952
C	-3.582654	-2.044313	-1.059259
N	-2.305572	-1.756044	-1.273126
H	-1.911605	-0.893308	-0.870183
C	-3.248878	1.078943	1.825561
C	-3.711874	1.453849	0.493572
H	-3.989463	0.905060	2.603414
C	2.620092	1.545393	-0.153726
C	3.275231	0.467280	0.413572
C	4.643291	0.627531	0.818890
C	5.323080	1.833966	0.495418
C	4.626475	2.863172	-0.184192
C	3.291163	2.758481	-0.493713
H	4.835318	-1.270638	1.855047
C	5.347263	-0.361224	1.559996
C	6.681190	1.999586	0.877104
H	5.159891	3.777731	-0.431384
C	7.339389	1.018354	1.572046

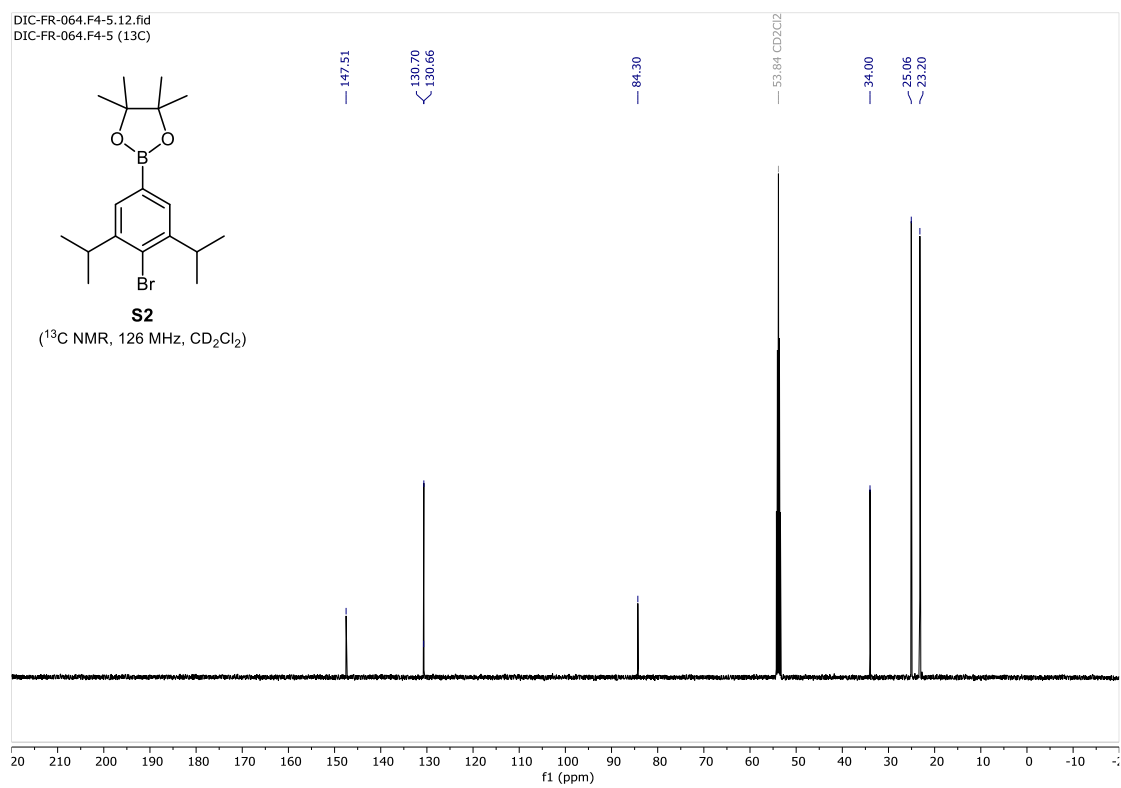
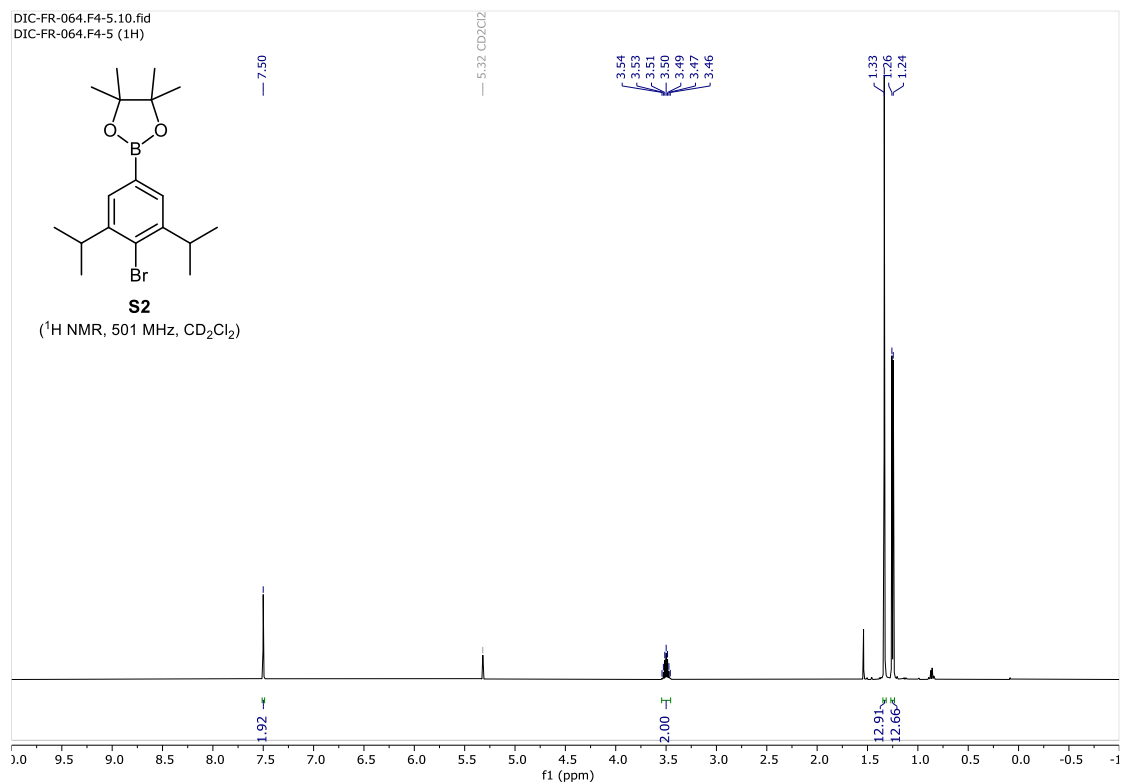
C	6.656690	-0.169886	1.925025
H	7.182876	2.927300	0.614210
H	8.376126	1.153652	1.864323
H	7.171684	-0.935715	2.497005
C	2.564438	-0.825849	0.621626
C	3.054695	-2.069829	0.097375
C	1.374573	-0.835187	1.316123
C	4.182398	-2.151884	-0.764471
C	2.357007	-3.270454	0.411753
C	0.648002	-2.020477	1.621233
C	4.607045	-3.362730	-1.255516
H	4.702604	-1.242961	-1.046786
C	2.831158	-4.508951	-0.096898
C	1.168209	-3.214243	1.182854
C	3.933992	-4.558834	-0.910269
H	5.466338	-3.401264	-1.918115
H	2.286902	-5.414197	0.159351
H	0.651020	-4.142958	1.411970
H	4.285904	-5.508642	-1.300770
C	-0.635520	-1.961746	2.365826
C	-0.762958	-1.208489	3.540782
C	-1.737780	-2.694089	1.909960
C	-1.961922	-1.200610	4.247323
C	-2.940184	-2.679434	2.614533
C	-3.054382	-1.934897	3.786535
H	-2.040579	-0.620870	5.162375
H	-3.788224	-3.249991	2.247689
C	2.604551	3.874237	-1.197963
C	3.201508	4.449697	-2.326132
C	1.396870	4.403098	-0.727320
C	2.605648	5.530488	-2.971372
C	0.805182	5.484843	-1.372704
C	1.404592	6.051784	-2.495885
H	3.078758	5.961570	-3.848742
H	-0.128459	5.887854	-0.991322
O	0.845213	0.373387	1.719520
O	1.298179	1.429040	-0.528188
P	0.081278	1.209530	0.540993
O	-0.942606	0.374239	-0.155323
O	-0.350639	2.499250	1.184760
S	-4.645025	-0.987208	-0.291811
O	-2.829389	2.454283	1.806676
H	-2.429903	0.359445	1.848204
H	-2.956762	1.392942	-0.284368

C	-4.970125	2.125961	0.197421	H	-6.426590	3.798532	-2.383275
C	-6.012368	2.203548	1.131240	H	-8.262781	3.942113	-0.721259
C	-5.126929	2.701487	-1.071020	H	-3.989878	-1.925866	4.338000
C	-7.191583	2.856914	0.797740	H	0.084951	-0.637135	3.904674
H	-5.901980	1.756145	2.113978	H	-1.648445	-3.269529	0.991246
C	-6.308092	3.353035	-1.400962	H	0.925617	3.976597	0.152447
H	-4.316835	2.627481	-1.791513	H	0.937863	6.894009	-2.997975
C	-7.339104	3.431784	-0.465512	H	4.131946	4.036849	-2.706829
H	-7.998082	2.919689	1.521132				

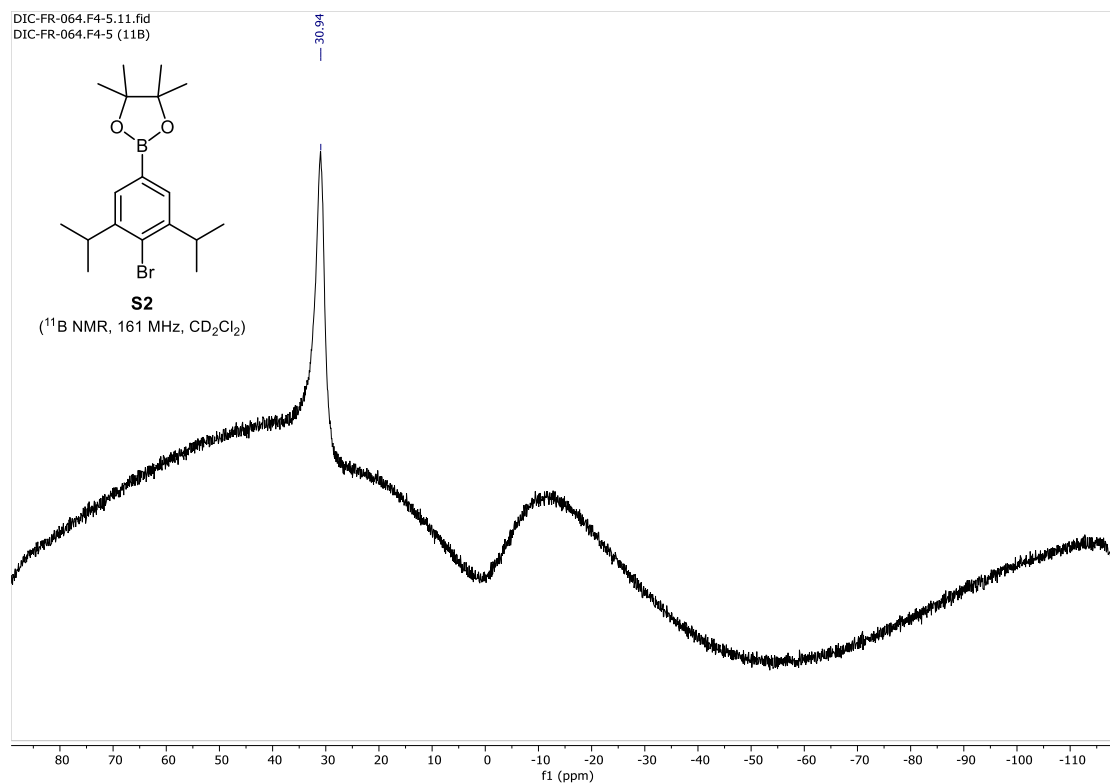
12. Complete Reference for Gaussian 09

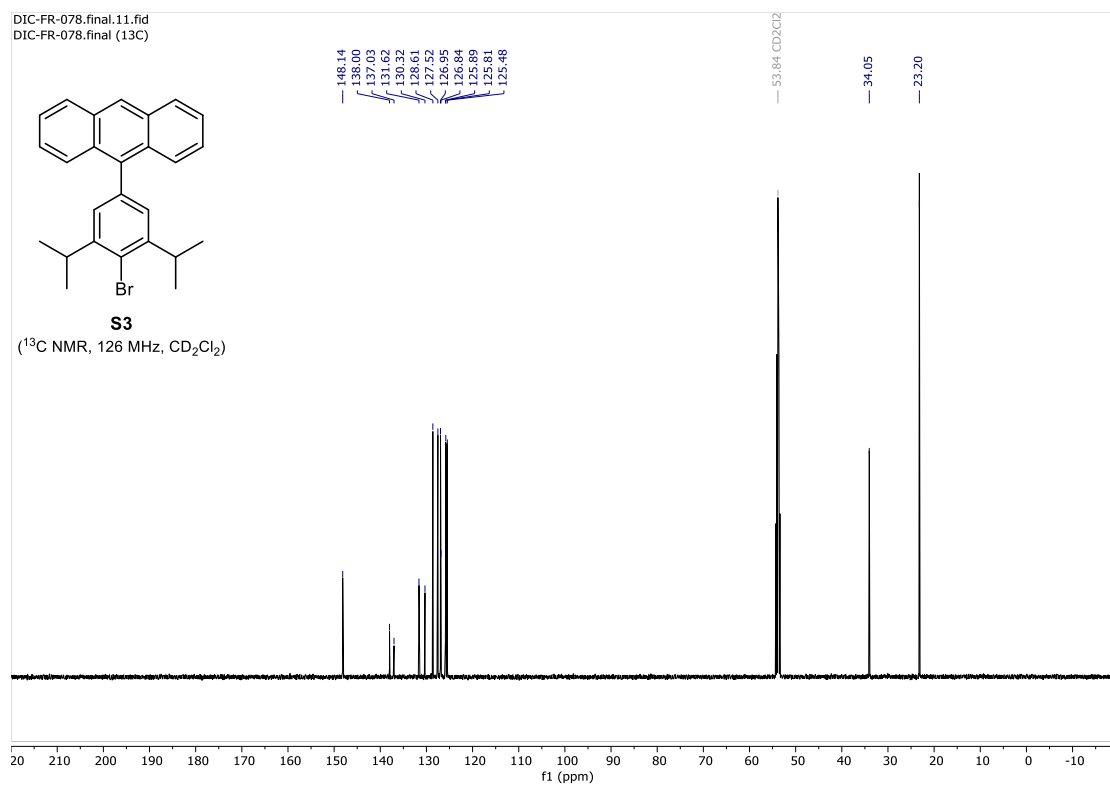
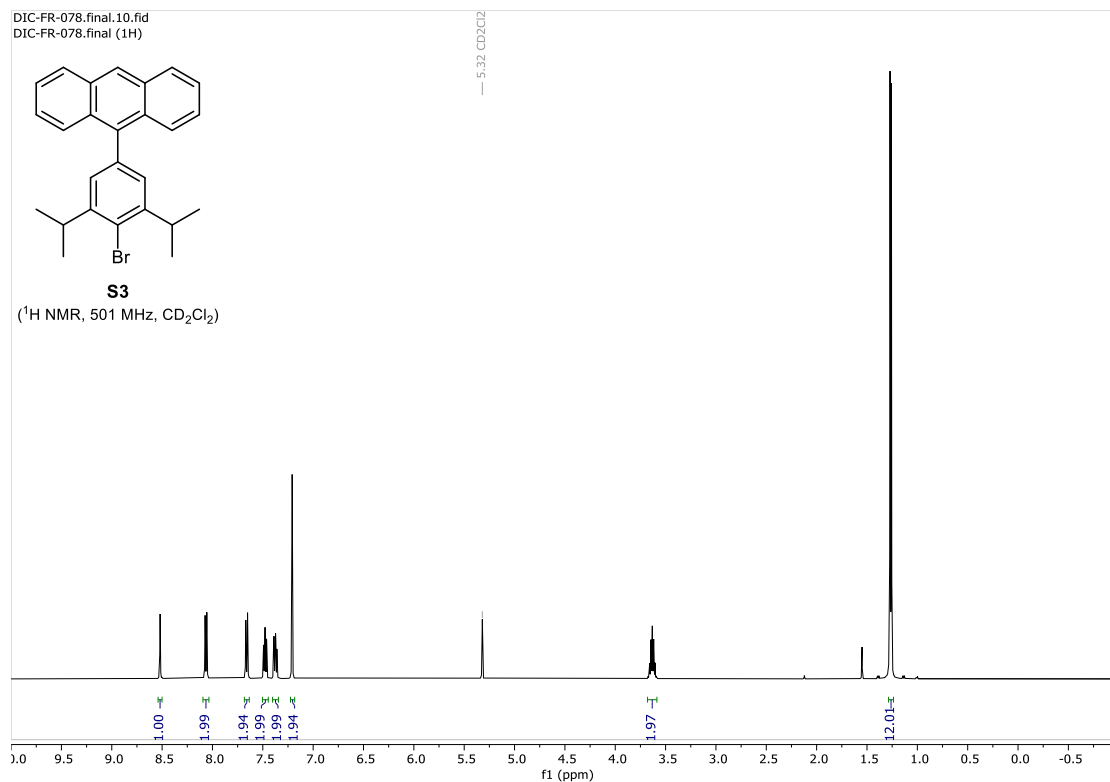
Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2013**.

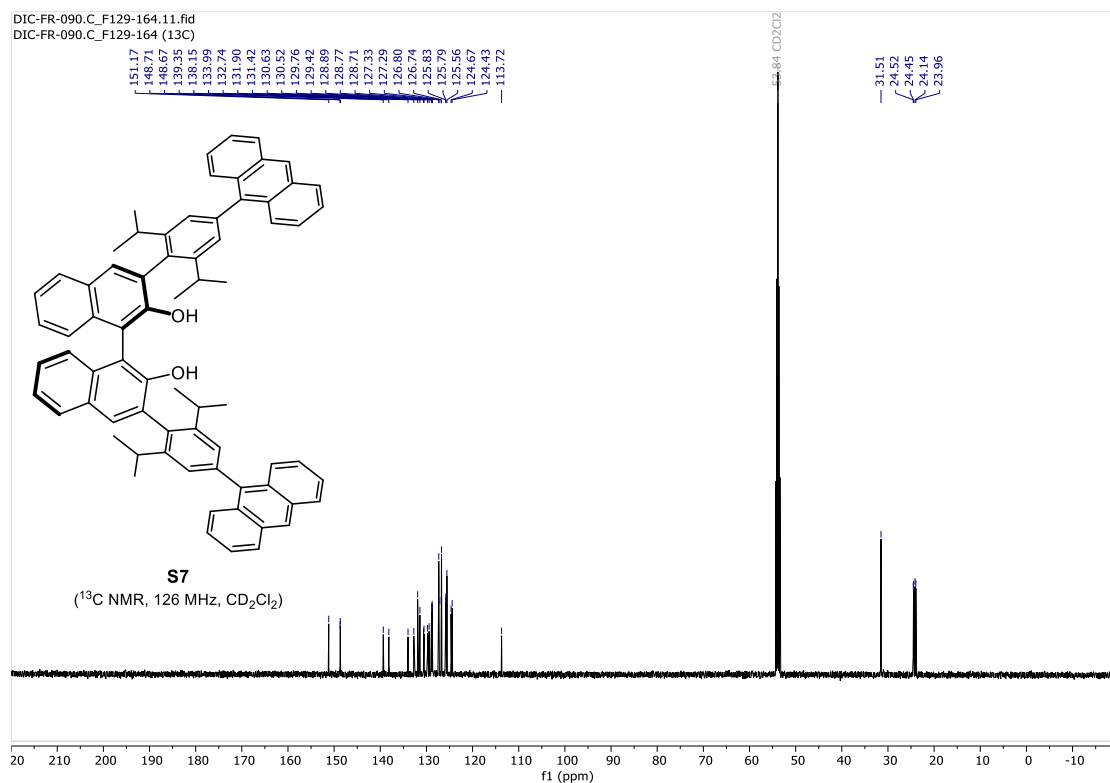
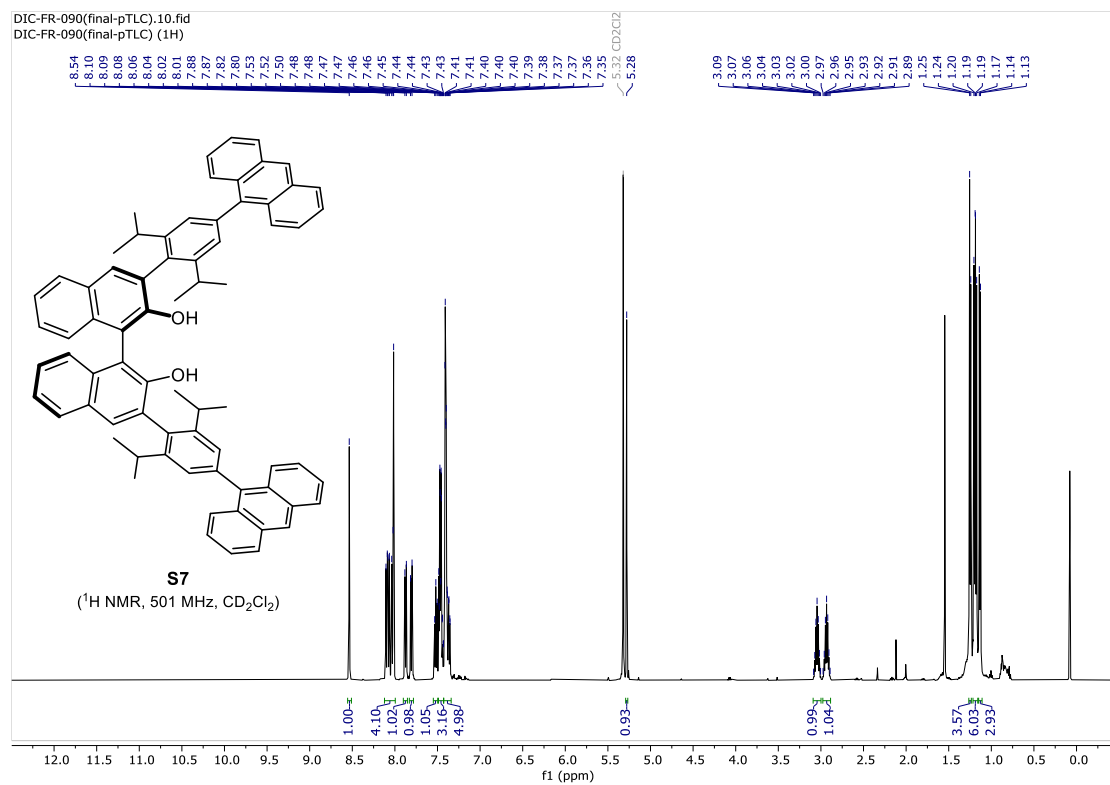
13.Copies of NMR Spectra



DIC-FR-064.F4-5.11.fid
DIC-FR-064.F4-5 (11B)

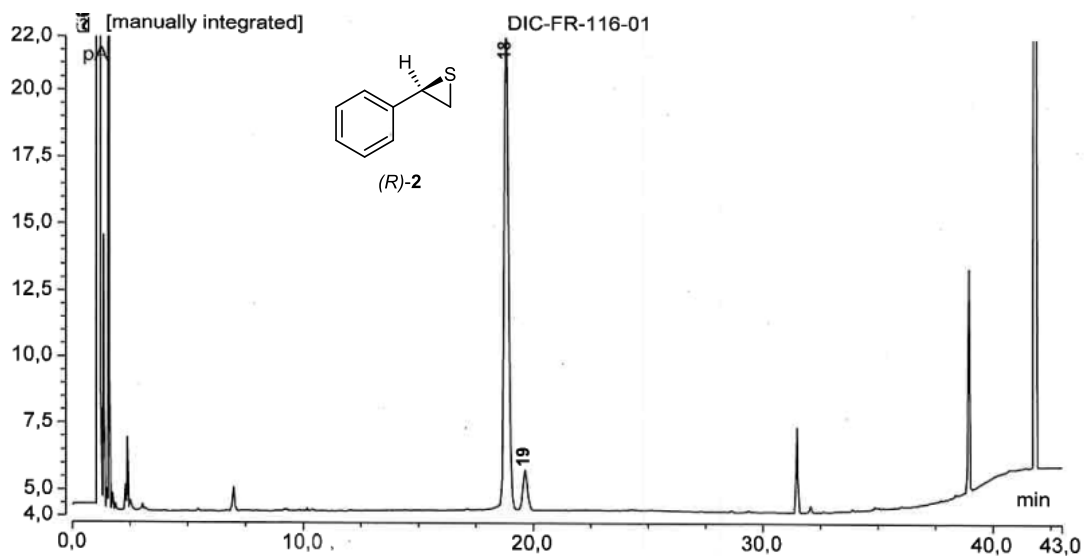






14.GC Traces

Thiirane (*R*)-2, obtained with catalyst (*R*)-C5



Sample: **DIC-FR-116-01**
 Sequenz: **8306 DIC-FR Kes**
 Sequenz date: **09.07.21**

Instrument: **GC_521**
 Measured: **09.07.21 11:48**
 Processing M.: **ee DIC-FR**
 Report-File: **ee 114-01**

chirale Messung, Verhältnis der Enantiomere

Zuordnung nach achiraler GCMS des Racemates 27223 DIC-FR-081-02 20/7633

ee unter Vorbehalt, Racemat nicht stabil (siehe Messungen auf BGB-176/BGB-15 G/618)

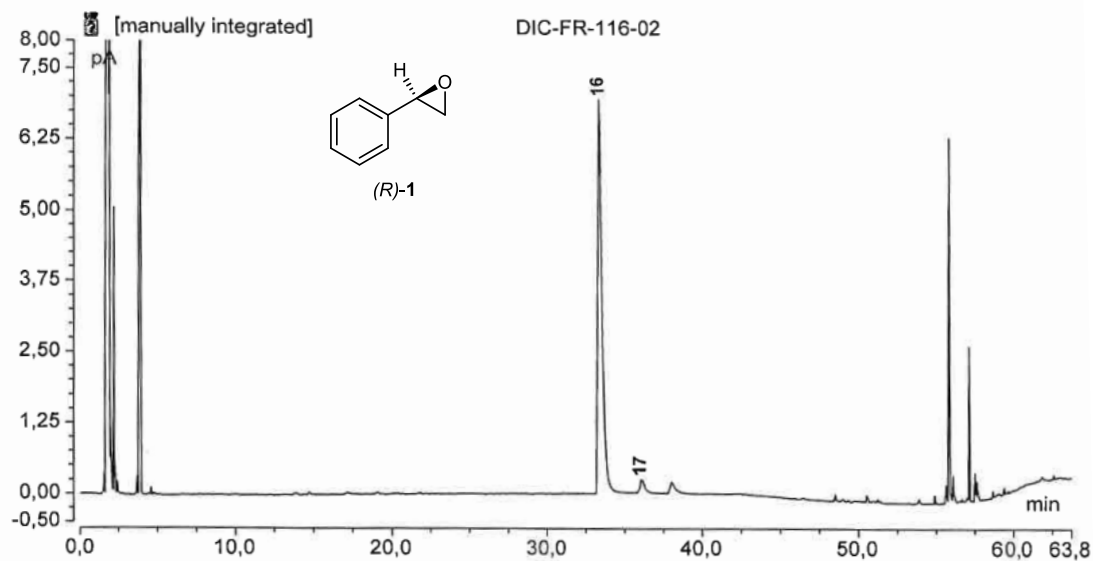
No.	Ret.Time min	Rel.Area %	Peak Name
18	18,80	92,22 .	
19	19,63	7,78 .	

Instrument parameters:

Column: 25,0 m Hydrodex-beta-TBDac-CD, 0.25/?df;G/625
 Temperature: 220/ 100, 25 min iso, 8/min 220, 3 min iso/350
 Gas: 0,60 bar Hydrogen
 Sample size: 1,0 µL

M. Masch

Epoxide (R)-1, obtained with catalyst (R)-C5



Sample: **DIC-FR-116-02** Instrument: **GC_313**
 Sequenz: **8306 DIC-FR Kes** Measured: **09.07.21 11:42**
 Sequenz date: **09.07.21** Processing M.: ee DIC-FR
 Report-File: ee 114-02

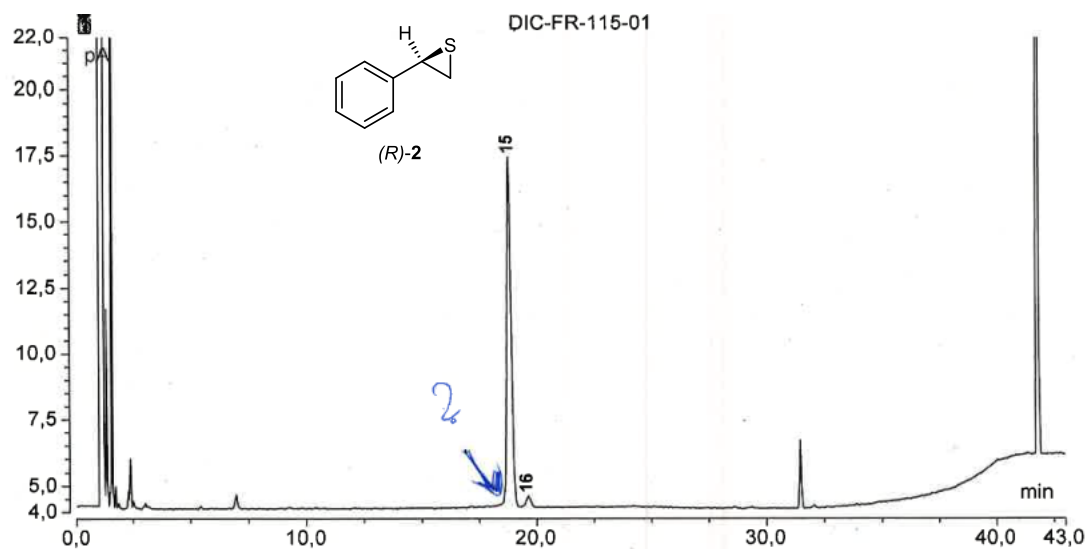
chirale Messung, Verhältnis der Enantiomere
 Zuordnung siehe achirale GCMS des Racemates 27222 DIC-FR-081-01 20/7633

No.	Ret.Time min	Rel.Area %	Peak Name
16	33,32	95,89 .	
17	36,08	4,11 .	

Instrument parameters:
 Column: 30,0 m BGB-176/BGB-15 0.25/0.25df;G/618
 Temperature: 220/ 70, 42 min iso 8/min 220, 3 min iso/ 350
 Gas: 0,60 bar H2
 Sample size: 1,0 µL

M. Masandh

Thiirane (*R*)-2, obtained with catalyst (*R*)-C6

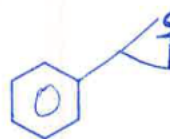


Sample: **DIC-FR-115-01**
 Sequenz: **8305 DIC-FR Ru**
 Sequenz date: **09.07.21**

Instrument: **GC_521**
 Measured: **09.07.21 08:49**
 Processing M.: **ee DIC-FR**
 Report-File: **ee- Verhältnis 115-01**

chirale Messung, Verhältnis der Enantiomere
 Zuordnung nach achiraler GCMS des Racemates 27223 DIC-FR-081-02 20/7633
 ee unter Vorbehalt, Racemat nicht stabil (siehe Messungen auf BGB-176/BGB-15 G/618)
 siehe Ausschnitt Plot

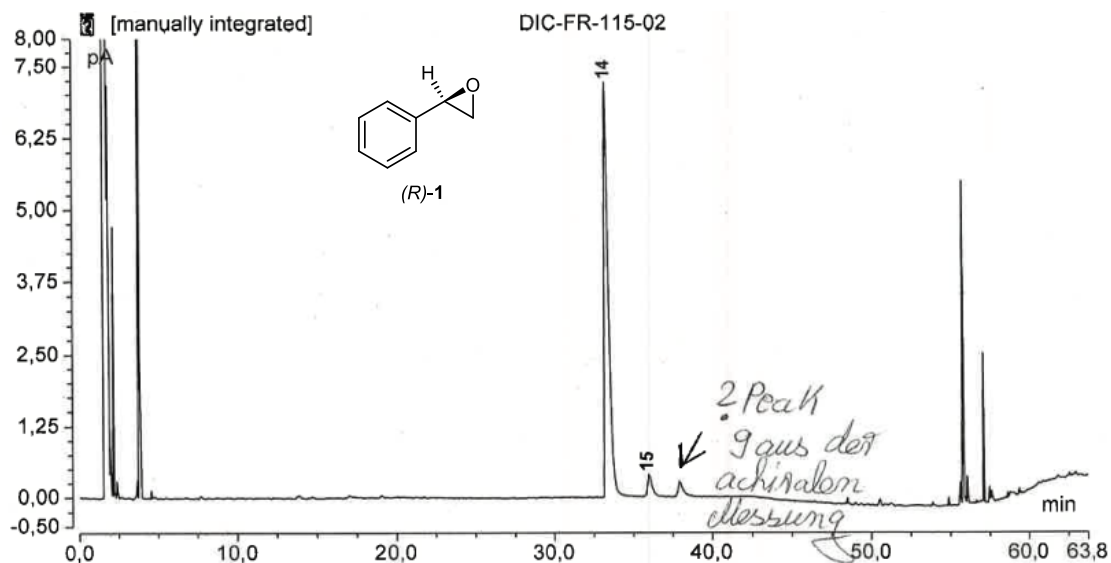
No.	Ret.Time min	Rel.Area %	Peak Name
15	18,80	96,77 .	
16	19,62	3,23 .	



Instrument parameters:
 Column: 25,0 m Hydrodex-beta-TBDAC-CD, 0.25/7df,G/625
 Temperature: 220/ 100, 25 min iso, 8/min 220, 3 min iso/350
 Gas: 0,60 bar Hydrogen
 Sample size: 1,0 µL

9.07.2021
 J. Rutke

Epoxide (R)-1, with catalyst (R)-C6



Sample: **DIC-FR-115-02**
 Sequenz: **8305 DIC-FR Ru**
 Sequenz date: **09.07.21**

Instrument: **GC_313**
 Measured: **09.07.21 09:14**
 Processing M.: 115-02
 Report-File: ee-Verhältnis 115-02

chirale Messung, Verhältnis der Enantiomere
 Zuordnung siehe achirale GCMS des Racemates 27222 DIC-FR-081-01 20/7633
 * in der achiralen Messung Umlagerung/Zersetzung

Zuordnung der Komponent Peak 9+10 aus der achiralen Messung und Klärung der Umlagerung für die chirale Messung wäre sinnvoll, bitte um Rückmeldung

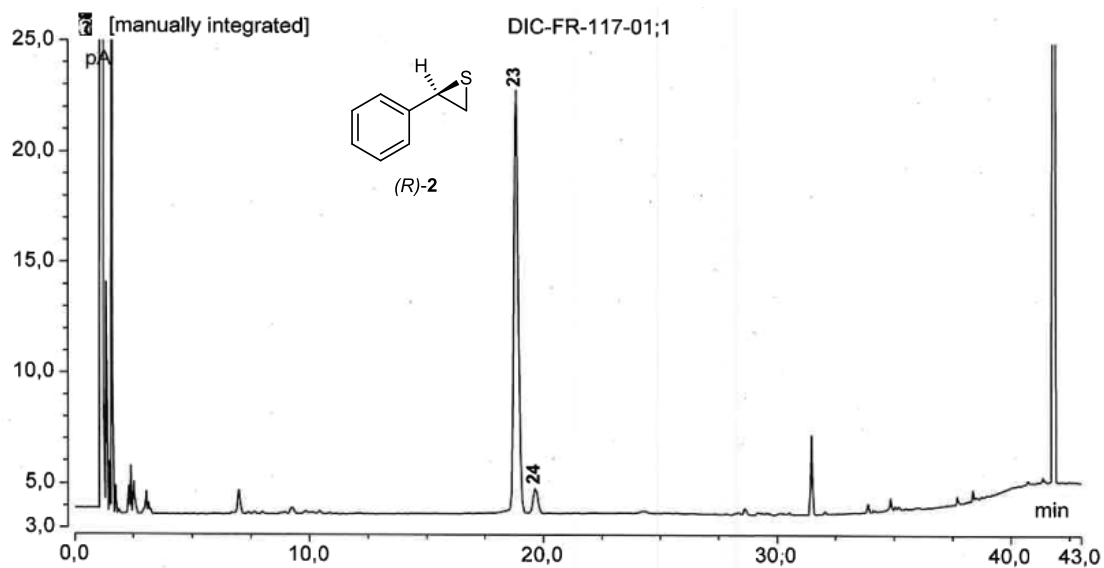
No.	Ret.Time min	Rel.Area %	Peak Name
14	33,28	94,92	* ? Umlagerung
15	35,98	5,08	*



Instrument parameters:
 Column: 30,0 m BGB-176/BGB-15 0.25/0.25df;G/618
 Temperature: 220/ 70, 42 min iso 8/min 220, 3 min iso/ 350
 Gas: 0,60 bar H2
 Sample size: 0,2 µL

9.07.2021
 J. Ruthe

Thiirane (*R*)-2, obtained with catalyst (*R*)-C7



Sample: **DIC-FR-117-01;1**
 Sequenz: **8307 DIC-FR Ru**
 Sequenz date: **09.07.21**

Instrument: **GC_521**
 Measured: **13.07.21 08:12**
 Processing M.: **ee DIC-FR**
 Report-File: **ee 117-01**

chirale Messung, Verhältnis der Enantiomere

Zuordnung nach achiraler GCMS des Racemates 27223 DIC-FR-081-02 20/7633

ee unter Vorbehalt, Racemat nicht stabil (siehe Messungen auf BGB-176/BGB-15 G/618)

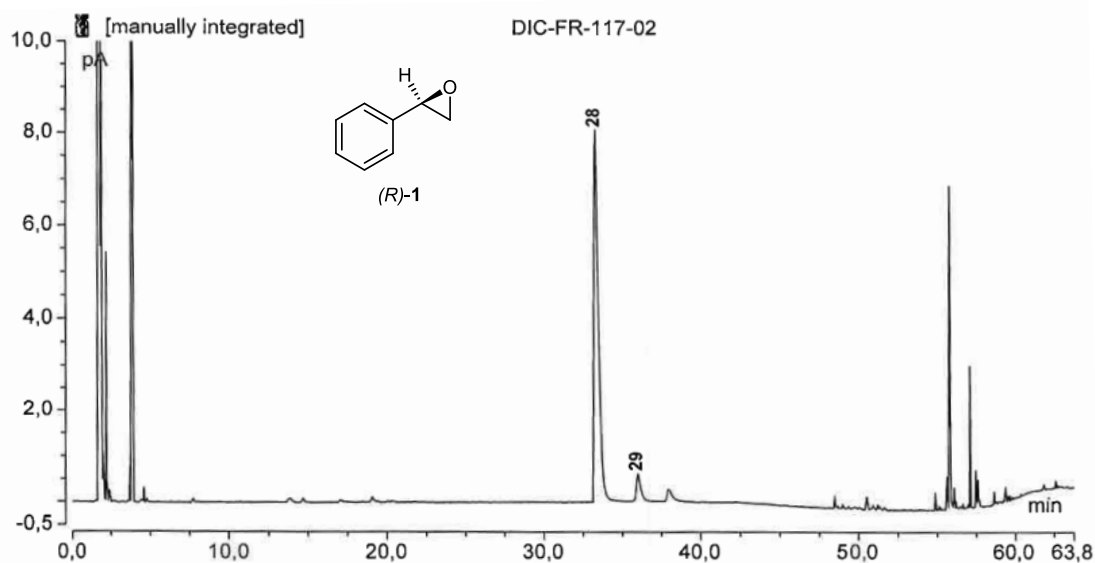
No.	Ret.Time min	Rel.Area %	Peak Name
23	18,81	94,02 .	
24	19,64	5,98 .	

Instrument parameters:

Column: 25,0 m Hydrodex-beta-TBDAC-CD 0.25/?df;G/625
 Temperature: 220/ 100, 25 min iso, 8/min 220, 3 min iso/350
 Gas: 0,60 bar Hydrogen
 Sample size: 1,0 µL

M. Mascher

Epoxide (R)-1, obtained with catalyst (R)-C7



Sample: **DIC-FR-117-02**
 Sequenz: **8307 DIC-FR Ru**
 Sequenz date: **09.07.21**

Instrument: **GC_313**
 Measured: **13.07.21 08:19**
 Processing M.: ee DIC-FR
 Report-File: ee 117-02

chirale Messung, Verhältnis der Enantiomere

Zuordnung siehe achirale GCMS des Racemates 27222 DIC-FR-081-01 20/7633

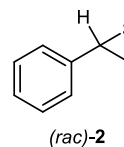
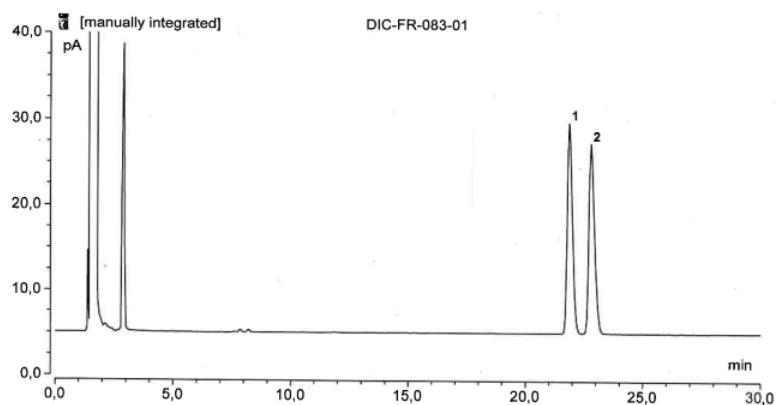
No.	Ret.Time min	Rel.Area %	Peak Name
28	33,28	92,69	.
29	36,00	7,31	.

Instrument parameters:

Column: 30,0 m BGB-176/BGB-15 0.25/0.25df;G/618
 Temperature: 220/ 70, 42 min iso 8/min 220, 3 min iso/ 350
 Gas: 0,60 bar H2
 Sample size: 1,0 µL

M. Masak

Racemic Samples

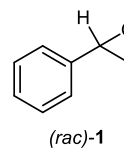
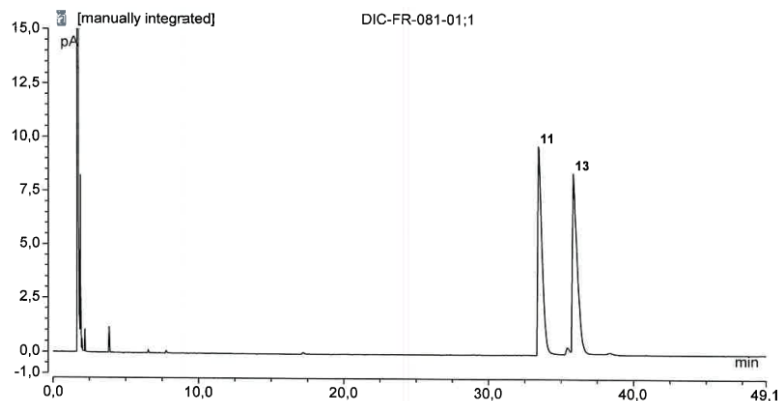


Sample: **DIC-FR-083-01** Instrument: **GC_413**
 Sequenz: **7822 DIC-FR VD** Measured: **23.11.20 14:30**
 Sequenz date: **23.11.20** Processing M.: ee DIC-FR
 Report-File: ee 083-01

chirale Messung des Racemates
 Zuordnung nach achiraler GCMS 27223 DIC-FR-081-02 20/7633

No.	Ret.Time min	Rel.Area %	Peak Name
1	21,85	49,94	.
2	22,79	50,06	.

Instrument parameters:
 Column: 25,0 m Hydrodex-beta-TBDAC-CD 0,25/2df G/681
 Temperature: 220/ 100 iso/ 350
 Gas: 0,60 bar Hydrogen
 Sample size: 1,0 µL



Sample: **DIC-FR-081-01;1** Instrument: **GC_313**
 Sequenz: **7633 DIC-FR SE** Measured: **09.09.20 11:29**
 Sequenz date: **09.09.20** Processing M.: ee DIC
 Report-File: Verhältnis 081-01

Racemat
 Verhältnis der Enantiomere
 Zuordnung achiral nach GCMS 27222 DIC-FR-081-01 20/7633
 Verunreinigungen im Bereich der Enantiomere!

No.	Ret.Time min	Rel.Area %	Peak Name
11	33,44	50,00	.
13	35,84	50,00	.



Instrument parameters:
 Column: 30,0 m BGB-176/BGB-15 0,25/0,25df G/618
 Temperature: 220/70 iso/350
 Gas: 0,60 bar H2
 Sample size: 0,2 µL

E. dlv

15. References

- [1] Eckhardt, M.; Frattini, S.; Hamprecht, D.; Himmelsbach, F.; Langkopf, E.; Lingard, I.; Peters, S.; Wagner, H. New indanyloxydihydrobenzofuranylacetic acids. U.S. Patent US 2013/0252937 A1, September 26, 2013.
- [2] Sasaki, S.; Murakami, F.; Murakami, M.; Watanabe, M.; Kato, K.; Sutoh, K.; Yoshifuji, M. Synthesis of Crowded Triarylphosphines Carrying Functional Sites. *J. Organomet. Chem.* **2005**, *690*, 2664–2672.
- [3] Cheng, X.; Goddard, R.; Buth, G.; List, B. Direct Catalytic Asymmetric Three-Component Kabachnik-Fields Reaction. *Angew. Chem. Int. Ed.* **2008**, *47*, 5079–5081.
- [4] Osakabe, H.; Saito, S.; Miyagawa, M.; Suga, T.; Uchikura, T.; Akiyama, T. Enantioselective Dehydroxyhydrogenation of 3-Indolylmethanols by the Combined Use of Benzothiazoline and Chiral Phosphoric Acid: Construction of a Tertiary Carbon Center. *Org. Lett.* **2020**, *22*, 2225–2229.
- [5] Cheon, C. H.; Yamamoto, H. A Brønsted Acid Catalyst for the Enantioselective Protonation Reaction. *J. Am. Chem. Soc.* **2008**, *130*, 9246–9247.
- [6] Romanov-Michailidis, F.; Guénée, L.; Alexakis, A. Enantioselective Organocatalytic Fluorination-Induced Wagner-Meerwein Rearrangement. *Angew. Chem. Int. Ed.* **2013**, *52*, 9266–9270.
- [7] Li, J.; Grosslight, S.; Miller, S. J.; Sigman, M. S.; Toste, F. D. Site-Selective Acylation of Natural Products with BINOL-Derived Phosphoric Acids. *ACS Catal.* **2019**, *9*, 9794–9799.
- [8] Terada, M.; Toda, Y. Double Bond Isomerization/Enantioselective Aza-Petasis-Ferrier Rearrangement Sequence as an Efficient Entry to Anti- and Enantioenriched Beta-Amino Aldehydes. *J. Am. Chem. Soc.* **2009**, *131*, 6354–6355.
- [9] Liao, S.; Leutzsch, M.; Monaco, M. R.; List, B. Catalytic Enantioselective Conversion of Epoxides to Thiiranes. *J. Am. Chem. Soc.* **2016**, *138*, 5230–5233.
- [10] Shaw, M. H.; Croft, R. A.; Whittingham, W. G.; Bower, J. F. Modular Access to Substituted Azocanes via a Rhodium-Catalyzed Cycloaddition-Fragmentation Strategy. *J. Am. Chem. Soc.* **2015**, *137* (25), 8054–8057.