Reactivity Profiles of Diazo Amides, Esters and Ketones in Transition Metal Free C-H Insertion Reactions

Sarah E. Cleary, [‡,§] Xin Li, [†,§] Li-Cheng Yang, [†] K. N. Houk,[‖] Xin Hong[†,*] and Matthias Brewer[‡,*]

[†]Department of Chemistry, Zhejiang University, Hangzhou 310027, China

[‡]Department of Chemistry, The University of Vermont, Burlington, Vermont 05405, United States

[‖]Department of Chemistry and Biochemistry, University of California, Los Angeles, California 90095, United States

Table of contents:

I) General Experimental Details

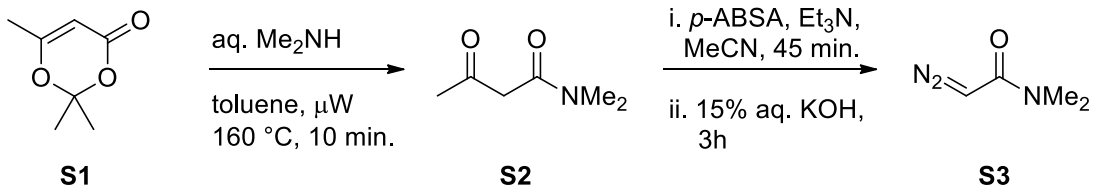
All reactions were performed under an atmosphere of nitrogen in flame-dried glassware, or in a Discover® SP microwave synthesizer in a capped tube when specified. Solvents were removed under vacuum using a rotary evaporator attached to a dry vacuum pump.

Tetrahydrofuran (THF), dichloromethane (CH_2Cl_2), acetonitrile (MeCN) and toluene were dried via a solvent dispensing system. Diisopropylamine (iPr$_2$NH) and triethylamine (Et_3N) were freshly distilled from CaH_2 prior to use. Scandium(III) triflate ($ScOTf_3$) was dried under vacuum at 200 °C for 1 hour prior to use. All other commercially available reagents were used without further purification. 1-Diazo-3-methylbutan-2-one was prepared following a known procedure.[1]

Flash column chromatography was performed on a CombiFlash® Rf 150 system using RediSep® Rf Gold silica columns, or on 50-200 μm neutral alumina (Sorbent Technologies). TLC analysis was carried out using silica gel on glass plates or neutral alumina on foil plates. Visualization of TLC plates was achieved using ultraviolet light and ceric ammonium molybdate.

^{1}H, ^{13}C, and ^{19}F NMR data was collected at room temperature on a 500 MHz spectrometer in $CDCl_3$. ^{1}H NMR chemical shifts are reported in ppm (δ units) downfield from tetramethylsilane, and ^{13}C NMR spectra are referenced to the $CDCl_3$ signal at 77.0 ppm. Exact mass analysis was performed on a Waters Xevo G2-XS LCMS-QTOF operated in positive ESI mode.

II) Preparation of 2-Diazo-*N*,*N*-dimethylacetamide (S3)



***N*,*N*-Dimethyl-3-oxobutanamide** (**S2**):[2] Prepared in accordance with Du *et al*. with the modification that 40% aqueous dimethylamine (Me_2NH) was used. Silica gel flash column chromatography provided **S2** as colorless oil (73% yield). ^{1}H NMR matched previously reported values.[2]

2-Diazo-*N*,*N*-dimethylacetamide (**S3**):[3] Prepared from β-ketoamide **S2** using the procedure specified by Bartlett *et al*. with the modification that *para*-acetamidobenzenesulfonyl azide (*p*-ABSA) was used in place of tosyl azide. After stirring in aqueous KOH for 3 hours, the solution was partitioned between 1:1 (v/v) CH_2Cl_2/Et_2O and 2.5N KOH saturated with NaCl. Layers were separated, and the organic layer was dried over Na_2SO_4, and solvent was removed under reduced pressure. The crude material was dissolved in EtOAc and eluted over a plug of neutral alumina. Alumina was washed with EtOAc, and filtrate was concentrated in vacuo to give pure α-diazo amide **S3** as a yellow oil that solidified upon standing in freezer (89% yield). ^{1}H NMR matched previously reported values.[3]

III) Preparation of β-hydroxy-α-diazo carbonyls

General Procedure A: A 0.28M solution of LDA (1.5 equiv) [freshly prepared by addition of *n*-butyllithium in hexanes (1.5 equiv) to a solution of *i*Pr_2NH (1.7 equiv) in THF (3 mL per mmol of *n*-butyllithium)] was added dropwise over 15 min down the inside wall of a chilled flask containing a cold (–78 °C) stirred solution of cyclohexanone (1 equiv) and α-diazo carbonyl (1.6 equiv) in THF (2 mL per mmol of ketone). The mixture was maintained at –78 °C for 30 minutes. AcOH (0.5 M in THF, 1.7 equiv) was added at –78 °C with rapid stirring under N_2, then the mixture was taken out of the cold bath, uncapped, and 10 mL water was

added. The layers were separated and the aqueous layer was extracted with 15 mL EtOAc. The organic layers were combined, washed with saturated aqueous $NaHCO_3$ (30 mL), water (30 mL), and brine (30 mL), then dried over anhydrous $CaCl_2$. The solvent was removed *in vacuo* to provide an oily residue that was further purified as indicated to afford the desired β-hydroxy-α-diazo carbonyl.

Methyl 2-diazo-2-(1-hydroxycyclohexyl)acetate (**20**):[4] Prepared from cyclohexanone (0.10 mL, 0.97 mmol) and methyl 2-diazoacetate[1] (159 mg, 1.59 mmol) following General Procedure A. The crude residue was dissolved in hexanes and filtered using a fritted funnel. The filtrate was concentrated to give 190 mg (99% yield) of the title compound as an orange-yellow oil. ^{1}H and ^{13}C NMR matched previously reported values.[4]

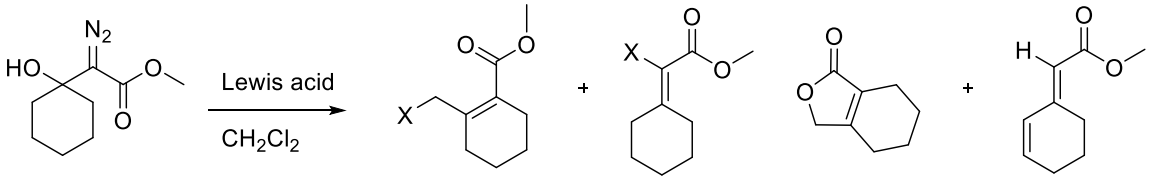
2-Diazo-2-(1-hydroxycylohexyl)-*N*,*N*-dimethylacetamide (**28**): Prepared from cyclohexanone (0.17 mL, 1.65 mmol) and 2-diazo-*N*,*N*-dimethylacetamide (**S3**, 290 mg, 2.56 mmol) following General Procedure A. The crude residue was dissolved in 1:1 hexanes/EtOAc and passed over a plug of neutral alumina. The alumina was washed with 1:1 hexanes/EtOAc (3 × 20 mL). The filtrate was concentrated in vacuo and further dried under reduced pressure on a high vacuum line to give 318 mg (91% yield) of the title compound as a yellow oil: R_f = 0.43 (7:1 hexanes/EtOAc on neutral alumina); ^{1}H NMR (500 MHz, $CDCl_3$): δ 5.10 (s, 1H), 2.97 (s, 6H), 1.62-1.79 (m, 6H), 1.43 (dq, J = 10.6, 4.9 Hz, 2H), 1.32 (tq, J = 11.6, 6.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 167.8, 72.6, 58.1, 37.3, 36.5, 25.2, 22.9. MS (ESI): Calculated for $[C_{10}H_{17}N_2NaO_2]^+$: 234.1218. Found: 234.1213.

IV) Reaction of β-hydroxy-α-diazo carbonyls with Lewis acids

General procedure B: Lewis acid (0.5 mmol) was dissolved in CH_2Cl_2 (6 mL) and the solution was maintained at the indicated temperature for 5 min. A solution of β-hydroxy-α-diazo carbonyl (0.5 mmol) in CH_2Cl_2 (2 mL) was added via syringe to the Lewis acid solution, and the syringe was rinsed with 2 mL CH_2Cl_2, which was also added to the Lewis

acid. The reaction was stirred for 10 min and was then cooled to 0 °C and quenched with 5% aqueous $NaHCO_3$ (10 mL). The layers were separated, and the aqueous layer was extracted three times using CH_2Cl_2 (10 mL). The combined organic layers were washed with H_2O and brine, dried over $MgSO_4$ and filtered. If quantitative NMR was used, a known quantity of the internal standard was dissolved in the organic filtrate, and the solvents were removed under reduced pressure. The crude residue was analyzed by qNMR when applicable, and purified by silica gel flash column chromatography.

Table S1. Treatment of 20 with Lewis acids following General Procedure B



20 **27** **25** **18** **24**

Entry	Lewis acid (1 equiv)	X	Yield 27 (%)	Yield 25 (%)	Yield 18 (%)	Yield 24 (%)
1	$Sc(OTf)_3$	--	--	--	24%[a]	17%[a]
2	$SnCl_4$	Cl	66%[b]	7%[b]	14%[b]	--

[a]Yield determined by quantitative ^{1}H NMR using 4-fluorobenzophenone as internal standard.
[b]Yield determined by ^{1}H NMR using 4-chlorobenzaldehyde as internal standard.

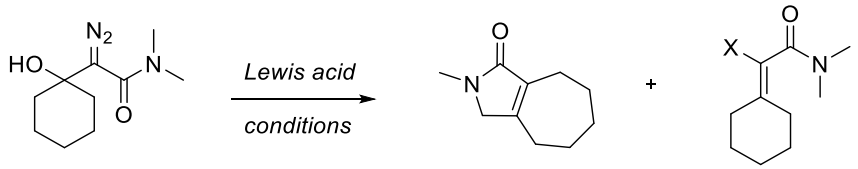
4, 5, 6, 7-Tetrahydroisobenzofuran-1(3*H*)-one (**18**):[5] Observed from the treatment of **20** with $Sc(OTf)_3$ or $SnCl_4$ following General Procedure B (summarized in entries 1 and 2, respectively, Table S1). Yields were determined using quantitative ^{1}H NMR. ^{1}H and ^{13}C NMR matched previously reported values.[5]

(*E*)-Methyl 2-(cyclohex-2-en-1-ylidene)acetate (**24**):[6] Observed from the treatment of **20** with $Sc(OTf)_3$ following General Procedure B (summarized in entry 1, Table S1). The yield of 17% was determined by quantitative ^{1}H NMR using 4-fluorobenzophenone as an internal standard. ^{1}H matched previously reported values.[6]

Methyl 2-chloro-2-cyclohexylideneacetate (**25**):[7] Observed in 7% yield from the treatment of **20** with $SnCl_4$ following General Procedure B (entry 2,Table S1). Yield was determined by quantitative ^1H NMR using 4-chlorobenzaldehyde as an internal standard. ^1H matched previously reported values.[7]

Methyl 2-(chloromethyl)cyclohex-1-enecarboxylate (**27**): Obtained from **20** (43 mg, 0.22 mmol) and 1M $SnCl_4$ (0.22 mL, 0.22 mmol) following General Procedure B. A yield of 66% was determined by quantitative ^1H NMR using 4-chlorobenzaldehyde as an internal standard (entry 2, Table S1). Due to the instability to chromatography, silica gel flash column chromatography (100% CH_2Cl_2) provided a diminished 5.2 mg (12 % yield) of the title compound, which was used for characterization: R_f = 0.88 (100% CH_2Cl_2); ^1H NMR (500 MHz, $CDCl_3$): δ 4.40 (s, 2H), 3.75 (s, 3H), 2.29-2.34 (m, 4H), 1.59-1.67 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 168.2, 143.3, 129.1, 51.7, 44.9, 29.0, 26.7, 21.9, 21.8. MS (ESI): Calculated for $[C_9H_{14}ClO_2]^+$: 189.0682. Found: 189.0665.

Table S2. Treatment of 28 with Lewis acids following General Procedure B



28 **29** **30a**, X = Cl; **30b**, X = OTf

Entry	Lewis Acid (1 equiv)	Solvent	Temp	Yield 29 (%)	Compound	Yield 30 (%)
1	$(C_6F_5)_3B$	CH_2Cl_2	rt	0%	-	-
2	$SnCl_4$	CH_2Cl_2	0 °C	Inseparable mixture	**30a**	33%
3	$Sc(OTf)_3$	CH_2Cl_2	rt	24%	**30b**	25% (47%)[a]
4	$Sc(OTf)_3$	MeCN	40 °C	24%	**30b**	0%
5	$Sc(OTf)_3$ (2 equiv)	CH_2Cl_2	rt	26%	**30b**	25%
6	$In(OTf)_3$	CH_2Cl_2	0 °C	17%	**30b**	28%
7	TMSOTf	CH_2Cl_2	0 °C	6%	**30b**	62%
8	$Eu(fod)_3$	CH_2Cl_2	40 °C	0%	-	-
9	$Dy(OTf)_3$	MeCN	30 °C	13%	**30b**	-

[a]Yield in parentheses was determined by ^{19}F NMR using 4-fluorobenzophenone as internal standard

2-Methyl-2,3,5,6,7,8-hexahydrocyclohepta[*c*]pyrrol-1(4*H*)-one (**29**): Obtained from **28** following General Procedure B. Results summarized in Table S2. R_f = 0.18 (hexanes/EtOAc 1:1 on silica gel); ^1H NMR (500 MHz, $CDCl_3$): δ 3.71 (s, 2H), 3.00 (s, 3H), 2.40 (td, *J* = 5.0, 1.2 Hz, 2H), 2.36 (dd, *J* = 6.7, 5.8 Hz, 2H), 1.78 (tt, *J* = 6.0, 3.8 Hz, 2H), 1.64 (dddd, *J* = 11.5, 7.4, 4.8, 2.1 Hz, 2H), 1.59 (ddt, *J* = 11.5, 7.6, 4.0 Hz, 2H); ^{13}C NMR (125 MHz, CDCl3) δ 172.7, 151.6, 134.8, 55.7, 31.1, 29.7, 29.1, 27.3, 27.2, 25.2. MS (ESI): Calculated for $[C_{10}H_{16}NO]^+$: 166.1232. Found: 166.1232.

2-Chloro-2-cylcohexylidene-*N*,*N*-dimethylacetamide (**30a**): Obtained from **28** (50.6 mg, 0.24 mmol) and 1 M $SnCl_4$ (0.24 mL, 0.24 mmol) in CH_2Cl_2 following General Procedure B (entry 2, Table S2). Silica gel flash column chromatography (hexanes/EtOAc, gradient

elution 0 to 50% EtOAc) gave 16.1 mg (33% yield) of the title compound as a colorless oil: R_f = 0.40 (hexanes/EtOAc 1:1 on silica gel); ^{1}H NMR (500 MHz, $CDCl_3$): δ 3.03 (s, 3H), 3.00 (s, 3H), 2.37 (t, *J* = 6.0 Hz, 2H), 2.16 (t, *J* = 5.2 Hz, 2H), 1.54-1.66 (m, 6H); ^{13}C NMR (125 Mhz, $CDCl_3$) δ 166.2, 139.3, 114.8, 37.9, 34.5, 31.7, 29.8, 27.2, 26.6, 26.0. MS (ESI): Calculated for $[C_{10}H_{17}ClNO]^+$: 202.0999. Found: 202.1001.

1-Cyclohexylidene-2-(dimethylamino)-2-oxoethyl trifluoromethanesulfonate (**30b**): Obtained from **28** following General Procedure B. Lewis acids and yields summarized in entries 3-7 and 9, Table S2. R_f = 0.10 (hexanes/EtOAc 1:1 on silica gel); ^{1}H NMR (500 MHz, CDCl3): δ 3.05 (s, 3H), 3.00 (s, 3H), 2.36 (br s, 2H), 2.21 (t, *J* = 5.9 Hz, 2H), 1.55-1.69 (m, 6H); ^{13}C NMR (125 MHz, CDCl3) δ 162.4, 138.3, 131.7, 118.4 (q, *J* = 321 Hz), 38.1, 34.8, 29.3, 28.0, 26.8, 26.5, 25.7; ^{19}F (471 MHz, CDCl3): δ −73.06 (s, 3F). MS (ESI): Calculated for $[C_{11}H_{17}F_3NO_4S]^+$: 316.0830. Found: 316.0829.

V) Computational details

All DFT calculations were conducted with the Gaussian 16 software package.[8] Geometry optimizations of all the minima and transition states were performed using B3LYP[9-10] functional with 6-311+G(d,p) basis set, including solvation energy corrections and Grimme's dispersion corrections.[11] To confirm whether each optimized stationary point is an energy minimum or a transition state, as well as evaluate the zero-point vibrational energy and thermal corrections at 298 K, the vibrational frequencies were computed at the same level of theory as for the geometry optimizations. The solvation energies were evaluated by a self-consistent reaction field (SCRF) using the PCM model.[12-14] Extensive conformational searches for the intermediates and transition states have been conducted to ensure that the lowest energy conformers were located. The 3D diagrams of molecules were generated using CYLView.[15]

VI) Computations on the effects of triflate anion on chemoselectivity.

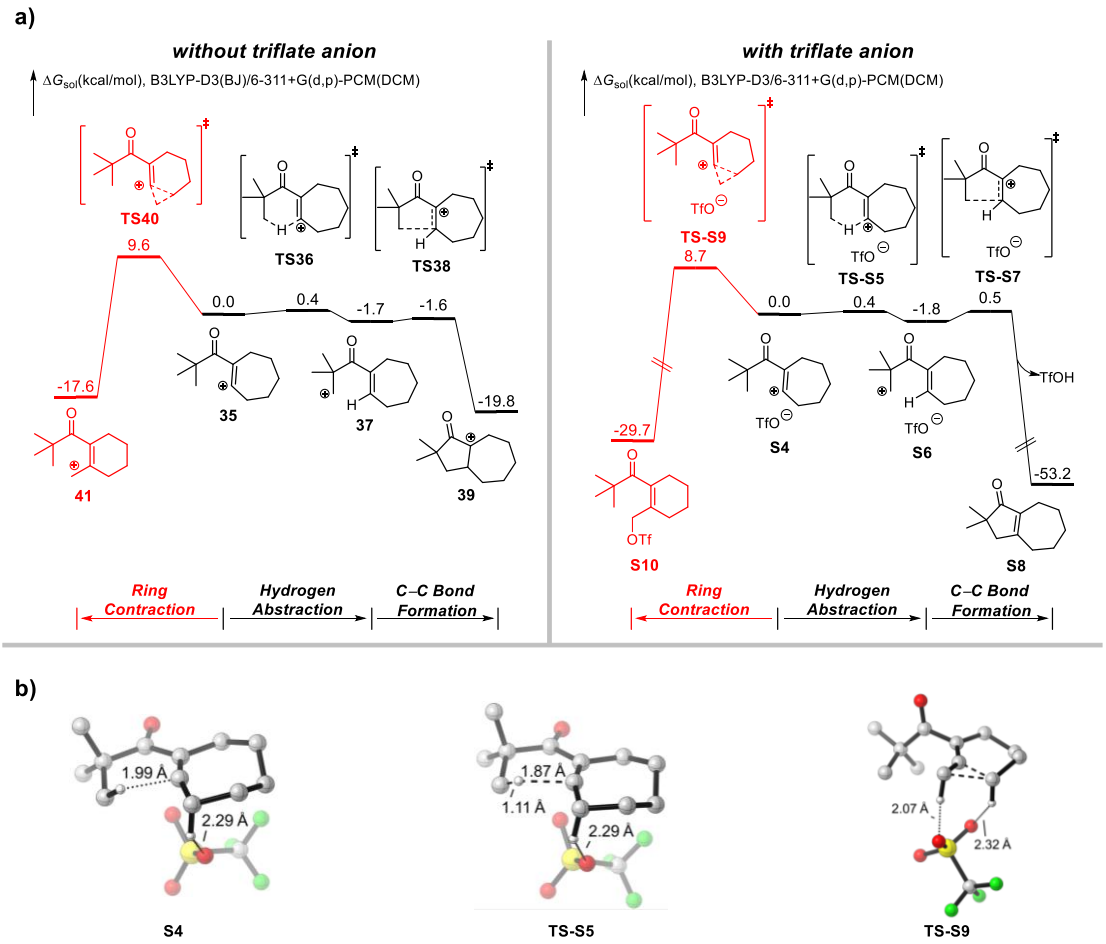


Figure S1. (a) Free energy diagram of chemoselectivity-determining processes of ketone vinyl cation, with and without triflate anion. (b) Optimized structures of key intermediate and transition states, trivial hydrogens are omitted for clarity.

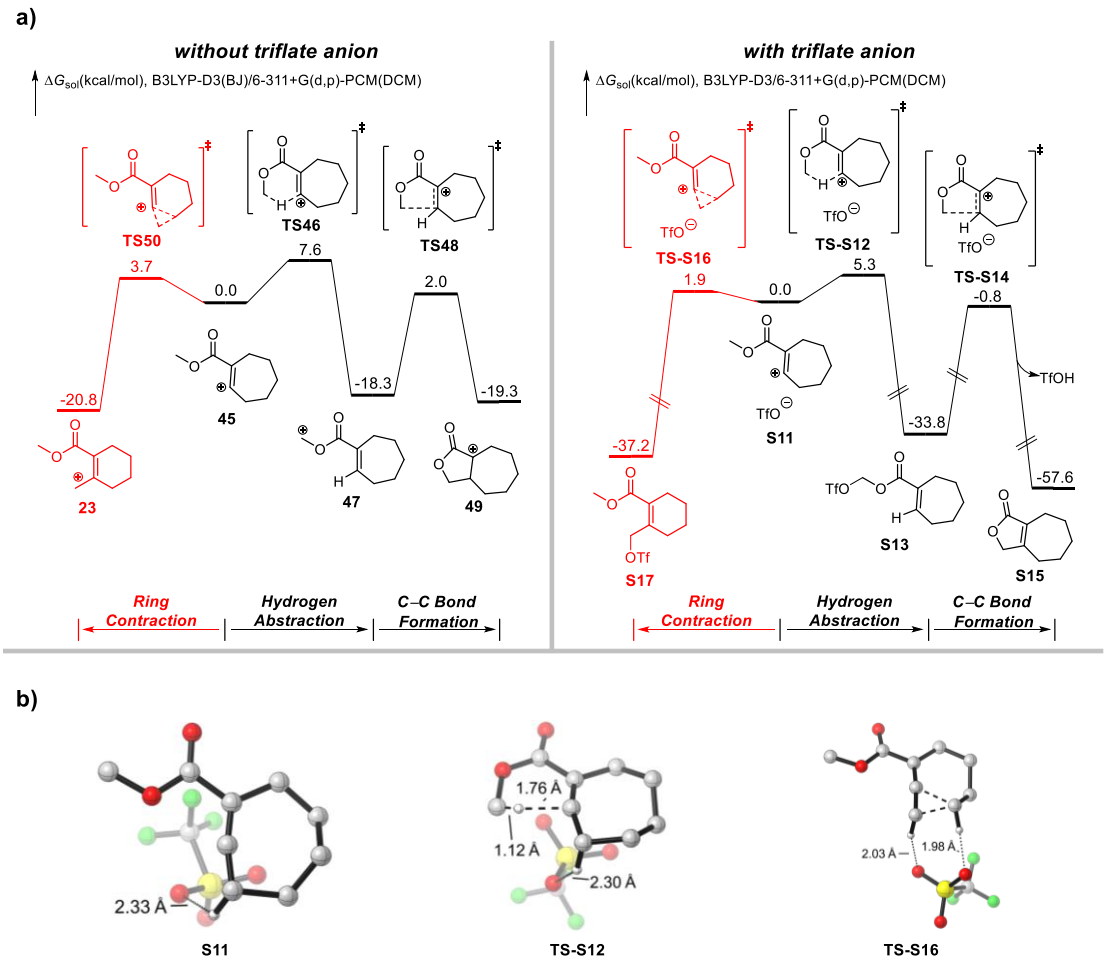


Figure S2. (a) Free energy diagram of chemoselectivity-determining processes of ester vinyl cation, with and without triflate anion. (b) Optimized structures of key intermediate and transition states, trivial hydrogens are omitted for clarity.

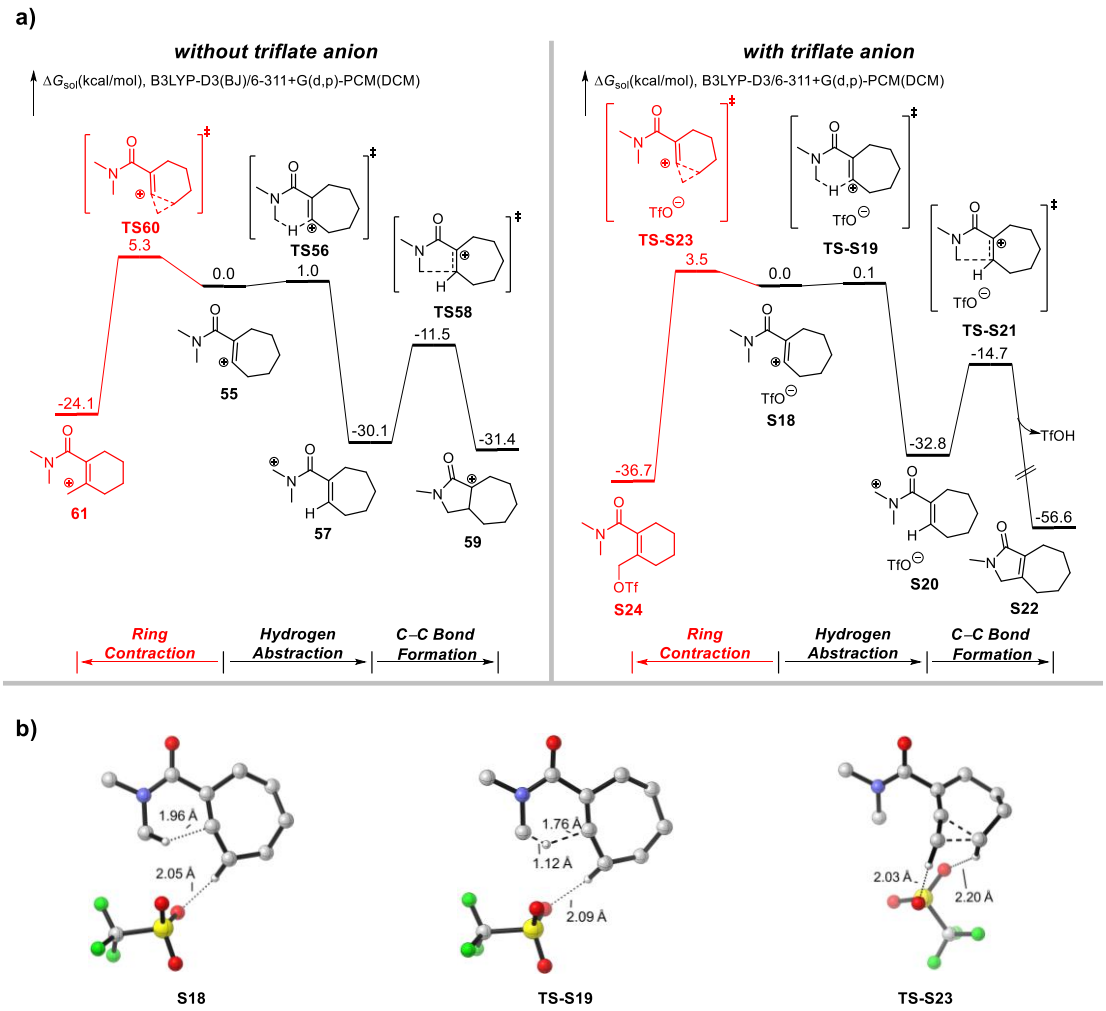


Figure S3. (a) Free energy diagram of chemoselectivity-determining processes of amide vinyl cation, with and without triflate anion. (b) Optimized structures of key intermediate and transition states, trivial hydrogens are omitted for clarity.

VII) Computations on the effects of DCM solvent on chemoselectivity.

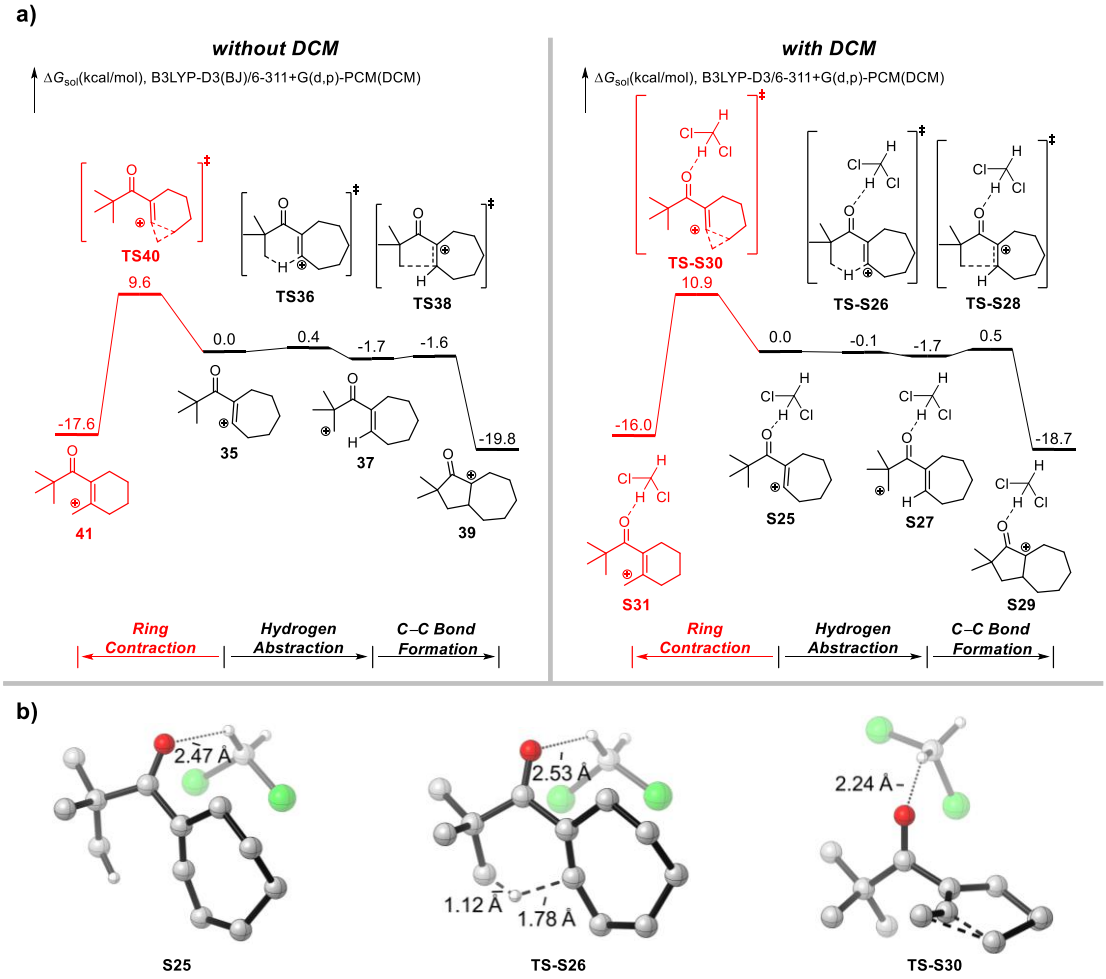


Figure S4. (a) Free energy diagram of chemoselectivity-determining processes of ketone vinyl cation, with and without DCM solvent. (b) Optimized structures of key intermediate and transition states, trivial hydrogens are omitted for clarity.

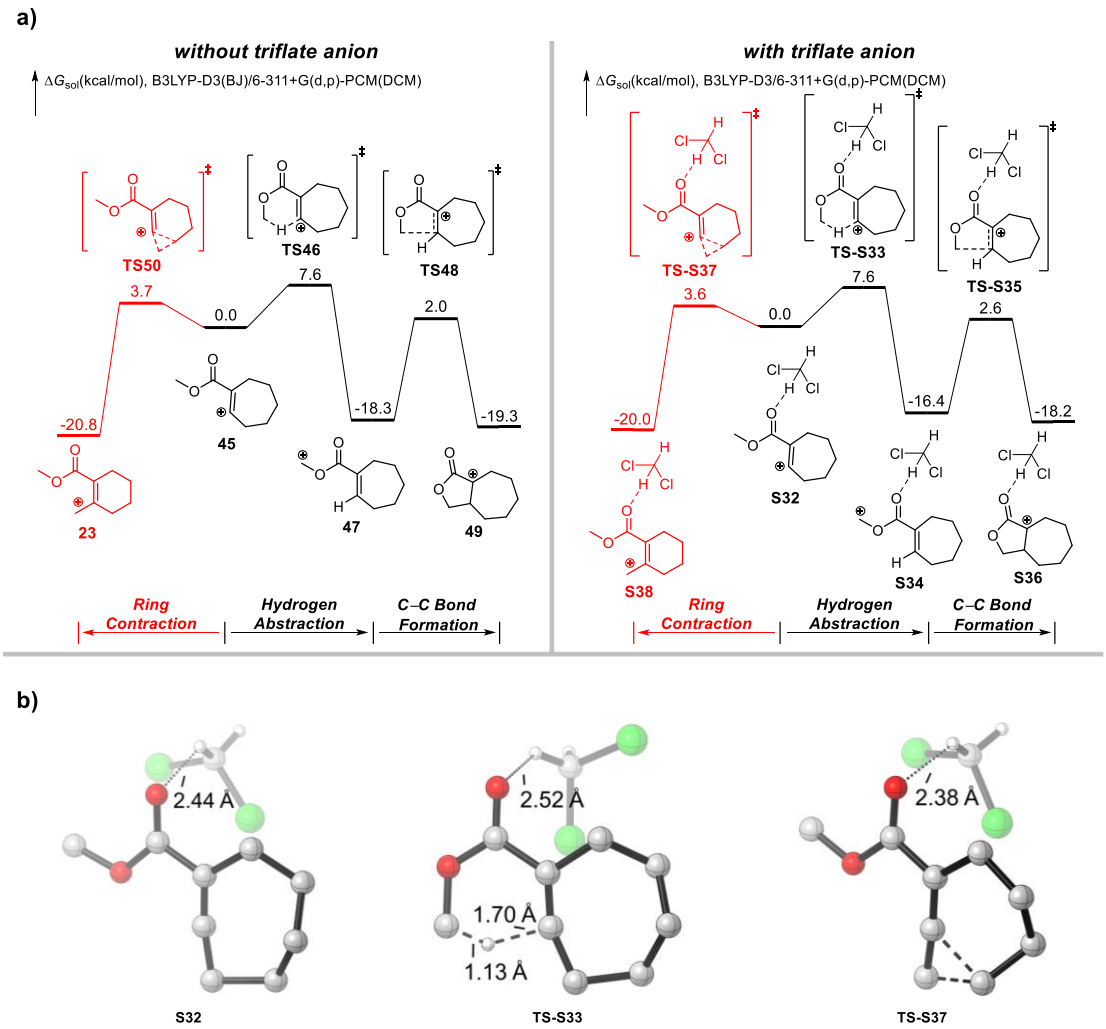


Figure S5. (a) Free energy diagram of chemoselectivity-determining processes of ester vinyl cation, with and without DCM solvent. (b) Optimized structures of key intermediate and transition states, trivial hydrogens are omitted for clarity.

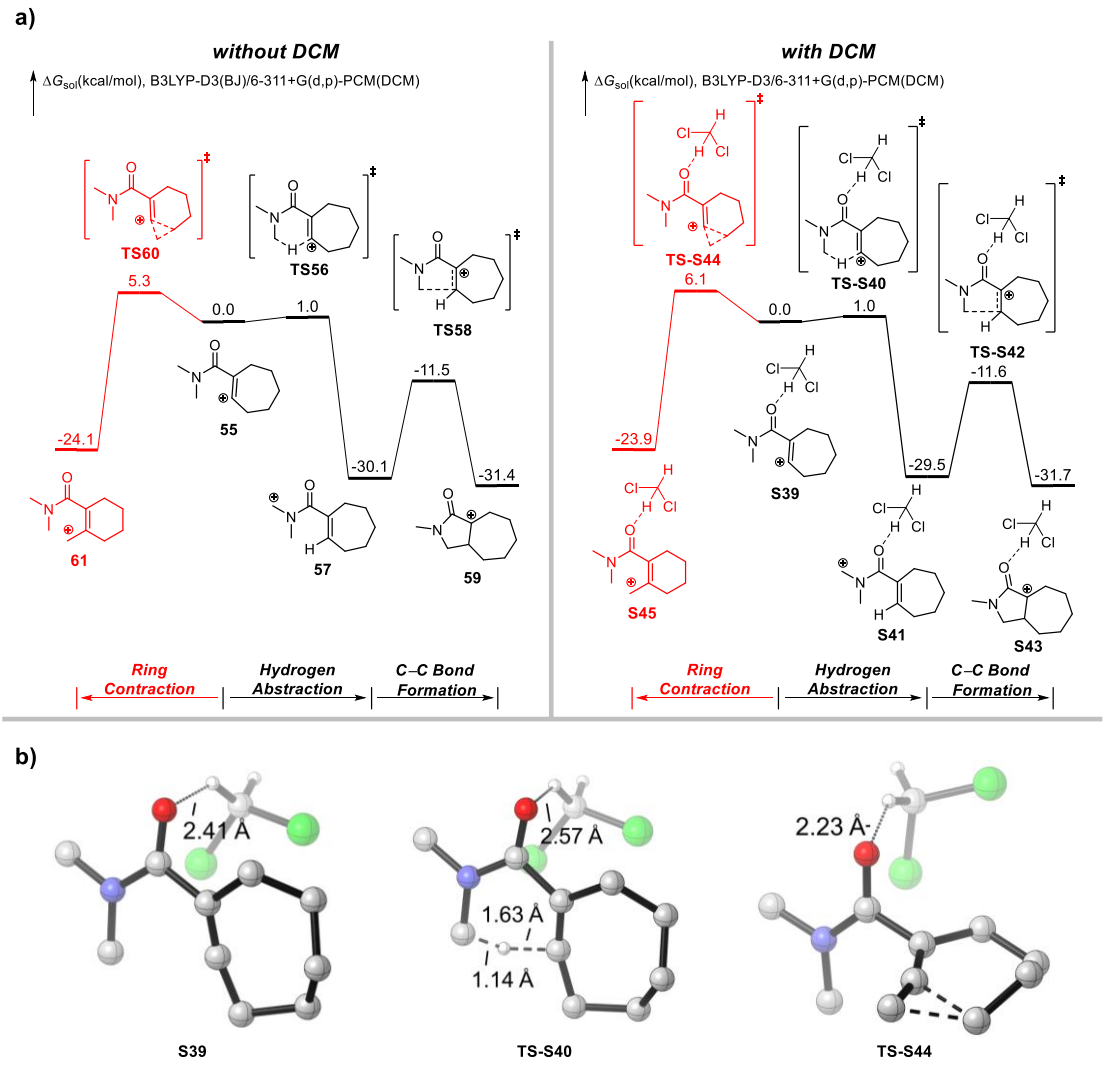


Figure S6. (a) Free energy diagram of chemoselectivity-determining processes of amide vinyl cation, with and without DCM solvent. (b) Optimized structures of key intermediate and transition states, trivial hydrogens are omitted for clarity.

VIII) Energies, enthalpies, and free energy of the calculated structures

Zero-point correction (ZPE), thermal correction to enthalpy (Δ*H*), thermal correction to Gibbs free energy (Δ*G*), energies (*E*), enthalpies (*H*), Gibbs free energies (*G*) (in Hartree) and imaginary frequencies of the transition states calculated at the B3LYP-D3/6-311+G(d,p)-PCM(Dichloromethane)

Structures	*ZPE*	*tcH*	*tcG*	*E*	*H*	*G*	Imaginary Frequency
21	0.203982	0.216666	0.164964	-501.134047	-500.917381	-500.969083	
23	0.203948	0.216410	0.165781	-501.179729	-500.963319	-501.013948	
31	0.294578	0.311531	0.250982	-653.455625	-653.144094	-653.204643	
TS32	0.291126	0.308727	0.247302	-653.427412	-653.118685	-653.180110	270.5*i*
33	0.283317	0.298707	0.242701	-543.879261	-543.580554	-543.636560	
TS34	0.281872	0.297047	0.241007	-543.874660	-543.577613	-543.633653	131.8*i*
35	0.282535	0.297845	0.242154	-543.888435	-543.590590	-543.646281	
TS36	0.282123	0.296666	0.242939	-543.888551	-543.591885	-543.645612	195.9*i*
37	0.283283	0.297684	0.244085	-543.893001	-543.595317	-543.648916	
TS38	0.282606	0.296691	0.243303	-543.892193	-543.595502	-543.648890	330.6*i*
39	0.284618	0.298597	0.246256	-543.924097	-543.625500	-543.677841	
TS40	0.281324	0.296285	0.241275	-543.872212	-543.575927	-543.630937	237.1*i*
41	0.282713	0.298166	0.241612	-543.915872	-543.617706	-543.674260	
42	0.216171	0.229974	0.176243	-610.725549	-610.495575	-610.549306	
TS43	0.211917	0.226722	0.170381	-610.696001	-610.469279	-610.525620	143.8*i*
TS44	0.203146	0.215288	0.165694	-501.130970	-500.915682	-500.965276	143.7*i*
45	0.204002	0.216544	0.166006	-501.146857	-500.930313	-500.980851	
45-trans	0.204309	0.216346	0.167787	-501.136136	-500.919790	-500.968349	
TS46	0.202893	0.214299	0.166708	-501.135428	-500.921129	-500.968720	199.8*i*
47	0.203369	0.216182	0.164992	-501.174958	-500.958776	-501.009966	
TS48	0.204957	0.215638	0.169899	-501.147605	-500.931967	-500.977706	239.9*i*
49	0.205353	0.216226	0.169812	-501.181391	-500.965165	-501.011579	
TS50	0.203056	0.215168	0.165529	-501.140546	-500.925378	-500.975017	220.9*i*
51	0.256540	0.272035	0.214702	-630.183623	-629.911588	-629.968921	
TS52	0.252900	0.268967	0.210567	-630.156932	-629.887965	-629.946365	317.4*i*
53	0.244973	0.259317	0.204105	-520.610163	-520.350846	-520.406058	
TS54	0.243758	0.257527	0.204209	-520.597426	-520.339899	-520.393217	164*i*
55	0.244168	0.258226	0.204577	-520.608293	-520.350067	-520.403716	
TS56	0.243407	0.256413	0.205420	-520.607597	-520.351184	-520.402177	187.8*i*
57	0.247425	0.260494	0.209222	-520.660942	-520.400448	-520.451720	
TS58	0.246089	0.258405	0.209013	-520.631002	-520.372597	-520.421989	342.9*i*
59	0.246786	0.259236	0.209500	-520.663232	-520.403996	-520.453732	
TS60	0.243142	0.257082	0.202872	-520.598208	-520.341126	-520.395336	148.6*i*
61	0.244979	0.258878	0.205792	-520.647911	-520.389033	-520.442119	
N2	0.005572	0.008877	-0.01286	-109.5608662	-109.5519892	-109.5737262	
TfOH	0.037683	0.046555	0.00412	-962.2381958	-962.1916408	-962.2340758	
S4	0.310119	0.334676	0.255167	-1505.735541	-1505.400865	-1505.480374	
TS-S5	0.309682	0.333501	0.255728	-1505.735534	-1505.402033	-1505.479806	78.3*i*
S6	0.310611	0.3343	0.25581	-1505.739025	-1505.404725	-1505.483215	
TS-S7	0.310297	0.333579	0.256156	-1505.73578	-1505.402201	-1505.479624	374.4*i*
S8	0.275174	0.28878	0.236602	-543.5676202	-543.2788402	-543.3310182	

TS-S9	0.308767	0.332996	0.252792	-1505.719231	-1505.386235	-1505.466439	279.4*i*
S10	0.314443	0.337832	0.260999	-1505.788692	-1505.45086	-1505.527693	
S11	0.231534	0.253281	0.17882	-1462.992023	-1462.738742	-1462.813203	
TS-S12	0.230792	0.251246	0.180457	-1462.98528	-1462.734034	-1462.804823	193.5*i*
S13	0.236478	0.256107	0.185471	-1463.052511	-1462.796404	-1462.86704	
TS-S14	0.231892	0.251784	0.18107	-1462.99549	-1462.743706	-1462.81442	179.1*i*
S15	0.196437	0.206728	0.16171	-500.8325948	-500.6258668	-500.6708848	
TS-S16	0.230563	0.251797	0.176326	-1462.986531	-1462.734734	-1462.810205	185.7*i*
S17	0.235823	0.25609	0.185181	-1463.057636	-1462.801546	-1462.872455	
S18	0.271057	0.294354	0.215585	-1482.4508	-1482.156446	-1482.235215	
TS-S19	0.270586	0.293055	0.215725	-1482.450714	-1482.157659	-1482.234989	129.3*i*
S20	0.274962	0.297225	0.221882	-1482.50933	-1482.212105	-1482.287448	
TS-S21	0.273306	0.294701	0.222001	-1482.479859	-1482.185158	-1482.257858	322.2*i*
S22	0.236209	0.248521	0.198949	-520.2902942	-520.0417732	-520.0913452	
TS-S23	0.271028	0.293995	0.215878	-1482.445472	-1482.151477	-1482.229594	166.6*i*
S24	0.275807	0.297931	0.222799	-1482.516512	-1482.218581	-1482.293713	
S25	0.31309	0.334029	0.262881	-1503.676934	-1503.342905	-1503.414053	
TS-S26	0.312182	0.33238	0.262481	-1503.676741	-1503.344361	-1503.41426	136.7*i*
S27	0.313532	0.333537	0.263934	-1503.680638	-1503.347101	-1503.416704	
TS-S28	0.312859	0.332635	0.261702	-1503.674903	-1503.342268	-1503.413201	367.4*i*
S29	0.315668	0.334985	0.268407	-1503.712323	-1503.377338	-1503.443916	
TS-S30	0.312088	0.332522	0.261698	-1503.658332	-1503.32581	-1503.396634	232.4*i*
S31	0.313627	0.334428	0.262636	-1503.702137	-1503.367709	-1503.439501	
S32	0.234474	0.252532	0.185456	-1460.933859	-1460.681327	-1460.748403	
TS-S33	0.233286	0.250249	0.186466	-1460.922817	-1460.672568	-1460.736351	202.6*i*
S34	0.234848	0.25258	0.187644	-1460.962113	-1460.709533	-1460.774469	
TS-S35	0.23538	0.251693	0.189311	-1460.9336	-1460.681907	-1460.744289	240.3*i*
S36	0.236747	0.252748	0.192867	-1460.970325	-1460.717577	-1460.777458	
TS-S37	0.233696	0.251307	0.185325	-1460.928011	-1460.676704	-1460.742686	215.4*i*
S38	0.234446	0.252456	0.185253	-1460.965481	-1460.713025	-1460.780228	
S39	0.275141	0.294555	0.225816	-1480.397572	-1480.103017	-1480.171756	
TS-S40	0.274228	0.292582	0.226783	-1480.396936	-1480.104354	-1480.170153	182.9*i*
S41	0.277749	0.296356	0.229606	-1480.448345	-1480.151989	-1480.218739	
TS-S42	0.276426	0.294332	0.229211	-1480.41943	-1480.125098	-1480.190219	311.8*i*
S43	0.277691	0.295538	0.230165	-1480.452472	-1480.156934	-1480.222307	
TS-S44	0.273995	0.293279	0.2244	-1480.38642	-1480.093141	-1480.16202	147.9*i*
S45	0.275467	0.294891	0.225692	-1480.435518	-1480.140627	-1480.209826	

IX) Cartesian Coordinates for the Optimized Structures

21

C	2.47389608	-1.37958541	-0.41085500
C	3.40557956	-0.16961813	-0.32410886
C	2.63915948	1.14327169	-0.50269566
C	1.49950619	1.29146519	0.51533543
C	0.61789651	0.04585714	0.46167075
C	1.33630835	-1.31417270	0.61652040
H	3.30438226	2.00006696	-0.36904363
H	3.91543245	-0.16881332	0.64543956
H	4.17933606	-0.24876400	-1.09045941
H	2.04816156	-1.46408862	-1.41509927
H	3.02203832	-2.30588936	-0.21713699
H	1.89207457	1.32192161	1.53717342
H	0.90218160	2.18359911	0.34329482
H	1.71698789	-1.30873771	1.64286841
H	0.64055720	-2.14383484	0.51198076
H	2.22880036	1.21081722	-1.51458187
C	-0.63676022	0.03079677	0.24846305
C	-2.02682225	0.25952780	0.01541244
C	-4.24792008	-0.47382784	-0.28600925
H	-4.72049255	-1.44952644	-0.28346255
H	-4.62301912	0.15186046	0.52067367
H	-4.35786588	0.01832188	-1.24973119
O	-2.23752735	1.45303673	-0.08545941
O	-2.82535599	-0.75758019	-0.05188161

23

C	2.33241647	1.02784793	-0.05259186
C	2.85072154	-0.30949739	-0.58738533
C	2.24600138	-1.46909512	0.20368223
C	0.72051379	-1.46156727	0.09675172
C	0.08758732	-0.13658782	0.14044627
C	0.82171339	1.06617281	0.04263885
H	2.61747120	-2.42853961	-0.15781391
H	2.59385811	-0.40911000	-1.64746058
H	3.93914927	-0.32958649	-0.51865332
H	2.73414305	1.20435853	0.95090435
H	2.66622229	1.85762255	-0.67766956
H	0.39003635	-1.87203899	-0.87842433
H	0.22697334	-2.12122950	0.82100179
H	2.53041089	-1.38918413	1.25680659
C	-1.40282354	-0.12795629	0.34770663
C	-3.53151756	-0.28686977	-0.67397649
H	-3.87668649	-0.39454997	-1.69668376
H	-3.81028508	-1.14805474	-0.07001154
H	-3.90477229	0.63305300	-0.22771364
O	-1.83524614	-0.08024043	1.47318756
O	-2.07495235	-0.21852369	-0.77735675
C	0.12351546	2.24172052	0.02476100
H	-0.95587552	2.28174510	0.10690111
H	0.63905214	3.19093477	-0.07023603

31

C	2.77259409	-1.60589021	-0.29836684

C	3.91775174	-0.59817361	-0.20021879
C	3.41847948	0.83769264	-0.35819170
C	2.27052623	1.15490250	0.64839403
C	1.20143720	0.13619305	0.45824492
C	1.63636442	-1.26258234	0.71088981
H	4.21889482	1.55866051	-0.18293205
H	4.41895634	-0.70736483	0.76739385
H	4.66310114	-0.81193634	-0.97071119
H	2.35181635	-1.61366275	-1.30753897
H	3.11557789	-2.61862281	-0.08014998
H	2.66091014	1.05469228	1.66551841
H	1.92677050	2.17966125	0.51987437
H	2.05664510	-1.29279056	1.72176015
H	0.82945728	-1.98369768	0.63977662
H	3.04959733	1.00262106	-1.37491161
C	-0.05446818	0.44188724	-0.01188253
C	-1.17403359	-0.56455252	-0.35048484
C	-2.61019261	-0.28813906	0.09122134
C	-3.28982518	0.60758377	-0.97525538
H	-3.23044149	0.15158956	-1.96496458
H	-4.34378190	0.71328153	-0.71018297
H	-2.86760578	1.61115721	-1.02793510
C	-2.63861441	0.38843540	1.47407957
H	-3.67634835	0.47821206	1.79999671
H	-2.10221742	-0.20515289	2.21768904
H	-2.21962271	1.39589460	1.46948276
C	-3.34991945	-1.63471882	0.15458691
H	-4.38369582	-1.45713651	0.45632557
H	-3.35146220	-2.13231519	-0.81516443
H	-2.88796996	-2.30350069	0.88355116
O	-0.82064977	-1.56232368	-0.92339051
N	-0.32246412	1.75757848	-0.22700892
N	-0.58218512	2.81418435	-0.44785583

TS32

C	-2.83001447	-1.61027507	0.28757241
C	-3.86365576	-0.52729594	0.59201491
C	-3.18578734	0.81633614	0.86571693
C	-2.25830756	1.23023495	-0.29434153
C	-1.26468469	0.13718386	-0.57775895
C	-1.90447523	-1.22282755	-0.87984318
H	-3.92638642	1.60726572	0.99985150
H	-4.54943998	-0.42559101	-0.25630685
H	-4.46552986	-0.81969077	1.45554059
H	-2.22122030	-1.81331065	1.17445487
H	-3.31761886	-2.54946632	0.01376915
H	-2.84865845	1.35868768	-1.20752648
H	-1.76495468	2.17277040	-0.07328207
H	-2.48356730	-1.07494030	-1.79730396
H	-1.15553135	-1.98306401	-1.07222151
H	-2.59906826	0.76356142	1.78809809
C	0.04279338	0.18563508	-0.54240656
C	1.27562795	-0.63832882	-0.51434291
C	2.49217107	-0.37750114	0.35812375
C	3.21130912	-1.72670042	0.54551220
H	3.52638275	-2.14748078	-0.40931556
H	4.09704070	-1.56588541	1.16220834

H	2.56792032	-2.45183288	1.04723292
C	2.07542092	0.17556757	1.73460887
H	2.96585047	0.25180887	2.36104300
H	1.62787145	1.16770622	1.68722108
H	1.37115961	-0.49552724	2.23110636
C	3.44974652	0.59164028	-0.37837208
H	4.35459028	0.69565241	0.22352855
H	3.73226864	0.19129935	-1.35358677
H	3.03435059	1.58729796	-0.52029791
O	1.11918506	-1.62066131	-1.20993781
N	0.53984331	2.07185010	-0.26924735
N	0.83907139	3.11039961	-0.44805702

33

C	-2.89200302	-1.42160697	0.37681640
C	-3.89584287	-0.26794460	0.33583308
C	-3.20341227	1.08370768	0.52628433
C	-2.09511519	1.31788363	-0.51341841
C	-1.14428408	0.12832284	-0.49833416
C	-1.77785051	-1.25707373	-0.66947635
H	-3.91945696	1.90359287	0.43070251
H	-4.42708176	-0.27762960	-0.62219206
H	-4.64640136	-0.40828391	1.11666838
H	-2.44126986	-1.49745443	1.37100529
H	-3.38682017	-2.37511076	0.17519739
H	-2.51419228	1.34716824	-1.52502158
H	-1.54880080	2.24085700	-0.33417845
H	-2.18772550	-1.26077676	-1.68480731
H	-1.03495717	-2.04897457	-0.59859468
H	-2.77143712	1.14946492	1.52941419
C	0.11807983	0.21553796	-0.29146993
C	1.45851506	0.63571339	-0.03871410
C	2.66505186	-0.22639707	0.10328777
C	3.88962331	0.64969560	0.38162284
H	3.77683717	1.20626197	1.31370773
H	4.77023643	0.01102264	0.46807090
H	4.06009728	1.36120504	-0.42833907
C	2.82230715	-1.01501849	-1.21849941
H	3.67298923	-1.69097112	-1.11557490
H	1.93840603	-1.61895196	-1.43794018
H	3.00967462	-0.34587326	-2.05998210
C	2.39075485	-1.20661473	1.26873674
H	3.25358875	-1.86656664	1.37278551
H	2.24531176	-0.67391414	2.21017651
H	1.51362245	-1.82972598	1.07657700
O	1.32570917	1.85262296	0.02803912

TS34

C	-3.19467374	-1.13500384	0.50227798
C	-3.68039090	0.30575971	0.33144529
C	-2.54887451	1.33284503	0.43914551
C	-1.47615901	1.17635021	-0.62905815
C	-1.02374698	-0.54692864	-0.49628584
C	-2.11262084	-1.51184978	-0.53622920
H	-2.94649870	2.34383104	0.31005955
H	-4.17867475	0.41603938	-0.63782768
H	-4.42864437	0.52483318	1.09536410

H	-2.78527000	-1.28033182	1.50542997
H	-4.02246186	-1.83474039	0.38196212
H	-1.81564887	1.15943660	-1.66354089
H	-0.70642818	1.95635625	-0.54512232
H	-2.53016297	-1.51671633	-1.54821976
H	-1.68677152	-2.49826212	-0.34156729
H	-2.08087697	1.30181870	1.42671806
C	0.01040857	0.11004560	-0.34507127
C	1.34190470	0.72215954	-0.12212308
C	2.46301975	-0.27427535	0.13190906
C	3.75863895	0.49869288	0.39819373
H	3.66586427	1.13569760	1.27941846
H	4.56769489	-0.21387509	0.56968945
H	4.02648675	1.12757958	-0.45223647
C	2.61070097	-1.16395094	-1.12340593
H	3.42778933	-1.86816208	-0.95544136
H	1.70736350	-1.74279307	-1.32735151
H	2.84919107	-0.56584547	-2.00522645
C	2.08442850	-1.14106223	1.35333601
H	2.90141383	-1.83654552	1.55422938
H	1.93156065	-0.52721753	2.24352286
H	1.18172267	-1.72988798	1.17646593
O	1.43979578	1.92592490	-0.15401128

35

C	-2.64266071	-1.34024723	0.46010867
C	-3.41080063	-0.21951690	-0.26225555
C	-3.06126441	1.19346160	0.21058759
C	-1.68414984	1.80465172	-0.28742726
C	-0.74269185	0.74887837	-0.15791789
C	-1.22586172	-1.61890774	-0.03079303
H	-3.79515930	1.90816261	-0.16632576
H	-3.29032644	-0.30332972	-1.34793309
H	-4.47532923	-0.35854203	-0.06119867
H	-2.61873415	-1.12635165	1.53341122
H	-3.19324421	-2.27689290	0.34523428
H	-1.75968228	2.12433767	-1.32978560
H	-1.44481199	2.66000027	0.34728300
H	-1.23163155	-2.01648504	-1.05027468
H	-0.73379088	-2.35590407	0.60649857
H	-3.06939953	1.23708793	1.30049595
C	-0.25466339	-0.42521364	-0.09339466
C	1.24632194	-0.80266423	-0.21202488
C	2.26562188	0.30072912	0.07387868
C	2.32171846	0.45604560	1.61262777
H	2.61382660	-0.48111476	2.08952316
H	3.06689321	1.21471593	1.85974850
H	1.36146031	0.77396787	2.02430111
C	1.81417889	1.60077756	-0.57300390
H	0.80071721	1.88866252	-0.22942859
H	2.44051304	2.43322285	-0.24593793
H	1.80676462	1.55280893	-1.66208814
C	3.63203836	-0.13655497	-0.47506691
H	4.37456705	0.62970013	-0.24633181
H	3.94727330	-1.07508374	-0.01855571
H	3.59652639	-0.27362632	-1.55733263
O	1.50790786	-1.94206375	-0.46616882

TS36

C	-2.63506441	-1.36221722	0.44998933
C	-3.41456222	-0.23468029	-0.24878104
C	-3.06804196	1.17205018	0.24434081
C	-1.70195438	1.79587896	-0.25694353
C	-0.74074641	0.75078184	-0.14830996
C	-1.22085065	-1.62502083	-0.05663679
H	-3.81115367	1.88845684	-0.11103571
H	-3.30053573	-0.30062091	-1.33648534
H	-4.47691879	-0.38315785	-0.04300084
H	-2.60340866	-1.16462267	1.52627006
H	-3.18151925	-2.30006466	0.32526893
H	-1.78704939	2.12629503	-1.29544967
H	-1.46393805	2.64839538	0.38202515
H	-1.23346294	-2.00446222	-1.08311402
H	-0.72163197	-2.37295754	0.56213639
H	-3.06614014	1.19637828	1.33509131
C	-0.25618357	-0.42769589	-0.10374569
C	1.24423780	-0.79555437	-0.22967185
C	2.25505762	0.31481800	0.06446469
C	2.33022452	0.43637667	1.60554901
H	2.63849635	-0.50839408	2.05638901
H	3.07014296	1.19753471	1.86040175
H	1.37172763	0.73355765	2.03654781
C	1.77496568	1.61871542	-0.54688823
H	0.74135328	1.85562161	-0.20921527
H	2.35618990	2.46642966	-0.17880373
H	1.77951528	1.60806355	-1.63671156
C	3.61872255	-0.09184604	-0.51439072
H	4.35391302	0.68082188	-0.28379412
H	3.95349385	-1.03363996	-0.07904646
H	3.56756698	-0.21065071	-1.59815106
O	1.51677475	-1.93031337	-0.49341065

37

C	-2.60808002	-1.36443102	0.36859678
C	-3.44759185	-0.17975475	-0.12634500
C	-2.96890537	1.19657144	0.34290346
C	-1.67947030	1.71738023	-0.32607474
C	-0.51955808	0.82519160	-0.08825729
C	-1.25255992	-1.55741417	-0.31720521
H	-3.73834248	1.94136180	0.12426046
H	-3.50822834	-0.19882259	-1.22128204
H	-4.46944266	-0.31406994	0.23818566
H	-2.45571382	-1.27969629	1.45002188
H	-3.17417624	-2.28524579	0.20715420
H	-1.82358147	1.79726488	-1.41053883
H	-1.46015177	2.72030704	0.04267672
H	-1.39529880	-1.66458554	-1.40079411
H	-0.78534963	-2.48305187	0.02303491
H	-2.83086829	1.19168241	1.42816926
C	-0.23614277	-0.46450027	-0.12867434
C	1.21604991	-0.85987853	-0.03500541
C	2.21920034	0.31803250	0.04732929
C	2.75594197	0.38306906	1.49131495
H	3.22138383	-0.56687482	1.75408884

H	3.50535949	1.17251410	1.56962693
H	1.95774911	0.58644658	2.20865756
C	1.50294738	1.56857883	-0.33817581
H	1.74494327	2.48809837	0.19782601
H	1.30011399	1.73747190	-1.39030798
C	3.35938002	0.05011411	-0.96037663
H	4.10752541	0.84127004	-0.89788620
H	3.82696441	-0.90136917	-0.70572682
H	2.98545333	-0.00540875	-1.98393334
O	1.56775957	-2.00957569	-0.02299371
H	0.40443279	1.50474530	0.34990654

TS38

C	2.59485655	1.36915688	0.33259494
C	3.44132011	0.16259601	-0.09081445
C	2.92436709	-1.20334750	0.37171172
C	1.64033355	-1.68783010	-0.32846070
C	0.45422896	-0.83304701	-0.02834533
C	1.25060055	1.53059527	-0.39269617
H	3.68924192	-1.95846636	0.17411059
H	3.55583489	0.15995853	-1.18163446
H	4.44547569	0.29535317	0.32089041
H	2.41609929	1.33595150	1.41259324
H	3.16644952	2.28048668	0.14077066
H	1.79095745	-1.68629846	-1.41482078
H	1.42855994	-2.71789937	-0.03701722
H	1.41635849	1.52958647	-1.48002971
H	0.80184540	2.49658799	-0.15509518
H	2.76272726	-1.19434949	1.45424866
C	0.22462945	0.48483350	-0.11774019
C	-1.22110935	0.88468650	0.02618199
C	-2.19161520	-0.31471126	0.02654794
C	-2.87354470	-0.41105086	1.40382541
H	-3.38239716	0.52683012	1.62602940
H	-3.61137160	-1.21514029	1.39680455
H	-2.15142791	-0.60688309	2.20038293
C	-1.37779417	-1.53645891	-0.29202197
H	-0.31861855	-1.38232320	0.64358018
H	-1.57963909	-2.44672176	0.27389202
H	-1.15897109	-1.75572183	-1.33182086
C	-3.23129704	-0.08312004	-1.09424010
H	-3.93920003	-0.91255477	-1.12617616
H	-3.77365349	0.83764326	-0.87648945
H	-2.75397839	0.01514739	-2.07092013
O	-1.57965834	2.03131004	0.10031021

39

C	2.61741793	1.32344164	0.40338607
C	3.37864979	0.14232773	-0.20253052
C	2.86829912	-1.24291680	0.20386628
C	1.51913887	-1.64469434	-0.39245491
C	0.29428368	-0.85644587	0.08783509
C	1.20881279	1.58002106	-0.14975396
H	3.59813511	-1.99021742	-0.11802770
H	3.38253706	0.22860934	-1.29532733
H	4.42129387	0.22978459	0.11342832
H	2.53333122	1.20086769	1.48847776

H	3.18178577	2.24250848	0.23647415
H	1.54582918	-1.55959662	-1.48399861
H	1.31618151	-2.69308008	-0.16405270
H	1.26295458	1.64785117	-1.26734166
H	0.79187725	2.54961977	0.13790061
H	2.82311599	-1.31182777	1.29699431
C	0.19388562	0.56942939	-0.05103109
C	-1.30554180	0.94143886	-0.10437919
C	-2.12607712	-0.32807099	0.03120641
C	-2.63540653	-0.39351404	1.49384066
H	-3.27726590	0.46143477	1.71113774
H	-3.21411995	-1.31011916	1.62027196
H	-1.81858903	-0.40388159	2.21936414
C	-1.09643572	-1.44314814	-0.25011526
H	-1.29116829	-2.34706815	0.32463620
H	-1.09939281	-1.71105612	-1.30925231
C	-3.31047102	-0.32534478	-0.94274741
H	-3.87149695	-1.25576141	-0.83599295
H	-3.97937175	0.50952375	-0.72865726
H	-2.97059251	-0.24347816	-1.97712305
O	-1.67008294	2.07783141	-0.25304232
H	0.35659299	-0.80268921	1.21831955

TS40

C	2.50542144	-1.51423151	-0.44846383
C	3.27496905	-0.31540695	0.09126041
C	2.65406795	1.01283397	-0.37615218
C	1.13479371	2.24350751	0.31482982
C	1.08021901	0.89473331	0.06055959
C	1.10241739	-1.59451998	0.15435049
H	3.21973798	1.83055369	0.08613988
H	3.33320332	-0.33711242	1.18183377
H	4.29957916	-0.29460217	-0.29131348
H	2.43910297	-1.44386392	-1.53795488
H	3.04921869	-2.43248005	-0.21953016
H	1.21781596	2.62325793	1.33210268
H	1.22083085	2.96371364	-0.49435615
H	1.13778919	-2.00090711	1.17189291
H	0.46662566	-2.27175294	-0.42007512
H	2.64961938	1.16855766	-1.45403120
C	0.44401075	-0.24682364	0.26417980
C	-1.00727085	-0.24237500	0.72766241
O	-1.18742916	-0.45992928	1.90494864
C	-2.12142866	-0.00962217	-0.28518374
C	-3.47194369	-0.35114166	0.35491895
H	-3.66736354	0.27446145	1.22718278
H	-4.26816585	-0.18650911	-0.37407104
H	-3.50557909	-1.39550381	0.67141702
C	-1.87652183	-0.88382958	-1.53140747
H	-0.91480415	-0.66405322	-2.00146517
H	-1.91249715	-1.94763982	-1.28538862
H	-2.65882679	-0.68196803	-2.26616480
C	-2.09625628	1.48310831	-0.69424762
H	-2.16733041	2.13867901	0.17736762
H	-1.19930679	1.73452946	-1.26192830
H	-2.95724222	1.68167242	-1.33633802

41

C	2.76879976	0.96825321	-0.22194173
C	3.17049895	-0.43796304	-0.67053870
C	2.60964762	-1.48152883	0.29373923
C	1.08220329	-1.41337736	0.32692300
C	0.50299419	-0.05927279	0.31929566
C	1.28516261	1.09429447	0.06386058
H	2.90709903	-2.48940775	0.00203755
H	2.79273298	-0.62816357	-1.68072879
H	4.25805936	-0.50647588	-0.71781439
H	3.30690792	1.22944664	0.69537461
H	3.04370772	1.71196504	-0.97211479
H	0.65607731	-1.90019193	-0.57035215
H	0.64035118	-1.98120757	1.15446279
H	2.99870884	-1.30889247	1.30120960
C	-0.95911485	0.04902975	0.69583063
O	-1.11914287	0.24199165	1.88249085
C	0.66999265	2.31294204	0.10112183
H	-0.37936341	2.43439855	0.33810122
H	1.23163910	3.22145156	-0.08675420
C	-2.06777000	-0.15245543	-0.32131436
C	-2.39944622	-1.66902906	-0.31267220
H	-3.24602531	-1.83604351	-0.98159728
H	-1.56960712	-2.28082678	-0.67112907
H	-2.67580423	-2.00358724	0.68846964
C	-3.30107135	0.64532519	0.13156487
H	-4.11527635	0.47095969	-0.57433016
H	-3.62981811	0.33652763	1.12391718
H	-3.09422689	1.71773510	0.15426175
C	-1.62661449	0.27662452	-1.73109773
H	-1.43476221	1.35002414	-1.78712933
H	-0.73090259	-0.24993543	-2.07107258
H	-2.42620653	0.04508347	-2.43679652

42

C	2.36373507	-1.55955420	-0.41335905
C	3.46746409	-0.50361842	-0.40463341
C	2.88961626	0.90510941	-0.52936289
C	1.81632282	1.17412483	0.56508812
C	0.77863207	0.10790758	0.49740569
C	1.29287453	-1.27521033	0.68197209
H	3.66584192	1.66505377	-0.42492208
H	4.04427778	-0.58264061	0.52320852
H	4.16141300	-0.68854888	-1.22870155
H	1.86989605	-1.58829838	-1.38905340
H	2.76612487	-2.55649010	-0.22607708
H	2.29563534	1.10284421	1.54659729
H	1.41478610	2.18045848	0.46413789
H	1.78890614	-1.30353626	1.65886240
H	0.50597241	-2.01943407	0.66203943
H	2.43043327	1.04203165	-1.51286746
C	-0.53680253	0.36753856	0.19735210
C	-1.69650429	-0.58224721	0.04876733
C	-4.03805819	-0.67462029	-0.30370331
H	-4.82251919	0.06408370	-0.43243818
H	-3.94803396	-1.30880631	-1.18380262
H	-4.20964126	-1.27837135	0.58551961

O	-1.58816877	-1.77872698	0.09623305
N	-0.88894410	1.68491140	0.01224437
N	-1.21957979	2.72786484	-0.14798874
O	-2.81848267	0.10020094	-0.13677111

TS43

C	-2.59730290	-1.46861306	0.44240355
C	-3.58241805	-0.30180643	0.37341923
C	-2.86124761	1.04124343	0.50669558
C	-1.74622629	1.19560353	-0.54433366
C	-0.80741231	0.02235671	-0.46778615
C	-1.48642180	-1.35809419	-0.61300355
H	-3.55830174	1.87155150	0.37555871
H	-4.12376535	-0.33530702	-0.57835571
H	-4.32671297	-0.39985486	1.16674321
H	-2.14233352	-1.52619591	1.43599332
H	-3.10787532	-2.41985757	0.26942466
H	-2.17854457	1.18120184	-1.55000543
H	-1.20602573	2.13054372	-0.41942230
H	-1.90185332	-1.35722698	-1.62610921
H	-0.76465032	-2.16451235	-0.53210077
H	-2.42539472	1.13993092	1.50561047
C	0.46603916	-0.00606533	-0.24749119
C	1.71117058	-0.74221249	-0.06115069
C	4.02730054	-0.77466018	0.35802208
H	3.93348924	-1.42567911	1.22483755
H	4.23696161	-1.35224815	-0.53995482
H	4.77953012	-0.01020792	0.51946090
O	1.60003855	-1.94440778	-0.14879798
N	1.12296489	1.99809740	-0.05222837
N	1.58895560	2.98287033	0.04949437
O	2.78113823	-0.03240302	0.17496320

TS44

C	-2.87124952	-1.00574892	0.52844285
C	-3.18401485	0.47503791	0.30716410
C	-1.94328607	1.36547983	0.41806542
C	-0.87392239	1.05590378	-0.61795064
C	-0.62414331	-0.69570080	-0.43437642
C	-1.81999696	-1.52880058	-0.47564587
H	-2.21404498	2.41185622	0.24529035
H	-3.63980852	0.61196955	-0.67930069
H	-3.92016549	0.80298801	1.04321968
H	-2.50199691	-1.16916703	1.54417294
H	-3.77111486	-1.60955822	0.40636582
H	-1.18990850	1.04884498	-1.65985032
H	-0.01682227	1.73322502	-0.53297740
H	-2.21636930	-1.50808820	-1.49591893
H	-1.51272382	-2.55215174	-0.25175222
H	-1.50679977	1.31493172	1.41906587
C	0.49485201	-0.20358612	-0.27913188
C	1.87685607	0.25931285	-0.07880674
C	4.06001551	-0.51631371	0.37688768
H	4.49998367	-1.49102285	0.55918887
H	4.48268390	-0.05244706	-0.51234556
H	4.17130245	0.13565249	1.24113203
O	2.18707319	1.42138219	-0.12974626

O	2.64273173	-0.78614630	0.15289234

45

C	2.18364337	-1.38844803	-0.29337747
C	2.88089119	-0.21565373	0.41946585
C	2.63755473	1.15797479	-0.20960457
C	1.20880652	1.93321840	0.04179574
C	0.37853699	0.82878223	-0.04002556
C	0.70659352	-1.58594783	0.04488924
H	3.31776598	1.89398509	0.22074812
H	2.64045221	-0.20261264	1.48715452
H	3.95984987	-0.37408658	0.35324709
H	2.29551681	-1.26826495	-1.37535826
H	2.69531857	-2.31573617	-0.02961634
H	1.20889234	2.39990834	1.02744555
H	1.09916793	2.65593213	-0.76687874
H	0.58408115	-1.96035592	1.06629187
H	0.24192481	-2.30870846	-0.62889151
H	2.77146542	1.12052674	-1.28875233
C	-0.15754351	-0.33194275	-0.02526609
C	-1.66782697	-0.46389487	0.00463120
C	-3.68845798	0.77995898	0.00504047
H	-4.05545007	0.31711427	0.91944670
H	-3.93547405	1.83652685	-0.02292896
H	-4.08114713	0.26396578	-0.86940517
O	-2.22085270	-1.52703900	0.03965093
O	-2.23385298	0.73648234	-0.01496227

TS46

C	1.96546834	-1.44841648	-0.28014677
C	2.74869522	-0.30414515	0.38394136
C	2.52031197	1.06278814	-0.25978328
C	1.15313524	1.79060098	0.06069125
C	0.12680529	0.80531087	-0.06649362
C	0.50395886	-1.59667464	0.12870523
H	3.26387049	1.77814467	0.09700356
H	2.54413915	-0.26326232	1.45948546
H	3.81431956	-0.52158924	0.28329564
H	2.02876789	-1.34608561	-1.36818685
H	2.44469118	-2.39795345	-0.03159676
H	1.15918914	2.18601587	1.08029090
H	1.03461775	2.60993312	-0.65026219
H	0.41829277	-1.88185006	1.18250603
H	0.01569968	-2.37366292	-0.46185624
H	2.61315163	0.98817847	-1.34403498
C	-0.40143820	-0.36445484	-0.01427614
C	-1.89599617	-0.65534591	-0.01719108
C	-2.21333054	1.70911941	0.08457758
H	-1.21387404	1.79319637	-0.43138497
H	-2.84925281	2.39088439	-0.47765777
H	-2.12098126	1.98762914	1.13220191
O	-2.31055370	-1.77471340	0.00443654
O	-2.71560444	0.40654959	-0.07163581

47

C	1.98538677	-1.36761825	-0.48213903
C	3.01767446	-0.24852968	-0.31548980

C	2.49126771	1.17740925	-0.49587459
C	1.45717850	1.62890340	0.56824060
C	0.09858437	1.06621958	0.35930881
C	0.86711021	-1.36902581	0.57145130
H	3.33111566	1.87296974	-0.43061809
H	3.47766055	-0.33497656	0.67608452
H	3.82031353	-0.41024055	-1.04075676
H	1.54124431	-1.32973618	-1.48215712
H	2.50084395	-2.32875954	-0.40581147
H	1.81772901	1.31443033	1.55734287
H	1.38994906	2.71598493	0.58020152
H	1.28585468	-1.23195662	1.57406079
H	0.36740366	-2.33764156	0.57443105
H	2.05916323	1.30055652	-1.49375055
C	-0.16808611	-0.26436554	0.35309234
C	-1.46092092	-0.76256018	0.13553441
C	-3.81825866	0.67245517	-0.38434138
H	-4.55576372	1.46304053	-0.56253210
H	-4.15242338	-0.37567533	-0.40106275
O	-2.21539973	-1.61631341	0.03256014
H	-0.71707204	1.75462855	0.19315623
O	-2.65660410	0.95787323	-0.17238394

TS48

C	1.80019271	-1.50686107	-0.14979162
C	2.82934919	-0.39582991	0.07953161
C	2.45075692	0.98233888	-0.46803280
C	1.22070666	1.62290347	0.21872884
C	-0.07011494	1.00060003	-0.21241392
C	0.46853172	-1.33812347	0.60893565
H	3.28932753	1.66609024	-0.31727767
H	3.03155234	-0.31131356	1.15391318
H	3.77002143	-0.70225747	-0.38633845
H	1.59031101	-1.61469564	-1.21847498
H	2.22981291	-2.45491130	0.18162745
H	1.32562477	1.51995049	1.30411718
H	1.18600824	2.68740017	-0.01171353
H	0.67752564	-1.06780733	1.65575073
H	-0.07559252	-2.28196201	0.64010597
H	2.28006007	0.92824796	-1.54790114
C	-0.43941534	-0.28772565	0.06871886
C	-1.86076218	-0.66804601	-0.15733526
C	-2.14101304	1.53752556	0.41080370
H	-0.61124470	1.54552975	-0.98876393
H	-2.34319533	2.52444013	0.00847975
H	-1.88816250	1.42110316	1.45804420
O	-2.36447231	-1.73098518	-0.26179652
O	-2.63890928	0.53864275	-0.26655231

49

C	1.81366983	-1.53750559	-0.36165794
C	2.70114383	-0.47115872	0.28877167
C	2.43652809	0.97354199	-0.14767543
C	1.11798968	1.57538139	0.33600222
C	-0.15397581	0.95076373	-0.27735891
C	0.35476023	-1.57759103	0.10403360
H	3.23776641	1.60522465	0.24383922

H	2.62487287	-0.54554440	1.37942730
H	3.73672132	-0.71530365	0.03994533
H	1.81660985	-1.42408549	-1.45136718
H	2.22785200	-2.52516804	-0.15328767
H	1.02971348	1.49533367	1.42307227
H	1.08323793	2.63734868	0.08580754
H	0.31916102	-1.66030048	1.22440825
H	-0.19754640	-2.47403713	-0.20076910
H	2.49542801	1.04762605	-1.23912957
C	-0.48194104	-0.42778645	-0.04673762
C	-2.00164592	-0.53984621	0.03445425
C	-1.47342696	1.70925429	-0.06863181
H	-1.71498087	2.39545738	-0.87596280
H	-1.48339226	2.23479039	0.88618142
O	-2.62615819	-1.55588729	0.13298173
H	0.02477794	0.87916848	-1.38346550
O	-2.50753906	0.69443579	-0.02752827

TS50

C	2.31679860	-1.36045059	-0.21087238
C	2.77904233	-0.07776518	0.47851197
C	2.27462352	1.18555079	-0.23376930
C	0.72837092	2.16291216	0.04438011
C	0.46469241	0.85136927	-0.09785969
C	0.82078776	-1.61736679	-0.04620330
H	2.76826198	2.05553491	0.20280426
H	2.50506087	-0.05593212	1.53623508
H	3.86819519	-0.00003140	0.42960061
H	2.57094828	-1.30052081	-1.27297861
H	2.86947953	-2.20749460	0.19801538
H	0.75720390	2.60308791	1.03711911
H	0.72156612	2.83814824	-0.80519183
H	0.61038473	-2.09117363	0.91847989
H	0.44686841	-2.30439688	-0.80748794
H	2.40907523	1.18020574	-1.31109169
C	-0.00973185	-0.36488480	-0.08098390
C	-1.50885486	-0.52370021	-0.00568387
C	-3.58903297	0.60270226	0.04309965
H	-3.98812822	0.03756201	-0.79800752
H	-3.89334539	0.14351932	0.98268042
H	-3.90611600	1.64015304	-0.00181979
O	-2.03360293	-1.60619348	0.07757729
O	-2.14146356	0.64600684	-0.03739894

51

C	2.07622927	-1.82055041	-0.09421989
C	3.35818160	-1.02529142	-0.34238522
C	3.05078478	0.42113143	-0.73075640
C	2.15842778	1.11047350	0.33623492
C	0.93705295	0.28952707	0.56062953
C	1.16825460	-1.12775503	0.95760842
H	3.96643570	1.00587157	-0.83397203
H	3.97875124	-1.03677250	0.56007901
H	3.93990776	-1.50328935	-1.13461834
H	1.51473526	-1.92978550	-1.02694566
H	2.29936398	-2.82631731	0.26621695
H	2.70879916	1.14257313	1.28327784

H	1.93362346	2.13713975	0.04934927
H	1.69225212	-1.11442252	1.92033151
H	0.23730344	-1.67554315	1.09330412
H	2.53567378	0.45231053	-1.69614938
C	-0.33254848	0.73243340	0.33081996
C	-1.63076765	-0.03640541	0.63188631
C	-1.81815344	-0.51073421	-1.81098054
H	-1.77652202	-1.53039896	-2.19868382
H	-2.51151785	0.07258801	-2.42033635
H	-0.82419967	-0.07751448	-1.88327101
C	-3.53014253	-1.27755003	-0.19326825
H	-4.26331452	-0.96880612	-0.93925620
H	-3.35503436	-2.35224449	-0.28694880
H	-3.89994933	-1.05663871	0.80362984
O	-1.96515832	-0.13081838	1.80377809
N	-0.52439878	2.02357899	-0.05372235
N	-0.77474357	3.06101961	-0.35868091
N	-2.28274837	-0.54445300	-0.42410462

TS52

C	-2.64131222	-1.57523197	0.46232889
C	-3.69610091	-0.47044987	0.53043245
C	-3.04691771	0.90514561	0.70260840
C	-2.02360963	1.19179859	-0.41231351
C	-1.02313090	0.07611792	-0.49946650
C	-1.61664478	-1.32997085	-0.65666488
H	-3.80001229	1.69557379	0.68265112
H	-4.29647281	-0.48013033	-0.38612974
H	-4.37993838	-0.66147713	1.36068536
H	-2.11485119	-1.65501428	1.41886131
H	-3.10678517	-2.54599514	0.27320212
H	-2.53713410	1.23086999	-1.37879488
H	-1.52770003	2.14814154	-0.25305064
H	-2.10389410	-1.32743578	-1.63753177
H	-0.84256878	-2.09275325	-0.67172401
H	-2.54492022	0.96296420	1.67338704
C	0.27301325	0.11888418	-0.40858044
C	1.53469673	-0.65743633	-0.44936120
C	3.77684126	-1.07648023	0.31323103
H	3.91955106	-1.37944052	-0.72120970
H	4.57019353	-0.39248310	0.61407010
H	3.80078760	-1.96214655	0.95339070
C	2.28808237	0.39031661	1.66773819
H	2.87244031	1.31230138	1.63846514
H	1.23474401	0.62539754	1.80492420
H	2.61517467	-0.20873228	2.51894817
O	1.56318727	-1.52268997	-1.32053339
N	0.83978408	1.97316213	-0.41921068
N	1.35119926	2.90233311	-0.69440808
N	2.49218084	-0.38722903	0.44524218

53

C	2.68203422	1.40049787	0.43733067
C	3.66518905	0.23280595	0.32633481
C	2.95506466	-1.11427349	0.48701705
C	1.81152979	-1.28355829	-0.52907511
C	0.88852001	-0.08644944	-0.46024400

C	1.53926697	1.28551819	-0.58688489
H	3.65576619	-1.94066573	0.34747676
H	4.16662901	0.26918982	-0.64746785
H	4.44277095	0.33288929	1.08721270
H	2.25610754	1.43771819	1.44506244
H	3.18956923	2.35317851	0.26783392
H	2.21673962	-1.30069343	-1.54715262
H	1.25269544	-2.20277603	-0.36663217
H	1.93445536	1.34155162	-1.60692447
H	0.81213619	2.08705956	-0.46397562
H	2.54917361	-1.20491463	1.49960944
C	-0.38478570	-0.16105408	-0.25339344
C	-1.73012427	-0.44620799	-0.03813841
C	-4.09932893	-0.46463109	0.32151004
H	-4.52732208	-0.12064415	1.26354894
H	-4.78405575	-0.24201024	-0.49724225
H	-3.91697290	-1.53562129	0.36869491
C	-2.84337364	1.69829187	0.00978348
H	-3.51262303	2.00607548	-0.79382454
H	-3.19315515	2.10725438	0.95788974
H	-1.84055000	2.06799758	-0.19713785
O	-1.47300324	-1.68613502	-0.01428653
N	-2.83085115	0.23530159	0.08959485

TS54

C	3.02850073	1.07970095	0.46049560
C	3.41365942	-0.39652236	0.34365363
C	2.22092175	-1.34474003	0.50991276
C	1.14647209	-1.17544848	-0.55033515
C	0.80164597	0.62216505	-0.48500255
C	1.96162269	1.49255965	-0.57959267
H	2.55750023	-2.38230610	0.42290934
H	3.88784242	-0.58030438	-0.62699192
H	4.15910983	-0.63179950	1.10557433
H	2.64413001	1.29236806	1.46158965
H	3.90138618	1.71447223	0.30333350
H	1.47912525	-1.19578811	-1.58631980
H	0.33426252	-1.90921476	-0.44351947
H	2.36090069	1.43236240	-1.59696789
H	1.61435616	2.51622647	-0.41747175
H	1.77058598	-1.24281011	1.50108333
C	-0.23673671	-0.01220110	-0.29283768
C	-1.59347471	-0.59033340	-0.09741240
C	-3.94257298	-0.14613176	0.26199326
H	-3.97747242	-1.22556837	0.15173392
H	-4.33584313	0.13833657	1.23988012
H	-4.54611395	0.32419595	-0.51764899
C	-2.34156585	1.75406415	0.21216076
H	-2.95424716	2.15732889	1.01844731
H	-1.30235660	1.98532545	0.43420914
H	-2.62943233	2.23078604	-0.72780442
O	-1.72509445	-1.80757802	-0.17678129
N	-2.55689364	0.30929462	0.14429235

55

C	2.40276771	-1.41088483	-0.27323073
C	3.14863509	-0.24962250	0.40746718

C	2.90450900	1.11683793	-0.23355841
C	1.49786118	1.82056976	0.04204202
C	0.55871800	0.77019657	-0.07324772
C	0.93773923	-1.59092043	0.11086375
H	3.61210869	1.84933658	0.15805149
H	2.92543180	-0.21791329	1.47933609
H	4.22083118	-0.44050734	0.32354108
H	2.48270862	-1.30388568	-1.35973867
H	2.90066759	-2.34886812	-0.01779064
H	1.48124521	2.25110685	1.04570457
H	1.36789482	2.59814938	-0.71233210
H	0.83941584	-1.88870801	1.15949498
H	0.46189528	-2.36165281	-0.49891551
H	3.03236623	1.05482541	-1.31434250
C	0.00330345	-0.37483493	-0.03372480
C	-1.50249365	-0.70929195	-0.02823083
C	-1.90275646	1.71891241	0.02372412
H	-1.08553855	1.87702557	-0.69525279
H	-2.71210240	2.35798478	-0.32845094
H	-1.60699998	2.04382607	1.02402662
C	-3.79106380	0.09591950	0.03565994
H	-4.26034311	0.51287702	-0.85754785
H	-3.96637602	-0.97487871	0.07512647
H	-4.21576731	0.57033150	0.92223306
O	-1.82256107	-1.88402416	-0.03699192
N	-2.34518956	0.33930345	-0.00391296

TS56

C	2.38261725	-1.41314646	-0.28219560
C	3.14046838	-0.24044002	0.36154939
C	2.85991076	1.11809672	-0.28325285
C	1.48580665	1.79828057	0.06370243
C	0.46553687	0.79276347	-0.08359354
C	0.93031137	-1.59597983	0.14803390
H	3.59811664	1.85059833	0.04981996
H	2.94770482	-0.20072202	1.43966345
H	4.21086345	-0.42742580	0.24906916
H	2.42865402	-1.31755681	-1.37197244
H	2.89456598	-2.34547813	-0.03301479
H	1.49258810	2.16611172	1.09372806
H	1.33959398	2.63873369	-0.61639804
H	0.87125072	-1.86867181	1.20788758
H	0.45482002	-2.40159675	-0.41496016
H	2.93533816	1.03800682	-1.36923475
C	-0.00746900	-0.40273710	-0.00129964
C	-1.50207337	-0.73458808	0.01186317
C	-1.79337068	1.67307669	0.10912467
H	-0.81894761	1.70209987	-0.48016202
H	-2.41217941	2.37888176	-0.44758794
H	-1.60065868	2.02899878	1.12135776
O	-1.86387642	-1.89412469	-0.00966564
N	-2.31730180	0.34802870	0.03570219
C	-3.76914004	0.18089231	-0.08585196
H	-3.98857321	-0.88311140	-0.09613173
H	-4.26502790	0.65014025	0.76462291
H	-4.11988209	0.64032524	-1.01228754

57

C	-2.17386758	1.40773636	-0.21962533
C	-3.21657372	0.28601084	-0.27925969
C	-2.69541520	-1.09239430	-0.69839324
C	-1.66627726	-1.71687705	0.27425536
C	-0.30054024	-1.12007141	0.16040231
C	-1.06265794	1.18971801	0.82298693
H	-3.54257905	-1.78045038	-0.76142712
H	-3.69356642	0.19707827	0.70474840
H	-4.00657353	0.58151267	-0.97649285
H	-1.71905246	1.55378612	-1.20538083
H	-2.68720086	2.34102540	0.02793376
H	-2.03044831	-1.58353517	1.30110137
H	-1.60004956	-2.79033068	0.09472092
H	-1.50986185	0.85173184	1.76477032
H	-0.56729413	2.13739162	1.03111501
H	-2.25826606	-1.04185915	-1.70115439
C	-0.01954238	0.17874627	0.40313282
C	1.30310154	0.71677793	0.11909001
C	2.75082985	-1.03693092	0.98439443
H	3.62533486	-1.67448416	0.92746121
H	2.13387151	-1.02728708	1.87449879
C	3.24491162	-0.20124121	-1.23746292
H	4.08678186	-0.88434124	-1.16650308
H	2.60193725	-0.46602906	-2.07636439
H	3.58685353	0.82596166	-1.34669898
O	1.62242822	1.85935502	-0.04580654
H	0.48274706	-1.78081051	-0.19243414
N	2.44628524	-0.28847366	-0.00171615

TS58

C	-2.24599505	1.42587787	-0.20874878
C	-3.20381455	0.24239102	-0.03678808
C	-2.69722017	-1.10642348	-0.55509745
C	-1.46290683	-1.64998423	0.20058142
C	-0.19713293	-0.94089899	-0.17908599
C	-0.94711967	1.35469147	0.62231720
H	-3.49392677	-1.84637306	-0.44742705
H	-3.46201796	0.14244305	1.02425523
H	-4.13523775	0.48207754	-0.55744079
H	-1.98526260	1.55118952	-1.26434466
H	-2.76155219	2.33981423	0.09530334
H	-1.63084883	-1.54831825	1.27746953
H	-1.33966752	-2.71200386	-0.01507268
H	-1.19385437	1.06465146	1.65678863
H	-0.47354199	2.33525873	0.68265631
H	-2.47294881	-1.04166681	-1.62502371
C	0.06234988	0.38500647	0.13547996
C	1.48243308	0.81999661	0.01471485
C	1.66784057	-1.42508642	0.63937736
H	0.34175230	-1.37217667	-1.02268923
H	2.02064244	-2.39004169	0.28832208
H	1.24866616	-1.39701917	1.63544927
C	3.61424119	-0.38208622	-0.49422760
H	3.73458181	-1.34850047	-0.98503263
H	3.69236587	0.42607972	-1.21682551
H	4.38122706	-0.26612969	0.27203709

O	1.88633978	1.94047930	-0.19201657
N	2.28547386	-0.32825400	0.12447546

59

C	-2.34814100	1.32610000	-0.43604900
C	-3.08579200	0.22847400	0.33963700
C	-2.67649300	-1.20568000	-0.00933100
C	-1.26079400	-1.61007000	0.39706900
C	-0.11944400	-0.87909800	-0.36383300
C	-0.90720900	1.58204800	0.00314300
H	-3.36289200	-1.89528600	0.48954500
H	-2.96547700	0.39636800	1.41624200
H	-4.15342700	0.33483200	0.13231800
H	-2.35323000	1.09819200	-1.50775000
H	-2.88302000	2.27041100	-0.31949600
H	-1.10318600	-1.46226500	1.46886800
H	-1.11376100	-2.67276800	0.19454100
H	-0.86214600	1.81782400	1.09235400
H	-0.46278400	2.49547100	-0.41859200
H	-2.80582800	-1.36989000	-1.08506100
C	0.07096400	0.53308500	-0.10294200
C	1.53149300	0.83680000	0.06621100
C	1.27619500	-1.50209800	-0.21662600
H	1.57508600	-2.07761300	-1.09567600
H	1.32220400	-2.16090300	0.65513300
C	3.59941300	-0.51181100	0.05560200
H	3.97144800	-1.00488800	-0.84489100
H	4.04293700	0.47645600	0.15022300
H	3.85811900	-1.11964100	0.92570700
O	2.01387800	1.94095000	0.25029200
H	-0.40878800	-0.88543900	-1.43637900
N	2.15893900	-0.36499400	-0.03095700

TS60

C	2.40236822	-1.27965454	-0.76145347
C	3.02427691	-0.27325149	0.20320523
C	2.46384583	1.14701948	0.00422311
C	0.99783610	2.04200633	0.79693843
C	0.74720795	0.81900468	0.27626339
C	0.93308807	-1.55733361	-0.44673930
H	3.03089401	1.82872764	0.64287220
H	2.91234984	-0.58249779	1.24477042
H	4.09514797	-0.17284726	0.00806208
H	2.50283902	-0.90052369	-1.78248373
H	2.96212165	-2.21520535	-0.71503684
H	1.17384605	2.16336765	1.86216061
H	0.94535969	2.94086637	0.19022417
H	0.83324743	-2.29820822	0.35276132
H	0.41374416	-1.97143160	-1.31537642
H	2.48591561	1.50472391	-1.02088950
C	0.19355423	-0.33769564	0.03070672
C	-1.25966619	-0.52572389	0.44529669
C	-3.60528123	0.01622533	0.17725569
H	-4.16405825	-0.59314561	-0.53798019
H	-3.64975016	-0.44653586	1.15874150
H	-4.05078318	1.01220047	0.21800352
O	-1.46337334	-1.27437642	1.39721268

N	-2.20922487	0.13458979	-0.24140179
C	-1.98128158	0.91061386	-1.45879363
H	-2.14961397	1.97434647	-1.27056471
H	-0.97010480	0.76855815	-1.82818147
H	-2.68125415	0.57615782	-2.22731372

61

C	-2.51023802	1.05088304	-0.05590356
C	-3.05499159	-0.22934404	0.58220825
C	-2.45532229	-1.45999524	-0.09710887
C	-0.93243893	-1.46607798	0.04885114
C	-0.27456690	-0.16141105	-0.16688074
C	-0.99863873	1.06426153	-0.15667426
H	-2.85267176	-2.37988327	0.33396692
H	-2.81554357	-0.24355706	1.65100719
H	-4.14284187	-0.24003129	0.49900874
H	-2.90759989	1.14681100	-1.07231463
H	-2.83628047	1.93454753	0.49493724
H	-0.65394644	-1.73500123	1.08571894
H	-0.44013982	-2.22792199	-0.56210503
H	-2.71282339	-1.46332212	-1.16042791
C	1.16582037	-0.19998500	-0.55291160
C	3.54928024	-0.21969601	-0.16061744
H	4.02869115	-1.08338379	0.30376440
H	3.55153844	-0.33533448	-1.24124917
H	4.09274131	0.68598539	0.11399443
O	1.22083509	-0.34534641	-1.78028099
C	-0.29113970	2.22571526	-0.22860676
H	0.78691784	2.24289778	-0.33279237
H	-0.79337549	3.18552636	-0.18778797
N	2.16732002	-0.11847946	0.31130967
C	1.96858672	0.03889662	1.75098822
H	0.90941826	0.12601615	1.98486285
H	2.37767543	-0.82613408	2.27566017
H	2.47694000	0.94236783	2.09213012

N2

N	0.00000000	0.00000000	0.54768300
N	0.00000000	0.00000000	-0.54768300

TfOH

H	0.23652171	-0.62692107	0.32420468
O	-0.42560525	-1.28627007	0.59619497
S	-1.67092203	-1.32832052	-0.42836669
O	-2.26538156	-2.63742061	-0.30260951
O	-1.29918192	-0.74810999	-1.70243456
C	-2.83113062	-0.10857839	0.42939101
F	-3.95946318	-0.04336010	-0.26909780
F	-3.08884145	-0.52547043	1.66274760
F	-2.25949670	1.09207518	0.47134031

S4

C	-0.69821474	3.28216846	-0.00341545
C	0.37313592	2.98896278	1.06230857
C	-0.19737170	2.59765978	2.42790758
C	-0.77304180	1.12732988	2.57406765
C	-1.48499364	0.88524743	1.37221035

C	-1.29378101	2.07154376	-0.71589392
H	0.58786020	2.63166911	3.18520679
H	1.06950103	2.22254950	0.71219901
H	0.95454395	3.90108472	1.21684636
H	-1.50258131	3.87295565	0.44776001
H	-0.25892704	3.90741232	-0.78466923
H	0.04904575	0.41150777	2.64418185
H	-1.40828024	1.09124126	3.46047220
H	-0.55005504	1.58150600	-1.34944483
H	-2.13191864	2.36526521	-1.35126818
H	-0.98404464	3.29565376	2.71914050
C	-1.83409561	0.92400340	0.14939599
C	-2.66901039	-0.12631863	-0.61715678
C	-3.18627985	-1.34997438	0.14512912
C	-4.66560371	-1.03783574	0.47563871
H	-5.23647032	-0.86294907	-0.43741310
H	-5.10056272	-1.89090700	1.00080039
H	-4.75733303	-0.15847055	1.11853967
C	-2.40147191	-1.58773084	1.42180892
H	-2.45214837	-0.70488419	2.08527303
H	-2.86191469	-2.38090231	2.01564699
H	-1.36227481	-1.84678066	1.22799665
C	-3.08665540	-2.57212311	-0.78474383
H	-3.50386052	-3.44490672	-0.27805617
H	-3.64842290	-2.40013009	-1.70334162
H	-2.04569186	-2.77112087	-1.04054557
O	-2.93696261	0.10674594	-1.76184677
O	-0.09867445	-1.09400241	-1.05599254
S	1.21154592	-1.14147315	-0.37154156
O	1.83236738	-2.47448103	-0.29793902
O	1.28053844	-0.34443163	0.87225643
C	2.33433858	-0.18827184	-1.54166075
F	3.58541442	-0.12364095	-1.06009972
F	2.37998933	-0.77112402	-2.74869608
F	1.89006173	1.07284030	-1.70686833

TS-S5

C	0.28913711	2.93554624	1.41656973
C	-0.39591321	3.27372833	0.08069012
C	0.57568772	3.44507242	-1.08986470
C	1.18118021	2.12575079	-1.71529934
C	1.51185659	1.28740909	-0.61398653
C	0.65217288	1.47035940	1.63794697
H	0.06533646	3.91168218	-1.93458921
H	-1.15293306	2.52483437	-0.16699025
H	-0.91612234	4.22731026	0.19909085
H	1.18542789	3.55499218	1.52913736
H	-0.37858370	3.20974715	2.23716597
H	0.42506926	1.61900667	-2.31988541
H	2.05032159	2.39417619	-2.31817428
H	-0.24556080	0.85418071	1.73634520
H	1.23831045	1.34773517	2.55106028
H	1.40531872	4.09063843	-0.79566250
C	1.45723308	0.75874131	0.54490645
C	2.03309303	-0.61278097	0.95636464
C	2.83671916	-1.39905601	-0.08441531
C	4.32214804	-1.08201105	0.21292100

H	4.58336645	-1.37649988	1.23039825
H	4.95168282	-1.63975033	-0.48360225
H	4.53870611	-0.01743177	0.09154165
C	2.47743391	-0.96998172	-1.49158711
H	2.60258745	0.12916043	-1.60274905
H	3.18345048	-1.37007027	-2.22292395
H	1.46263720	-1.24804575	-1.76682304
C	2.55032049	-2.89738247	0.11329144
H	3.15364297	-3.47652077	-0.58881760
H	2.80602812	-3.20271630	1.12837259
H	1.49548539	-3.10895010	-0.06353549
O	1.89385747	-0.96062691	2.09479694
O	-0.45573994	-1.40253452	0.04525192
S	-1.53748905	-0.95411154	-0.85818883
O	-2.07315076	-1.99102171	-1.75599855
O	-1.30333037	0.36402597	-1.48618535
C	-2.95881187	-0.60774355	0.32401434
F	-4.04397973	-0.18318758	-0.34199854
F	-3.29421069	-1.70941171	1.01159114
F	-2.61918891	0.34727668	1.21126123

S6

C	2.41281359	0.76515504	1.31841395
C	3.52064256	0.13669115	0.46287181
C	3.22046576	-1.26072170	-0.08601800
C	2.14148922	-1.32127603	-1.18825537
C	0.81203330	-0.90199947	-0.68429078
C	1.16632914	1.23140175	0.55534478
H	4.12950155	-1.67411727	-0.53054783
H	3.76608836	0.81063624	-0.36728412
H	4.42323559	0.06616193	1.07657698
H	2.11168602	0.06514960	2.10535286
H	2.82211710	1.64357630	1.82440739
H	2.41121232	-0.65302813	-2.01546701
H	1.46157044	1.89945594	-0.26389150
H	0.51807840	1.81300657	1.21279283
H	2.93360756	-1.93125810	0.72886266
C	0.31640095	0.13969143	-0.03772261
C	-1.17557318	0.25387405	0.06406462
C	-1.96364699	-0.89668154	-0.60031688
C	-2.50628202	-1.79747903	0.52938534
H	-3.14885418	-1.20968906	1.18546210
H	-3.08383780	-2.61685375	0.10158760
H	-1.69874051	-2.22864320	1.12252657
C	-1.04971486	-1.63711905	-1.51786656
H	-1.14377357	-2.72547157	-1.55587657
H	-0.80531680	-1.18114737	-2.47085012
C	-3.11747447	-0.28949613	-1.42881616
H	-3.71733898	-1.08448266	-1.87400642
H	-3.74854359	0.29961953	-0.76270690
H	-2.74373571	0.35952488	-2.22297520
O	-1.71724665	1.17160788	0.62768305
H	0.04067335	-1.84036995	-0.82799446
H	2.07557054	-2.33533048	-1.57842514
O	-1.28897409	-4.69610980	-0.58481563
S	0.13282278	-5.09927939	-0.65147060
O	0.95776830	-4.19423097	-1.48520597

O	0.38731049	-6.53562957	-0.82505614
C	0.76086185	-4.73429445	1.08416288
F	2.05877112	-5.04737059	1.20353957
F	0.62847548	-3.41838211	1.36304288
F	0.07452944	-5.42148098	2.00624001

TS-S7

C	2.49329803	1.64283454	0.35616478
C	3.60146550	0.60484682	0.14343297
C	3.31809219	-0.78924257	0.71219115
C	2.23274299	-1.58883063	-0.02689210
C	0.86826579	-0.99249783	0.08968235
C	1.22188201	1.44412984	-0.48368584
H	4.23379822	-1.38391095	0.66166466
H	3.82286930	0.52204172	-0.92766623
H	4.51247201	0.98368079	0.61556820
H	2.21853170	1.67895376	1.41587980
H	2.88621828	2.63093437	0.10325205
H	2.47397801	-1.65048364	-1.09460012
H	1.49409261	1.36013322	-1.54646593
H	0.57162606	2.31738518	-0.40532692
H	3.05342328	-0.71113996	1.77211468
C	0.40150394	0.24595781	-0.15970548
C	-1.09945185	0.34054749	-0.17171894
C	-1.77626995	-1.04000708	-0.15914669
C	-2.61667926	-1.19019151	1.12106006
H	-3.35304768	-0.38798984	1.17582410
H	-3.14166274	-2.14700986	1.10981186
H	-1.99470782	-1.14676636	2.01864299
C	-0.67121985	-2.05911784	-0.24785550
H	0.19067281	-1.59006414	0.80826703
H	-0.73420591	-2.94014081	0.39052932
H	-0.28661132	-2.34461924	-1.22651540
C	-2.66345871	-1.14636417	-1.42091378
H	-3.15492565	-2.11995577	-1.44929245
H	-3.42323281	-0.36454489	-1.38266283
H	-2.07688736	-1.02328375	-2.33317378
O	-1.69604168	1.38775170	-0.22812937
H	2.19966506	-2.61560848	0.33603662
O	0.86239353	-3.56174930	-2.48302571
S	1.04376493	-4.83192946	-1.74031421
O	1.04319095	-4.67270515	-0.26960701
O	2.06654235	-5.73768915	-2.28420275
C	-0.57745138	-5.72911296	-2.06027608
F	-0.60531258	-6.91571429	-1.43548037
F	-1.61519376	-4.99758070	-1.60733496
F	-0.76396036	-5.94155591	-3.37123055

S8

C	-1.78483071	2.38921460	1.38053553
C	-1.78745405	3.25704869	0.11611713
C	-1.22173965	2.60120154	-1.14954535
C	-2.06928496	1.45596769	-1.73337373
C	-2.07386980	0.20257284	-0.91449973
C	-2.75322336	1.19696993	1.35108532
H	-1.12653936	3.36902792	-1.92361567
H	-2.81315167	3.59328358	-0.08449339

H	-1.20430871	4.16158655	0.31840504
H	-0.76941598	2.02228182	1.57084519
H	-2.05204951	3.02254809	2.23266793
H	-3.10556473	1.80394718	-1.84377792
H	-3.75842268	1.56162264	1.10133937
H	-2.82448775	0.75904153	2.35011384
H	-0.20914371	2.23148011	-0.95125878
C	-2.36829198	0.10350184	0.40053687
C	-2.26300438	-1.30008687	0.81656305
C	-1.84226934	-2.15942929	-0.38939922
C	-0.49410433	-2.82966259	-0.08470147
H	-0.57708591	-3.46994813	0.79637443
H	-0.17702592	-3.44440505	-0.93148883
H	0.28230028	-2.08328095	0.10541036
C	-1.73403079	-1.12722626	-1.53147762
H	-0.73020952	-1.09383233	-1.97017250
H	-2.41960572	-1.34686160	-2.35803624
C	-2.92074946	-3.21846540	-0.65966257
H	-2.63732471	-3.83814849	-1.51474251
H	-3.04531375	-3.86568520	0.21129703
H	-3.88463463	-2.75144625	-0.88059399
O	-2.47152516	-1.74162613	1.93903576
H	-1.71513906	1.22196896	-2.74096833

TS-S9

C	2.51061993	-1.44880182	-0.84296550
C	3.31877132	-0.34858987	-0.16445057
C	2.70516737	1.03247220	-0.44443744
C	1.18468609	2.21808336	0.40680142
C	1.15846086	0.89471375	0.03361172
C	1.11996219	-1.58306637	-0.21980733
H	3.29157392	1.79324455	0.08293835
H	3.40501177	-0.52029992	0.91135710
H	4.33338961	-0.29464490	-0.57044676
H	2.41467421	-1.21729771	-1.90648035
H	3.03715867	-2.40161498	-0.75948609
H	1.25967249	2.51293037	1.45250903
H	1.25554842	2.97644197	-0.37300859
H	1.16620141	-2.13336773	0.72710139
H	0.45512557	-2.15481390	-0.87168077
H	2.64349004	1.29223394	-1.49918110
C	0.49615523	-0.24907946	0.08892386
C	-0.95464528	-0.27946800	0.53715924
O	-1.16596440	-0.69459568	1.65723528
C	-2.04660443	0.15865289	-0.43194339
C	-3.41342420	-0.28038926	0.10571438
H	-3.62418588	0.17298152	1.07567822
H	-4.19194892	0.02695683	-0.59601808
H	-3.46242926	-1.36539449	0.22024364
C	-1.78242038	-0.46111317	-1.81876202
H	-0.80979821	-0.16950405	-2.21886763
H	-1.83929562	-1.55198954	-1.78141035
H	-2.54522042	-0.10773439	-2.51604869
C	-2.00182751	1.70234696	-0.54345584
H	-2.09473740	2.17523955	0.43770896
H	-1.09354390	2.05490507	-1.03102135
H	-2.84371617	2.03033525	-1.15726886

O	0.98617718	3.23901207	-2.40709879
S	0.73980150	2.30553391	-3.53355059
O	-0.59266956	2.41139028	-4.14769972
O	1.22500657	0.93057491	-3.29262937
C	1.90348230	2.94624769	-4.86345826
F	1.81825185	2.19708857	-5.97380457
F	1.60805993	4.21372042	-5.19091118
F	3.17765306	2.91271455	-4.43591058

S10

C	-3.11864281	0.74010319	0.22468341
C	-3.28313277	-0.71706221	0.66016743
C	-2.48727388	-1.63877348	-0.26413958
C	-0.99301864	-1.31300107	-0.18773287
C	-0.72374819	0.17489493	-0.24862522
C	-1.68572275	1.09539572	-0.09312781
H	-2.64475493	-2.68781247	-0.00170745
H	-2.91926499	-0.83313878	1.68734509
H	-4.34158742	-0.98813963	0.66307143
H	-3.73262820	0.94256671	-0.66285256
H	-0.57113518	-1.71483993	0.74133101
H	-0.45070227	-1.80570437	-1.00110141
H	-2.83518840	-1.50869531	-1.29470459
C	0.70362825	0.56861504	-0.52699321
O	1.03069295	0.89880127	-1.65281618
C	-1.39383621	2.55350724	-0.20408671
H	-0.42439852	2.78211166	-0.63658210
H	-2.17866063	3.08813761	-0.73798521
C	1.73428899	0.49739468	0.61423417
C	2.45297812	-0.86630579	0.48368719
H	3.22899349	-0.93570413	1.25040373
H	1.76758406	-1.70462647	0.62315819
H	2.92517661	-0.96368105	-0.49609311
C	2.75516383	1.63243064	0.43043702
H	3.52346324	1.55809136	1.20388754
H	3.23615556	1.57772448	-0.54617551
H	2.27492240	2.60993181	0.52461214
C	1.07574431	0.61590607	1.99778633
H	0.55843671	1.57012836	2.11140710
H	0.35533153	-0.18268666	2.18304261
H	1.84765449	0.55430169	2.76901278
H	-3.48517863	1.41465463	1.00510689
O	-1.37384210	3.07959391	1.20213935
S	-1.76138958	4.59301729	1.52032536
O	-2.04923351	4.66662004	2.93649669
O	-2.66445630	5.13334619	0.52060653
C	-0.09130207	5.43350852	1.25967901
F	-0.21442045	6.73310399	1.51167663
F	0.81308256	4.90226616	2.07645140
F	0.29801526	5.25879525	-0.00446858

S11

C	-3.23284408	-1.36667201	-1.23192745
C	-3.45843883	-2.26024903	0.00196533
C	-2.18534233	-2.60102363	0.78173456
C	-1.52533528	-1.48188223	1.78852100
C	-1.75007324	-0.36592475	1.00589964

C	-3.10752033	0.13153269	-0.95425951
H	-2.38577899	-3.39709652	1.49969550
H	-4.22500671	-1.84281051	0.66400577
H	-3.84834961	-3.22011472	-0.34609879
H	-2.33443695	-1.70519818	-1.75154694
H	-4.07270032	-1.49217743	-1.91825274
H	-2.07267476	-1.46613317	2.73163059
H	-4.07494100	0.56704804	-0.68436150
H	-2.74347350	0.66018064	-1.83792730
H	-1.38453787	-2.88164074	0.10302121
C	-2.16134039	0.51565312	0.17630301
C	-1.75636749	1.95950903	0.34802886
C	-0.45110034	3.42955299	1.67071645
H	-1.27670915	4.11351479	1.86150766
H	0.17330096	3.31820938	2.55173177
H	0.13662463	3.76985002	0.81959038
O	-2.12448372	2.82930190	-0.39388453
O	-0.96571828	2.09804645	1.40641483
H	-0.46843012	-1.72872099	1.89196893
O	1.22209816	-0.69970451	0.66149913
S	1.33440485	-1.12252677	-0.75194510
O	0.09345620	-1.70063552	-1.31109739
O	2.57642402	-1.83248767	-1.10015366
C	1.49135506	0.51013887	-1.67227271
F	1.61681754	0.30689198	-2.99231025
F	0.40252058	1.28119339	-1.47743057
F	2.56225926	1.19997409	-1.25133219

TS-S12

C	4.47495507	1.24951683	0.29841038
C	3.61711630	2.52309692	0.20579986
C	2.70247373	2.56697114	-1.01864290
C	1.40260165	1.66348396	-0.98212213
C	1.80795940	0.40328343	-0.45684741
C	3.79219334	0.02187044	0.89298673
H	2.29453701	3.57124428	-1.14848705
H	3.04052318	2.66024180	1.12482685
H	4.29015959	3.37981461	0.12133206
H	4.87375392	1.00421520	-0.69182973
H	5.33824852	1.45024526	0.93720408
H	0.65237127	2.09106990	-0.30974209
H	1.01289629	1.59047200	-1.99868395
H	3.53775478	0.19354139	1.94337154
H	4.44258874	-0.85241948	0.83514369
H	3.26449634	2.30824030	-1.91747482
C	2.46430754	-0.42561652	0.26871346
C	2.01639426	-1.83339925	0.64250936
C	-0.08562356	-1.26235008	-0.31487622
H	0.46496316	-0.58673993	-1.02267992
H	-0.79729603	-1.78821414	-0.94880104
H	-0.55742797	-0.68104202	0.47317823
O	2.74378241	-2.57480718	1.23442118
O	0.80932500	-2.21684891	0.20839679
O	-0.33306424	1.54836282	1.69542995
S	0.52726711	0.97619270	2.75525310
O	1.78060259	1.71390138	3.00051809
O	0.67716889	-0.49374537	2.68094659

C	-0.47095956	1.23821001	4.32525389
F	0.18600976	0.75779676	5.39115889
F	-0.70023592	2.54499801	4.52774399
F	-1.65549582	0.61291703	4.24492625

S13

C	-1.99761271	0.51237370	-1.27573285
C	-3.26502696	0.88074224	-0.49578937
C	-3.53882607	0.05780586	0.76800399
C	-2.47370132	0.20471268	1.87627569
C	-1.20498433	-0.54618894	1.59952208
C	-0.68494035	0.73343143	-0.50254693
H	-4.50047705	0.37366449	1.18381804
H	-3.20921764	1.94122431	-0.21780553
H	-4.12713025	0.78527730	-1.16423890
H	-2.04895095	-0.53192892	-1.60308014
H	-1.96580379	1.12328188	-2.18335422
H	-2.24518440	1.27156103	2.00232432
H	-0.71775422	1.71668487	-0.01733730
H	0.14833081	0.75584794	-1.20414666
H	-3.64249941	-1.00155314	0.50915443
C	-0.40545327	-0.32080261	0.54303419
C	0.76922832	-1.17875521	0.31043944
C	1.89065170	-3.09105854	1.17717625
H	2.69092827	-3.11136135	1.90999561
H	2.25562548	-3.12188471	0.15369137
O	1.43955426	-1.20059864	-0.69408213
H	-0.93793938	-1.33974135	2.28686293
O	1.07097614	-1.98707458	1.39673967
H	-2.89011215	-0.14060281	2.82424280
O	-0.25356425	-3.88107077	-0.57523342
S	0.03917712	-4.86408862	0.44897510
O	-0.99045738	-5.51399525	1.22616221
O	1.13368886	-4.30063297	1.49389960
C	1.07480123	-6.22169331	-0.36039368
F	1.41309981	-7.13165400	0.54468932
F	0.35579935	-6.78885705	-1.32308478
F	2.17399949	-5.67929713	-0.88232324

TS-S14

C	2.76768811	1.72442348	-1.15365537
C	2.46950810	2.73511985	-0.04081906
C	1.27974766	2.40002293	0.86117062
C	1.46447469	1.13264251	1.72795872
C	1.36421232	-0.12589864	0.92844488
C	3.26787706	0.35030663	-0.67367042
H	1.11424878	3.23016768	1.55270651
H	3.36763368	2.85968670	0.57678083
H	2.28023416	3.70726577	-0.50560513
H	1.88243373	1.58370577	-1.78192585
H	3.54630018	2.13826249	-1.79948414
H	2.44399785	1.17063469	2.21808817
H	4.06240144	0.49070780	0.07361273
H	3.71766676	-0.19673067	-1.50214080
H	0.36431742	2.29622147	0.27508318
C	2.22223228	-0.52046649	-0.04648973
C	2.14195441	-1.91696839	-0.52684318

C	1.17312247	-2.26877957	1.54775666
H	0.38209116	-0.63860359	1.02471105
H	0.21542508	-2.40621741	2.03739851
H	2.08464968	-2.13406218	2.11964303
O	2.66618728	-2.45034532	-1.44458425
O	1.22824056	-2.65980432	0.31167951
H	0.69389915	1.11456210	2.49692747
O	-1.80994724	1.18046768	1.33228855
S	-2.34191752	-0.05227257	0.72435476
O	-3.77239159	-0.31775949	0.92910333
O	-1.45711087	-1.23597989	0.90413912
C	-2.19465822	0.27378283	-1.12243265
F	-2.62615126	-0.77764285	-1.83363795
F	-2.91502833	1.34675400	-1.47859635
F	-0.91056300	0.50345802	-1.45837472

S15

C	-2.77450289	1.10480377	1.52949427
C	-3.27678119	1.97569199	0.37041017
C	-2.39191246	1.99174833	-0.88291934
C	-2.40136433	0.69990116	-1.71550462
C	-1.81497708	-0.49290021	-1.03296918
C	-2.88503532	-0.40990582	1.30889633
H	-2.72684957	2.80326976	-1.53589314
H	-4.29186175	1.66221879	0.09391688
H	-3.36421812	3.00513688	0.73209146
H	-1.73189686	1.36065262	1.75082097
H	-3.35290983	1.35262281	2.42488195
H	-3.43687473	0.46049423	-1.99270819
H	-3.93082018	-0.66497959	1.09312164
H	-2.62890306	-0.93418475	2.23283457
H	-1.36016435	2.22608434	-0.59769685
C	-2.01776839	-0.94903127	0.21421562
C	-1.22537442	-2.18188612	0.38266498
C	-0.86641942	-1.41430827	-1.73614079
H	0.06023344	-0.91342180	-2.03081503
H	-1.31073323	-1.87967297	-2.62077551
O	-1.12336913	-2.90868286	1.34544505
O	-0.55229361	-2.44085985	-0.78136444
H	-1.86897053	0.87137683	-2.65570778

TS-S16

C	-1.73000767	2.83094221	0.30900494
C	-0.43170230	2.03852624	0.46876979
C	-0.51229957	0.97189451	1.56585338
C	-1.00283095	-0.73791788	1.40362085
C	-1.96468626	-0.01346234	0.80357133
C	-2.85299736	2.02146698	-0.33540239
H	0.50381996	0.58745690	1.73790237
H	-0.09934620	1.59472972	-0.47225157
H	0.36848058	2.70708491	0.79591854
H	-2.04576256	3.18815250	1.29376297
H	-1.54207351	3.71608967	-0.30114925
H	-0.25415651	-1.24322265	0.78907696
H	-2.75096863	2.01695625	-1.42560614
H	-3.83154449	2.45674080	-0.12356236
H	-0.96959079	1.32199754	2.48612867

C	-2.87474083	0.57316930	0.07936023
C	-3.98217464	-0.28873107	-0.46883893
C	-4.89920980	-2.46950555	-0.53892596
H	-5.88843008	-2.13713307	-0.22662806
H	-4.84875712	-2.52908399	-1.62536376
H	-4.65201553	-3.42576010	-0.08773363
O	-4.83341643	0.14653793	-1.20483934
O	-3.89294672	-1.54921055	-0.04873384
H	-1.11787243	-1.06644461	2.43171417
O	2.35980331	-0.09286704	1.56112428
S	2.67032002	-0.97852827	0.41279906
O	1.46770869	-1.55268623	-0.23523109
O	3.78553694	-1.91209259	0.62131325
C	3.31793097	0.21848243	-0.88416937
F	3.63402573	-0.42836086	-2.01539987
F	2.38917881	1.14536785	-1.17941681
F	4.41337919	0.85429341	-0.44378616

S17

C	2.78210320	2.46556288	-0.52552356
C	3.40414550	1.13952863	-0.95914624
C	2.69135413	-0.02137048	-0.26662856
C	1.21564373	-0.04995009	-0.66259747
C	0.56275203	1.31391448	-0.62418776
C	1.27200845	2.45257922	-0.51651037
H	3.15885510	-0.97574736	-0.52048176
H	3.30703768	1.02830850	-2.04488354
H	4.47268156	1.13838089	-0.73097916
H	3.12975206	2.73954137	0.47969717
H	3.11054192	3.27871447	-1.18259541
H	1.10397321	-0.45731303	-1.67594496
H	0.64828420	-0.71734630	-0.01013251
H	2.77545658	0.09858652	0.81955601
C	-0.93011306	1.26490329	-0.67306932
C	-2.91976165	2.33158805	-1.40339586
H	-3.15723731	3.25229140	-1.92763090
H	-3.28593444	1.46381611	-1.95137706
H	-3.34468904	2.34117310	-0.39995014
O	-1.58704285	0.36031894	-0.19923970
O	-1.47697516	2.29832537	-1.33308054
C	0.65276722	3.80655921	-0.35058277
H	-0.36373699	3.79113975	0.02200477
H	1.27893389	4.44680532	0.27007713
O	0.64241328	4.42971642	-1.70694988
S	-0.47374926	5.49047487	-2.11446384
O	-1.61745780	5.44668315	-1.22244072
O	-0.61839594	5.42800832	-3.55278808
C	0.44644196	7.09084011	-1.72759427
F	-0.34312631	8.12541025	-2.00347329
F	0.76813341	7.10993338	-0.43256283
F	1.55432348	7.16716730	-2.45831094

S18

C	-4.72946583	-1.43468532	-0.36923189
C	-4.12594052	-2.72684612	0.21088846
C	-2.71076131	-3.04717409	-0.27590186
C	-1.54004185	-2.17845122	0.33398963

C	-1.98391503	-0.84000760	0.28453570
C	-4.25817550	-0.11867918	0.24805492
H	-2.43921109	-4.06654079	0.00473565
H	-4.15518949	-2.70516638	1.30644382
H	-4.76196685	-3.56032982	-0.09668742
H	-4.55300596	-1.40772490	-1.44949836
H	-5.81332901	-1.46289269	-0.23304168
H	-1.30045653	-2.47661270	1.35752980
H	-4.54221076	-0.05389735	1.30225732
H	-4.70400719	0.73482005	-0.26836412
H	-2.65905124	-2.96901739	-1.36306804
C	-2.74736219	0.17895323	0.19231094
C	-2.34114589	1.64911273	0.07808305
C	-0.02642087	0.82984086	0.06658229
H	0.16080812	0.39815524	-0.91805545
H	0.90841029	1.21414675	0.47187725
H	-0.30426375	0.03388476	0.78079779
C	-0.52793104	3.25967400	-0.07576223
H	0.06548269	3.35993776	-0.98691512
H	-1.37977022	3.93204900	-0.11876758
H	0.09433800	3.50649663	0.78678209
O	-3.21949747	2.49470161	0.01782127
N	-1.01576514	1.88411919	0.04516601
H	-0.64406041	-2.31233580	-0.29122740
O	1.49582168	-1.50059477	1.51473462
S	2.14000187	-2.20356312	0.38542962
O	1.32783847	-2.21283830	-0.85623150
O	2.78921177	-3.48151102	0.71806605
C	3.58038566	-1.08022787	-0.06374322
F	4.26468621	-1.57162048	-1.10746628
F	3.14486879	0.14944194	-0.39507698
F	4.42661820	-0.95362838	0.96975672

TS-S19

C	-4.43641769	-1.62109259	-0.42627828
C	-3.55799741	-2.77521839	0.08783974
C	-2.12372271	-2.77314010	-0.44749409
C	-1.14472802	-1.71345846	0.17245144
C	-1.82618726	-0.46440565	0.19048530
C	-4.22771424	-0.25754336	0.23126056
H	-1.64298720	-3.72913471	-0.23005252
H	-3.55467767	-2.79378008	1.18400482
H	-4.01670221	-3.71355103	-0.23318662
H	-4.30402743	-1.52208028	-1.50876338
H	-5.48582954	-1.88009927	-0.26512347
H	-0.82668680	-1.99064396	1.18103091
H	-4.47845739	-0.29499480	1.29570750
H	-4.87013235	0.49729446	-0.22809430
H	-2.12928706	-2.64040083	-1.53120988
C	-2.82074394	0.34518278	0.14120560
C	-2.72644401	1.86539721	0.05975675
C	-0.32246454	1.48394481	-0.09125675
H	-0.07171648	1.14584055	-1.09683940
H	0.54230993	1.95653349	0.37282715
H	-0.47409901	0.59216716	0.57226687
C	-1.23617446	3.79291375	-0.05899652
H	-0.68927538	4.05945355	-0.96508084

H	-2.19816691	4.29769477	-0.05052605
H	-0.65387824	4.09207426	0.81517414
O	-3.74706302	2.53240108	0.07794453
N	-1.46844909	2.34744420	-0.03074604
H	-0.24900352	-1.64667628	-0.46062254
O	1.65697513	-0.40014151	1.37325819
S	2.44843133	-0.92165811	0.23819246
O	1.67499640	-1.04426081	-1.02135861
O	3.33154005	-2.05726212	0.54645258
C	3.64378034	0.48099766	-0.13787985
F	4.42449654	0.17890405	-1.18556418
F	2.97556356	1.61267592	-0.43095569
F	4.43484169	0.73053397	0.91639683

S20

C	2.00491164	1.71949621	0.51428751
C	3.38774788	1.10808376	0.26006959
C	3.48119617	-0.41701623	0.37883887
C	2.64189689	-1.19708955	-0.65854176
C	1.17837987	-1.21055139	-0.35451167
C	0.92320386	1.29662410	-0.49577615
H	4.52580840	-0.71231050	0.24654822
H	3.72326648	1.40345809	-0.74217127
H	4.09893294	1.55254530	0.96365175
H	1.66595138	1.47460152	1.52685351
H	2.09909675	2.80867408	0.47164786
H	2.79938053	-0.74613349	-1.64713401
H	1.33012464	1.36812581	-1.51131497
H	0.08533975	1.99165127	-0.44211971
H	3.19177370	-0.73477627	1.38610795
C	0.40439133	-0.10782412	-0.28674323
C	-0.97151194	-0.22422573	0.17940662
C	-1.70588881	-2.12145155	-1.15229921
H	-2.34538015	-2.97747840	-1.30374637
H	-1.15884313	-1.69639636	-1.98126653
C	-2.41078455	-2.06005486	1.16266658
H	-3.04347592	-2.88381024	0.84606683
H	-1.68701813	-2.41138224	1.89629530
H	-3.00719850	-1.24640206	1.56750270
O	-1.63906231	0.63018037	0.69907851
H	0.74398935	-2.17247657	-0.12341629
N	-1.66320833	-1.55494440	-0.00335955
H	2.99753069	-2.22655187	-0.71665698
O	0.04015071	-4.13784580	0.98979887
S	0.11382031	-4.89182105	-0.27734082
O	1.24425373	-5.81722393	-0.42008944
O	-0.16573184	-4.05486106	-1.47642658
C	-1.39158352	-6.01595826	-0.20214013
F	-1.46779611	-6.79379810	-1.28943217
F	-1.35128676	-6.80264610	0.88006868
F	-2.52049438	-5.27819713	-0.13962397

TS-S21

C	-2.21892022	0.44786850	-1.31482932
C	-3.33825705	0.23368324	-0.28908007
C	-3.17443145	-0.97225462	0.64112941
C	-1.95556904	-0.87979676	1.58936150

C	-0.67219298	-1.14498709	0.86309591
C	-0.84625907	0.82797024	-0.72201695
H	-4.06678934	-1.05508971	1.26728139
H	-3.44358726	1.14271973	0.31623139
H	-4.27983498	0.11809870	-0.83429478
H	-2.10204372	-0.44556733	-1.93594471
H	-2.51253768	1.25927722	-1.98571244
H	-1.92932697	0.11249745	2.05192499
H	-0.98276774	1.61541695	0.03493644
H	-0.19881619	1.24515463	-1.49407097
H	-3.10374463	-1.89772117	0.06298503
C	-0.12165266	-0.29467597	-0.06853954
C	1.29666695	-0.54288137	-0.43181917
C	1.20557020	-1.41608655	1.74071708
H	-0.37961384	-2.21091217	0.81317328
H	1.27326187	-2.34736823	2.29239570
H	1.04037320	-0.51273207	2.31083464
C	2.92518144	-2.32418346	0.21967215
H	2.54703427	-3.32935091	0.41016625
H	3.15405390	-2.20419993	-0.83579732
H	3.81468468	-2.12503237	0.81547624
O	1.86708481	-0.16855181	-1.43279102
N	1.87131049	-1.35964124	0.56294504
H	-2.06090815	-1.61767347	2.38607105
O	-2.06840095	-4.14233475	-0.52116009
S	-0.67765183	-4.62550363	-0.56905503
O	-0.49136951	-6.08067076	-0.65357766
O	0.22898088	-3.94271894	0.39607626
C	-0.05029132	-3.99078997	-2.22486094
F	1.24675549	-4.29142558	-2.39280740
F	-0.74196387	-4.53007638	-3.23767898
F	-0.17753149	-2.65253841	-2.29808813

S22

C	2.74551314	-1.27892855	1.58894424
C	3.50227968	-1.94047307	0.42957221
C	2.83201274	-1.84511182	-0.94743303
C	2.83697721	-0.44819674	-1.58831631
C	2.00979222	0.57532861	-0.87482292
C	2.73114874	0.25602542	1.57176789
H	3.34888202	-2.52496791	-1.63221565
H	4.51288549	-1.51549164	0.36877221
H	3.63218543	-3.00118418	0.66832280
H	1.71306907	-1.64730156	1.60554535
H	3.20594971	-1.59959617	2.52907589
H	3.87338175	-0.08768249	-1.64308613
H	3.76715830	0.62042868	1.55044557
H	2.29764354	0.62901798	2.50346868
H	1.79801248	-2.20145377	-0.87436480
C	1.97072099	0.86606653	0.43632997
C	1.00793288	1.98470704	0.65002782
C	1.06960180	1.48487468	-1.61977288
H	0.28831524	0.91540151	-2.13979315
H	1.59803690	2.08265798	-2.37377799
C	-0.47902227	3.34559729	-0.82035076
H	-1.38501478	2.92030719	-1.26311057
H	-0.73314641	3.80402481	0.13439965

H	-0.08827867	4.11573271	-1.49228944
O	0.70606162	2.51736969	1.71972231
N	0.50981215	2.31941527	-0.57845222
H	2.49058704	-0.52758948	-2.62325673

TS-S23

C	1.41032530	2.73129451	-1.32874473
C	1.09625567	3.33759558	0.03795797
C	0.32063960	2.36190477	0.93758491
C	0.90825921	1.08711770	2.17826877
C	1.53101392	1.02575265	0.98287842
C	2.45952935	1.62357416	-1.25105076
H	-0.00491949	2.89434096	1.83263024
H	1.99507180	3.70191332	0.54121989
H	0.42437712	4.19212929	-0.07912184
H	0.48535461	2.33709534	-1.75759795
H	1.76645138	3.51518398	-1.99972338
H	1.38291853	1.58878657	3.01668803
H	-0.01789119	0.53276076	2.34142043
H	3.47241107	2.03858954	-1.23357658
H	2.40798811	0.97185747	-2.12739188
H	-0.51382727	1.86872092	0.44890711
C	2.33521862	0.77912913	-0.01087972
C	3.35499707	-0.33560603	0.16946508
O	4.53382206	-0.00375575	0.28428978
C	3.84572357	-2.69498743	0.40986524
H	3.42895036	-3.38028210	1.15076575
H	4.01677470	-3.24361161	-0.52067395
H	4.78826139	-2.29275501	0.77000154
C	1.52310777	-2.00443270	-0.09156905
H	1.04895185	-2.39349411	0.81303206
H	0.93597547	-1.17226973	-0.46616793
H	1.53255803	-2.79340464	-0.84653551
O	-1.69923501	-0.49288220	1.83692272
S	-1.99256922	-0.79147447	0.41476852
O	-2.09288441	-2.22094367	0.08282269
O	-1.21626971	0.02907416	-0.54191668
C	-3.74584444	-0.14874970	0.20340635
F	-4.17503717	-0.33727446	-1.05385342
F	-4.59131161	-0.77804016	1.03324881
F	-3.80228154	1.16770090	0.46953313
N	2.90188342	-1.60204364	0.18794161

S24

C	-0.42146144	2.65611661	0.15158227
C	-1.51258755	3.49554231	0.81882406
C	-2.79350937	3.46505592	-0.01826232
C	-3.32823001	2.03475008	-0.13672762
C	-2.23753735	1.03021067	-0.41530738
C	-0.93214623	1.31426914	-0.31585965
H	-3.56017868	4.10983681	0.41830361
H	-1.72211076	3.09199974	1.81623247
H	-1.16384069	4.52202700	0.95581851
H	-0.00290611	3.19479167	-0.70924204
H	0.41718273	2.49687784	0.83778720
H	-3.84599347	1.74400508	0.78713199
H	-4.07758904	1.96645210	-0.93167729

H	-2.57850097	3.85450298	-1.01942443
C	-2.70503134	-0.31962340	-0.89779581
C	-3.35601111	-2.60670020	-0.35964744
H	-4.31005203	-2.83464593	0.12422202
H	-3.47914794	-2.63425538	-1.43834018
H	-2.61580668	-3.35179533	-0.05782669
O	-2.89815620	-0.49712743	-2.10536580
C	0.09881608	0.28762943	-0.64610336
H	-0.27170245	-0.50861531	-1.28564307
N	-2.89991632	-1.27973568	0.03671414
C	-2.75881689	-1.07021764	1.47321536
H	-2.27372101	-0.12018450	1.67686806
H	-3.73997415	-1.08609189	1.95766637
H	-2.15061916	-1.87023150	1.90110317
H	1.00107053	0.72612411	-1.06977407
O	0.53534959	-0.33222108	0.65551749
S	0.82593018	-1.89378688	0.76242903
O	0.10893512	-2.64225591	-0.25355614
O	0.74437633	-2.23980084	2.16566690
C	2.65128731	-1.94172282	0.28830935
F	3.08063128	-3.19937500	0.33555738
F	2.79569393	-1.46686975	-0.94994241
F	3.35824288	-1.19599698	1.13149634

S25

C	-3.00304961	-0.93889625	-1.31825899
C	-3.57772504	-0.21193846	-0.08879445
C	-3.34484913	-0.93081446	1.24282736
C	-1.88137831	-0.85295784	1.88359256
C	-1.03613468	-1.02845608	0.76768576
C	-1.51458967	-0.74220150	-1.59040183
H	-3.96452986	-0.48669597	2.02348907
H	-3.21410206	0.81901405	-0.03936888
H	-4.66073576	-0.14755294	-0.21430719
H	-3.22082264	-2.00837118	-1.23587385
H	-3.52428034	-0.58787306	-2.21173623
H	-1.72353796	0.12822727	2.33776163
H	-1.79660728	-1.64346012	2.63007591
H	-1.29858049	0.28308178	-1.90139026
H	-1.17740694	-1.41151603	-2.38444367
H	-3.60299377	-1.98604073	1.15216095
C	-0.55775336	-0.97704540	-0.40737539
C	0.95673553	-0.93115074	-0.76009739
C	1.89592085	-1.78832253	0.07874234
C	1.62866284	-3.25739196	-0.32904126
H	1.82302959	-3.41072649	-1.39211598
H	2.30005600	-3.90358694	0.23978470
H	0.60167545	-3.55796137	-0.11265836
C	1.59797696	-1.59020242	1.56402117
H	0.57467889	-1.89840350	1.82211188
H	2.24052813	-2.24664774	2.15524903
H	1.75657540	-0.56112086	1.88456525
C	3.34405107	-1.39322265	-0.24383979
H	4.02364514	-2.02453854	0.33095100
H	3.55703706	-1.52905568	-1.30455740
H	3.53295801	-0.35049566	0.01580467
O	1.26494420	-0.26439504	-1.70573956

H	1.17294928	2.17846314	-1.37037697
C	0.93090669	2.78050307	-0.50297861
H	1.17192599	3.82776125	-0.63619371
Cl	-0.83789601	2.65361192	-0.21634201
Cl	1.88509084	2.16233265	0.88336551

TS-S26

C	-3.02912340	0.62583387	1.31523427
C	-3.56032946	-0.08538877	0.05814024
C	-3.35765211	0.69576876	-1.24256288
C	-1.90105400	0.70615849	-1.85885392
C	-1.01888778	0.92091486	-0.75844792
C	-1.53389232	0.49594620	1.58987792
H	-3.96138613	0.25964298	-2.04080845
H	-3.13823575	-1.09184333	-0.02743360
H	-4.63816988	-0.21577788	0.17730033
H	-3.30028330	1.68535190	1.26852609
H	-3.53553985	0.21824991	2.19328710
H	-1.67976812	-0.25840127	-2.32435616
H	-1.84716022	1.49800222	-2.60718463
H	-1.27101905	-0.53098548	1.85719344
H	-1.24147859	1.13673231	2.42459884
H	-3.66998735	1.73232708	-1.10847343
C	-0.58227517	0.84482194	0.43925545
C	0.91534311	0.92118963	0.81757774
C	1.79489979	1.80596597	-0.06601093
C	1.45283113	3.26887067	0.30746388
H	1.63675783	3.45382951	1.36719899
H	2.09241446	3.93580245	-0.27382281
H	0.41207882	3.51178488	0.08509685
C	1.46724624	1.53454209	-1.52211467
H	0.35995320	1.55078365	-1.68376440
H	1.81731493	2.33693174	-2.17375108
H	1.83156925	0.57043181	-1.87035631
C	3.27023294	1.49957267	0.23237087
H	3.90338370	2.13398965	-0.38996631
H	3.49647515	1.70107689	1.27988876
H	3.50475644	0.45556766	0.02144004
O	1.27345580	0.32677194	1.79373568
H	1.27873739	-2.17163183	1.38401914
C	1.11664355	-2.79962212	0.51600931
H	1.43178401	-3.82336042	0.67501406
Cl	-0.64265336	-2.81239571	0.15580979
Cl	2.07708111	-2.12772193	-0.84089527

S27

C	-2.70535272	-1.51432349	1.60932866
C	-3.57392013	-1.72357065	0.36194557
C	-3.89294314	-0.45614618	-0.43600940
C	-2.71057553	0.14251857	-1.22797506
C	-1.59964233	0.55541383	-0.33852784
C	-1.21959760	-1.24365432	1.35129625
H	-4.66488728	-0.68104431	-1.17617428
H	-3.10416014	-2.46544798	-0.29512789
H	-4.52480737	-2.15782614	0.68201918
H	-3.12065547	-0.70202712	2.21542543
H	-2.75737056	-2.41657412	2.22382922

H	-2.31647945	-0.59939683	-1.93302846
H	-3.05496856	0.99362536	-1.81720393
H	-0.79332100	-2.05046245	0.74220215
H	-0.66614827	-1.24182321	2.29197944
H	-4.30223170	0.31050518	0.22845903
C	-0.88847815	0.04611979	0.65111848
C	0.36463057	0.77699981	1.05556360
C	0.63643681	2.09244471	0.28796893
C	0.22160994	3.25977547	1.20867057
H	0.79364902	3.21914291	2.13558167
H	0.42949700	4.20905111	0.71210083
H	-0.84162489	3.22186308	1.45732774
C	-0.16430944	2.06535415	-0.96930061
H	-1.34680099	1.73468865	-0.55648035
H	-0.58954284	3.00299001	-1.33283399
H	0.16874163	1.41492885	-1.77092693
C	2.13793193	2.16709411	-0.06551116
H	2.36007913	3.11748504	-0.55217702
H	2.71368416	2.09644045	0.85752279
H	2.43541194	1.35131164	-0.72407408
O	1.09272595	0.36811745	1.92334984
H	2.36661239	-1.52227641	1.26097185
C	2.83248221	-1.89017778	0.35460324
H	3.02627983	-2.95535071	0.38035269
Cl	1.69209228	-1.57894587	-1.00579044
Cl	4.38896381	-1.03713127	0.13946267

TS-S28

C	2.47983809	1.48086185	0.31276603
C	3.34552057	0.32614030	-0.20474517
C	2.89675795	-1.07492912	0.22176363
C	1.60260984	-1.57833436	-0.44428534
C	0.39964815	-0.77863901	-0.06975909
C	1.10148312	1.62997137	-0.34720964
H	3.67789478	-1.79363713	-0.03781355
H	3.40568493	0.37487331	-1.29879174
H	4.36373252	0.47655164	0.16403789
H	2.34898049	1.38824517	1.39612922
H	3.01143711	2.42016643	0.14284282
H	1.70972020	-1.53322344	-1.53483400
H	1.43742442	-2.62471511	-0.18215703
H	1.22088081	1.69400184	-1.43887256
H	0.63013946	2.56602364	-0.04385743
H	2.78109891	-1.11330784	1.30947456
C	0.12448472	0.53478400	-0.09014867
C	-1.32838663	0.87306387	0.11710173
C	-2.25572011	-0.35758888	0.08627017
C	-2.88452284	-0.54852474	1.47943977
H	-3.42861522	0.35276784	1.76164833
H	-3.58297450	-1.38661694	1.45925347
H	-2.12649042	-0.74426491	2.24210938
C	-1.40891744	-1.52932319	-0.32250465
H	-0.33037283	-1.38228730	0.60052965
H	-1.56206639	-2.47528668	0.19767370
H	-1.21493800	-1.68352775	-1.37917975
C	-3.34137336	-0.11077543	-0.98614205
H	-4.03079333	-0.95513859	-1.02168866

H	-3.89519569	0.78950199	-0.71749003
H	-2.90379009	0.02821010	-1.97644985
O	-1.72437396	2.00179411	0.26086688
H	-2.24794620	3.42641554	-1.50557817
C	-1.96155084	3.50521667	-2.54605331
H	-1.81518842	2.53640287	-3.00853835
Cl	-3.27404606	4.34514076	-3.43151740
Cl	-0.40207322	4.38889626	-2.62309916

S29

C	-2.01223054	-2.45015096	-0.21655676
C	-3.49966403	-2.17945139	0.01248940
C	-3.82142282	-1.01348565	0.95141171
C	-3.50920381	0.37549706	0.39110922
C	-2.02343851	0.74294898	0.28927222
C	-1.23687629	-1.38667364	-1.01170077
H	-4.88971186	-1.04048543	1.18065241
H	-3.99581661	-2.01985064	-0.95199016
H	-3.93426257	-3.09082117	0.43161970
H	-1.49789565	-2.58508960	0.74002387
H	-1.89660971	-3.38425455	-0.76903057
H	-3.94937188	0.48922141	-0.60542374
H	-3.96791051	1.13760875	1.02484946
H	-1.80969882	-1.15388860	-1.94775004
H	-0.26903271	-1.73589586	-1.37820226
H	-3.30091833	-1.15310792	1.90597432
C	-1.11852104	-0.04622251	-0.51286738
C	0.05547456	0.86056612	-0.94353259
C	-0.19662900	2.26401744	-0.42573285
C	0.70025203	2.49015783	0.81773962
H	1.75280252	2.37613566	0.55615151
H	0.53346586	3.50567224	1.18093505
H	0.47212580	1.79340702	1.62569882
C	-1.68918048	2.22570246	-0.03439550
H	-1.91535114	2.87025569	0.81299532
H	-2.31589029	2.53567656	-0.87355427
C	0.13061768	3.30598321	-1.50312673
H	-0.09145357	4.30434882	-1.12164399
H	1.18830096	3.26206176	-1.76685590
H	-0.46079223	3.14123792	-2.40533174
O	0.96743178	0.44252261	-1.61027864
H	-1.56077021	0.53092490	1.28830703
H	2.31633301	-1.10071733	-0.43557913
C	2.56456959	-1.24180986	0.61050404
H	2.99790333	-2.21333155	0.81387392
Cl	3.72911020	0.01887832	1.09273142
Cl	1.02347429	-1.14281511	1.54842496

TS-S30

C	-2.17060372	-2.35187285	1.20862386
C	-3.13347980	-2.56918708	0.04826197
C	-3.91571621	-1.28506638	-0.28087156
C	-3.56665085	0.37927235	-1.47056019
C	-2.75570706	-0.15395850	-0.49743890
C	-1.04641386	-1.38638047	0.83106961
H	-4.55226873	-1.48880584	-1.15061389
H	-2.61206490	-2.92943863	-0.84152898

H	-3.90078006	-3.30695269	0.30007207
H	-2.72204051	-1.96268095	2.06948860
H	-1.73806255	-3.30723587	1.51083984
H	-3.36743793	0.20740794	-2.52732561
H	-4.49559445	0.88214967	-1.21437736
H	-0.28181638	-1.89124021	0.22971662
H	-0.53097635	-1.01691092	1.71932026
H	-4.54751643	-0.91118379	0.52359405
C	-1.53522155	-0.22739277	0.00706959
C	-0.51608592	0.85523212	-0.32154364
O	0.25917116	0.59830824	-1.21747668
C	-0.51631600	2.15765884	0.46697465
C	0.78748586	2.91988186	0.20476883
H	0.91892503	3.13038666	-0.85739465
H	0.76369067	3.86857354	0.74496234
H	1.65296758	2.35327466	0.54992707
C	-0.68210214	1.86857280	1.97120038
H	-1.60642301	1.32585803	2.18302533
H	0.16132396	1.29562173	2.36109657
H	-0.72338009	2.81671118	2.51138672
C	-1.72126840	2.99592312	-0.02864966
H	-1.67385328	3.16343686	-1.10719928
H	-2.67451985	2.52774350	0.22120803
H	-1.69214695	3.96879319	0.46677931
H	2.40130409	-0.01659211	-1.01562722
C	3.22960352	-0.22111760	-0.34830926
H	3.78775237	-1.10829045	-0.62115227
Cl	4.34716144	1.17841851	-0.40034942
Cl	2.54461719	-0.48570627	1.29311653

S31

C	4.01581886	-0.61827185	1.09726444
C	4.30167854	-1.18808372	-0.29294129
C	3.09561933	-1.97907700	-0.79656410
C	1.86712982	-1.07506016	-0.89881399
C	1.68863787	-0.11254347	0.19871600
C	2.69279904	0.11882525	1.17175327
H	3.29011407	-2.41618771	-1.77656980
H	4.52740970	-0.37396617	-0.98978180
H	5.18598112	-1.82507961	-0.24870753
H	3.98420132	-1.43298165	1.82828987
H	4.80987054	0.05998222	1.41456456
H	1.91794944	-0.45050004	-1.80987769
H	0.92742519	-1.62617636	-1.03323966
H	2.87758678	-2.80413994	-0.11238581
C	0.33288529	0.55250559	0.29432754
O	-0.42696700	-0.04659365	1.02738648
C	2.42832949	1.00161289	2.17938158
H	1.47834618	1.51065972	2.28019771
H	3.16975902	1.20552313	2.94420197
C	-0.00758571	1.79283661	-0.50933545
C	-0.48331622	1.31517304	-1.90766576
H	-0.81381059	2.19326772	-2.46611195
H	0.31561536	0.84290909	-2.48121095
H	-1.31940409	0.62075419	-1.82907851
C	-1.15358135	2.53611779	0.19418686
H	-1.42620114	3.40990158	-0.40065772

H	-2.03226073	1.89944295	0.29628637
H	-0.85592697	2.87863690	1.18770773
C	1.22700974	2.69768956	-0.67174948
H	1.57206036	3.09389002	0.28560547
H	2.06291523	2.17847476	-1.14891483
H	0.96238890	3.54388864	-1.30769084
H	-2.26188752	-1.45514979	0.85395137
C	-2.85530823	-1.82770784	0.02896214
H	-3.52813699	-2.62714822	0.31349633
Cl	-3.83759233	-0.46840439	-0.60220795
Cl	-1.72263034	-2.47973507	-1.20632458

S32

C	2.13479309	-1.39163845	-0.26608968
C	2.77443100	-0.08435542	0.23544969
C	2.37586313	1.16799862	-0.54807454
C	0.90511335	1.86019623	-0.29565848
C	0.16854541	0.69512387	-0.16978732
C	0.70659627	-1.65169162	0.20740194
H	3.01699208	2.00496939	-0.26973624
H	2.60101054	0.05567169	1.30735503
H	3.85657346	-0.16793767	0.11100866
H	2.16145027	-1.40816312	-1.36014801
H	2.74004630	-2.23424797	0.07276422
H	0.92629023	2.45880900	0.61600004
H	0.68378893	2.45260666	-1.18391134
H	0.68201345	-1.88511327	1.27650856
H	0.26368116	-2.49326557	-0.32816362
H	2.44391844	0.99272665	-1.61986885
C	-0.26530765	-0.49111702	0.02735949
C	-1.75316174	-0.74359137	0.15195888
C	-3.87907091	0.30721767	0.12245540
H	-4.16242833	-0.09692217	1.09260545
H	-4.22244332	1.33076820	0.01075503
H	-4.25515796	-0.32170421	-0.68211902
O	-2.20588543	-1.84184476	0.32836868
O	-2.42767449	0.39054888	0.03475028
H	-2.53661545	-3.13340158	-1.71154298
C	-2.51479665	-2.85701787	-2.75890561
H	-2.45100533	-3.71172661	-3.42077067
Cl	-4.02579576	-1.97174219	-3.13349453
Cl	-1.05147643	-1.84553777	-3.02415866

TS-S33

C	1.52203408	-1.79852126	-0.38040668
C	2.54520287	-0.73544858	0.05096487
C	2.35444904	0.62990654	-0.60897588
C	1.16430842	1.52686841	-0.08168559
C	0.01825096	0.67806251	-0.00755130
C	0.15511758	-1.73111154	0.28937801
H	3.22927021	1.25850003	-0.43082565
H	2.56446457	-0.63609940	1.14202687
H	3.53789520	-1.08509027	-0.24161649
H	1.38982289	-1.76360580	-1.46605116
H	1.92162922	-2.78864871	-0.14980329
H	1.39005057	1.93758865	0.90625790
H	1.02621991	2.34530925	-0.79128313

H	0.23459820	-1.90183379	1.36786993
H	-0.50690854	-2.49524989	-0.11899947
H	2.23400402	0.51359483	-1.68696302
C	-0.63058132	-0.41831991	0.15088828
C	-2.14170356	-0.53944278	0.24509687
C	-2.17383627	1.84462459	0.33613022
H	-1.22849697	1.80072322	-0.27635213
H	-2.77896199	2.58783912	-0.18065362
H	-1.94663448	2.12496281	1.36238250
O	-2.68179699	-1.60574606	0.27557110
O	-2.83679940	0.60711661	0.26230242
H	-2.92537165	-2.64531713	-2.00817809
C	-2.23024640	-2.73013700	-2.83488072
H	-2.71580199	-2.97354945	-3.77174900
Cl	-1.42069192	-1.13556280	-3.03318080
Cl	-1.06464751	-4.03471745	-2.45095418

S34

C	-2.01500557	1.46663960	-0.08497478
C	-2.91187233	0.25589166	-0.36137600
C	-2.20764214	-0.98870345	-0.90858524
C	-1.19145199	-1.63830821	0.06647472
C	0.10256585	-0.90981393	0.14068383
C	-0.95741296	1.24382897	1.00819914
H	-2.96104464	-1.74787113	-1.13165794
H	-3.43735739	-0.01378656	0.56267391
H	-3.68355576	0.55485584	-1.07677130
H	-1.52055105	1.79113452	-1.00599766
H	-2.64743143	2.29772479	0.23888790
H	-1.64166850	-1.66604126	1.06773209
H	-1.00055534	-2.66857412	-0.23135825
H	-1.40993254	0.75636691	1.87829631
H	-0.57896558	2.20551686	1.35413294
H	-1.70624612	-0.75883426	-1.85393947
C	0.21140947	0.37754078	0.54911188
C	1.44506577	1.06264113	0.52840119
C	3.88633210	0.24369332	-0.19727280
H	4.72053837	-0.38734319	-0.51314719
H	4.06001645	1.30916476	-0.00135556
O	2.00346214	2.05564127	0.69289540
H	0.99459900	-1.43107226	-0.17469810
O	2.78311941	-0.25258632	-0.03863681
H	2.57142647	3.07745478	-2.63445457
C	2.49367935	2.21368680	-3.28342520
H	2.40102649	2.48286414	-4.32818512
Cl	3.99893595	1.24811541	-3.10198207
Cl	1.03117232	1.29078154	-2.81088675

TS-S35

C	1.80774619	-1.60921189	-0.05672699
C	2.75926156	-0.40931435	-0.09103462
C	2.22443014	0.84649769	-0.78402735
C	1.02245128	1.50252609	-0.06126620
C	-0.25020837	0.75209522	-0.29026576
C	0.52543886	-1.41523686	0.77746290
H	3.01897968	1.59519099	-0.82318838
H	3.05073106	-0.15354472	0.93460009

H	3.67520989	-0.71853862	-0.60223371
H	1.52868325	-1.90199185	-1.07256946
H	2.33663794	-2.46004569	0.37911653
H	1.23357083	1.54446559	1.01226546
H	0.89228747	2.52500341	-0.41520276
H	0.79011273	-0.98657008	1.75648371
H	0.05643816	-2.37773795	0.98056398
H	1.95165419	0.62328024	-1.82039745
C	-0.49638485	-0.51031939	0.17670658
C	-1.88970444	-1.02183358	0.09566082
C	-2.33026047	1.20591516	0.43567992
H	-0.89084953	1.15732024	-1.07553386
H	-2.64626820	2.11855919	-0.05802786
H	-1.98593178	1.23491142	1.46194938
O	-2.30585945	-2.12734027	0.13429207
O	-2.77632115	0.09720932	-0.08469523
H	-2.29913771	-3.25196721	-2.27337982
C	-2.23393784	-2.63947152	-3.16459312
H	-2.22267649	-3.22531989	-4.07519565
Cl	-3.66181518	-1.56056642	-3.20552816
Cl	-0.69018288	-1.71902853	-3.08526510

S36

C	-1.32132638	-1.83188105	0.40076649
C	-2.40869475	-0.87409407	-0.09631047
C	-2.28581612	0.58002925	0.37084660
C	-1.09023275	1.35715067	-0.18051365
C	0.28421752	0.90806933	0.38418922
C	0.07190954	-1.62601165	-0.19995825
H	-3.18720327	1.11696656	0.06448962
H	-2.44784200	-0.90622491	-1.19118458
H	-3.36910112	-1.26098466	0.25306879
H	-1.22775059	-1.78044806	1.49069703
H	-1.60990946	-2.85677352	0.16287343
H	-1.04729479	1.29972298	-1.27124933
H	-1.18504611	2.41252213	0.08348299
H	-0.00915886	-1.54790869	-1.31863050
H	0.74854205	-2.47747789	-0.08162839
H	-2.26640068	0.61422774	1.46577449
C	0.77666180	-0.40385740	0.03500755
C	2.27519028	-0.29752706	-0.22167492
C	1.47443190	1.84679590	0.11636130
H	1.72465814	2.48371092	0.96028156
H	1.31703028	2.44988717	-0.77707780
O	3.01329066	-1.21035805	-0.46587926
H	0.13618917	0.82359806	1.48110248
O	2.61735663	0.98679910	-0.13430937
H	3.42947891	-2.49423227	1.52895104
C	2.81085567	-2.74925667	2.38170878
H	3.38650428	-3.00117564	3.26385937
Cl	1.83097083	-1.28738804	2.79190391
Cl	1.78517370	-4.14324465	1.94597260

TS-S37

C	2.32664517	-1.28000266	-0.31749760
C	2.64619337	-0.11125718	0.61332144
C	2.06774894	1.21797212	0.10858570

C	0.43215609	2.00438427	0.46859853
C	0.28598100	0.72769402	0.07144405
C	0.85220211	-1.67508522	-0.29029883
H	2.46615591	2.03055061	0.71859364
H	2.32806389	-0.30344351	1.64082040
H	3.72599681	0.05662639	0.64129663
H	2.62387842	-1.01188146	-1.33544379
H	2.92987246	-2.14254408	-0.03026054
H	0.37931456	2.25059645	1.52561124
H	0.40522892	2.82532726	-0.24087559
H	0.63813819	-2.32712364	0.56224505
H	0.57433206	-2.23915614	-1.18265853
H	2.24834934	1.41911815	-0.94289048
C	-0.08015442	-0.50485753	-0.15185562
C	-1.55987831	-0.79357503	-0.16585972
C	-3.73404883	0.13968943	-0.13773489
H	-4.03989026	-0.40167932	-1.03179961
H	-4.03761887	-0.40273415	0.75589241
H	-4.13863556	1.14721469	-0.13698977
O	-1.98949221	-1.92220311	-0.19218464
O	-2.29255233	0.31316351	-0.14093504
H	-2.17059814	-2.92144261	1.96544646
C	-2.15740691	-2.55474964	2.98491758
H	-2.00070667	-3.33685462	3.71734624
Cl	-0.79374130	-1.39003156	3.12296295
Cl	-3.73917566	-1.78401368	3.32046557

S38

C	2.51618283	2.16715343	-1.08885427
C	2.98530392	0.79584934	-1.58065699
C	2.55759044	-0.29689907	-0.60152128
C	1.03610236	-0.32939232	-0.45911411
C	0.37398902	0.98007193	-0.42396384
C	1.04335374	2.18489157	-0.73461392
H	2.89864034	-1.27800561	-0.93357098
H	2.56094418	0.59203996	-2.56953669
H	4.07024783	0.80339876	-1.69319615
H	3.07844595	2.45041047	-0.19272608
H	2.70538364	2.93847800	-1.83751776
H	0.56769629	-0.83248424	-1.32902781
H	0.68316205	-0.93423764	0.38454392
H	3.00461764	-0.11590977	0.38033422
C	-1.06796793	0.98050934	0.00909668
C	-3.33046227	0.87720730	-0.68490137
H	-3.82660412	0.89330133	-1.64942629
H	-3.54629868	-0.04232820	-0.14623972
H	-3.59842492	1.74613998	-0.08740157
O	-1.32393577	1.01147868	1.18931276
O	-1.90330893	0.92675453	-1.00093426
C	0.32108701	3.34582760	-0.70306820
H	-0.72923981	3.37531699	-0.43961750
H	0.78785250	4.29515527	-0.94165355
H	-1.80964704	-0.86824861	2.56881107
C	-2.33830647	-1.79426052	2.37968283
H	-2.11634172	-2.56806759	3.10404386
Cl	-4.09474508	-1.45258222	2.44351209
Cl	-1.82185682	-2.39102759	0.76219567

S39

C	-2.79688716	-0.61872935	-1.12767945
C	-3.74490824	0.14311913	-0.18495884
C	-3.27687531	0.19543398	1.27043184
C	-2.09508331	1.21285648	1.62935473
C	-1.19762271	1.06200800	0.55563505
C	-1.56157421	0.13181602	-1.61632955
H	-4.08536219	0.54616779	1.91388450
H	-3.94867111	1.15112800	-0.56219570
H	-4.70320785	-0.38100711	-0.17898721
H	-2.48537975	-1.54824303	-0.64328474
H	-3.34908693	-0.90727940	-2.02481918
H	-2.47702099	2.23295486	1.70231575
H	-1.66489974	0.89157452	2.58094620
H	-1.83832094	0.94953228	-2.28875976
H	-0.88326024	-0.53740424	-2.14987019
H	-2.96733309	-0.79478333	1.60449310
C	-0.64928129	0.78713380	-0.55653693
C	0.81199375	1.01708718	-0.98339995
C	1.08776009	2.46036047	1.00144470
H	1.20191404	1.76410952	1.83652565
H	1.68381731	3.34865606	1.20731048
H	0.05297015	2.80756958	0.92378936
C	2.95332915	2.06109526	-0.58691298
H	3.57661406	1.52013964	0.12957452
H	3.13473515	1.67729302	-1.58605699
H	3.19470617	3.12342049	-0.54857457
O	1.21176431	0.40215370	-1.95913135
N	1.53711246	1.87904077	-0.25138455
H	2.12293939	-1.61800600	-1.00764741
C	1.92829598	-2.18709446	-0.10645995
H	2.52932980	-3.08448744	-0.02993828
Cl	2.31427996	-1.14084118	1.30204863
Cl	0.20190329	-2.67355600	-0.12819392

TS-S40

C	2.22862825	-1.71118722	1.02192209
C	3.50825359	-1.16089139	0.37168187
C	3.31142527	-0.63727385	-1.05200943
C	2.63323366	0.77293838	-1.20059236
C	1.47140259	0.77419063	-0.35274750
C	1.26443066	-0.68148593	1.60210884
H	4.27913077	-0.50664572	-1.54101369
H	3.96554365	-0.39121079	1.00390922
H	4.23224421	-1.97667012	0.31057110
H	1.69820430	-2.33478150	0.29614678
H	2.50589175	-2.36891774	1.84892918
H	3.32172827	1.56265660	-0.88695027
H	2.37523606	0.91646446	-2.25102272
H	1.71595170	-0.17117976	2.46076730
H	0.34910018	-1.16063417	1.95408332
H	2.73472097	-1.35545384	-1.63764907
C	0.78981148	0.44462661	0.68885145
C	-0.49422684	1.14971415	1.12166977
C	0.11950236	2.77834709	-0.56250159
H	0.53615537	1.87061356	-1.11153440

H	-0.44282414	3.27514717	-1.35480739
H	0.94900497	3.39604580	-0.21944793
O	-1.20507907	0.64842632	1.97229686
N	-0.74320558	2.31358386	0.47557803
C	-2.02552189	2.99690997	0.67260952
H	-2.48889317	2.59744573	1.57063775
H	-1.85055324	4.06557486	0.79219838
H	-2.67759476	2.82250385	-0.18649136
H	-2.70855754	-0.59115822	0.30035046
C	-2.55444307	-1.06339647	-0.66274375
H	-3.43350417	-1.58469068	-1.02104716
Cl	-2.15265298	0.22049190	-1.85610281
Cl	-1.22976751	-2.25695449	-0.48749447

S41

C	2.14479639	1.43618728	0.21623207
C	3.13142410	0.28067684	0.41574005
C	2.53167118	-1.02709379	0.94205021
C	1.51761947	-1.70003666	-0.01356739
C	0.17583480	-1.04245392	-0.01678596
C	1.05668023	1.17437620	-0.84029851
H	3.34304574	-1.74029991	1.10964785
H	3.63592101	0.07813968	-0.53722619
H	3.91087438	0.60601011	1.11159059
H	1.67051997	1.69013200	1.16883379
H	2.70874224	2.31861137	-0.09886572
H	1.92900237	-1.67970526	-1.03111106
H	1.39721269	-2.74818901	0.26171153
H	1.51884093	0.74714379	-1.73774235
H	0.60641932	2.12039529	-1.13934142
H	2.05507409	-0.85969651	1.91336501
C	-0.04114302	0.23922675	-0.38326413
C	-1.35140942	0.84473228	-0.20065311
C	-2.80130938	-0.92502634	-1.02192744
H	-3.70184484	-1.52656805	-0.97780202
H	-2.12171652	-1.01468261	-1.86058379
C	-3.42574995	0.12360548	1.07455197
H	-4.29401323	-0.52374277	0.99140654
H	-2.85880215	-0.09629715	1.97827569
H	-3.71907504	1.17133550	1.07861602
O	-1.62521149	2.00968192	-0.12016393
H	-0.64854985	-1.63705272	0.35857011
N	-2.54176205	-0.10030150	-0.08431430
H	-0.74839799	3.17782710	1.84213094
C	-0.94659335	2.95953322	2.88448450
H	-0.36598495	3.57250590	3.56271150
Cl	-2.68302730	3.27010388	3.19421832
Cl	-0.49949723	1.24190261	3.17729286

TS-S42

C	-2.27842198	1.44997959	0.05075625
C	-3.10040726	0.16706142	-0.09397816
C	-2.48981957	-0.90357218	-1.00109804
C	-1.21017087	-1.55346712	-0.43168755
C	0.00482151	-0.67984028	-0.51800742
C	-0.93330264	1.31559458	0.78487906
H	-3.21870862	-1.70531913	-1.14237761

H	-3.28317452	-0.26422306	0.89791737
H	-4.08077456	0.43989530	-0.49474510
H	-2.09990663	1.88864921	-0.93366124
H	-2.86475778	2.18006816	0.61414248
H	-1.39080258	-1.81416363	0.61680209
H	-1.00078632	-2.48086189	-0.96559797
H	-1.09776789	0.81935950	1.75694825
H	-0.53358287	2.30341846	1.02011208
H	-2.28320933	-0.48773699	-1.99242455
C	0.14491585	0.54504889	0.11093404
C	1.53749242	1.07346797	0.19953019
C	1.83586583	-1.22928746	0.46173877
H	0.67832327	-0.89193336	-1.34764683
H	2.30774547	-2.09252533	0.00221240
H	1.26551618	-1.40389390	1.36221816
C	3.82141323	0.10655866	-0.16081760
H	4.09696012	-0.75226412	-0.77338756
H	3.94363902	1.02756618	-0.72242253
H	4.44355781	0.13031900	0.73405402
O	1.88205783	2.23307637	0.20024302
N	2.41327709	-0.02563928	0.22916016
H	2.06663425	2.88432589	-2.26617734
C	1.60675280	2.40702472	-3.12318107
H	1.81531949	2.91727912	-4.05514198
Cl	2.26973216	0.73931796	-3.25094915
Cl	-0.16487488	2.40448996	-2.86713957

S43

C	1.88831230	1.77105421	0.32519835
C	2.84366050	0.68140415	-0.17195237
C	2.55417043	-0.73735507	0.32802811
C	1.25230694	-1.36426682	-0.17340375
C	-0.03574617	-0.73916182	0.41561605
C	0.47526383	1.73179071	-0.26287348
H	3.37223216	-1.38844754	0.00852713
H	2.86112267	0.68653629	-1.26811350
H	3.85206145	0.95462518	0.14951064
H	1.80701986	1.74338493	1.41679441
H	2.30015547	2.74983017	0.07259347
H	1.19246129	-1.31976910	-1.26449238
H	1.22685818	-2.41992113	0.10563236
H	0.53120586	1.65795095	-1.37766588
H	-0.09037166	2.65856242	-0.12436802
H	2.56392853	-0.75018432	1.42412105
C	-0.38354147	0.61175005	0.01165514
C	-1.86583534	0.71627312	-0.20326491
C	-1.33134940	-1.54796684	0.22931327
H	-1.60709883	-2.11957135	1.11743006
H	-1.23617470	-2.24192155	-0.61056984
C	-3.74981534	-0.87518197	-0.16326161
H	-4.10753378	-1.25500959	0.79712821
H	-4.29803867	0.02457953	-0.43191789
H	-3.89490474	-1.64314506	-0.92551794
O	-2.47622790	1.74431741	-0.45371628
H	0.14285850	-0.62639838	1.50378788
N	-2.34103688	-0.54478274	-0.06123382
H	-2.54151417	3.10352749	1.43009573

C	-1.95955366	3.30821314	2.32149377
H	-2.55163781	3.68292544	3.14711018
Cl	-1.22895251	1.74474720	2.85052996
Cl	-0.71469452	4.52602111	1.91600387

TS-S44

C	-2.42748471	-1.41238187	0.44397876
C	-3.03384426	-0.29290412	-0.39838119
C	-2.48332845	1.09029876	-0.00606366
C	-1.01857801	2.08055853	-0.66654745
C	-0.76095109	0.80595717	-0.29363559
C	-0.94926190	-1.64159044	0.13417630
H	-3.04823997	1.84782217	-0.55446321
H	-2.89714150	-0.46454770	-1.46855639
H	-4.10906192	-0.22103235	-0.21619468
H	-2.55672375	-1.16843968	1.50232315
H	-2.97800992	-2.33719006	0.26387540
H	-1.18418896	2.32736657	-1.71171878
H	-0.97658151	2.90125258	0.04282185
H	-0.82423607	-2.28724655	-0.74034723
H	-0.44384721	-2.15006096	0.95873288
H	-2.51760318	1.31056173	1.05682471
C	-0.20870853	-0.37195496	-0.18397170
C	1.24902491	-0.50993464	-0.59707554
C	3.59718258	-0.10664637	-0.19369845
H	4.06891067	-0.93356950	0.34433041
H	3.65986217	-0.29010977	-1.26248776
H	4.11461417	0.82141549	0.05307933
O	1.46388961	-1.10109702	-1.65484066
N	2.19397335	0.01569286	0.19869394
C	1.96165618	0.50412699	1.55583110
H	2.29780469	1.53974810	1.64258031
H	0.90821036	0.44972995	1.81188668
H	2.52593781	-0.11132243	2.26093203
H	2.22777069	-3.17219509	-1.31673544
C	2.21550142	-4.03305116	-0.65827007
H	3.04582630	-4.71077824	-0.81382523
Cl	2.31611027	-3.41903242	1.03007279
Cl	0.69641818	-4.93783203	-0.95960807

S45

C	-2.49252053	1.18039520	-0.14520063
C	-3.10202863	-0.09610856	0.43972683
C	-2.57432019	-1.32243341	-0.30382274
C	-1.05340241	-1.41744163	-0.18001629
C	-0.32574813	-0.14176928	-0.31140412
C	-0.98204249	1.11880950	-0.23973637
H	-3.01579350	-2.24028521	0.08671042
H	-2.85464316	-0.17347541	1.50433098
H	-4.18939951	-0.04396448	0.36733226
H	-2.88077466	1.33720806	-1.15759098
H	-2.77482173	2.05703025	0.43999251
H	-0.77080608	-1.78478383	0.82505122
H	-0.61343043	-2.15676576	-0.85490764
H	-2.84210138	-1.26073017	-1.36276904
C	1.12085118	-0.23393388	-0.67240282
C	3.48624558	-0.40544033	-0.21361233

H	3.88625956	-1.34365937	0.17421247
H	3.52313092	-0.41436344	-1.29948430
H	4.07703646	0.42847810	0.16852833
O	1.21061031	-0.30890834	-1.90503875
C	-0.21246806	2.24274438	-0.23646219
H	0.86627599	2.20804165	-0.32865818
H	-0.66437839	3.22332146	-0.14018153
N	2.09779297	-0.25156574	0.22192592
C	1.85822861	-0.19885579	1.66266999
H	0.80381984	-0.02797739	1.87017796
H	2.16364500	-1.14063972	2.12242194
H	2.43505743	0.61934805	2.09640254
H	1.86830456	-2.29435830	-2.94544453
C	1.63937074	-3.33498634	-2.75175493
H	2.23179149	-4.02505903	-3.33950004
Cl	1.98199859	-3.64999029	-1.01515948
Cl	-0.08853794	-3.59901781	-3.15563235

X) References

(1).Yates, P.; Garneau, F. X.; Lokensgard, J. P., Preparation and spectra of mercuribis (α-diazo ketones). *Tetrahedron* **1975,** *31*, 1979-1983.

(2).Du, H.; Rodriguez, J.; Bugaut, X.; Constantieux, T., Organocatalytic Enantio- and Diastereoselective Conjugate Addition to Nitroolefins: When β-Ketoamides Surpass β-Ketoesters. *Chemistry – A European Journal* **2014,** *20* (27), 8458-8466.

(3).Bartlett, P. A.; Carruthers, N. I.; Winter, B. M.; Long, K. P., .alpha.-Diazophosphonic acids as potential photoaffinity labeling reagents: synthesis, stability, and photochemistry. *J. Org. Chem.* **1982,** *47* (7), 1284-1291.

(4).Chen, D.-F.; Wu, P.-Y.; Gong, L.-Z., Rhodium/Chiral Urea Relay Catalysis Enables an Enantioselective Semipinacol Rearrangement/Michael Addition Cascade. *Org. Lett.* **2013,** *15* (15), 3958-3961.

(5).Pellicciari, R.; Natalini, B.; Sadeghpour, B. M.; Marinozzi, M.; Snyder, J. P.; Williamson, B. L.; Kuethe, J. T.; Padwa, A., The reaction of alpha-diazo-beta-hydroxy esters with boron trifluoride etherate: Generation and rearrangement of destabilized vinyl cations. A detailed experimental and theoretical study. *J. Am. Chem. Soc.* **1996,** *118* (1), 1-12.

(6).Paquette, L. A.; Zon, G., Silver(I) ion-catalyzed rearrangements of strained .sigma. bonds. XXII. Kinetic deuterium isotope and electronic effects in the silver(I) promoted type .gamma. isomerization of 1-alkyltricyclo[4.1.0.0.2,7]heptanes. Mechanistic analysis of the formation of bicyclo[3.2.0]hept-6-enes. *J. Am. Chem. Soc.* **1974,** *96* (1), 224-233.

(7).Takai, K.; Hotta, Y.; Oshima, K.; Nozaki, H., Wittig-type Reaction of Dimetallated Carbodianion Species as Produced by Zinc Reduction of gem-Polyhalogen Compounds in the Presence of Lewis Acids. *Bull. Chem. Soc. Jpn.* **1980,** *53* (6), 1698-1702.

(8).Frisch, M. J. T., G. W.; Schlegel, H. B.; Scuseria, G. E.;; Robb, M. A. C., J. R.; Scalmani, G.; Barone, V.; Mennucci,; B.; Petersson, G. A. N., H.; Caricato, M.; Li, X.; Hratchian, H.; P.; Izmaylov, A. F. B., J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.;; Ehara, M. T., K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima,; T.; Honda, Y. K., O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.;; Peralta, J. E. O., F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin,; K. N.; Staroverov, V. N. K., R.; Normand, J.; Raghavachari, K.;; Rendell, A. B., J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega,; N.; Millam, J. M. K., M.; Knox, J. E.; Cross, J. B.; Bakken, V.;; Adamo, C. J., J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.;; Austin, A. J. C., R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.;; Morokuma, K. Z., V. G.; Voth, G. A.; Salvador, P.;; Dannenberg, J. J. D., S.; Daniels, A. D.; Farkas, O.;; Foresman, J. B. O., J. V.; Cioslowski, J.; Fox, D. J.; , *Gaussian 09, revision C.01;* . Gaussian Inc.: Wallingford, CT, 2010.

(9).Becke, A. D., Density-functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.* **1993,** *98* (7), 5648-5652.

(10).Lee, C.; Yang, W.; Parr, R. G., Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. *Phys. Rev. B* **1988,** *37* (2), 785-789.

(11).Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H., A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *J. Chem. Phys.* **2010,** *132* (15), 154104.

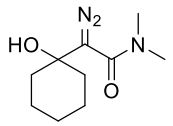
(12).Tomasi, J.; Mennucci, B.; Cammi, R., Quantum mechanical continuum solvation models. *Chem. Rev.* **2005,** *105* (8), 2999-3093.

(13).Cancès, E.; Mennucci, B., Comment on "Reaction field treatment of charge penetration" [J. Chem. Phys. 112, 5558 (2000)]. *J. Chem. Phys.* **2001,** *114* (10), 4744-4745.

(14).Chipman, D. M., Reaction field treatment of charge penetration. *J. Chem. Phys.* **2000,** *112* (13), 5558-5565.

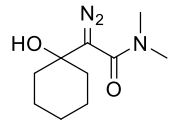
(15).Legault, C. Y., CYLView. *CYLView* **2009,** *1.0b*, http://www.cylview.org.

^{1}H NMR ($CDCl_3$, with 0.03% v/v TMS, 500 MHz)



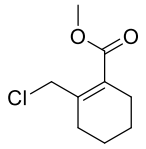
28

^{13}C NMR ($CDCl_3$, with 0.03% v/v TMS, 125 MHz)

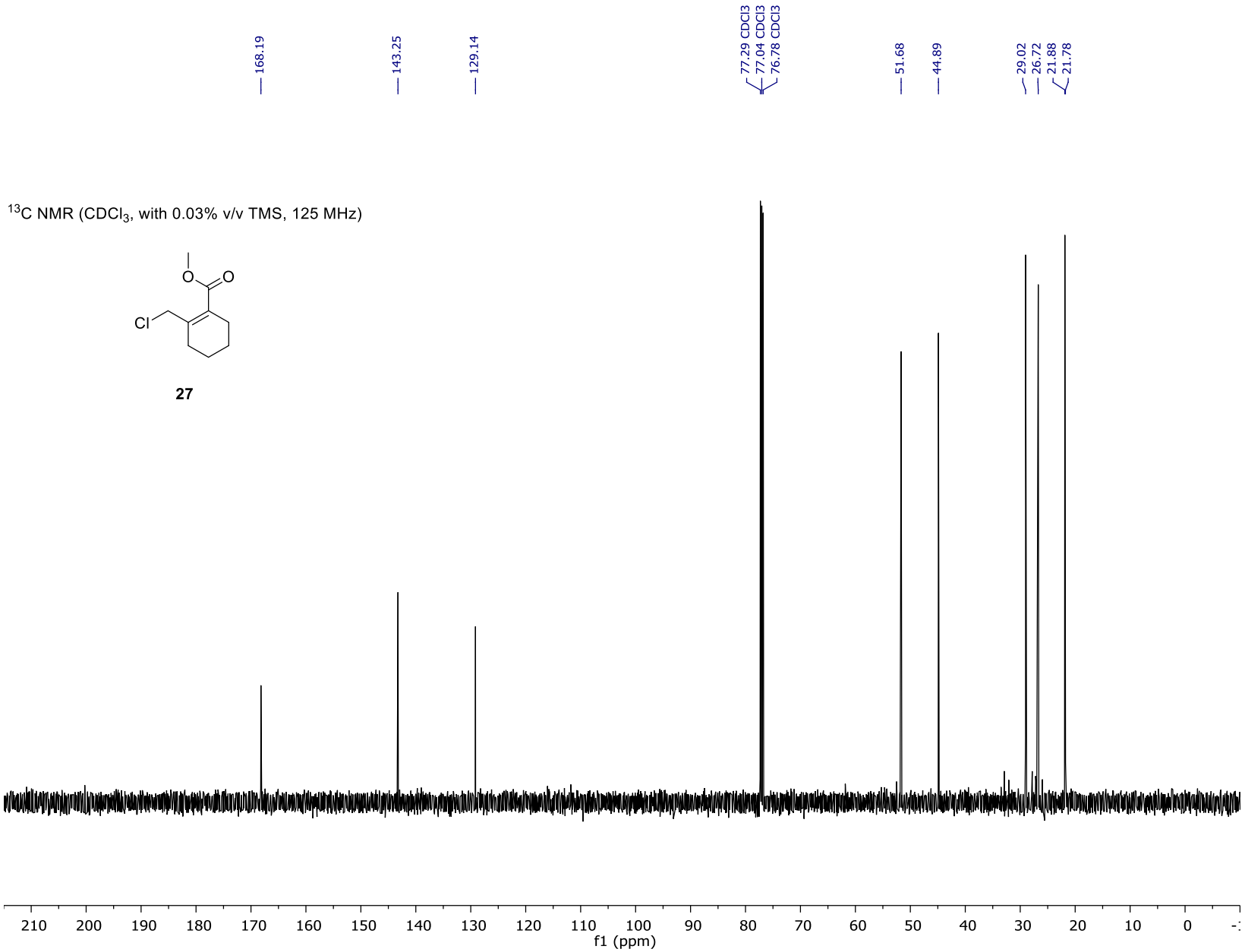


28

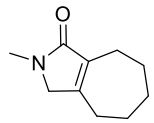
^{1}H NMR ($CDCl_3$, with 0.03% v/v TMS, 500 MHz)



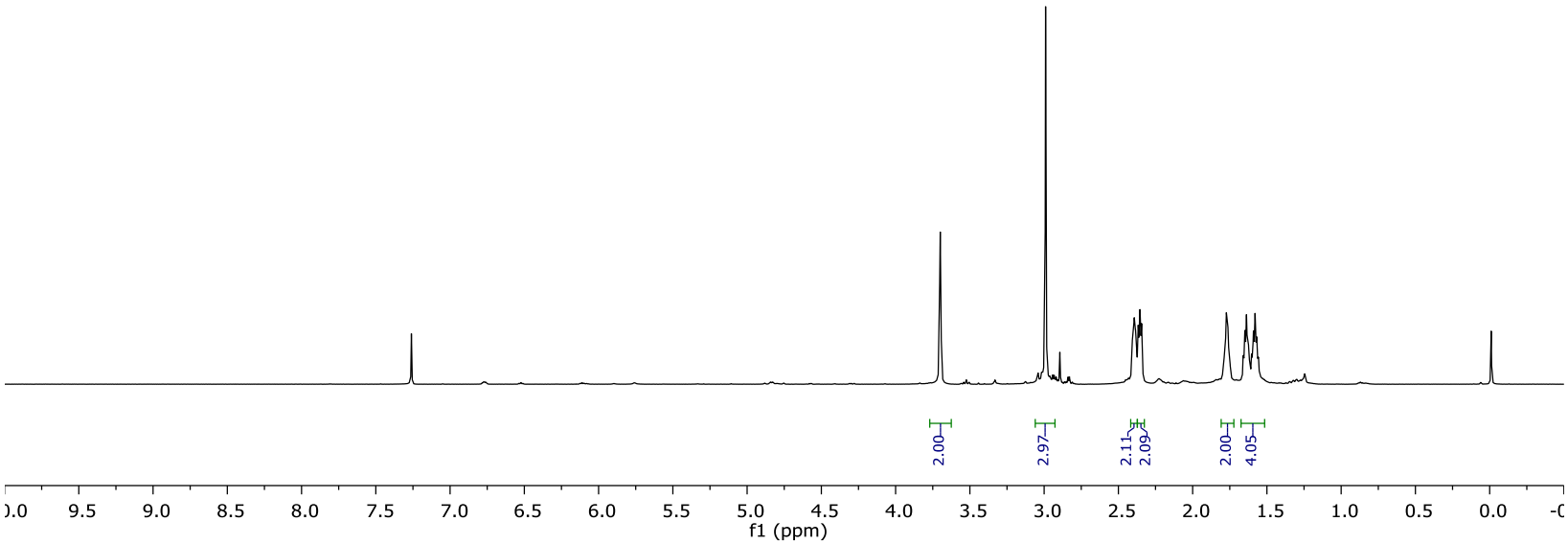
27

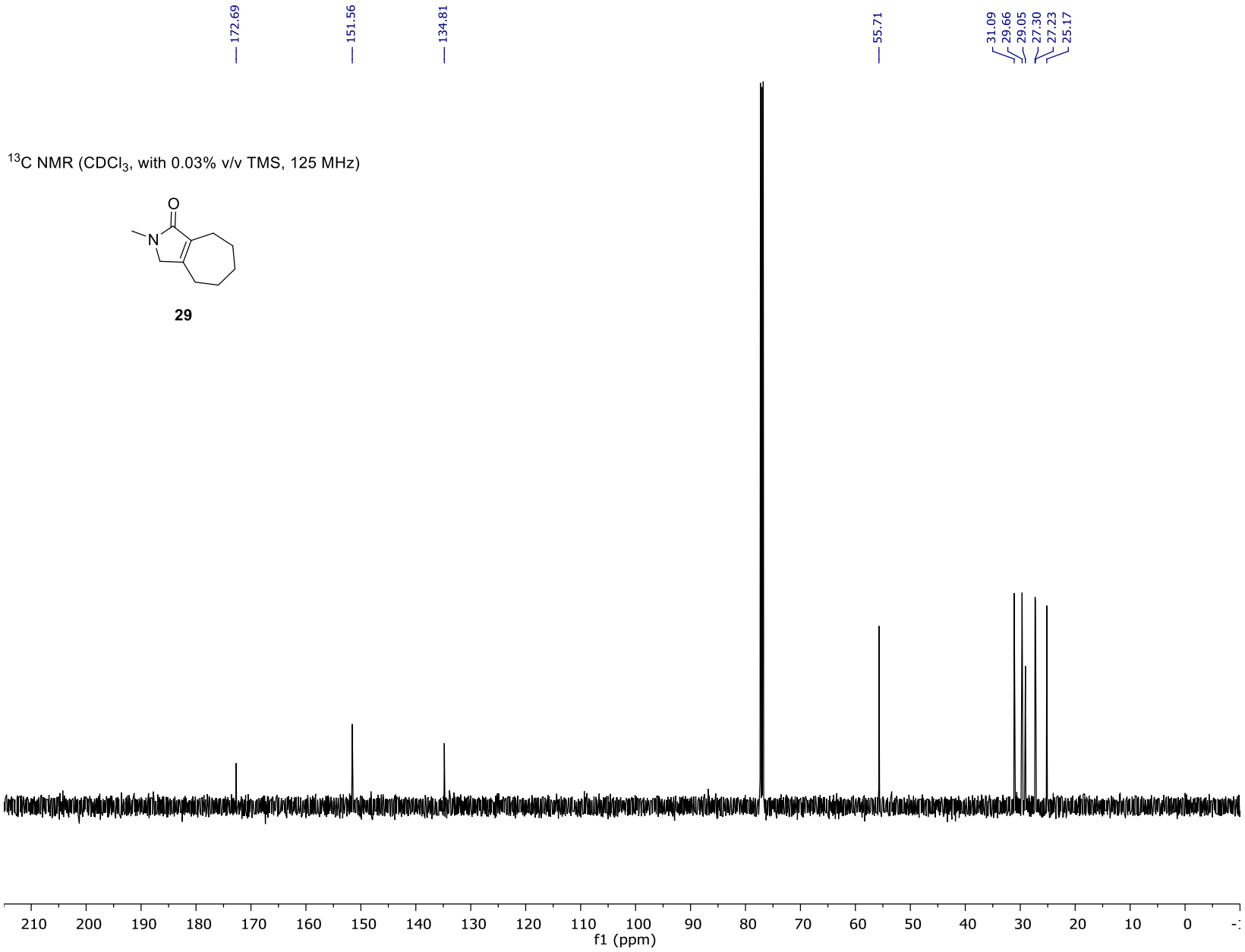

168.19
143.25
129.14
77.29 CDCl3
77.04 CDCl3
76.78 CDCl3
51.68
44.89
29.02
26.72
21.88
21.78
13C NMR (CDCl3, with 0.03% v/v TMS, 125 MHz)
O
O
Cl
27
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

^{1}H NMR ($CDCl_3$, with 0.03% v/v TMS, 500 MHz)

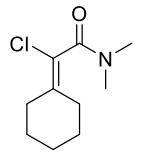


29

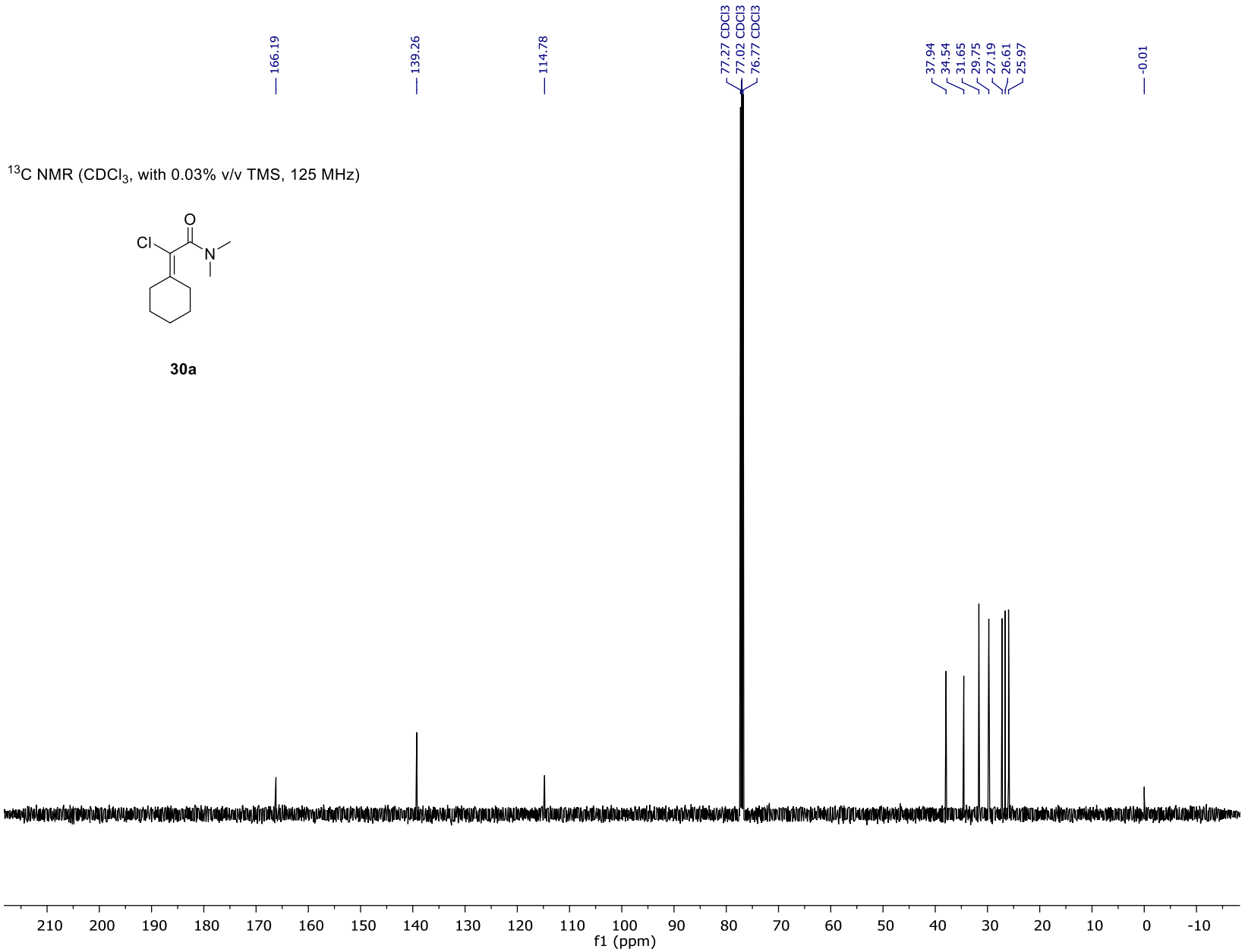



172.69
151.56
134.81
55.71
31.09
29.66
29.05
27.30
27.23
25.17
^{13}C NMR ($CDCl_3$, with 0.03% v/v TMS, 125 MHz)
O
N
29
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

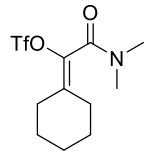
^{1}H NMR ($CDCl_3$, with 0.03% v/v TMS, 500 MHz)



30a

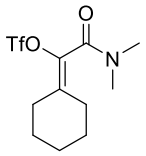

166.19
139.26
114.78
77.27 CDCl3
77.02 CDCl3
76.77 CDCl3
37.94
34.54
31.65
29.75
27.19
26.61
25.97
-0.01
13C NMR (CDCl3, with 0.03% v/v TMS, 125 MHz)
O
Cl
N
30a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

^{1}H NMR ($CDCl_3$, with 0.03% v/v TMS, 125 MHz)

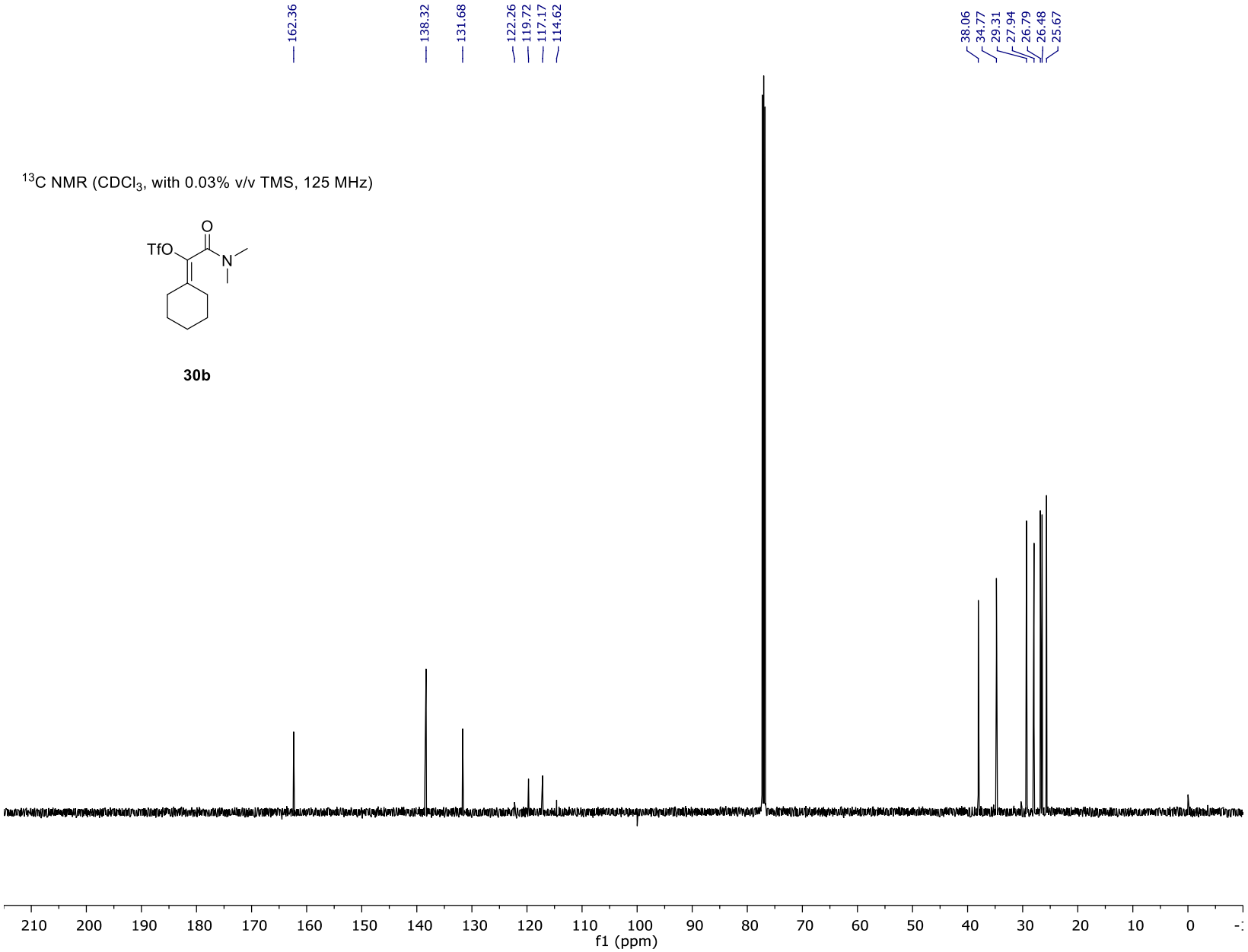


30b

^{19}F NMR ($CDCl_3$, 471 MHz)



30b


162.36
138.32
131.68
122.26
119.72
117.17
114.62
38.06
34.77
29.31
27.94
26.79
26.48
25.67
^{13}C NMR ($CDCl_3$, with 0.03% v/v TMS, 125 MHz)
TfO
O
N
30b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)