

Electronic Supplementary Information

Thiolate–Palladium(IV) or Sulfonium–Palladate(0)? A Theoretical Study on the Mechanism of Palladium-catalyzed C–S Bond Formation Reactions

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1. Complete reference for Gaussian 09

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

Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2013**.

2. The value of Hammett plots

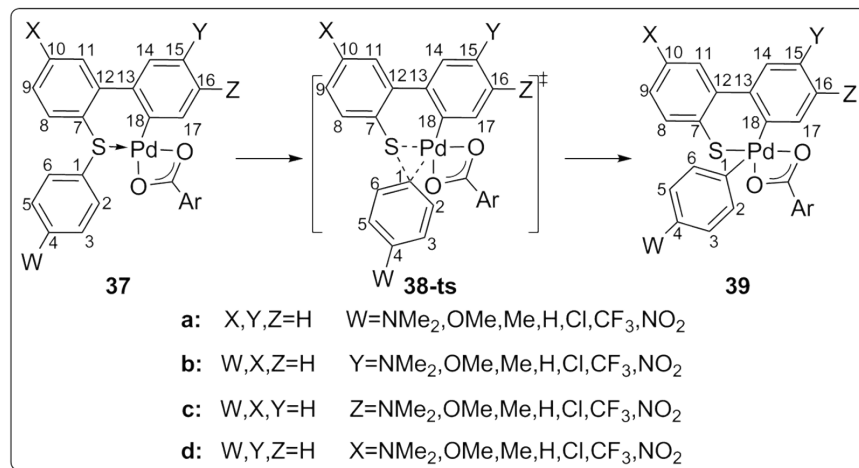


Fig. S1. Diarylsulfane with various substituents at different positions

Table S1 The value of Hammett plots for different substitution positions in 4-position.

W	σ	$\Delta H(\text{kcal/mol})$	$\lg k$	$\lg k_X/k_H$
NO ₂	0.78	19.8	-3.465740	0.59
CF ₃	0.54	21.5	-3.762937	0.29
Cl	0.23	22.8	-4.002448	0.05
H	0.00	23.1	-4.052350	0.00
Me	-0.17	23.9	-4.181621	-0.13
OMe	-0.27	24.9	-4.363944	-0.31
NMe ₂	-0.83	26.3	-4.611617	-0.56

Table S2 The value of Hammett plots for different substitution positions in 15-position.

Y	σ	$\Delta H(\text{kcal/mol})$	$\lg k$	$\lg k_X/k_H$
NO ₂	0.78	24.5	-4.290806	-0.24
CF ₃	0.54	23.9	-4.181512	-0.13

Cl	0.23	23.6	-4.142268	-0.09
H	0.00	23.1	-4.052350	0.00
Me	-0.17	23.0	-4.022905	0.03
OMe	-0.27	23.1	-4.040731	0.01
NMe ₂	-0.83	22.3	-3.905552	0.15

Table S3 The value of Hammett plots for different substitution positions in 16-position.

Z	σ	$\Delta H(\text{kcal/mol})$	$\lg k$	$\lg k_X/k_H$
NO ₂	0.78	24.1	-4.220556	-0.17
CF ₃	0.54	23.8	-4.169322	-0.12
Cl	0.23	23.6	-4.135711	-0.08
H	0.00	23.1	-4.052350	0.00
Me	-0.17	23.2	-4.057907	-0.01
OMe	-0.27	23.1	-4.051353	0.00
NMe ₂	-0.83	22.5	-3.936464	0.12

Table S4 The value of Hammett plots for different substitution positions in 10-position.

X	σ	$\Delta H(\text{kcal/mol})$	$\lg k$	$\lg k_X/k_H$
NO ₂	0.78	23.1	-4.051385	0.00
CF ₃	0.54	23.1	-4.041577	0.01
Cl	0.23	22.8	-3.997748	0.05
H	0.00	23.1	-4.052350	0.00
Me	-0.17	22.8	-3.998057	0.05
OMe	-0.27	22.7	-3.971806	0.08
NMe ₂	-0.83	22.3	-3.911050	0.14

3. Absolute calculation energies, enthalpies, and free energies

Table S5. Absolute calculation energies, enthalpies, and free energies

Geometry	E _(elec-B3-LYP) ¹	E _(solv, M06-L) ²	G _(corr-B3-LYP) ³	H _(corr-B3-LYP) ⁴	IF ⁵
1	-1125.651728	-1125.867668	0.267641	0.346303	
2	-1092.520190	-1092.634120	0.217741	0.280015	
3-ts	-2218.141078	-2218.482354	0.503584	0.622022	-1152.45
4	-1718.728094	-1718.975986	0.353548	0.443572	
5-ts	-1718.679273	-1718.937173	0.353237	0.441607	-228.07
6	-1718.694200	-1718.951830	0.352408	0.442753	
7-ts	-1718.665541	-1718.929889	0.350244	0.440878	-161.00
8	-1718.737279	-1718.986292	0.350608	0.443268	
9	-860.294472	-860.375050	0.127143	0.171800	
10	-858.403208	-858.571669	0.201573	0.26875	
11-ts	-1357.865805	-1358.120696	0.356082	0.448181	-1112.33
12-ts	-2218.142418	-2218.494739	0.502647	0.622941	-133.34
13-ts	-1718.649495	-1718.914630	0.349391	0.441629	-121.22
14	-1718.667167	-1718.925691	0.350139	0.443563	
15-ts	-1718.647416	-1718.914231	0.352408	0.440804	-153.87
16-ts	-2218.143264	-2218.484437	0.502017	0.621955	-1031.07
17	-1718.709989	-1718.961218	0.3517	0.443209	
18-ts	-1718.646177	-1718.902081	0.35161	0.440531	-261.51
19	-1718.658525	-1718.913441	0.350994	0.441618	
20-ts	-1718.629115	-1718.893665	0.349272	0.439377	-293.86
21	-1180.313907	-1180.570780	0.013359	0.072192	
22	-350.195533	-350.2404295	0.147797	0.193374	
23-ts	-1530.498440	-1530.812908	0.175933	0.263408	-1084.57
24	-1003.695251	-1003.902315	0.150146	0.220278	
25	-989.871753	-989.9896734	0.134014	0.186079	
26	-1993.607306	-1993.936358	0.307194	0.409159	
27-ts	-1993.552610	-1993.901823	0.303486	0.407633	-72.40
28	-1993.582816	-1993.930587	0.308572	0.410059	
29-ts	-1993.573732	-1993.914531	0.307414	0.408451	-174.58
30	-1993.639044	-1993.965917	0.309995	0.411153	
31	-979.422882	-979.5144109	0.220384	0.282871	
32	-1540.983020	-1541.320159	0.092477	0.17327	
33-ts	-1540.979596	-1541.313273	0.088811	0.168663	-829.44
34	-360.660112	-360.7468884	0.06217	0.099328	
35-ts	-1993.537345	-1993.889457	0.308056	0.409286	-51.78
36	-1993.540308	-1993.887789	0.306111	0.410263	
ArCO₂H	-499.438953	-499.541081	0.136158	0.182962	

ArCO₂⁻	-498.8738062	-499.0365967	0.121604	0.168751	
Ph	-232.243825	-232.277532	0.073335	0.106130	
TFA	-526.775929	-526.901434	0.007574	0.046309	
CF₃CO₂⁻	-526.230372	-526.440640	-0.003516	0.032032	
37 _(W=NMe₂, X=Y=Z=H)	-1852.696746	-1852.967881	0.420489	0.521494	
37 _(W=OMe, X=Y=Z=H)	-1833.250708	-1833.520304	0.382843	0.479003	
37 _(W=Me, X=Y=Z=H)	-1758.046284	-1758.299285	0.378733	0.473049	
37 _(W=Cl, X=Y=Z=H)	-2178.319212	-2178.58032	0.34141	0.435046	
37 _(W=CF₃, X=Y=Z=H)	-2055.760242	-2056.077809	0.352274	0.45195	
37 _(W=NO₂, X=Y=Z=H)	-1923.221478	-1923.525043	0.351209	0.448606	
37 _(Y=NMe₂, W=X=Z=H)	-1852.691157	-1852.961053	0.421397	0.521506	
37 _(Y=OMe, W=X=Z=H)	-1833.24823	-1833.517155	0.382664	0.47897	
37 _(Y=Me, W=X=Z=H)	-1758.04519	-1758.297708	0.37774	0.473074	
37 _(Y=Cl, W=X=Z=H)	-2178.320868	-2178.581689	0.341439	0.435149	
37 _(Y=CF₃, W=X=Z=H)	-2055.763857	-2056.081729	0.352141	0.452016	
37 _(Y=NO₂, W=X=Z=H)	-1923.227898	-1923.532092	0.35182	0.448846	
37 _(Z=NMe₂, W=X=Y=H)	-1852.694506	-1852.965391	0.421195	0.521474	
37 _(Z=OMe, W=X=Y=H)	-1833.249666	-1833.518761	0.383237	0.47898	
37 _(Z=Me, W=X=Y=H)	-1758.045805	-1758.298761	0.377966	0.472959	
37 _(Z=Cl, W=X=Y=H)	-2178.321522	-2178.582708	0.341767	0.435155	
37 _(Z=CF₃, W=X=Y=H)	-2055.763602	-2056.08134	0.352612	0.452067	
37 _(Z=NO₂, W=X=Y=H)	-1923.226862	-1923.530933	0.352419	0.448776	
37 _(X=NMe₂, W=Y=Z=H)	-1852.69357	-1852.963968	0.420008	0.52142	
37 _(X=OMe, W=Y=Z=H)	-1833.249045	-1833.518122	0.382495	0.478923	
37 _(X=Me, W=Y=Z=H)	-1758.045622	-1758.29842	0.37777	0.472987	
37 _(X=Cl, W=Y=Z=H)	-2178.319697	-2178.580551	0.341536	0.435106	
37 _(X=CF₃, W=Y=Z=H)	-2055.761896	-2056.079474	0.352604	0.452001	
37 _(X=NO₂, W=Y=Z=H)	-1923.175759	-1923.489614	0.351879	0.446768	
38-ts _(W=NMe₂, X=Y=Z=H)	-1852.644042	-1852.924015	0.421163	0.519562	-225.09
38-ts _(W=OMe, X=Y=Z=H)	-1833.199721	-1833.478689	0.3824	0.477046	-225.78
38-ts _(W=Me, X=Y=Z=H)	-1757.996716	-1758.259355	0.378484	0.471143	-224.22
38-ts _(W=Cl, X=Y=Z=H)	-2178.271047	-2178.542107	0.341484	0.433227	-225.42
38-ts _(W=CF₃, X=Y=Z=H)	-2055.713681	-2056.041714	0.352214	0.450071	-223.03
38-ts _(W=NO₂, X=Y=Z=H)	-1923.177088	-1923.49179	0.352263	0.446867	-220.94
38-ts _(Y=NMe₂, W=X=Z=H)	-1852.643383	-1852.923556	0.420785	0.519522	-234.29
38-ts _(Y=OMe, W=X=Z=H)	-1833.199997	-1833.478509	0.382727	0.477067	-232.22
38-ts _(Y=Me, W=X=Z=H)	-1757.996743	-1758.25915	0.378071	0.471096	-230.29
38-ts _(Y=Cl, W=X=Z=H)	-2178.271586	-2178.542105	0.34163	0.433231	-228.54
38-ts _(Y=CF₃, WXZ=H)	-2055.714005	-2056.041756	0.352505	0.450065	-227.06
38-ts _(Y=NO₂, WXZ=H)	-1923.177449	-1923.490997	0.352165	0.446767	-223.38
38-ts _(Z=NMe₂, W=X=Y=H)	-1852.646496	-1852.92759	0.42056	0.519467	-228.28

38-ts (Z=OMe, W=X=Y=H)	-1833.200675	-1833.47996	0.383047	0.477018	-229.13
38-ts (Z=Me, W=X=Y=H)	-1757.997199	-1758.259981	0.377695	0.471077	-231.51
38-ts (Z=Cl, W=X=Y=H)	-2178.271831	-2178.543147	0.34194	0.4332	-228.70
38-ts (Z=CF ₃ , W=X=Y=H)	-2055.714015	-2056.041403	0.352607	0.450042	-226.51
38-ts (Z=NO ₂ , W=X=Y=H)	-1923.176594	-1923.490547	0.352165	0.446767	-225.75
38-ts (X=NMe ₂ , WYZ=H)	-1852.64588	-1852.926572	0.42061	0.519587	-222.02
38-ts (X=OMe, W=Y=Z=H)	-1833.200906	-1833.480131	0.38273	0.477048	-225.22
38-ts (X=Me, W=Y=Z=H)	-1757.997107	-1758.260139	0.378001	0.471061	-226.98
38-ts (X=Cl, W=Y=Z=H)	-2178.271075	-2178.542248	0.341237	0.433154	-228.81
38-ts (X=CF ₃ , W=Y=Z=H)	-2055.712942	-2056.040719	0.350691	0.449996	-231.01
38-ts (X=NO ₂ , W=Y=Z=H)	-1923.175759	-1923.489614	0.351879	0.446768	-234.20

¹The electronic energy was calculated by B3-LYP in gas phase. ²The electronic energy was calculated by M06-L in solvation, toluene and acetic acid were used as the solvents to represent the mechanisms of the reactions reported by Chatani and Anbarasan, respectively. ³The thermal correction to Gibbs free energy calculated by B3-LYP in gas phase. ⁴The thermal correction to enthalpy calculated by B3-LYP in gas phase. ⁵The B3-LYP calculated imaginary frequencies for the transition states.

4. B3-LYP geometries for all the compounds and transition state

1				H	3.46665200	2.91351200	0.52493700
C	-6.02300200	-1.04857500	0.59314400	H	3.14981300	1.94423900	1.94986900
C	-4.62499700	-1.08103200	0.59925300	H	4.67339100	2.84504500	1.82414500
C	-3.92557100	0.00013700	-0.00008700	C	3.94178600	-2.25755600	-1.26191200
C	-4.62434900	1.08171500	-0.59945100	H	3.46809200	-2.91345400	-0.52488700
C	-6.02236900	1.05005300	-0.59339900	H	3.15068100	-1.94426300	-1.94975600
C	-6.71883600	0.00093600	-0.00014900	H	4.67472300	-2.84430600	-1.82417200
H	-6.56904800	-1.86337500	1.06076900	C	2.44830600	-0.00024300	0.00011100
H	-6.56793200	1.86517700	-1.06101500	O	1.75664800	1.08429500	-0.00623100
H	-7.80573400	0.00124900	-0.00017700	O	1.75722200	-1.08513900	0.00649300
C	-3.94059800	2.25794100	-1.26191900	Pd	0.00000100	-0.00069300	0.00005900
H	-3.46646800	2.91347400	-0.52486100	2			
H	-3.14973800	1.94429000	-1.94987300	C	0.85772300	1.87952200	0.46554100
H	-4.67326000	2.84517300	-1.82403300	C	-0.03093200	0.80402000	0.33168400
C	-3.94192700	-2.25760700	1.26181300	C	-1.40674200	1.05302900	0.11543100
H	-3.46819300	-2.91348200	0.52479000	C	-1.83112300	2.38799000	0.00950500
H	-3.15086500	-1.94436600	1.94972700	C	-0.94198600	3.45415300	0.12215500
H	-4.67492300	-2.84437100	1.82398400	C	0.40806800	3.19423500	0.35704100
C	-2.44831000	-0.00028500	-0.00006200	H	1.90990400	1.68637500	0.64364200
O	-1.75664800	1.08427100	0.00616400	H	-2.88862000	2.57907300	-0.15196300
O	-1.75720200	-1.08516600	-0.00623700	H	-1.30218300	4.47556400	0.03747200
C	6.02293800	-1.04860700	-0.59331600	H	1.11650200	4.01191000	0.46100900
C	4.62493200	-1.08102100	-0.59935400	C	-2.42534300	-0.02872500	-0.00755800
C	3.92557600	0.00014900	0.00006100	C	-3.25967400	-0.08412700	-1.13611100
C	4.62441600	1.08168200	0.59942200	C	-2.61357600	-0.97878000	1.00941800
C	6.02243400	1.04997800	0.59330400	C	-4.24443300	-1.06530400	-1.25059200
C	6.71883600	0.00085900	-0.00002000	H	-3.12091900	0.64096900	-1.93362400
H	6.56893700	-1.86341000	-1.06099300	C	-3.59845800	-1.96047100	0.89525600
H	6.56804500	1.86506500	1.06093100	H	-1.99702100	-0.93610700	1.90275000
H	7.80573400	0.00113000	-0.00004700	C	-4.41632700	-2.00826800	-0.23513300
C	3.94071400	2.25789200	1.26196600	H	-4.87474400	-1.09552400	-2.13559500

H	-3.73072400	-2.68418300	1.69520800
H	-5.18279000	-2.77361200	-0.32344200
S	0.54151800	-0.90274400	0.42753900

C	2.29041100	-0.77345000	0.04527300	C	6.53509800	-1.94505600	-1.09149700
C	3.23252100	-1.07002000	1.03808100	C	6.58806300	-1.45587700	-2.39356700
C	2.72311100	-0.47233400	-1.25481100	H	5.54195900	-0.37916000	-3.93316300
C	4.59626400	-1.06530100	0.73318600	H	7.38074700	-2.49319700	-0.68436700
H	2.89437300	-1.30315500	2.04319000	H	7.47598200	-1.61548100	-2.99990200
C	4.08572600	-0.45318300	-1.54931500	C	5.42641900	-2.29982700	1.12182700
H	1.99049000	-0.25505300	-2.02608900	H	5.50050600	-1.50256300	1.86757000
C	5.02465300	-0.75319500	-0.55753200	H	4.51652800	-2.86197400	1.35583700
H	5.32157100	-1.29926500	1.50788900	H	6.28174600	-2.97110600	1.24713800
H	4.41507800	-0.21586300	-2.55743400	C	3.19290800	0.19513600	-2.80671900
H	6.08549800	-0.74598200	-0.79273400	H	2.35432000	-0.47223700	-3.02828100
3-ts				H	2.80167600	0.98742500	-2.16116700
C	0.43437000	3.77903500	-0.81427300	H	3.52645400	0.65212500	-3.74395800
C	0.05856800	2.97242800	0.26925500	C	3.08721900	-0.82302800	0.00830400
C	1.04962500	2.37776700	1.07874300	O	3.23075500	-0.53099300	1.23881400
C	2.39904200	2.62218600	0.77740500	O	1.94633200	-0.94197500	-0.54777800
C	2.76859900	3.41684000	-0.30657500	H	2.02967400	-0.27188700	1.70490700
C	1.77947000	3.99276700	-1.10625700	4			
H	-0.33228600	4.23617700	-1.43107900	C	-3.74189500	1.19253900	1.10072700
H	3.16287800	2.16639400	1.39992000	C	-3.02237700	0.18564400	0.45675100
H	3.81998100	3.58782900	-0.51999700	C	-3.12027300	-1.16616900	0.84950500
H	2.05162200	4.61987900	-1.95116000	C	-3.94791300	-1.44433700	1.95166700
C	0.71739000	1.53760700	2.27443800	C	-4.66019700	-0.44580800	2.61243300
C	0.28973200	2.17036000	3.44823400	C	-4.56396200	0.87669400	2.18286600
C	0.89073800	0.12451700	2.26475300	H	-3.66114700	2.22044400	0.76539100
C	0.03001000	1.43348200	4.60581000	H	-4.00678100	-2.46719000	2.30970200
H	0.16620300	3.25011500	3.45628000	H	-5.28140000	-0.70208100	3.46595800
C	0.63360200	-0.59280400	3.45648000	H	-5.11492700	1.66530500	2.68730500
C	0.21048600	0.04784000	4.61712200	C	-2.40901400	-2.27220900	0.15149800
H	-0.30192400	1.94646400	5.50487900	C	-3.05669000	-3.52093600	0.04214000
H	0.77590800	-1.67072200	3.46229800	C	-1.11137100	-2.14277800	-0.39438600
H	0.02172400	-0.52277600	5.52237600	C	-2.44245800	-4.61198000	-0.56444200
S	-1.67213600	2.72581100	0.69208000	H	-4.07112900	-3.62425400	0.41718200
C	-2.48826500	2.80195700	-0.90558700	C	-0.49885300	-3.24809500	-0.99830000
C	-2.29382300	1.79165900	-1.86034100	C	-1.15281100	-4.47922800	-1.08032500
C	-3.39481000	3.83779000	-1.16316000	H	-2.97174200	-5.55809100	-0.63837800
C	-2.99091400	1.83445000	-3.06746200	H	0.50943400	-3.15039800	-1.39070900
H	-1.60452500	0.97763800	-1.65565700	H	-0.65633900	-5.32585300	-1.54802200
C	-4.10187800	3.86457000	-2.36828200	S	-1.97207200	0.55526300	-0.97579000
H	-3.54234900	4.61747900	-0.42181400	C	-1.76174300	2.34305000	-0.91666100
C	-3.89806800	2.86736000	-3.32276600	C	-0.82046900	2.95204900	-0.07887900
H	-2.83423700	1.05080000	-3.80389500	C	-2.55193500	3.10869200	-1.78295600
H	-4.80536800	4.67021900	-2.56108800	C	-0.68633500	4.34079500	-0.10395300
H	-4.44539600	2.89142200	-4.26119500	H	-0.18644500	2.34746500	0.55983200
Pd	0.21011700	-0.90231400	0.52270900	C	-2.40932200	4.49720700	-1.79754500
C	-5.79431500	-2.30759700	0.24257900	H	-3.26852100	2.62132100	-2.43750000
C	-4.53062200	-1.75147400	0.46856400	C	-1.47868100	5.11235000	-0.95782100
C	-3.40450100	-2.37603100	-0.12705500	H	0.04714300	4.81786400	0.53962800
C	-3.55268600	-3.54293500	-0.92055700	H	-3.02119000	5.09395400	-2.46792800
C	-4.83726500	-4.06867500	-1.09496400	H	-1.36481200	6.19269600	-0.97440900
C	-5.95100300	-3.45721500	-0.52635500	Pd	0.00145200	-0.48573200	-0.37510500
H	-6.66491000	-1.82801800	0.68221100	C	6.19989100	-0.76242600	-0.00926600
H	-4.95938900	-4.97071000	-1.68891800	C	4.83193700	-0.92297300	-0.25717800
H	-6.94141600	-3.87746900	-0.68177900	C	3.92910100	0.00370800	0.31580200
C	-2.39258200	-4.26343700	-1.57373000	C	4.39513600	1.06166900	1.13177200
H	-1.99778300	-3.69876800	-2.42394100	C	5.76969900	1.16503700	1.37118900
H	-1.55417000	-4.40946200	-0.88614800	C	6.66898800	0.26676300	0.80244300
H	-2.71888400	-5.24473300	-1.93278000	H	6.90176000	-1.46051700	-0.45865800
C	-4.43918500	-0.50509800	1.32159000	H	6.13470700	1.96537900	2.01006000
H	-3.98585700	-0.71920300	2.29439400	H	7.73454000	0.36894700	0.99178200
H	-3.82237800	0.27031700	0.85873300	C	3.46915300	2.07519000	1.76888900
H	-5.44019500	-0.09522700	1.48982300	H	3.07123500	2.77153500	1.02392800
C	-2.04941800	-1.80728400	0.08272300	H	2.60590700	1.60040000	2.24657200
O	-1.14153800	-1.87019500	-0.81876800	H	4.00633300	2.65129300	2.52940300
O	-1.72634000	-1.23410500	1.18849700	C	4.38484900	-2.06898800	-1.13877700
C	5.50027000	-0.76392300	-2.91751900	H	3.89897500	-2.85489000	-0.55193900
C	4.33887500	-0.55623900	-2.16429500	H	3.65907600	-1.75000200	-1.89372900
C	4.30562200	-1.04408100	-0.83477800	H	5.24611000	-2.50525400	-1.65498600
C	5.40960500	-1.74183300	-0.28543800	C	2.46450500	-0.13200600	0.05430000

O	1.74099700	0.88468900	-0.20031800	C	-1.47650800	1.54934400	0.32315700
O	1.91073200	-1.28961000	0.08382300	C	-2.91417800	3.68074000	1.40984200
5-ts				H	-4.65852100	2.61321100	0.78907600
C	-4.18448600	-1.49047600	-1.46963400	C	-0.80433100	2.63483600	0.90309500
C	-3.26147100	-0.50572900	-1.06792100	C	-1.52010500	3.70024600	1.45115800
C	-3.67268600	0.59704500	-0.28024000	H	-3.48848100	4.51322800	1.80697800
C	-5.02695600	0.60360500	0.12734600	H	0.28105000	2.64581800	0.93951600
C	-5.93575800	-0.36557700	-0.27623300	H	-0.98695200	4.53555700	1.89701800
C	-5.51960500	-1.41506800	-1.09998500	S	-1.65030500	-0.26786300	-2.07029000
H	-3.83198700	-2.32312800	-2.07124200	C	-0.41472900	-1.28478800	0.70587300
H	-5.36757100	1.38080400	0.80164700	C	-0.84512800	-1.11672700	2.01922100
H	-6.96562800	-0.31002600	0.06517800	C	-0.06864600	-2.52957600	0.18624200
H	-6.21878500	-2.18155300	-1.42120700	C	-0.92709500	-2.25027800	2.83884900
C	-2.78408900	1.70940300	0.14628800	H	-1.10194500	-0.14118800	2.41192900
C	-3.39093100	2.95269100	0.45228000	C	-0.16246900	-3.64770200	1.02451500
C	-1.38145200	1.63115800	0.30264200	H	0.27707500	-2.63559600	-0.83469300
C	-2.67698100	4.02865100	0.96029400	C	-0.59111300	-3.51097700	2.34540000
H	-4.44962700	3.08203800	0.25511700	H	-1.25528900	-2.13222000	3.86841600
C	-0.66753900	2.70729000	0.85412000	H	0.10416400	-4.62501000	0.63054700
C	-1.30742400	3.89946100	1.18995600	Pd	-0.12800500	0.31323200	-0.50242600
H	-3.18879500	4.96321100	1.17289000	C	5.89284900	-0.02551800	1.18390100
H	0.40276000	2.62011100	1.00819900	C	4.49789500	0.02490200	1.08706200
H	-0.73092800	4.72205600	1.60489700	C	3.91692600	0.15040000	-0.19805200
S	-1.61274300	-0.78935100	-1.62242400	C	4.72459600	0.23762600	-1.35807400
C	-0.79579500	-1.66978100	0.38130700	C	6.11483200	0.20965400	-1.20472600
C	-1.66346300	-1.63563800	1.46949700	C	6.69802500	0.07248700	0.05225600
C	0.08946600	-2.72813300	0.17272300	H	6.34855800	-0.13973200	2.16419600
C	-1.60536300	-2.67745100	2.40288400	H	6.74369900	0.29185400	-2.08752100
H	-2.36612400	-0.82248000	1.60430400	H	7.78022700	0.04171700	0.14984500
C	0.12707400	-3.75901500	1.11554700	C	4.15171300	0.37668100	-2.75200800
H	0.74531400	-2.74530200	-0.68911200	H	3.69641900	-0.55901500	-3.09088900
C	-0.71485000	-3.73710000	2.23034500	H	3.36729900	1.13881800	-2.80311800
H	-2.26466400	-2.64804100	3.26655100	H	4.94172600	0.65279200	-3.45757500
H	0.81677000	-4.58545100	0.96450000	C	3.68040400	-0.07635500	2.35690800
Pd	-0.07096300	0.26163400	-0.35152400	H	3.24476800	0.89093300	2.62732200
C	6.00595100	0.22748700	1.14396500	H	2.84544900	-0.77658100	2.25888400
C	4.60786600	0.25160800	1.09133900	H	4.31350700	-0.41126000	3.18485700
C	3.98096300	0.19269500	-0.17583500	C	2.43265500	0.18620800	-0.33857000
C	4.74516500	0.12430400	-1.36481800	O	1.84095800	-0.44762700	-1.26853500
C	6.14043200	0.12948100	-1.26084400	O	1.72229300	0.87237500	0.48656600
C	6.76952700	0.17387000	-0.01928700	H	-0.66130000	-4.38391500	2.98840600
H	6.49722100	0.25585200	2.11335900	7-ts			
H	6.73656300	0.09387500	-2.16922700	C	4.34805300	-0.32048700	-1.95507900
H	7.85484200	0.16669400	0.04174100	C	3.51421600	-0.22245100	-0.83326600
C	4.11800000	0.06299500	-2.74095900	C	3.27884500	-1.34930300	-0.00815900
H	3.67707400	-0.92005000	-2.93444800	C	3.87293700	-2.57139100	-0.35962700
H	3.31145500	0.79340800	-2.86114000	C	4.69798300	-2.66581000	-1.47688600
H	4.87341700	0.25906000	-3.50862300	C	4.94512300	-1.53901600	-2.26931300
C	3.83179100	0.32234600	2.38891800	H	4.51783500	0.55335600	-2.57663300
H	3.38523100	1.31147900	2.53221000	H	3.67764300	-3.45556200	0.24000800
H	3.00756500	-0.39757200	2.41872200	H	5.14553900	-3.62112200	-1.73544600
H	4.49466000	0.11822500	3.23594100	H	5.58925600	-1.61451100	-3.14062400
C	2.49102300	0.19872100	-0.26282600	C	2.47027000	-1.13662100	1.20215700
O	1.87434100	-0.59244200	-1.04585600	C	2.57159300	-1.95211200	2.34692600
O	1.80314100	1.00908100	0.45556200	C	1.63584700	-0.00866100	1.30074000
H	-0.68087300	-4.54494800	2.95576300	C	1.90843600	-1.62394700	3.52385900
6				H	3.22290200	-2.82080300	2.31798900
C	-4.05427700	-1.47013400	-1.81482200	C	0.99165300	0.36269700	2.47740200
C	-3.22636900	-0.45512200	-1.30067900	C	1.12944300	-0.46465000	3.59365700
C	-3.67905000	0.35887600	-0.23477400	H	2.01279300	-2.26235300	4.39624200
C	-4.94567500	0.06973600	0.31147600	H	0.33600100	1.22289200	2.51459100
C	-5.76037000	-0.93177500	-0.20363200	H	0.60188600	-0.20952300	4.50818400
C	-5.31927100	-1.69698200	-1.28689900	S	2.74224900	1.31298600	-0.38831800
H	-3.68416500	-2.08546200	-2.62942200	C	-0.13687300	2.37220300	-0.29815100
H	-5.28703300	0.63270100	1.17419900	C	0.35521200	3.29740800	0.61621100
H	-6.72954100	-1.12447800	0.24768400	C	-1.13940500	2.69584100	-1.21141200
H	-5.94414000	-2.48529000	-1.69730000	C	-0.18474300	4.58978800	0.62005500
C	-2.88552400	1.48597900	0.30501100	H	1.14705900	3.04394500	1.31365500
C	-3.57496900	2.59526500	0.84720800	C	-1.65898200	3.99647500	-1.19778900

H	-1.52706700	1.95908700	-1.90609300	C	4.07053700	-1.82026100	1.56715700
C	-1.18793400	4.93995900	-0.28366300	H	3.47019600	-1.20616800	2.24616200
H	0.19349100	5.31900000	1.33183000	H	3.40483300	-2.59784700	1.17977400
H	-2.44332000	4.25829700	-1.90329700	H	4.86319600	-2.30041900	2.15016100
H	-1.60138000	5.94449900	-0.27586200	C	3.78414300	1.68512100	-2.19055200
Pd	0.57329600	0.50019800	-0.44255600	H	2.82531800	1.29284100	-2.54475300
C	-4.44291600	-3.25310200	-0.83334500	H	3.55706400	2.58914300	-1.61722100
C	-3.26975000	-2.53780700	-0.56469200	H	4.38099500	1.96884000	-3.06348600
C	-3.37725800	-1.19920200	-0.13032600	C	2.47979500	0.13331000	-0.00594400
C	-4.64155000	-0.58985300	0.02781200	O	1.71431600	-0.84899100	0.25365700
C	-5.78763700	-1.33314000	-0.27747600	O	1.98537400	1.32043800	0.00001900
C	-5.69441700	-2.65672800	-0.70114100	9			
H	-4.36805500	-4.28973300	-1.15362600	C	-0.96136900	-0.00002500	-2.63826600
H	-6.76359600	-0.86508800	-0.17181800	C	-0.73190900	0.00000000	-1.26037300
H	-6.59511200	-3.22341300	-0.92383500	C	0.57760500	0.00000100	-0.72760200
C	-4.79346700	0.83422800	0.51666200	C	1.66715100	0.00000600	-1.61236200
H	-4.50648900	0.92074400	1.56911000	C	1.44414300	0.00000500	-2.98515300
H	-4.15242600	1.53102900	-0.03494400	C	0.13639400	-0.00002700	-3.49567900
H	-5.83107200	1.16642800	0.40730600	H	-1.97299800	-0.00005800	-3.03359700
C	-1.93411500	-3.23075100	-0.73120900	H	2.68233100	0.00003900	-1.22443000
H	-1.39485800	-2.85150500	-1.60555300	H	2.28875900	0.00004700	-3.66829200
H	-1.28182800	-3.07497100	0.13552600	H	-0.02400300	-0.00007500	-4.57022800
H	-2.07659400	-4.30933100	-0.85607800	C	0.57760500	0.00000100	0.72760200
C	-2.14013900	-0.39753500	0.21006200	C	1.66715100	0.00000600	1.61236200
O	-2.03149200	0.18638400	1.28511100	C	-0.73190900	0.00000000	1.26037300
O	-1.23510100	-0.38068500	-0.74811300	C	1.44414300	0.00000500	2.98515300
8				H	2.68233100	0.00003900	1.22443000
C	-3.87399600	0.76914200	-0.57716900	C	-0.96136900	-0.00002500	2.63826600
C	-3.16616900	-0.37952400	-0.23216500	C	0.13639400	-0.00002700	3.49567900
C	-3.41513400	-1.62976900	-0.83239700	H	2.28875900	0.00004700	3.66829200
C	-4.40618100	-1.71255200	-1.81980800	H	-1.97299800	-0.00005800	3.03359700
C	-5.11474500	-0.56993800	-2.18294300	H	-0.02400300	-0.00007500	4.57022800
C	-4.85170300	0.66119200	-1.56729700	S	-1.97077300	0.00003600	0.00000000
H	-3.66326800	1.71959000	-0.09933800	10			
H	-4.61933800	-2.66357000	-2.29971200	C	2.83499400	0.09079000	-0.05971700
H	-5.88076100	-0.63510800	-2.95029500	C	3.96487900	-0.57076100	0.42968300
H	-5.41179000	1.54422400	-1.86061000	C	2.94717600	1.27321700	-0.78975200
C	-2.56265800	-2.69197500	-0.30353400	C	5.23717000	-0.05205500	0.15525600
C	-2.52273600	-4.04639100	-0.65963900	H	3.87489100	-1.48279300	1.02521500
C	-1.68088500	-2.23308800	0.69415700	C	4.22208300	1.78574100	-1.05299800
C	-1.61561100	-4.89703900	-0.03197400	H	2.05714900	1.78104400	-1.15104300
H	-3.19252700	-4.43014000	-1.42392700	C	5.36169700	1.12531800	-0.58461700
C	-0.76792600	-3.07143600	1.32793300	H	6.12013900	-0.56390100	0.52927900
C	-0.74212300	-4.41477900	0.95215900	H	4.32294100	2.70348200	-1.62713600
H	-1.58290800	-5.94603100	-0.31185900	H	6.34794900	1.53161700	-0.79165300
H	-0.08351300	-2.68831600	2.07751700	Pd	1.19153400	-0.87233900	0.31668400
H	-0.03410200	-5.08852000	1.42538200	C	-4.36612000	1.82273300	0.26168200
S	-1.91986000	-0.50004200	1.04952300	C	-3.02633200	1.43871500	0.38405900
C	-0.91673100	2.35162200	0.58468100	C	-2.66661500	0.12385700	0.00088300
C	-1.60315100	2.77838800	1.73015200	C	-3.63187900	-0.78035100	-0.50578300
C	-0.84890100	3.20019800	-0.52937400	C	-4.95319000	-0.33845800	-0.63104800
C	-2.21536000	4.03844100	1.75790500	C	-5.32255100	0.94805600	-0.24691200
H	-1.66117400	2.14139900	2.60954300	H	-4.65686500	2.82397300	0.56888800
C	-1.46776600	4.45405500	-0.49878100	H	-5.69969900	-1.01906700	-1.03222900
H	-0.30616400	2.89151900	-1.41903500	H	-6.35667600	1.26871100	-0.34300800
C	-2.15357100	4.87600600	0.64325700	C	-3.29602500	-2.19357700	-0.92951300
H	-2.73946100	4.36005400	2.65509900	H	-2.40148700	-2.23530700	-1.55912100
H	-1.40724600	5.10315300	-1.36943900	H	-3.09548700	-2.83120900	-0.06300200
H	-2.63072500	5.85229000	0.66532800	H	-4.13024000	-2.62505400	-1.49157500
Pd	0.05495500	0.61579300	0.48728700	C	-2.03478200	2.43847100	0.93935000
C	5.89134100	0.45423700	-1.62415300	H	-1.38730400	1.99819000	1.70433600
C	4.53681000	0.67563300	-1.35104400	H	-1.37441900	2.82326500	0.15570600
C	3.92798300	-0.06737500	-0.31153900	H	-2.56531500	3.28468500	1.38706200
C	4.67297000	-1.00431500	0.44375900	C	-1.25489600	-0.33037500	0.14175800
C	6.03037300	-1.17176800	0.14852900	O	-0.94937300	-1.48473500	0.55849700
C	6.63732100	-0.45555300	-0.87967900	O	-0.29560100	0.48248700	-0.17764500
H	6.36328600	1.00983900	-2.43063300	11-ts			
H	6.61375000	-1.87757700	0.73457400	C	0.52773800	2.26453000	-0.34015800
H	7.69105700	-0.60608100	-1.10041300				

C	0.73439900	3.03252600	0.83021700	C	0.15243200	-0.12857300	4.39463500
C	-0.02054400	2.91308900	-1.47156600	H	1.64679300	0.09689500	5.93350600
C	0.39776800	4.38424000	0.87286500	H	-1.12819700	-0.49263700	2.66610700
H	1.17573400	2.56216200	1.70596300	H	-0.61851500	0.38018100	4.96615200
C	-0.34690200	4.26606600	-1.43484200	S	0.69563800	-2.01015100	0.80950100
H	-0.17958500	2.34662100	-2.38561400	C	-0.32075100	-1.56246900	-2.32894100
C	-0.14527900	4.99862700	-0.25972800	C	-0.25082100	-2.97175100	-2.20208600
H	0.56035300	4.96060500	1.77983500	C	0.10852100	-0.98583000	-3.54819500
H	-0.75905200	4.75265100	-2.31488600	C	0.24386300	-3.76408100	-3.23381100
H	-0.40496000	6.05385400	-0.22997000	H	-0.62833200	-3.44223700	-1.29794700
Pd	-0.17984600	0.29415700	0.03286200	C	0.61102400	-1.77691800	-4.57973900
C	-6.25784800	-0.52451500	0.55828900	H	0.03803200	0.09035600	-3.67524400
C	-4.93387600	-0.07361300	0.53212400	C	0.68490500	-3.16383300	-4.42000200
C	-3.92501600	-0.97435400	0.10639200	H	0.27554700	-4.84532500	-3.12708000
C	-4.24742500	-2.29620100	-0.29273500	H	0.93869000	-1.31845400	-5.50887100
C	-5.59018000	-2.68756700	-0.26954300	H	1.07378300	-3.78139000	-5.22578100
C	-6.58851400	-1.81563000	0.15617300	Pd	0.45848800	-0.25011100	-0.73959100
H	-7.03717900	0.15278400	0.89777600	C	2.26249900	5.57805300	-1.76563900
H	-5.85004100	-3.69372000	-0.58790900	C	1.93962500	4.21932900	-1.83755300
H	-7.62489400	-2.14283500	0.17544700	C	1.43051700	3.58779500	-0.67587800
C	-3.21408800	-3.29895100	-0.75859900	C	1.23715700	4.31101200	0.52766800
H	-2.51874200	-2.86951300	-1.48635300	C	1.55464700	5.67322900	0.53802700
H	-2.60440200	-3.65977800	0.07549000	C	2.06830100	6.30298500	-0.59263700
H	-3.70929400	-4.15823900	-1.22174800	H	2.66807100	6.07031600	-2.64567000
C	-4.64936600	1.34422900	0.97916100	H	1.39617800	6.24311000	1.44979100
H	-3.80399400	1.39887500	1.67176100	H	2.31661100	7.36068800	-0.56012800
H	-4.39614400	1.98776000	0.13084200	C	0.68414500	3.68552400	1.78981200
H	-5.52982500	1.76190000	1.47766200	H	-0.19246500	3.06097900	1.59271300
C	-2.50887900	-0.53069900	0.07937600	H	1.42320500	3.03916300	2.27369800
O	-1.54423500	-1.31837100	0.36893900	H	0.39514200	4.46809500	2.49843800
O	-2.19546000	0.67748700	-0.24142300	C	2.16486000	3.48936900	-3.14389800
C	6.30259000	-1.11693100	0.48122000	H	2.66514400	2.52659600	-2.99937200
C	5.15873000	-0.32797600	0.31884400	H	1.21708600	3.27795600	-3.64954800
C	3.93700000	-0.97305800	0.01326500	H	2.78135500	4.09836600	-3.81248500
C	3.86852400	-2.37759000	-0.14213400	C	1.09374200	2.14456100	-0.71709300
C	5.04717600	-3.11808200	0.00365100	O	1.34889400	1.36776600	0.27074500
C	6.25318300	-2.49914900	0.32005900	O	0.52975900	1.60888900	-1.73885100
H	7.24338200	-0.63421100	0.73276700	C	-5.90700300	1.31708900	1.30508500
H	5.01030800	-4.19611400	-0.13003600	C	-4.59715000	1.06867000	0.87829400
H	7.15518200	-3.09364300	0.43997200	C	-4.29880900	-0.17692900	0.28948600
C	2.58900700	-3.11177500	-0.48051800	C	-5.29956300	-1.15749100	0.13293800
H	1.91295600	-3.15498200	0.37913700	C	-6.59324200	-0.87981700	0.59003300
H	2.03363200	-2.62638600	-1.28981300	C	-6.90064700	0.34956800	1.16962300
H	2.81570000	-4.13617700	-0.79224200	H	-6.14542400	2.28111200	1.74929900
C	5.27902400	1.17033100	0.49619000	H	-7.36687800	-1.63693100	0.48229800
H	5.17769000	1.69455400	-0.45902200	H	-7.91222200	0.55423600	1.51170000
H	4.50426200	1.57269000	1.15754200	C	-4.99931100	-2.49446600	-0.50849600
H	6.25353900	1.42092000	0.92660100	H	-4.67718700	-2.36764300	-1.54642100
C	2.69623500	-0.15115300	-0.15446300	H	-4.18799600	-3.01798900	0.01332900
O	1.62799100	-0.57297100	0.40498300	H	-5.88206300	-3.14203600	-0.48906500
O	2.74793300	0.92235400	-0.83040700	C	-3.53932700	2.13837200	1.04267800
H	1.57769900	1.52266500	-0.64280500	H	-2.76119000	1.82281100	1.74533900
12-ts				H	-3.03640900	2.35549800	0.09234400
C	3.08108200	-3.16785900	-0.20087100	H	-3.98358900	3.06975500	1.40910700
C	2.41973300	-2.48788200	0.81937200	C	-2.88060500	-0.46480100	-0.17283000
C	3.05858500	-2.12997700	2.02279900	O	-2.73480000	-0.69004700	-1.42001300
C	4.40578700	-2.47233400	2.19378600	O	-1.95784500	-0.46177500	0.68072800
C	5.08002900	-3.14822300	1.17848100	H	-1.28918300	-1.06842200	-1.78330100
C	4.42478200	-3.49403000	-0.01085600	13-ts			
H	2.56825100	-3.42720900	-1.12189500	C	-3.61562700	-0.03254800	2.41916600
H	4.92344600	-2.20962400	3.11198200	C	-3.00132300	-0.47335300	1.24759600
H	6.12582800	-3.40987500	1.31159700	C	-3.12325400	-1.79462000	0.77344500
H	4.96400600	-4.01925600	-0.79375800	C	-3.90988300	-2.69061600	1.51535000
C	2.16603900	-1.42715200	2.94276200	C	-4.55405200	-2.25501600	2.66923400
C	2.43984800	-0.93337500	4.22375400	C	-4.41854500	-0.93131900	3.11812900
C	0.86827500	-1.25680200	2.42133300	H	-3.47977200	0.98626700	2.77063000
C	1.43348500	-0.28692300	4.93975900	H	-4.01006000	-3.72279200	1.19228800
H	3.42932200	-1.05268300	4.65615300	H	-5.16284100	-2.95277200	3.23702500
C	-0.15091100	-0.61663500	3.12174400	H	-4.93091700	-0.60814100	4.01931800

C	-2.41334600	-2.03179100	-0.47743000	H	-0.21610800	2.58652900	0.11914700
C	-2.50441600	-3.14792000	-1.31860500	C	-4.00104800	3.44429100	-0.11709900
C	-1.62008900	-0.93537600	-0.89255500	H	-4.31515400	1.31418700	-0.23643400
C	-1.87351000	-3.13614100	-2.56028600	C	-3.06059400	4.47370400	-0.00699900
H	-3.09690300	-4.00719800	-1.01665900	H	-0.96744000	4.97355600	0.16085700
C	-1.06906200	-0.87071900	-2.18320000	H	-5.06025000	3.67701400	-0.18130300
C	-1.17981200	-1.99756600	-2.99699700	H	-3.39200000	5.50808600	0.01283200
H	-1.95192800	-4.00156000	-3.21143900	Pd	0.53837900	-0.09989400	-0.08249600
H	-0.55344700	0.01825300	-2.53014800	C	6.73468100	-1.46876200	-0.00835200
H	-0.72073400	-1.98687100	-3.98121100	C	5.33500700	-1.45142800	-0.03314700
S	-1.75593600	0.46084500	0.33579900	C	4.67131000	-0.20427000	-0.03319900
C	-2.64532100	1.87642900	-0.36042600	C	5.40661500	1.00178300	-0.02233200
C	-1.85743200	2.98884000	-0.66893400	C	6.80499200	0.93869200	-0.02471200
C	-4.01893200	1.85269600	-0.61978300	C	7.46922000	-0.28543700	-0.01079600
C	-2.46585600	4.10781100	-1.23915400	H	7.25035100	-2.42638200	0.00661400
H	-0.78958400	2.97014300	-0.46397700	H	7.37545800	1.86483300	-0.03136900
C	-4.61166100	2.98088400	-1.18683400	H	8.55613400	-0.31716700	-0.00217800
H	-4.61153900	0.97651200	-0.37789000	C	4.73283100	2.35679700	-0.01793900
C	-3.83912600	4.10482900	-1.49524700	H	3.95815000	2.42967300	-0.78936100
H	-1.86549800	4.98054500	-1.47851900	H	4.23495300	2.54588900	0.93789700
H	-5.67838200	2.97926200	-1.39222700	H	5.46814900	3.14911500	-0.19556400
H	-4.30919400	4.97831800	-1.93792000	C	4.58377200	-2.76482600	-0.04984600
Pd	0.36303400	0.00154500	0.14318600	H	3.79794600	-2.79593100	0.71300500
C	6.61350500	-0.84719100	-0.43537100	H	4.08449100	-2.92103000	-1.01074300
C	5.21525000	-0.89835100	-0.47806200	H	5.27009800	-3.59908100	0.13148000
C	4.47807600	0.07591200	0.23184900	C	3.16484100	-0.16025200	-0.04401700
C	5.13947600	1.07445300	0.98111800	O	2.55964600	0.59627800	0.77867500
C	6.53889800	1.07251900	1.01738800	O	2.52802300	-0.88031300	-0.87513800
C	7.27538600	0.12511500	0.31057600	15-ts			
H	7.18591000	-1.58644900	-0.99110900	C	-2.03675900	-2.60070900	-0.84795400
H	7.05257600	1.82991700	1.60526100	C	-2.62660000	-1.34972200	-0.71165200
H	8.36215800	0.14397400	0.34144700	C	-4.01402100	-1.14282200	-0.78451500
C	4.38780800	2.13699600	1.75325000	C	-4.83983200	-2.25611200	-0.97581500
H	3.91061500	2.85313700	1.07718600	C	-4.26859600	-3.52490800	-1.08820900
H	3.58597800	1.70873300	2.36440200	C	-2.88013700	-3.70026800	-1.02967900
H	5.07041300	2.68043300	2.41544500	H	-0.95511000	-2.70783400	-0.82554100
C	4.54494200	-1.98755500	-1.28686700	H	-5.91739200	-2.13630200	-1.04330100
H	4.04822200	-2.71341500	-0.63599100	H	-4.91171300	-4.38758600	-1.23619800
H	3.76904800	-1.58702500	-1.94846000	H	-2.45321400	-4.69280400	-1.13718900
H	5.28232300	-2.51347400	-1.90297200	C	-4.38008500	0.27455800	-0.70064800
C	2.97313000	0.04893100	0.18910900	C	-5.64912300	0.85651300	-0.79701300
O	2.33874700	1.12760000	-0.04512200	C	-3.26578800	1.11841000	-0.55684600
O	2.36345800	-1.04789700	0.38605200	C	-5.77485500	2.24551300	-0.75129600
14				H	-6.53090200	0.23295800	-0.91462700
C	-2.17450400	-0.50983100	2.64835200	C	-3.36972000	2.50300800	-0.54415900
C	-2.49029700	-0.66260200	1.30529600	C	-4.64657300	3.06555100	-0.63121000
C	-3.53289900	-1.48497000	0.85068100	H	-6.76037200	2.69577200	-0.82588300
C	-4.29521100	-2.17417300	1.80076300	H	-2.48612500	3.13208900	-0.48672200
C	-4.00505100	-2.02061400	3.15718700	H	-4.75952200	4.14551300	-0.61704800
C	-2.95557900	-1.19629000	3.58193200	S	-1.69868600	0.18113700	-0.50711100
H	-1.33721600	0.10983700	2.95547400	C	-1.26977700	0.26364100	1.36262700
H	-5.10523600	-2.82635300	1.48687800	C	-1.16371800	-0.92837600	2.09276800
H	-4.59784900	-2.55590600	3.89325500	C	-1.26241900	1.50647600	2.01425600
H	-2.73695600	-1.09786600	4.64090600	C	-1.00804200	-0.86569800	3.47768600
C	-3.64732100	-1.50754500	-0.61333400	H	-1.18655800	-1.88866100	1.59206900
C	-4.53333200	-2.24073800	-1.41183700	C	-1.10439000	1.54649600	3.39974000
C	-2.70584800	-0.68072700	-1.24501900	H	-1.35405800	2.42842400	1.45338900
C	-4.45982200	-2.12599100	-2.80051500	C	-0.97677800	0.36606700	4.13477100
H	-5.26920300	-2.89780600	-0.95691900	H	-0.90919500	-1.78958600	4.04063400
C	-2.60376100	-0.57062400	-2.62498800	H	-1.07572800	2.50987500	3.90099100
C	-3.50517600	-1.29855900	-3.40600400	H	-0.85443700	0.40599300	5.21305900
H	-5.14627200	-2.69540000	-3.42039000	Pd	0.43608000	0.34942200	-0.33748700
H	-1.83859600	0.05219600	-3.07958500	C	6.71048400	0.70123700	-1.18675500
H	-3.45551600	-1.23017900	-4.48862100	C	5.31789100	0.84416600	-1.18490600
S	-1.56012800	0.10993100	-0.05392900	C	4.54974400	0.00035600	-0.35186400
C	-2.22036700	1.83322500	-0.06260100	C	5.17604200	-0.95929300	0.47356300
C	-1.27003100	2.84673900	0.05227300	C	6.57295800	-1.05060000	0.46044100
C	-3.58625300	2.11305900	-0.14675000	C	7.33895600	-0.23320200	-0.36719000
C	-1.69995600	4.17612900	0.07692400	H	7.30556300	1.33860800	-1.83689600

H	7.06042900	-1.77811600	1.10572800	C	6.01193600	0.94007400	-0.04129000
H	8.42256900	-0.32370400	-0.37301100	C	5.02230400	-0.07133000	-0.12489700
C	4.38864000	-1.88392100	1.37659600	C	5.37469100	-1.41706300	-0.39582100
H	3.64030700	-1.34185800	1.96517100	C	6.72567900	-1.72316600	-0.59125300
H	3.84049900	-2.63100800	0.79423300	C	7.70818900	-0.74099900	-0.50002600
H	5.06033300	-2.40206500	2.06968000	H	8.11876900	1.34022600	-0.14449600
C	4.68485400	1.88857300	-2.07830300	H	7.00538900	-2.74935500	-0.81527800
H	3.85939000	1.47576700	-2.66851300	H	8.75334500	-1.00148100	-0.64640900
H	4.26122000	2.70694700	-1.48841800	C	4.36022400	-2.53526200	-0.50277000
H	5.42782400	2.30041800	-2.76992100	H	3.96497500	-2.81082200	0.48010900
C	3.04812100	0.12788500	-0.34322800	H	3.49758900	-2.25518800	-1.11477600
O	2.33705900	-0.92187300	-0.45097100	H	4.82606700	-3.42057300	-0.94749900
O	2.52451900	1.27920400	-0.22911900	C	5.69344100	2.39057000	0.25032100
16-ts				H	5.22493000	2.87733000	-0.61064500
C	-0.72725800	-4.30004300	-1.74587400	H	4.99484500	2.50178000	1.08524500
C	-1.49240900	-3.26561300	-1.18864900	H	6.61196600	2.93298700	0.49617300
C	-2.87796700	-3.44871000	-0.96072400	C	3.59459900	0.29003700	0.07078400
C	-3.43174900	-4.69906500	-1.28685400	O	2.78807600	-0.50320300	0.68768200
C	-2.66594500	-5.72359500	-1.84160100	O	3.11144800	1.39224600	-0.35675200
C	-1.30708000	-5.52340300	-2.08009800	17			
H	0.33405500	-4.13693500	-1.90602500	C	4.36791800	-0.83845500	-1.86498200
H	-4.49482100	-4.84997400	-1.12220700	C	3.26563100	-0.73683600	-1.00175600
H	-3.13421100	-6.67140300	-2.09305000	C	3.07008800	-1.68747100	0.02480500
H	-0.69879500	-6.31206400	-2.51387400	C	4.01852100	-2.72135000	0.13164000
C	-3.78198900	-2.40947800	-0.38902100	C	5.11713400	-2.81510600	-0.71975400
C	-4.56232300	-2.71215600	0.73894700	C	5.29855400	-1.86513100	-1.72342000
C	-3.92889400	-1.14839100	-0.98730400	H	4.48237600	-0.11040900	-2.66256900
C	-5.45711300	-1.77760600	1.26081600	H	3.88300000	-3.45773400	0.91851400
H	-4.45422400	-3.68283200	1.21594800	H	5.82721500	-3.62818500	-0.59687200
C	-4.82469700	-0.21510900	-0.46695300	H	6.14785800	-1.92382700	-2.39784400
H	-3.34640400	-0.90208400	-1.86876100	C	1.94510000	-1.69841900	1.00530600
C	-5.59071800	-0.52543900	0.65874400	C	1.06758400	-2.79433500	1.03551500
H	-6.04641500	-2.02791500	2.13909400	C	1.80885300	-0.69762200	1.97943000
H	-4.92173100	0.75652100	-0.94257200	C	0.06983300	-2.88043200	2.00691400
H	-6.28728500	0.20400800	1.06341900	H	1.16606900	-3.57658000	0.28770300
S	-0.62494800	-1.72212600	-0.85894000	C	0.81496500	-0.78913800	2.95544600
C	-0.54616700	-1.62477500	0.91743500	H	2.49423200	0.14364300	1.98425800
C	-0.24216400	-0.34777100	1.47395600	C	-0.05809100	-1.87804100	2.97109500
C	-0.74220300	-2.73400700	1.74867800	H	-0.60375500	-3.73311100	2.01227500
C	-0.12677800	-0.25543300	2.88555400	H	0.72530900	-0.00626400	3.70329500
C	-0.61921700	-2.59508100	3.12992300	H	-0.83185400	-1.94614400	3.73079300
H	-0.97556800	-3.70332000	1.32118500	S	2.13865400	0.60844700	-1.46376800
C	-0.31257900	-1.35706100	3.70964000	C	2.34198000	1.95359000	-0.25941200
H	0.08522700	0.71571800	3.32669500	C	1.07103300	2.15840700	0.26418800
H	-0.76646600	-3.46659900	3.76328600	C	3.45513300	2.71930400	0.06793900
H	-0.23017300	-1.26206200	4.78854700	C	0.87555600	3.19382100	1.18014800
Pd	1.20461900	0.81069800	0.44544400	C	3.25121200	3.74963500	0.99360200
C	-3.61394800	5.38323300	-0.07502200	H	4.43440800	2.52621200	-0.36178600
C	-2.96240200	4.24033700	0.40146300	C	1.97881000	3.98390700	1.53343500
C	-1.94441900	3.66572200	-0.39622500	H	-0.10333700	3.38324500	1.61183100
C	-1.59930300	4.21872600	-1.65200200	H	4.08657100	4.37816700	1.28980000
C	-2.30032200	5.34666700	-2.09462800	H	1.84535100	4.79938400	2.24047200
C	-3.29341800	5.93150000	-1.31415800	Pd	-0.06787000	0.73871700	-0.49892000
H	-4.38554700	5.84270200	0.53744500	C	-6.24901600	0.56078500	-0.28809400
H	-2.05450200	5.77033500	-3.06495900	C	-4.88458500	0.86785900	-0.33883300
H	-3.81809100	6.81384700	-1.67148500	C	-3.95348800	-0.19879700	-0.37074300
C	-0.52569300	3.63737400	-2.54662200	C	-4.39095800	-1.54539300	-0.34239400
H	0.47531600	3.83711000	-2.15189300	C	-5.76495900	-1.79918800	-0.26629100
H	-0.61038100	2.55010000	-2.64385300	C	-6.68998200	-0.75898400	-0.24500800
H	-0.59482000	4.07400600	-3.54797100	H	-6.97127500	1.37326700	-0.27973000
C	-3.36407300	3.68708800	1.75216600	H	-6.10844300	-2.83002400	-0.22945100
H	-3.88828800	2.73178400	1.65301100	H	-7.75398100	-0.97664400	-0.19629800
H	-2.49795100	3.50186600	2.39658100	C	-3.44085100	-2.72276200	-0.37894900
H	-4.02236000	4.39407200	2.26677300	H	-3.01527200	-2.85716200	-1.37845400
C	-1.22704600	2.44448700	0.09796900	H	-2.59303800	-2.59120600	0.29981300
O	0.04148800	2.41307600	-0.03714700	H	-3.97052000	-3.64033900	-0.10170200
O	-1.90105800	1.50872000	0.62477100	C	-4.47526800	2.32459800	-0.37719700
H	-1.03919700	0.58011300	1.01724800	H	-4.03362000	2.63973900	0.57335500
C	7.35044600	0.57529200	-0.22140700	H	-3.72368800	2.52266600	-1.14764100

	H	-5.34799400	2.95443200	-0.57833400	C	-0.56334600	-0.43893600	1.51440400	
	C	-2.49156600	0.09241300	-0.44756600	C	-0.40076100	0.54452500	2.48692900	
	O	-1.70724200	-0.60809800	-1.15787000	C	-0.69828900	-1.78768200	1.83452700	
	O	-1.99861900	1.08054200	0.22022100	C	-0.37783100	0.15315100	3.83112500	
18-ts					H	-0.28040500	1.58712600	2.22031800	
	C	3.32534400	-2.19073100	-1.98569300	C	-0.66951400	-2.15433800	3.18601000	
	C	2.78431600	-1.14157000	-1.21373800	H	-0.81418900	-2.54328900	1.06799100	
	C	1.57390700	-1.34735200	-0.52816700	C	-0.51399000	-1.19021200	4.18208500	
	C	0.91802200	-2.58840000	-0.66815200	H	-0.25014000	0.91242200	4.59828100	
	C	1.46098800	-3.61119500	-1.43475700	H	-0.77012100	-3.20444800	3.44800000	
	C	2.68348800	-3.41624800	-2.08638000	H	-0.49637700	-1.48480600	5.22765300	
	H	4.25278000	-2.01693800	-2.52467600	S	-3.99874800	-0.06582000	0.20146800	
	H	-0.03214200	-2.74623000	-0.17184900	C	-3.12876400	-1.20345400	-0.85102500	
	H	0.93034000	-4.55479500	-1.52389600	C	-1.74928400	-1.16985400	-1.09011500	
	H	3.12152100	-4.20727500	-2.68825100	C	-3.90410200	-2.22633600	-1.42477000	
	C	1.43220000	-0.71175300	1.45250200	C	-1.16288600	-2.14961400	-1.90703600	
	C	0.64889300	-1.54616600	2.26641800	C	-3.31417800	-3.19969500	-2.22688200	
	C	2.59294100	-0.12608700	1.96681200	H	-4.97616100	-2.24197400	-1.24760000	
	C	1.03016300	-1.78151600	3.58750800	C	-1.94177900	-3.15856500	-2.47891600	
	H	-0.26062900	-1.99593300	1.88622200	H	-0.08949600	-2.13777900	-2.07886100	
	C	2.96611300	-0.37873500	3.29049600	H	-3.93012500	-3.98001400	-2.66545700	
	H	3.21240900	0.51931200	1.36120900	H	-1.47320600	-3.90689400	-3.11218900	
C	2.19193600	-1.20360900	4.10478700	Pd	-0.38417900	0.12059300	-0.41383500		
H	0.41162000	-2.42334900	4.20936800	C	5.76498900	-1.03281700	0.17650600		
H	3.86942500	0.08433600	3.67872300	C	4.36597100	-1.04693900	0.14659000		
H	2.48768300	-1.39402700	5.13262500	C	3.69105400	0.08769700	-0.36592800		
S	3.80009500	0.30713600	-1.19458500	C	4.41388000	1.20456400	-0.85061900		
C	2.75618500	1.72039700	-0.90809500	C	5.81195200	1.15840600	-0.82372600		
C	1.44187900	1.71037200	-0.42871200	C	6.48619500	0.05441400	-0.30905400		
C	3.40197800	2.94763000	-1.15896300	H	6.29095500	-1.89246300	0.58399100		
C	0.79420300	2.93642700	-0.20374600	H	6.37430300	2.00508100	-1.20927700		
C	2.75193800	4.15250900	-0.92358500	H	7.57291600	0.04136100	-0.28664600		
H	4.41872800	2.94428400	-1.54472500	C	3.74447500	2.43961200	-1.41423500		
C	1.44064800	4.14901600	-0.44346600	H	2.95421300	2.19167900	-2.13046000		
H	-0.23341900	2.94145900	0.14486200	H	3.27438300	3.03273100	-0.62367200		
H	3.26449400	5.08908400	-1.12484800	H	4.48196900	3.06686000	-1.92509400		
H	0.91457100	5.08298300	-0.26565300	C	3.64595600	-2.26680200	0.68006100		
Pd	0.24995100	0.15345600	-0.04157700	H	2.82571300	-2.00333700	1.35471900		
C	-5.92955200	1.11829200	0.32384500	H	3.20383600	-2.85303900	-0.13160000		
C	-4.53218800	1.15015300	0.38731800	H	4.34683400	-2.90666300	1.22592700		
C	-3.80748300	0.06637900	-0.16344700	C	2.19767000	0.10644100	-0.39444700		
C	-4.47682300	-1.01919400	-0.77741300	O	1.55229500	1.16669600	-0.08699300		
C	-5.87433400	-0.99193600	-0.83877000	O	1.54131900	-0.93945400	-0.72724200		
				20-ts					
C	-6.59884600	0.06203200	-0.28844500	C	-3.82304300	-1.63740900	1.91923000		
H	-6.49522100	1.93843100	0.75869200	C	-3.15383900	-0.83234800	0.98848500		
H	-6.39655200	-1.81311100	-1.32318500	C	-2.04934600	-0.05182000	1.38296900		
H	-7.68474200	0.06049900	-0.33716300	C	-1.72086900	0.00963300	2.75307200		
C	-3.74770000	-2.19778500	-1.38582100	C	-2.41165000	-0.76526000	3.68163100		
H	-2.89873500	-1.88615400	-2.00233500	C	-3.44333500	-1.61292100	3.25840700		
H	-3.34593300	-2.85902600	-0.61125400	H	-4.67128400	-2.23712500	1.60034400		
H	-4.43041200	-2.77946400	-2.01344500	H	-0.89511400	0.63223800	3.09276200		
C	-3.86438500	2.33209400	1.05633600	H	-2.13525800	-0.71993300	4.73117200		
H	-3.08365300	2.02341500	1.75925000	H	-3.97701800	-2.22489400	3.97988100		
H	-3.38384500	2.98502100	0.32081500	C	-0.46007900	-1.07554300	-1.05759000		
H	-4.60476000	2.92064800	1.60740800	C	-0.48917300	-2.40598000	-0.65611000		
C	-2.31639800	0.06436400	-0.09546000	C	-0.43053500	-0.68687300	-2.39165700		
O	-1.67181900	-0.99106600	0.20636700	C	-0.52106500	-3.39139800	-1.65126000		
O	-1.65535800	1.13723600	-0.34652300	H	-0.48118400	-2.67848200	0.39304500		
19				C	-0.46485500	-1.69056100	-3.36829000		
	C	-3.90044100	2.63521000	0.08556000	H	-0.37404800	0.35826800	-2.67394800	
	C	-3.12607900	1.46657800	-0.02066400	C	-0.51369300	-3.03641700	-3.00131600	
	C	-1.74661900	1.57198100	-0.23796600	H	-0.54616500	-4.43785300	-1.35807700	
	C	-1.15968800	2.84194600	-0.35435900	H	-0.44568600	-1.40726500	-4.41753900	
	C	-1.93687900	3.99833500	-0.25471700	H	-0.53825200	-3.80767300	-3.76610600	
	C	-3.30957700	3.89107400	-0.02467400	S	-3.79081600	-0.63528000	-0.65066200	
	H	-4.97242100	2.54867500	0.24136700	C	-3.13694700	0.99556800	-0.86017800	
	H	-0.08612100	2.92810700	-0.50173700	C	-2.03817300	1.39033900	-0.07157800	
	H	-1.46719000	4.97327600	-0.35243100	C	-3.78968500	1.92216700	-1.68343700	
	H	-3.92466900	4.78316700	0.05559900					

C	-1.70096600	2.75888000	-0.02118500	C	-0.51087200	1.36998900	-0.01207600
C	-3.40063000	3.25872700	-1.66900200	C	-0.40139900	2.06703800	1.23251000
H	-4.63312300	1.60281600	-2.28962900	C	-0.27595600	3.45398700	1.22930300
C	-2.37625600	3.68400700	-0.81347700	C	-0.21396200	4.18317900	0.03327000
H	-0.88056300	3.09911300	0.60804500	H	-0.25265700	4.05761300	-2.11602400
H	-3.92169600	3.97715800	-2.29526500	H	-0.21750200	3.98446800	2.17733800
H	-2.09342400	4.73214800	-0.77588200	C	-0.45704700	1.31980900	2.54200000
Pd	-0.31179700	0.33147500	0.33368300	H	-1.26820300	0.58232300	2.54257300
C	5.93080600	1.38395900	0.19432500	H	0.47577600	0.77055200	2.71827000
C	4.53244400	1.43485600	0.20142200	H	-0.61214900	2.00167600	3.38388700
C	3.81023600	0.21887000	0.22817300	C	-0.50132400	1.40687800	-2.56704200
C	4.48575300	-1.02387300	0.23488700	H	0.42487800	0.85794300	-2.77606900
C	5.88510400	-1.02417900	0.19919400	H	-1.31732800	0.67475800	-2.57998100
C	6.60645500	0.16644800	0.18605800	H	-0.66483200	2.11772300	-3.38294300
H	6.49223300	2.31506200	0.18904500	C	-0.09838900	5.68603900	0.05804400
H	6.41099400	-1.97575300	0.18705000	H	0.41969600	6.06334900	-0.82931400
H	7.69325300	0.14576000	0.16907900	H	-1.09428100	6.14929200	0.07645000
C	3.76007800	-2.35146500	0.26395200	H	0.43813400	6.03249700	0.94703400
H	3.30237400	-2.53055900	1.24184400	Pd	0.27255000	-0.55010100	-0.05166100
H	2.94947600	-2.39584600	-0.47035500	C	4.19213300	-1.37578700	0.02688000
H	4.45880300	-3.16762500	0.05252600	C	2.67315900	-1.14805300	-0.04973400
C	3.85509000	2.78813000	0.19612700	O	2.25939400	0.06083800	-0.03793600
H	3.33964500	2.97087500	-0.75138500	O	1.88247700	-2.12002500	-0.08192900
H	3.09728600	2.87094100	0.98331300	F	4.84146100	-0.51986300	-0.77772000
H	4.59321700	3.58153700	0.35239500	F	4.51196000	-2.62438500	-0.32650500
C	2.31020100	0.24788900	0.24744600	F	4.60879300	-1.16766200	1.29108000
O	1.66737500	-0.52100600	1.03557800	C	-3.85714500	-1.95594800	0.02827300
O	1.67501000	1.04265200	-0.51844100	C	-2.63370600	-1.01210400	-0.03816800
21				O	-1.50916700	-1.56858400	-0.06589900
Pd	0.00000200	-0.00001000	-0.04830800	O	-2.87597800	0.22708200	-0.01481200
C	3.94698600	0.00013200	0.03604100	H	-1.73977900	0.82233200	-0.01250200
C	2.41352300	0.00033900	-0.03990500	F	-4.92758300	-1.39357100	-0.54430800
O	1.76847900	-1.09263100	-0.04931300	F	-4.13953600	-2.19892700	1.32149000
O	1.76819200	1.09314500	-0.04922600	F	-3.60306900	-3.11780600	-0.58058800
F	4.31681100	-0.00951700	1.32724600	24			
F	4.44108800	1.09468300	-0.54874200	C	3.90658900	0.73007700	-0.00347000
F	4.44117300	-1.08573400	-0.56492700	C	2.53799500	1.01352700	0.00016700
C	-3.94698700	-0.00006700	0.03609000	C	1.62057900	-0.03167500	0.00638500
C	-2.41351300	-0.00024000	-0.03977000	C	2.00217500	-1.37809300	0.01555200
O	-1.76837700	1.09269400	-0.04920600	C	3.38406400	-1.62220900	0.00670500
O	-1.76825200	-1.09307700	-0.04908800	C	4.34364200	-0.59805200	-0.00544500
F	-4.31704100	0.00534800	1.32717600	H	4.62932600	1.54492800	0.00027700
F	-4.44106800	-1.09272200	-0.55241000	H	3.72160300	-2.65745200	0.01221600
F	-4.44101400	1.08776800	-0.56144700	C	1.01516100	-2.52083100	0.03520000
22				H	0.37407800	-2.48122400	0.92228100
C	-0.95847100	-1.00448700	-0.01236500	H	0.34772100	-2.48891000	-0.83211900
C	-1.37151100	0.32822900	-0.00083700	H	1.53893600	-3.48166100	0.03229000
C	-0.39102100	1.33311600	0.01151500	C	1.99011300	2.43568200	-0.01646900
C	0.96956700	1.02369700	0.00930900	H	2.11540300	2.92114300	-0.98987700
C	1.35002700	-0.32797200	0.00079400	H	0.89590900	2.52560700	0.22852500
C	0.40198100	-1.35152800	-0.00853000	H	2.45770900	3.06072000	0.75261800
H	-1.70800500	-1.79424800	-0.02289700	C	5.81798900	-0.93123000	-0.03881800
H	-0.69960200	2.37729900	0.02031200	H	6.14508900	-1.18651800	-1.05557000
H	2.40877200	-0.58227600	0.00123700	H	6.42744600	-0.08640500	0.29820600
C	2.01864200	2.11263000	-0.00632300	H	6.04950300	-1.79087200	0.59975500
H	2.52364000	2.16629600	-0.98018800	Pd	-0.13593700	0.82676100	0.01439200
H	1.57875400	3.09574100	0.19014400	C	-3.94012200	-0.51409100	-0.01537100
H	2.79529000	1.93382000	0.74697000	C	-2.53416500	0.11418300	-0.02280200
C	-2.83941300	0.69110300	0.00045500	O	-2.38471400	1.35294700	-0.00215100
H	-3.11267400	1.25282700	0.90294600	O	-1.55081700	-0.70482600	-0.02786800
H	-3.09773100	1.32227900	-0.85925900	F	-4.16534000	-1.10293800	1.17452700
H	-3.47194500	-0.20167000	-0.03954800	F	-4.04218700	-1.44915200	-0.97484500
C	0.82028600	-2.80460500	0.00600100	F	-4.88464000	0.40997300	-0.21749200
H	0.61729600	-3.26900900	0.98034300	25			
H	0.27469800	-3.38719200	-0.74589500	N	-1.32746800	-0.01666400	-0.40782400
H	1.89099000	-2.91496400	-0.19427100	C	-1.88119000	1.18358400	0.08660400
23-ts				C	-1.90132800	-1.17869400	0.15250900
C	-0.29552600	3.49512500	-1.18577900	C	-3.01122100	0.80658700	1.04166100
C	-0.42181000	2.10910700	-1.23393600	H	-3.94391200	1.23556100	0.66177900

H	-2.81698800	1.27327100	2.01217300	F	-4.59769400	-2.85090500	0.43569700
C	-3.02018000	-0.72920300	1.08945600	27-ts			
H	-2.82246400	-1.13575400	2.08608900	C	-0.81485200	3.97802600	-0.80369500
H	-3.96048000	-1.17113500	0.74511400	C	-0.60536700	2.59671800	-0.88358200
O	-1.50854200	2.29646100	-0.20049700	C	-0.55012300	1.89145500	0.33809700
O	-1.55130500	-2.31177900	-0.07626400	C	-0.90442400	2.47629200	1.57080000
S	-0.05593300	-0.05972100	-1.58751800	C	-1.11582600	3.85918100	1.58448800
C	1.40163000	-0.01950200	-0.54297000	C	-1.06750400	4.62699400	0.41347200
C	1.94940900	1.21199800	-0.15751600	H	-0.81339300	4.55744500	-1.72504100
C	2.01407500	-1.22025100	-0.15909400	H	-1.34307300	4.34274500	2.53263300
C	3.10970600	1.23701600	0.61743400	S	2.12785800	-0.25347600	1.25229500
H	1.45791100	2.13186900	-0.45760900	C	3.29599700	0.11616000	0.00844500
C	3.17627300	-1.18503000	0.61316600	C	4.48718000	-0.64631200	-0.02352900
H	1.57228800	-2.16506500	-0.45938500	C	3.11546400	1.17307500	-0.91323500
C	3.72302000	0.04109400	1.00010600	C	5.46819200	-0.35927900	-0.96310700
H	3.53605500	2.18959600	0.91993000	H	4.61854400	-1.45795400	0.68529400
H	3.65352900	-2.11406900	0.91281000	C	4.10549800	1.44950600	-1.84867300
H	4.62888300	0.06485800	1.60010700	H	2.21174700	1.76975600	-0.86815900
26				C	5.27677100	0.68397000	-1.87836000
N	-0.48926700	2.59527500	0.18278000	H	6.37973800	-0.94849900	-0.99221800
C	-0.99557700	3.64031900	0.99779000	H	3.96821100	2.26202800	-2.55581000
C	-1.09626300	2.52050700	-1.09225800	H	6.04495800	0.90226200	-2.61474200
C	-2.06414500	4.36154700	0.18438100	C	-0.99698900	1.67814200	2.85058300
H	-1.75397700	5.40348100	0.05461800	H	-1.54150900	0.73889200	2.70748400
H	-2.99219600	4.37030600	0.76313500	H	0.00047300	1.41103500	3.22499600
C	-2.17557100	3.59170600	-1.14197800	H	-1.50438900	2.25577900	3.62966800
H	-3.13643900	3.07910500	-1.25504800	C	-0.45274400	1.93377400	-2.23369000
H	-2.02789200	4.21249900	-2.03016900	H	0.46778500	1.34350100	-2.30767100
O	-0.61685200	3.88680800	2.11561800	H	-1.27839000	1.23797500	-2.40950400
O	-0.78730900	1.73656800	-1.95897300	H	-0.44429900	2.68431100	-3.03030800
S	0.61997200	1.42291000	0.81893600	C	-1.29732600	6.11751000	0.45819400
C	2.15272500	1.80253700	-0.04030200	H	-1.76484200	6.47994400	-0.46333800
C	2.40020600	1.40915000	-1.36030300	H	-1.93632600	6.40008500	1.30111200
C	3.11744800	2.49502500	0.70259700	H	-0.34746200	6.65773900	0.57460100
C	3.62787400	1.72768200	-1.93953200	N	0.57074700	-2.11231600	0.53882500
H	1.64077100	0.87876400	-1.92019200	C	0.77171800	-2.93979400	-0.55106700
C	4.34377600	2.80174400	0.11133100	C	0.23732800	-2.79147100	1.70102800
H	2.90736100	2.79014400	1.72617300	C	0.49116700	-4.38461500	-0.10956200
C	4.59717200	2.41907500	-1.20713200	H	1.41572600	-4.96458900	-0.20790200
H	3.82875000	1.42879800	-2.96420400	H	-0.24399700	-4.82733700	-0.78750200
H	5.09720700	3.33734000	0.68146100	C	0.00456100	-4.26119700	1.34531400
H	5.55300900	2.65744500	-1.66527400	H	-1.07005400	-4.44469100	1.43988200
C	2.59083600	-3.07312700	-1.05410600	H	0.52462300	-4.90789000	2.05769100
C	1.47528600	-2.22545400	-0.99369400	O	1.11623100	-2.57746000	-1.66247600
C	1.14101800	-1.65930500	0.24861100	O	0.15278700	-2.28045400	2.80307300
C	1.87065400	-1.95798600	1.41047700	Pd	0.08766900	0.00725100	0.38573500
C	2.97410600	-2.81739300	1.29604700	C	-3.74962000	-1.23777500	-1.24447000
C	3.35428100	-3.38018400	0.07541700	C	-2.49828300	-1.27273100	-0.32182300
H	2.85919500	-3.51125600	-2.01450100	O	-1.72367400	-0.27600100	-0.59491000
H	3.54448100	-3.05372400	2.19320300	O	-2.39726000	-2.15221000	0.51892000
C	1.50324600	-1.40379400	2.77166300	F	-4.57680700	-0.24062000	-0.86093100
H	1.71258300	-0.32885900	2.85271500	F	-4.43438200	-2.38803600	-1.18893300
H	0.43723500	-1.53885400	2.98597700	F	-3.41185200	-1.01812500	-2.53170200
H	2.07359700	-1.90460400	3.56085300	28			
C	0.64738000	-1.99681200	-2.24164500	C	-2.35615800	-3.02633000	-0.88688400
H	-0.30427700	-2.53895600	-2.17890700	C	-1.54882700	-1.88141900	-1.02749900
H	0.39535900	-0.94130200	-2.39193900	C	-1.17437900	-1.25905000	0.16682800
H	1.17768000	-2.35253700	-3.13178100	C	-1.54040700	-1.68888100	1.44392600
C	4.53155200	-4.32471100	-0.01420200	C	-2.34331300	-2.84213100	1.49309700
H	4.21723500	-5.36916500	0.11609600	C	-2.75949600	-3.52368600	0.34980400
H	5.02791900	-4.25617300	-0.98858500	H	-2.66789300	-3.53389700	-1.79750600
H	5.27690600	-4.11188500	0.75990600	H	-2.64913800	-3.20173200	2.47316900
Pd	-0.51125300	-0.53746300	0.31730800	S	1.30901100	0.98822900	1.69478300
C	-4.36369500	-1.68458300	-0.18485100	C	3.00693200	0.71147400	1.30297200
C	-2.93021900	-1.18923600	0.08098900	C	3.67957400	-0.40429200	1.83732900
O	-2.00425700	-2.05578400	0.04303100	C	3.72382700	1.67186000	0.56030500
O	-2.72583600	0.03606800	0.27619200	C	5.05039700	-0.55112600	1.63481100
F	-4.53278400	-1.87068700	-1.51031700	H	3.11954100	-1.14675400	2.39504700
F	-5.27508700	-0.79288400	0.23074700	C	5.09417100	1.51718900	0.36626800

H	3.19768500	2.52564000	0.14560200	H	-2.00510900	0.39572800	2.32977500
C	5.75788300	0.40766400	0.90271900	H	-0.39391800	1.07617300	2.06837800
H	5.56732000	-1.41204500	2.04891200	H	-1.68419300	2.06954700	2.78239000
H	5.64660200	2.26299400	-0.19838500	C	-1.23293200	1.20904500	-3.10865900
H	6.82790600	0.29255400	0.75218900	H	-0.14639300	1.34429500	-3.14819200
C	-1.15410600	-1.03901700	2.75074500	H	-1.42780900	0.13752600	-3.24529900
H	-0.08479900	-1.15945000	2.94767900	H	-1.67663600	1.73607800	-3.95918300
H	-1.37736800	0.03108700	2.75071600	C	-4.14887900	4.53354300	-0.72059500
H	-1.70697500	-1.50179900	3.57333300	H	-3.59196900	5.47823700	-0.78551600
C	-1.16566000	-1.47472400	-2.43504600	H	-4.79830400	4.48044900	-1.60093100
H	-1.13216000	-0.39345100	-2.56944600	H	-4.77975700	4.58827200	0.17231900
H	-0.18773700	-1.88756600	-2.70611000	Pd	0.33417700	-0.02271700	-0.54394000
H	-1.89848100	-1.87609800	-3.14155500	C	3.43234700	2.34062700	1.16613900
C	-3.64862900	-4.74170100	0.45002300	C	2.28792700	1.32428200	0.93140900
H	-3.53746500	-5.39090200	-0.42446700	O	1.92602200	0.60498100	1.86308500
H	-3.41783200	-5.33311800	1.34245000	O	1.79894000	1.40471400	-0.25355700
H	-4.70671600	-4.45526700	0.51338700	F	2.90265700	3.56648300	1.40345400
N	1.34567700	-0.30441500	-1.09405300	F	4.24938700	2.44926900	0.10456500
C	1.88809000	0.49463400	-2.08251000	F	4.17855500	2.00840000	2.23087100
C	2.01779600	-1.50716400	-0.93162300	30			
C	2.99063800	-0.28049300	-2.80302100	C	-3.92299400	-0.73051600	-2.04224000
H	3.90817400	0.31553700	-2.79408700	C	-2.81597400	0.09587400	-1.83206900
H	2.70342800	-0.41791400	-3.85095000	C	-2.26061700	0.13769800	-0.53021400
C	3.09973000	-1.59725500	-2.01857600	C	-2.78496300	-0.63854400	0.52877400
H	2.92100100	-2.49002000	-2.62616700	C	-3.89993100	-1.43615800	0.24970400
H	4.06811200	-1.72930200	-1.52615100	C	-4.48029900	-1.50294700	-1.01952200
O	1.52773500	1.64113000	-2.30702600	H	-4.35954400	-0.76905000	-3.03745600
O	1.80388800	-2.34079100	-0.07201200	H	-4.31720700	-2.03569900	1.05546900
Pd	-0.13754500	0.53094400	-0.02465700	S	-0.80662800	1.19243200	-0.37688700
C	-3.69717400	2.54835600	-0.02050600	C	-1.04224000	2.17756500	1.12069400
C	-2.38551800	1.75570900	-0.16422700	C	-2.28685900	2.78167900	1.33656000
O	-2.02814800	1.30150600	-1.26767700	C	0.04128400	2.43764000	1.96477900
O	-1.70725500	1.58238600	0.90536900	C	-2.45191700	3.63226100	2.42924100
F	-3.46357200	3.73415000	0.56555800	H	-3.11898200	2.58037500	0.66863400
F	-4.55722600	1.85641000	0.75041200	C	-0.13920100	3.30324700	3.04728800
F	-4.26942900	2.76341400	-1.20868400	H	1.01619200	1.99225700	1.78426900
29-ts				C	-1.37996900	3.89457500	3.28669000
N	1.50585100	-1.76116000	-0.88385600	H	-3.41985300	4.09316500	2.60554800
C	0.82475800	-2.83985700	-1.25668400	H	0.70120200	3.50610900	3.70484700
C	2.89554000	-2.03656100	-0.85942800	H	-1.51280300	4.55929200	4.13549300
C	1.71721300	-4.03968200	-1.55248400	C	-2.22958400	-0.64556100	1.93279300
H	1.55536100	-4.36046300	-2.58663300	H	-1.13890000	-0.70147100	1.94286800
H	1.42507400	-4.87397200	-0.90675400	H	-2.52275100	0.25313900	2.48693000
C	3.12582400	-3.49724400	-1.27855200	H	-2.60970500	-1.51436800	2.47751000
H	3.64534600	-4.02400000	-0.47244000	C	-2.26617500	0.90248700	-2.98904200
H	3.77983200	-3.52102900	-2.15533700	H	-2.36590600	1.98015500	-2.81014700
O	-0.43925900	-2.94783100	-1.37729700	H	-1.20293000	0.70912700	-3.16946000
O	3.74958900	-1.24027200	-0.55658000	H	-2.81517100	0.66417900	-3.90456300
S	-1.51591500	-1.16585600	-0.83971600	C	-5.65582600	-2.41195600	-1.28637900
C	-2.08072000	-1.90600400	0.67095700	H	-6.28540400	-2.02726000	-2.09539800
C	-1.24357800	-2.06532500	1.78906900	H	-5.31560900	-3.41236700	-1.58508600
C	-3.39764100	-2.39315600	0.68460600	H	-6.27980800	-2.53357700	-0.39487500
C	-1.73380900	-2.72326200	2.91417300	N	2.11036400	1.26795800	-0.97448000
H	-0.23442700	-1.66394400	1.77291200	C	2.09255900	1.55388200	-2.32770400
C	-3.87962300	-3.03577900	1.82353700	C	3.04699900	1.99788500	-0.26814100
H	-4.02937700	-2.27133500	-0.19019300	C	3.17318800	2.60276900	-2.61747500
C	-3.04794600	-3.20424800	2.93371400	H	2.69859100	3.48884000	-3.05193700
H	-1.09291800	-2.84964500	3.78169300	H	3.86050900	2.20474700	-3.37048100
H	-4.89908200	-3.40949100	1.84165700	C	3.83324100	2.86826700	-1.25510200
H	-3.42443100	-3.70958800	3.81864800	H	4.88687800	2.57218700	-1.21857600
C	-2.68920900	2.79535600	-1.83486000	H	3.78139800	3.91295500	-0.93301900
C	-1.78902700	1.73226800	-1.80431900	O	1.33555300	1.05613300	-3.14621000
C	-1.36730200	1.21435900	-0.54066000	O	3.20562200	1.95744200	0.94250600
C	-1.88847900	1.77240800	0.66327600	Pd	1.03800700	-0.21254000	-0.16931200
C	-2.78384200	2.84061900	0.57018400	C	1.88472200	-3.94505900	0.97549100
C	-3.20123100	3.36235800	-0.65982900	C	1.56203700	-2.52163400	0.49412900
H	-2.99184400	3.20412000	-2.79674000	O	0.37621700	-2.08857900	0.61967400
H	-3.15840700	3.28975000	1.48781400	O	2.48065500	-1.79426000	0.02356100
C	-1.46392700	1.30291900	2.03235400	F	2.05704000	-3.93163200	2.31118700

F	3.00252600	-4.40698800	0.40599200	H	0.83768700	4.16369900	-1.20100100
F	0.87551400	-4.77995100	0.68766000	C	-0.12507400	3.89971400	0.77313200
31				H	0.83694500	4.18619900	1.20940600
C	2.59560800	-1.30741600	-0.10857800	H	-0.88258500	4.55732700	1.21212600
C	1.35440800	-1.05324600	-0.70072500	O	-0.56589700	2.03407900	-2.29310800
C	0.83294000	0.25809500	-0.63366700	O	-0.48628700	2.01640500	2.30301600
C	1.54871900	1.28836300	0.01246400	Pd	0.27972400	-0.18768700	-0.01482300
C	2.78900400	0.98078300	0.58468800	C	4.10567700	-1.18858400	0.00299800
C	3.33119400	-0.30568800	0.53273700	C	2.61305100	-0.83080200	-0.04569700
H	2.99853800	-2.31729900	-0.15223200	O	1.72956600	-1.73395700	-0.04064000
H	3.34288200	1.77058800	1.08781600	O	2.26647500	0.39626700	-0.05011000
S	-0.71814600	0.64514200	-1.45576000	F	4.54469500	-1.05665000	1.26621800
C	-1.98221200	0.15978600	-0.27802000	F	4.80495300	-0.36077500	-0.78347000
C	-3.31111300	0.20928700	-0.72787000	F	4.30316900	-2.44664400	-0.39578500
C	-1.71532700	-0.23675600	1.03795400	C	-3.81183600	-1.67885600	0.01119200
C	-4.35451100	-0.12993900	0.13123300	C	-2.60526400	-0.71088600	0.03324800
H	-3.52518500	0.51140700	-1.74995800	O	-1.46234500	-1.24170400	0.01472300
C	-2.76881400	-0.58069600	1.88877500	O	-2.88259300	0.51814000	0.04278600
H	-0.69189500	-0.27770900	1.39639000	H	-1.81367000	1.16312600	0.02360900
C	-4.09017500	-0.52854900	1.44434300	F	-3.43759600	-2.93517600	0.25834600
H	-5.37868800	-0.08668800	-0.23041000	F	-4.38482800	-1.62677000	-1.20260400
H	-2.54839600	-0.88858800	2.90787200	F	-4.71294400	-1.30469500	0.92846100
H	-4.90506600	-0.79577500	2.11114500	34			
C	1.01490600	2.69906400	0.11249900	N	0.00000100	0.95893100	-0.00001900
H	0.89935300	3.15845900	-0.87547200	H	-0.00000100	1.97231600	-0.00008500
H	0.02724600	2.72146000	0.58591000	C	-1.17856700	0.21445100	0.00004600
H	1.69214500	3.32531400	0.70161900	C	1.17856800	0.21445200	-0.00007300
C	0.60632400	-2.17850500	-1.37566500	C	-0.77019900	-1.25981700	0.00007700
H	-0.36497700	-2.35483300	-0.89940900	H	-1.20525100	-1.74522100	-0.87911300
H	0.40378900	-1.95063700	-2.42781100	H	-1.20523800	-1.74519300	0.87928800
H	1.18231500	-3.10785300	-1.32839500	C	0.77019700	-1.25981900	0.00006000
C	4.68563600	-0.60441800	1.13194000	H	1.20524000	-1.74512500	0.87931000
H	4.71485400	-1.60422200	1.57902000	H	1.20524100	-1.74529400	-0.87909300
H	5.47293600	-0.56946200	0.36696100	O	-2.29719300	0.67752600	0.00007300
H	4.95097700	0.12257500	1.90646600	O	2.29719400	0.67752400	-0.00017800
32				35-ts			
N	-0.57738000	1.67231000	-0.00113100	N	-3.05545700	-0.87049900	-0.75686200
C	-0.49008500	2.47529200	-1.15969100	C	-3.25431300	-1.36955300	-2.02489100
C	-0.50049800	2.45236500	1.17342900	C	-4.22874400	-0.54291200	-0.12016100
C	-0.51865800	3.94864800	-0.74666300	C	-4.76693700	-1.49248300	-2.29108200
H	-1.39734600	4.42812600	-1.19011600	H	-5.01342800	-2.54887800	-2.44163000
H	0.36171900	4.44184400	-1.17050800	H	-5.01071400	-0.97116300	-3.22222200
C	-0.53302700	3.93333600	0.78976000	C	-5.41763900	-0.88588500	-1.04037300
H	0.33330900	4.42642900	1.24144300	H	-5.98381100	0.03028100	-1.24116200
H	-1.42553000	4.39523200	1.22453600	H	-6.09076300	-1.56688600	-0.51000800
O	-0.42464900	2.03732200	-2.28823700	O	-2.37320200	-1.66216900	-2.82056100
O	-0.44137500	1.99207100	2.29359200	O	-4.33182200	-0.06622500	1.00422500
Pd	0.32135700	-0.15878900	-0.01369200	C	-0.76788800	-1.70838900	0.89369800
C	4.15699400	-1.12146900	0.00695900	C	-1.80575100	-1.83822500	1.82260800
C	2.65883800	-0.78712400	-0.04326400	C	0.28964600	-2.62092500	0.83615000
O	1.78915800	-1.70277400	-0.03463300	C	-1.75370900	-2.89701000	2.72833200
O	2.29639400	0.43550000	-0.05187500	H	-2.63460800	-1.13459800	1.83096800
F	4.58964700	-0.99880200	1.27344700	C	0.31875400	-3.67709200	1.74928300
F	4.84795800	-0.27576800	-0.76701800	H	1.08706500	-2.50526800	0.10950700
F	4.37448600	-2.37265000	-0.40529700	C	-0.69761000	-3.81400600	2.69472900
C	-3.78594100	-1.78719600	0.00528700	H	-2.55031700	-3.00864500	3.45841700
C	-2.59776000	-0.80156100	0.01825500	H	1.13886100	-4.38787700	1.71471100
O	-1.44427800	-1.24790100	0.02388200	H	-0.67268300	-4.63816200	3.40209800
O	-2.94922600	0.44104000	0.00055800	C	-1.75257800	3.47879200	-0.06667200
H	-2.09845500	1.01844300	-0.00823100	C	-1.60003600	2.16748400	-0.52942100
F	-3.36658200	-3.03041600	0.22594400	C	-1.02331300	1.21258200	0.35116600
F	-4.38201300	-1.72705100	-1.19435000	C	-0.56138100	1.58839500	1.64752200
F	-4.67036600	-1.44284300	0.94837400	C	-0.75784100	2.91283900	2.03529700
33-ts				C	-1.36336000	3.87048300	1.21180400
N	-0.67250900	1.67246700	0.00611600	H	-2.19698800	4.21083200	-0.73683100
C	-0.46727200	2.47011700	-1.17287300	H	-0.40447000	3.21328400	3.01873600
C	-0.43139200	2.46220100	1.18359500	C	0.17280500	0.68540700	2.61559600
C	-0.13026500	3.90071200	-0.76226400	H	-0.49953400	-0.01860200	3.11395000
H	-0.87223000	4.57685300	-1.19887700	H	0.96006700	0.10206200	2.13048800

H	0.64524000	1.29765100	3.38879700	S	0.71102000	0.35999100	-0.17481100
C	-2.09824700	1.87487300	-1.92992400	ArCO₂H			
H	-1.69060900	0.96875400	-2.38018500	C	1.86676300	-1.30057300	-0.05633700
H	-3.18917200	1.76770000	-1.92321400	C	0.46826200	-1.24792100	-0.07087500
H	-1.85670800	2.71708000	-2.58660800	C	-0.15814600	0.02186900	-0.01147400
C	-1.57410600	5.28130500	1.70067700	C	0.61290000	1.20973000	0.05507300
H	-0.67282700	5.67425600	2.18460300	C	2.00702700	1.09921600	0.09073400
H	-1.84417900	5.95456600	0.88185200	C	2.63324800	-0.14227900	0.03270100
H	-2.38160100	5.31823900	2.44335900	H	2.35655000	-2.26899900	-0.11623400
Pd	1.30844100	0.23550100	-0.86529500	H	2.60440500	2.00452000	0.15887700
C	5.31233700	-0.20850800	-0.30421500	H	3.71805500	-0.20732600	0.05181400
C	3.80082700	0.00800400	-0.50462200	C	0.00080900	2.59281800	0.10344500
O	3.40329000	0.83101900	-1.36667200	H	-0.45300700	2.86009600	-0.85542100
O	3.01538200	-0.69677100	0.19958900	H	-0.79563900	2.66846000	0.85026400
F	5.68578100	-1.34936000	-0.91751900	H	0.76955300	3.33362700	0.34459900
F	5.60958600	-0.31794200	1.00172700	C	-0.28859600	-2.55572400	-0.18001300
F	6.02626600	0.79983800	-0.81803900	H	-0.77736100	-2.81803300	0.76341600
S	-0.77301800	-0.42530700	-0.36970100	H	-1.07405500	-2.51845700	-0.94103600
36				H	0.40079300	-3.36353000	-0.44426300
N	2.76783100	1.03610100	-0.84498700	C	-1.64465100	0.15978100	-0.05131700
C	2.67822600	1.98929600	-1.83876100	O	-2.25730600	1.05237200	-0.60486100
C	4.06179000	0.64245700	-0.57919500	O	-2.30320700	-0.81503400	0.63016500
C	4.09370500	2.33982500	-2.32693800	H	-3.25088500	-0.61056900	0.51393700
H	4.26739900	3.40946900	-2.17178700	ArCO₂⁻			
H	4.15220400	2.15842800	-3.40508000	C	-1.91744000	1.19889600	-0.08140900
C	5.01490900	1.43771000	-1.49424900	C	-0.51652000	1.21523200	-0.07274700
H	5.59976200	0.73084600	-2.09205300	C	0.20277600	0.00018700	0.00011500
H	5.72254400	1.98715300	-0.86515300	C	-0.51582200	-1.21529600	0.07299700
O	1.63988700	2.47560200	-2.25963900	C	-1.91675400	-1.19975800	0.08141600
O	4.41309200	-0.18533200	0.24865100	C	-2.62409900	-0.00063300	-0.00009800
C	0.98842000	1.27702700	1.35354300	H	-2.45859200	2.14332200	-0.14584000
C	2.13897100	1.07548500	2.12256200	H	-2.45739300	-2.14446800	0.14593000
C	0.02324300	2.22269900	1.70546900	H	-3.71333800	-0.00095600	-0.00014500
C	2.29963300	1.82849400	3.28451700	C	0.21598300	-2.53809700	0.14379400
H	2.89431100	0.35978500	1.80947100	H	0.97289900	-2.57973700	-0.64359000
C	0.20421600	2.97080500	2.87074100	H	0.75811300	-2.64239100	1.09386800
H	-0.85689400	2.36810400	1.08549000	H	-0.48140200	-3.38183500	0.05818000
C	1.33648700	2.77143700	3.66094200	C	0.21469700	2.53839300	-0.14360700
H	3.18664500	1.68144000	3.89399800	H	0.97562000	2.57763300	0.64002200
H	-0.54201000	3.70707600	3.15381200	H	0.75159400	2.64559700	-1.09638700
H	1.47465600	3.35506300	4.56668900	H	-0.48234600	3.38177700	-0.05197100
C	1.97156900	-3.45788200	-0.71179000	C	1.75703400	0.00031600	-0.00007100
C	1.68821500	-2.10518000	-0.92393300	O	2.29581200	-0.71601500	-0.88049500
C	1.10740700	-1.38033700	0.14206200	O	2.29615200	0.71671700	0.88019500
C	0.70373700	-2.02031400	1.34240600	Ph			
C	1.02272300	-3.37381100	1.48060500	C	-1.05874700	-0.91124000	0.00000500
C	1.68028700	-4.10545300	0.48807500	C	0.25992300	-1.37238900	0.00006900
H	2.42785000	-4.01939600	-1.52382400	C	1.31857200	-0.46125700	-0.00005600
H	0.71913100	-3.87798500	2.39491500	C	1.05866900	0.91132700	0.00000800
C	-0.11540800	-1.38161900	2.44415600	C	-0.25980700	1.37240700	0.00006200
H	0.47989400	-0.72453100	3.08468300	C	-1.31861200	0.46115200	-0.00005800
H	-0.95222500	-0.79751200	2.04899000	H	-1.88222100	-1.62029100	-0.00006600
H	-0.53724600	-2.16708100	3.07741000	H	0.46192800	-2.44014400	0.00007800
C	2.00530900	-1.54130200	-2.29275600	H	2.34433200	-0.81995600	-0.00015500
H	1.41213300	-0.66334900	-2.55602800	H	1.88231600	1.62016600	0.00000700
H	3.06190600	-1.26203000	-2.36385700	H	-0.46205900	2.44010900	0.00001800
H	1.81662100	-2.30852600	-3.05052300	H	-2.34429100	0.82010600	-0.00006300
C	2.04456800	-5.55360100	0.70331100	TFA			
H	1.32827800	-6.05394500	1.36323100	C	-0.60090700	0.00069100	-0.00000900
H	2.08169300	-6.10332700	-0.24264400	C	0.93413900	-0.15998300	-0.00010300
H	3.03446400	-5.63915800	1.17081300	O	1.49806000	-1.22228000	-0.00000800
Pd	-1.38515000	0.40403600	-0.80630000	O	1.52046100	1.04599500	-0.00010800
C	-5.38299200	-0.01793500	-0.19980400	H	2.48551700	0.89531500	0.00004300
C	-3.87499900	0.10788100	-0.48663200	F	-1.18834800	-1.19614300	-0.00053100
O	-3.48888700	0.43062700	-1.63509600	F	-0.99667900	0.68025400	-1.08981200
O	-3.08094100	-0.08298500	0.48694200	F	-0.99642600	0.67930200	1.09051600
F	-5.82310400	1.12091400	0.37359600	CF₃CO₂⁻			
F	-5.63117100	-1.03390100	0.64280500	C	-0.51315900	0.00002500	-0.00971000
F	-6.08024200	-0.21991600	-1.32415000	C	1.06622600	0.00029200	-0.02584200

O	1.56221000	1.14469500	-0.01151300	C	-2.77557300	-1.05174800	0.50840500
O	1.56161900	-1.14442500	-0.01203000	C	-2.50186700	-2.40677500	0.79160600
F	-0.99833100	-0.00745500	1.27148100	C	-3.21888600	-2.98576200	1.85408100
F	-1.07305300	-1.08190100	-0.61953400	C	-4.17371000	-2.27420800	2.57718100
F	-1.07406400	1.08890500	-0.60731900	C	-4.44342400	-0.94559100	2.25290200
37 (W=NMe ₂ ,X=Y=Z=H)							
C	3.23518300	1.77326300	1.25696700	H	-3.94291000	0.70096100	0.95987800
C	2.08965400	2.11452200	0.53776300	H	-2.99658000	-4.01132600	2.13108300
C	1.34885800	3.27933800	0.82951000	H	-4.69843200	-2.75677000	3.39693100
C	1.79702900	4.05778900	1.91166200	H	-5.18726000	-0.37952700	2.80634200
C	2.93106400	3.71919700	2.64686100	C	-1.52194800	-3.22235200	0.02195200
C	3.65892600	2.57739000	2.31525700	C	-1.80914300	-4.58798300	-0.18754000
H	3.79178500	0.87988000	0.99569600	C	-0.31118100	-2.70725000	-0.49570900
H	1.22131200	4.93345400	2.19435500	C	-0.92701700	-5.42584200	-0.86230800
H	3.23810800	4.34329000	3.48145400	H	-2.75621700	-4.98821500	0.16357100
H	4.54662700	2.30282800	2.87812300	C	0.57354400	-3.56049700	-1.16797700
C	0.15573600	3.70504600	0.04718400	C	0.27642200	-4.91303600	-1.34758400
C	-0.05889400	5.08612100	-0.14642800	H	-1.18220800	-6.47138200	-1.01240700
C	-0.78248900	2.79988100	-0.49991000	H	1.51593900	-3.16635400	-1.53774600
C	-1.16886600	5.56414200	-0.83572200	H	0.98081900	-5.55779700	-1.86739200
H	0.67668100	5.79222800	0.22887300	S	-1.87458100	-0.28927700	-0.86867500
C	-1.89971200	3.29101300	-1.18784300	C	-2.12074700	1.47234600	-0.64289900
C	-2.10053500	4.66311500	-1.35252900	C	-1.42840600	2.21179500	0.33028100
H	-1.30059900	6.63404200	-0.97310800	C	-3.00489500	2.11959500	-1.50961200
H	-2.63221000	2.59190300	-1.58156300	C	-1.63892100	3.57763400	0.43618600
H	-2.97809500	5.02201300	-1.88475300	H	-0.71443400	1.72050600	0.98175500
S	1.54139900	1.10178400	-0.86451200	C	-3.21750900	3.49608400	-1.40867500
C	2.39973900	-0.45404800	-0.66736500	H	-3.53241100	1.55070700	-2.26968200
C	2.00427400	-1.42734200	0.26021400	C	-2.53324000	4.23068500	-0.43080300
C	3.47699100	-0.72404300	-1.52089600	H	-1.10965300	4.16957100	1.17577100
C	2.68227800	-2.63464200	0.34406600	H	-3.90675000	3.97733200	-2.09241600
H	1.14701100	-1.25079100	0.90052100	Pd	0.31268900	-0.81715700	-0.35455700
C	4.15945100	-1.93156800	-1.44352900	C	6.35620600	0.60106700	-0.08568000
H	3.78328000	0.01519700	-2.25574000	C	5.07744900	0.08573200	-0.32591700
C	3.78423100	-2.92127000	-0.50155900	C	3.97474100	0.68550700	0.32693800
H	2.33819500	-3.36788900	1.06280300	C	4.15926100	1.77328000	1.21286400
H	4.98314200	-2.10549000	-2.12466900	C	5.45972500	2.23685400	1.43971100
Pd	-0.69591500	0.81060000	-0.37331300	C	6.55143300	1.66289200	0.79339200
C	-5.84230900	-2.67538600	-0.10054100	H	7.20740100	0.15631200	-0.59518900
C	-4.83005700	-1.74218000	-0.35211000	H	5.61220700	3.06196700	2.13100600
C	-3.59023900	-1.89609100	0.31097300	H	7.55364300	2.04294000	0.97478100
C	-3.37961700	-2.96069400	1.21832600	C	3.01216300	2.44389500	1.93730000
C	-4.43025100	-3.85345700	1.45661500	H	2.41011600	3.04907200	1.25223700
C	-5.65119200	-3.71959900	0.80031600	H	2.33207400	1.71593900	2.39168800
H	-6.79303000	-2.57342300	-0.61795700	H	3.39554100	3.09464300	2.72998700
H	-4.28232200	-4.66512900	2.16478300	C	4.93203400	-1.07603600	-1.28495100
H	-6.45293300	-4.42858200	0.99105100	H	4.69461100	-2.00274500	-0.75316500
C	-2.07183700	-3.16304000	1.95279600	H	4.12466500	-0.91576800	-2.00682000
H	-1.28921200	-3.52150700	1.27671400	H	5.86345300	-1.22468700	-1.84083000
H	-1.70092800	-2.23234300	2.39463400	C	2.59531800	0.16903500	0.07553600
H	-2.19973800	-3.89555600	2.75662200	O	1.61354800	0.96162400	-0.09464300
C	-5.10141100	-0.62101100	-1.33170000	O	2.38153600	-1.09588200	0.02715300
H	-5.22063300	0.33653500	-0.81497700	O	-2.65870200	5.56906700	-0.24281800
H	-4.28138600	-0.48961500	-2.04501900	C	-3.52177200	6.29983900	-1.10360100
H	-6.01680000	-0.82598100	-1.89632400	H	-3.45437200	7.33936900	-0.77928500
C	-2.48441200	-0.92407800	0.04988600	H	-3.20160500	6.22354800	-2.15048400
O	-1.28706700	-1.31924200	-0.12219800	H	-4.56110600	5.95825300	-1.01486100
O	-2.73519600	0.33316200	-0.00138800	37 (W=Me,X=Y=Z=H)			
N	4.46300900	-4.11886000	-0.41176400	C	-3.74639000	0.58496900	1.22039000
C	5.49640000	-4.43961900	-1.38336000	C	-2.95009900	-0.32058900	0.51917200
H	5.91961000	-5.41685400	-1.14556700	C	-2.90599500	-1.68957000	0.85847700
H	5.10769200	-4.47532700	-2.41218800	C	-3.67200000	-2.09026800	1.96731100
H	6.31289600	-3.70695500	-1.35297800	C	-4.45946200	-1.19259700	2.68509200
C	3.97338300	-5.16566000	0.47204400	C	-4.50409500	0.14843300	2.30762500
H	4.64855400	-6.02132100	0.41979700	H	-3.77443800	1.62788300	0.92521100
H	3.94753000	-4.82521500	1.51465300	H	-3.62142900	-3.12718000	2.28388800
H	2.96390800	-5.50739800	0.19873800	H	-5.02921500	-1.54125300	3.54179300
37 (W=OMe,X=Y=Z=H)							
C	-3.74139000	-0.33372100	1.21428000	H	-5.11557300	0.85891500	2.85650100
				C	-2.11044200	-2.69231100	0.09846400
				C	-2.63661000	-3.99309800	-0.04880000

C	-0.84675400	-2.41440200	-0.47055300	C	-1.59274200	3.66063900	0.10868700
C	-1.93586900	-4.99337300	-0.71514300	H	-0.52110800	1.86290300	0.60466700
H	-3.62566200	-4.21028100	0.34511700	C	-3.45272400	3.40287200	-1.43871300
C	-0.14642800	-3.42866100	-1.13562200	H	-3.82661500	1.39697400	-2.12125900
C	-0.67989600	-4.71378600	-1.25490000	C	-2.64181000	4.20459000	-0.63423600
H	-2.37222800	-5.98332100	-0.81688300	H	-0.96409200	4.30338300	0.71522300
H	0.83675800	-3.21709100	-1.54645900	H	-4.25703900	3.84477900	-2.01660800
H	-0.11639400	-5.48801700	-1.76975000	Pd	0.30115000	-0.80825500	-0.38015700
S	-1.97875600	0.20600100	-0.92019400	C	6.35697500	0.53403800	-0.05202000
C	-1.94422200	1.99977900	-0.79918500	C	5.07414500	0.03722100	-0.30820000
C	-1.05450800	2.67619900	0.04328000	C	3.97209500	0.65476800	0.32961100
C	-2.82209600	2.71830400	-1.61869000	C	4.16125800	1.74113400	1.21646800
C	-1.06308300	4.06927900	0.06672400	C	5.46547600	2.18526900	1.45972000
H	-0.35015600	2.12188100	0.65365900	C	6.55658800	1.59405100	0.82826400
C	-2.81713900	4.11243900	-1.58105500	H	7.20799400	0.07609700	-0.54984800
H	-3.50537600	2.19104700	-2.27814200	H	5.62146900	3.00872900	2.15210800
C	-1.93822700	4.81003100	-0.74185600	H	7.56189800	1.95919900	1.02226800
H	-0.36846600	4.59043800	0.72097900	C	3.01624100	2.43139600	1.92567200
H	-3.50460200	4.66437400	-2.21731300	H	2.44368000	3.05892700	1.23503500
Pd	0.09937800	-0.65898200	-0.39328700	H	2.30994400	1.71667900	2.36022900
C	6.30080500	-0.39029700	-0.01815700	H	3.39944000	3.06596100	2.73130300
C	4.95342500	-0.66098000	-0.28257400	C	4.92467500	-1.12375700	-1.26752100
C	3.96966400	0.15633800	0.32267100	H	4.66996400	-2.04691700	-0.73752500
C	4.33695400	1.21586000	1.18549200	H	4.12798400	-0.95425800	-1.99905300
C	5.69603400	1.43082700	1.43906800	H	5.86036300	-1.28476300	-1.81250600
C	6.67362600	0.64089100	0.83974100	C	2.59008000	0.15604000	0.06328800
H	7.06376800	-1.00334100	-0.49136500	O	1.61783600	0.95988400	-0.11861400
H	5.98578700	2.23267300	2.11371200	O	2.36035100	-1.10567900	0.01331100
H	7.72520900	0.82903100	1.04104300	Cl	-2.94120400	5.93002200	-0.56433800
C	3.32286200	2.11603100	1.85807900	37 (W=CF ₃ ,X=Y=Z=H)			
H	2.86594200	2.80381800	1.13948100	C	2.30897600	2.70021200	1.34564100
H	2.50421500	1.54740300	2.31108700	C	1.14239700	2.68741800	0.58127900
H	3.80564700	2.70582200	2.64407600	C	0.06795500	3.56307700	0.84620400
C	4.61237700	-1.80273100	-1.21562800	C	0.21556700	4.42622700	1.94619100
H	4.19768700	-2.65389500	-0.66637600	C	1.37016300	4.43989300	2.72586900
H	3.86185200	-1.51658900	-1.95943300	C	2.42397900	3.57959400	2.42291700
H	5.50995000	-2.13716800	-1.74588000	H	3.12605400	2.02802500	1.10944400
C	2.52332400	-0.09837600	0.04698800	H	-0.61121200	5.07957000	2.20607100
O	1.71213600	0.85921400	-0.16677800	H	1.43997400	5.11600500	3.57316000
O	2.07664500	-1.30166900	0.02477800	H	3.33030500	3.58002900	3.02147800
C	-1.90808900	6.31976800	-0.73194400	C	-1.17000000	3.60839800	0.02067500
H	-1.13705600	6.70022100	-1.41489300	C	-1.79175300	4.85744400	-0.18843400
H	-2.86565300	6.74308000	-1.05177100	C	-1.76575500	2.46157200	-0.55200900
H	-1.67807800	6.70970400	0.26522400	C	-2.96945800	4.97290100	-0.92008200
37 (W=Cl,X=Y=Z=H)				H	-1.32364900	5.75364900	0.20927500
C	-3.68271000	-0.25671900	1.27055000	C	-2.95320600	2.58620900	-1.28325400
C	-2.75618200	-1.00405600	0.54369400	C	-3.55925900	3.83136800	-1.46431200
C	-2.48408700	-2.35451900	0.84933000	H	-3.41962100	5.95054700	-1.06892900
C	-3.16699800	-2.90146100	1.94997400	H	-3.42058100	1.69757200	-1.69803800
C	-4.08554200	-2.16197400	2.69209100	H	-4.48452200	3.90566600	-2.03019300
C	-4.35030400	-0.83712300	2.34963000	S	0.96417500	1.58634500	-0.85127000
H	-3.88390500	0.77455700	1.00325800	C	2.29558400	0.38757500	-0.64977700
H	-2.94580000	-3.92341500	2.24096300	C	2.15371600	-0.75207000	0.14930700
H	-4.58505100	-2.61968000	3.54119000	C	3.47551200	0.61343400	-1.36894700
H	-5.06412200	-0.24889700	2.91903700	C	3.20777900	-1.66011500	0.23524800
C	-1.53655900	-3.19310300	0.06477300	H	1.22468200	-0.94252000	0.67425000
C	-1.83991900	-4.55933300	-0.11356600	C	4.52660900	-0.29730700	-1.27517700
C	-0.33845200	-2.69591300	-0.49737400	H	3.57111400	1.49497000	-1.99539400
C	-0.98562500	-5.41289400	-0.80440600	C	4.39151800	-1.43252000	-0.47220600
H	-2.77733300	-4.94700200	0.27558100	H	3.10736000	-2.54561000	0.85382000
C	0.51768800	-3.56319800	-1.18708200	H	5.44727900	-0.12475500	-1.82206900
C	0.20416700	-4.91579700	-1.33753900	Pd	-1.07247400	0.59588400	-0.39006300
H	-1.25197800	-6.45876700	-0.93018800	C	-4.92580100	-4.26819400	-0.06129700
H	1.45021300	-3.18158000	-1.59322900	C	-4.23919200	-3.07889100	-0.32999300
H	0.88592600	-5.57314300	-1.87139400	C	-3.01229600	-2.84390500	0.33483100
S	-1.89471200	-0.29890300	-0.89053500	C	-2.49554300	-3.78186800	1.25984000
C	-2.16801400	1.47343400	-0.73945300	C	-3.23196400	-4.94387500	1.51415200
C	-1.35355200	2.28797800	0.05531600	C	-4.43418300	-5.19216000	0.85689500
C	-3.20823300	2.03115200	-1.49317100	H	-5.86100800	-4.46473200	-0.57949600

H	-2.85088800	-5.66220200	2.23567500	O	-2.62977500	0.65434300	0.02495600
H	-4.98754700	-6.10544800	1.06010800	N	3.94556400	-4.73920600	-0.46009400
C	-1.19037400	-3.57454700	1.99752800	O	4.90727800	-5.00439400	-1.17865600
H	-0.33276000	-3.71503400	1.33163600	O	3.41713300	-5.51883900	0.32921500
H	-1.10611900	-2.56406100	2.41033900	37 (X=NMe ₂ , W=Y=Z=H)			
H	-1.10602500	-4.28850900	2.82316500	C	-3.28022300	1.46511500	0.13143900
C	-4.83135900	-2.10920400	-1.32968100	C	-2.48211500	0.45043000	-0.39387400
H	-5.23865100	-1.22427300	-0.83053400	C	-2.74774500	-0.89887200	-0.08249200
H	-4.08596300	-1.74836000	-2.04567500	C	-3.79537700	-1.16744000	0.80802700
H	-5.63833800	-2.59196600	-1.89025600	C	-4.59848400	-0.15560400	1.37824100
C	-2.25060300	-1.59006800	0.05801000	C	-4.32606600	1.17779500	1.00109900
O	-0.98512200	-1.60209600	-0.09335000	H	-3.09124700	2.49960700	-0.13426900
O	-2.86803400	-0.46829200	-0.03035000	H	-3.96140600	-2.20036000	1.08346900
C	5.50235100	-2.45053900	-0.41744200	H	-4.91684100	1.99858300	1.38856100
F	5.33930300	-3.40765900	-1.35686700	C	-1.98224100	-2.03187300	-0.67669100
F	6.71016600	-1.88516800	-0.63197600	C	-2.67342900	-3.22504300	-0.97523600
F	5.54877600	-3.07361800	0.77919300	C	-0.59651700	-1.97829200	-0.95134600
37 (W=NO ₂ , X=Y=Z=H)				C	-2.02294700	-4.33730100	-1.50009100
C	3.47945000	1.23077300	1.23131100	H	-3.74753300	-3.26377600	-0.81631400
C	2.38752300	1.73475400	0.52412700	C	0.05129900	-3.10502000	-1.47487600
C	1.81066000	2.98460000	0.83432200	C	-0.65014700	-4.28220700	-1.74318300
C	2.36418200	3.67873800	1.92495100	H	-2.58768100	-5.23828800	-1.72448200
C	3.44346400	3.17907900	2.65017100	H	1.12174900	-3.06716200	-1.65629800
C	4.00976500	1.95479200	2.29952700	H	-0.12562800	-5.14603500	-2.14428600
H	3.91833500	0.27768900	0.95849800	S	-1.13763000	0.80633300	-1.55206400
H	1.91250600	4.61998800	2.22105400	C	-0.81084900	2.56046000	-1.30176800
H	3.83424400	3.74344100	3.49192200	C	-0.08301300	3.03211300	-0.20338000
H	4.85362900	1.55420800	2.85353300	C	-1.28528900	3.44443600	-2.27806000
C	0.68400000	3.58047700	0.06464900	C	0.15623200	4.40115900	-0.08227300
C	0.66238100	4.98017300	-0.11307300	H	0.30937600	2.33550900	0.52885600
C	-0.37463400	2.82146100	-0.48379000	C	-1.03996800	4.81268000	-2.14626700
C	-0.37510300	5.61440600	-0.78880700	H	-1.83942900	3.06310900	-3.13069600
H	1.49073600	5.57329900	0.26424900	C	-0.32135500	5.29031700	-1.04880900
C	-1.41778300	3.46873300	-1.15742600	H	0.72655700	4.77098400	0.76500500
C	-1.42638200	4.85716500	-1.30681100	H	-1.40699800	5.50062700	-2.90263000
H	-0.35830300	6.69350200	-0.91433300	H	-0.12643500	6.35463100	-0.94999400
H	-2.24324700	2.88309100	-1.55189700	Pd	0.59968000	-0.41161100	-0.63796500
H	-2.24902000	5.34018300	-1.82808500	C	6.58651000	-1.16101900	0.85638400
S	1.68985900	0.83982100	-0.89347900	C	5.28311200	-1.20573900	0.34856000
C	2.34393900	-0.83016100	-0.70728500	C	4.34780400	-0.24796500	0.80557800
C	1.76385300	-1.75837200	0.16611000	C	4.71556200	0.72647700	1.76256700
C	3.43481700	-1.18468400	-1.51222800	C	6.02343100	0.71518700	2.25959400
C	2.29144100	-3.04512600	0.24800200	C	6.95638800	-0.21511400	1.80868900
H	0.89390200	-1.48808100	0.75329600	H	7.31609500	-1.88358200	0.49921700
C	3.96610300	-2.47024600	-1.43305300	H	6.30946200	1.45087500	3.00732700
H	3.86515000	-0.45976300	-2.19590300	H	7.97095400	-0.20259100	2.19894100
C	3.38474500	-3.37665500	-0.54976600	C	3.74924300	1.76870400	2.28300800
H	1.86499800	-3.78866400	0.90981700	H	3.53547400	2.52611600	1.52230000
H	4.81003600	-2.77568100	-2.03890600	H	2.78685600	1.33071900	2.56801900
Pd	-0.56158600	0.83644300	-0.37402700	H	4.17066900	2.26808700	3.16153000
C	-6.15529100	-1.83576900	-0.05284100	C	4.93845200	-2.26440800	-0.67653500
C	-5.01968000	-1.05549300	-0.29720000	H	4.30533200	-3.04518300	-0.24324700
C	-3.79891100	-1.43159700	0.31325400	H	4.38544000	-1.85082300	-1.52598000
C	-3.72938800	-2.56359400	1.16042500	H	5.85206000	-2.73197100	-1.05792100
C	-4.89810600	-3.29643200	1.39323200	C	2.95272200	-0.26138700	0.26870800
C	-6.10176100	-2.94300300	0.78925000	O	2.36367500	0.81656300	-0.06507400
H	-7.09335900	-1.56367600	-0.52996200	O	2.32743600	-1.37427200	0.13769700
H	-4.85658500	-4.15775800	2.05510200	N	-5.60539000	-0.46040800	2.27946100
H	-6.99731700	-3.53060200	0.97430200	C	-5.95457800	-1.84750600	2.53225300
C	-2.45160600	-3.00757600	1.83950800	H	-6.76579000	-1.88462100	3.26162100
H	-1.75331500	-3.44725000	1.12040600	H	-6.28759000	-2.37134700	1.62260800
H	-1.92786400	-2.17345100	2.31800900	H	-5.10576000	-2.40327400	2.95097700
H	-2.67394300	-3.75580500	2.60694300	C	-6.49335200	0.59000300	2.74479700
C	-5.14855800	0.13961900	-1.21698500	H	-7.06825500	1.05286200	1.92711500
H	-5.09913500	1.07927900	-0.65797400	H	-7.20106800	0.16964000	3.46161700
H	-4.34582100	0.17621200	-1.96046600	H	-5.93509500	1.38447800	3.25677500
H	-6.10495500	0.10334700	-1.74833900	37 (X=OMe, W=Y=Z=H)			
C	-2.56760000	-0.62801300	0.05827900	C	-3.49261200	1.26255300	0.33432500
O	-1.43632500	-1.18497300	-0.13136700	C	-2.68910500	0.25560200	-0.19053300

C	-2.87251800	-1.09562900	0.18713900	H	-4.03231300	-3.47009700	-0.05776300
C	-3.86176500	-1.36181700	1.13878700	C	-0.35351000	-3.19616100	-1.19548100
C	-4.66412000	-0.35140100	1.68463300	C	-1.03872900	-4.40373000	-1.34501600
C	-4.48410300	0.97251400	1.27490900	H	-2.92000800	-5.42637900	-1.05739200
H	-3.35383900	2.29081800	0.01912300	H	0.68404000	-3.12711800	-1.50997400
H	-4.01049600	-2.37333400	1.49987600	H	-0.53607100	-5.26040400	-1.78715000
H	-5.08799500	1.77878700	1.67399200	S	-1.69588000	0.66176300	-1.21863100
C	-2.08206600	-2.21744400	-0.39221800	C	-1.42126800	2.43711200	-1.08980100
C	-2.72724400	-3.45602900	-0.59264400	C	-0.55552200	2.98681400	-0.13729300
C	-0.71607300	-2.11115300	-0.73945500	C	-2.08001400	3.25502100	-2.01576000
C	-2.04838400	-4.56046400	-1.09698700	C	-0.36532700	4.36866900	-0.10849200
H	-3.78748600	-3.54003400	-0.37106000	H	-0.02081000	2.34134700	0.55039300
C	-0.03938900	-3.23064600	-1.24114600	C	-1.88134100	4.63637900	-1.97702200
C	-0.69419900	-4.45151700	-1.41543000	H	-2.73929300	2.81324100	-2.75710600
H	-2.57674300	-5.49832000	-1.24535200	C	-1.02657000	5.19235000	-1.02324100
H	1.01755900	-3.15192000	-1.47940900	H	0.31028900	4.79957600	0.62477100
H	-0.14784400	-5.30861100	-1.80139500	H	-2.39098600	5.27360400	-2.69405800
S	-1.42472300	0.61214200	-1.43785100	H	-0.86909100	6.26703700	-0.99753200
C	-1.17529200	2.39090700	-1.30317400	Pd	0.18881700	-0.46088400	-0.49421000
C	-0.40825100	2.95794200	-0.27886400	C	6.33215700	-0.93502500	0.32331300
C	-1.74875200	3.19431000	-2.29606300	C	4.98221300	-1.04938500	-0.02767200
C	-0.23075900	4.34131300	-0.24749800	C	4.06657200	-0.10680500	0.49675800
H	0.06210700	2.32415700	0.46452100	C	4.50118400	0.92085400	1.36682000
C	-1.56399600	4.57765200	-2.25418300	C	5.85668500	0.97827200	1.70859300
H	-2.33124200	2.73992900	-3.09211400	C	6.76938400	0.06409100	1.18861900
C	-0.80729700	5.15037000	-1.23021500	H	7.04504500	-1.64548000	-0.08771000
H	0.36940400	4.78495400	0.54170300	H	6.19617000	1.75511200	2.38924600
H	-2.00759100	5.20314200	-3.02357600	H	7.82051700	0.13042000	1.45776900
H	-0.65977500	6.22641100	-1.20199400	C	3.55984700	1.94920300	1.95604900
Pd	0.41342900	-0.47533800	-0.55905800	H	3.23300300	2.66776000	1.19784600
C	6.49312000	-0.86421100	0.66559000	H	2.65338600	1.49025400	2.36429100
C	5.16958500	-0.99923700	0.23125400	H	4.05762600	2.49791100	2.76224200
C	4.21276800	-0.05902900	0.68101300	C	4.56833300	-2.16439400	-0.96352200
C	4.58032000	0.98704100	1.55969100	C	4.02015400	-2.94725200	-0.42993600
C	5.91062200	1.06544200	1.98589600	H	3.90761100	-1.80958000	-1.76095100
C	6.86393700	0.15352600	1.54023600	H	5.45204300	-2.61530200	-1.42651800
H	7.23811100	-1.57303000	0.31286300	C	2.62203500	-0.19271600	0.12465000
H	6.19792700	1.85671100	2.67395000	O	1.95088900	0.85016600	-0.16461200
H	7.89504500	0.23600100	1.87454600	O	2.03358600	-1.33295600	0.09185400
C	3.59264000	2.01336600	2.07181300	C	-5.68588000	-0.66340800	3.24067400
H	3.30500600	2.71532500	1.28276200	H	-6.70926100	-0.72438700	2.84672300
H	2.66801300	1.54991500	2.43154600	H	-5.45392300	-1.62981700	3.69949300
H	4.03382300	2.58088500	2.89761200	H	-5.68857300	0.09504100	4.03120300
C	4.82700800	-2.13295500	-0.71097600	37 (X=Cl, W=Y=Z=H)			
H	4.25432500	-2.91379600	-0.20065200	C	-3.43456200	1.38017400	0.46695000
H	4.21417700	-1.79730800	-1.55366100	C	-2.67996600	0.36788900	-0.12546600
H	5.74260300	-2.58092600	-1.11056300	C	-2.89488100	-0.99170600	0.18766500
C	2.79577600	-0.16702600	0.21896900	C	-3.87406300	-1.27811900	1.15395700
O	2.13580700	0.86281900	-0.13479300	C	-4.61516900	-0.26244900	1.75051400
O	2.22123100	-1.31374800	0.17222700	C	-4.41121100	1.07264100	1.41332300
O	-5.57971800	-0.76347000	2.60574600	H	-3.26594600	2.41678600	0.19797100
C	-6.40472700	0.21522900	3.21796200	H	-4.03592800	-2.30489000	1.46005800
H	-7.04133500	-0.32678200	3.91944400	H	-4.99415800	1.85773400	1.88196800
H	-5.81016100	0.95762400	3.76663000	C	-2.15108600	-2.10667400	-0.45958800
H	-7.03506600	0.73062700	2.48106900	C	-2.83712500	-3.31450200	-0.70709300
37 (X=Me, W=Y=Z=H)				C	-0.78777600	-2.02199000	-0.82393200
C	-3.60492600	1.31460500	0.72706800	C	-2.19899000	-4.41169400	-1.27600200
C	-2.86562300	0.30059400	0.11837000	H	-3.89619700	-3.37954400	-0.47330400
C	-3.03858700	-1.05055900	0.48125500	C	-0.15310500	-3.13470200	-1.39037800
C	-3.95637600	-1.31674800	1.51198300	C	-0.84722700	-4.32593100	-1.61173400
C	-4.70019500	-0.31916800	2.14842600	H	-2.75676900	-5.32561100	-1.46050600
C	-4.51466000	1.00501200	1.73601900	H	0.90190500	-3.07533200	-1.64225600
H	-3.46952700	2.34700500	0.42431400	H	-0.33281900	-5.17889400	-2.04727900
H	-4.06750700	-2.34445000	1.84541100	S	-1.43448100	0.74156200	-1.38690400
H	-5.07481400	1.80658600	2.21141900	C	-1.15341300	2.51163600	-1.21105000
C	-2.31206100	-2.17137100	-0.17691700	C	-0.31476200	3.03418600	-0.21979400
C	-2.98960800	-3.39631900	-0.35409200	C	-1.77548100	3.35305400	-2.14169200
C	-0.97350000	-2.07852200	-0.62242700	C	-0.11607800	4.41386500	-0.15649000
C	-2.36721800	-4.49963900	-0.92940000	H	0.19429300	2.37105500	0.47068500

C	-1.56888400	4.73162000	-2.06718600	H	8.03011300	-0.34786300	2.42058400
H	-2.41193200	2.93200500	-2.91440000	C	3.83516500	1.67809300	2.41163100
C	-0.74186400	5.26114800	-1.07452500	H	3.66718900	2.46827000	1.67292600
H	0.53838300	4.82433800	0.60698100	H	2.85448100	1.24784800	2.63986400
H	-2.05014500	5.38730200	-2.78708100	H	4.22753900	2.13649500	3.32508700
H	-0.57805800	6.33380000	-1.02117000	C	5.08688800	-2.27837000	-0.63128600
Pd	0.38794700	-0.42721800	-0.58001100	H	4.42869800	-3.06428500	-0.24753400
C	6.45509000	-1.04409100	0.59282900	H	4.57345500	-1.83231100	-1.48911500
C	5.12721300	-1.12165700	0.15798600	H	6.00960700	-2.74548400	-0.99025900
C	4.19965900	-0.17372900	0.65145900	C	3.09132300	-0.27703000	0.30237000
C	4.59993900	0.82264700	1.57293700	O	2.51757600	0.81894600	-0.00276100
C	5.93292100	0.84309400	1.99727200	O	2.46281300	-1.37713900	0.09189800
C	6.85771600	-0.07649400	1.50930600	C	-5.56073600	-0.52742400	2.09252000
H	7.17811200	-1.75832900	0.20696600	F	-6.70761800	-0.63494400	1.38063200
H	6.24513900	1.59512000	2.71762800	F	-5.37276200	-1.71109000	2.71453300
H	7.89153300	-0.03895800	1.84316300	F	-5.77875300	0.40521500	3.04595100
C	3.64514500	1.85547600	2.13198700	37 (X=NO ₂ , W=Y=Z=H)			
H	3.38445600	2.60396300	1.37696500	C	-3.27850800	1.42141000	0.33284300
H	2.70428000	1.40727600	2.46777000	C	-2.52559400	0.41088100	-0.27074100
H	4.10216900	2.36846700	2.98436400	C	-2.76757700	-0.95829600	-0.01048700
C	4.75037600	-2.20322100	-0.83125500	C	-3.78142600	-1.25792700	0.91086000
H	4.15866600	-2.99020300	-0.35301600	C	-4.51775000	-0.24298100	1.51208600
H	4.14434100	-1.81481600	-1.65601200	C	-4.28638400	1.10090700	1.23685900
H	5.65209700	-2.65782200	-1.25404200	H	-3.08040500	2.46149700	0.10204500
C	2.77974900	-0.22108600	0.19197000	H	-3.98736500	-2.28406500	1.18625000
O	2.14403000	0.84142900	-0.10791800	H	-4.87855900	1.86558400	1.72321700
O	2.17292800	-1.34830000	0.09162900	C	-2.01111100	-2.06015200	-0.66358100
Cl	-5.82093900	-0.67575000	2.95905900	C	-2.69731500	-3.25481000	-0.96751400
37 (X=CF ₃ , W=Y=Z=H)				C	-0.63428400	-1.97687300	-0.97276700
C	-3.05732900	1.50400700	0.10525700	C	-2.04611100	-4.34069000	-1.54285500
C	-2.29185200	0.49364300	-0.47756000	H	-3.76397200	-3.31927900	-0.77153000
C	-2.57047500	-0.87207700	-0.25264000	C	0.01306300	-3.07832700	-1.54587900
C	-3.63466800	-1.16563700	0.61468700	C	-0.68218000	-4.25645600	-1.82629200
C	-4.39755500	-0.16204800	1.20993600	H	-2.60267000	-5.24507600	-1.77176300
C	-4.11392100	1.17914100	0.95236000	H	1.07740900	-3.02190600	-1.75536300
H	-2.83033800	2.54515300	-0.09289900	H	-0.15843300	-5.10159800	-2.26573600
H	-3.84569800	-2.20161300	0.85344200	S	-1.24174400	0.80076700	-1.48338500
H	-4.69937900	1.96435900	1.41828700	C	-0.96990200	2.57006400	-1.28776200
C	-1.80154700	-1.97713600	-0.88643800	C	-0.12484800	3.08267900	-0.29684300
C	-2.49360200	-3.15103600	-1.25191400	C	-1.60207200	3.41918200	-2.20493800
C	-0.40901000	-1.91737800	-1.12286500	C	0.06869300	4.46259800	-0.21919100
C	-1.83513300	-4.23948700	-1.81451300	H	0.39348700	2.41382600	0.38123400
H	-3.57055100	-3.19538200	-1.11539700	C	-1.40085900	4.79735400	-2.11464400
C	0.24558900	-3.02091500	-1.68395000	H	-2.24163000	3.00499800	-2.97882800
C	-0.45681700	-4.17893200	-2.02417300	C	-0.56826600	5.31801700	-1.12162600
H	-2.39719400	-5.12690300	-2.09184000	H	0.72737500	4.86667000	0.54395800
H	1.32030900	-2.98222700	-1.83710500	H	-1.89003300	5.45978300	-2.82283100
H	0.07247900	-5.02605400	-2.45317200	H	-0.40884400	6.39059900	-1.05632600
S	-0.93467000	0.88155600	-1.61293300	Pd	0.54068200	-0.39843800	-0.63317300
C	-0.63492800	2.63871600	-1.35694100	C	6.54032200	-1.11082500	0.78449700
C	0.16255300	3.10851900	-0.30731200	C	5.23221600	-1.16261400	0.29030500
C	-1.19703600	3.52475300	-2.28463800	C	4.29413100	-0.21562200	0.76605800
C	0.38043000	4.48136600	-0.18305200	C	4.66406900	0.75414200	1.72800100
H	0.62644100	2.41143500	0.38155400	C	5.97726700	0.74857700	2.21032900
C	-0.97322600	4.89561500	-2.14747100	C	6.91249500	-0.17010300	1.74094900
H	-1.80072500	3.14405100	-3.10325800	H	7.27200700	-1.82395100	0.41339000
C	-0.18690700	5.37307200	-1.09680200	H	6.26563200	1.47937200	2.96173300
H	1.00331900	4.85157100	0.62601900	H	7.93094300	-0.15274900	2.12042300
H	-1.40846000	5.58607300	-2.86414100	C	3.69758600	1.78479700	2.27078000
H	-0.00911300	6.43994900	-0.99481600	H	3.48151600	2.55696600	1.52546500
Pd	0.77805500	-0.37022700	-0.69553800	H	2.73676800	1.34139300	2.55187700
C	6.68634300	-1.24462200	0.99693700	H	4.12191300	2.26884600	3.15622500
C	5.40300900	-1.25618100	0.43911100	C	4.88836500	-2.21578500	-0.74073300
C	4.46296000	-0.29978000	0.89107500	H	4.26935900	-3.00813600	-0.30804500
C	4.80585300	0.63934500	1.89235500	H	4.32268300	-1.80128100	-1.58131000
C	6.09359600	0.59413600	2.43730900	H	5.80328100	-2.66935300	-1.13513800
C	7.03119400	-0.33413600	1.99211900	C	2.89604300	-0.23591700	0.24527100
H	7.42005600	-1.96534600	0.64489700	O	2.28108700	0.84025600	-0.05188100
H	6.36010500	1.30141700	3.21872600	O	2.28297300	-1.35358100	0.08624000

N	-5.56956300	-0.60241100	2.47603400	C	-3.85808500	0.39276500	2.11032800
O	-6.19748300	0.31729600	3.00034700	C	-4.15927200	1.60698700	2.72337300
O	-5.76000000	-1.79756900	2.69667100	C	-3.62442100	2.79132000	2.21923700
37 (Y=NM ₂ , W=X=Z=H)							
C	-2.16305500	3.25700100	1.05673500	H	-2.35844800	3.66846200	0.71698500
C	-2.03487100	2.00180600	0.46117900	H	-4.25769300	-0.52771700	2.52358000
C	-2.77927100	0.88822400	0.90580100	H	-4.80439300	1.62380800	3.59720900
C	-3.62400100	1.09608200	2.01077400	H	-3.85233600	3.74554700	2.68557700
C	-3.74890500	2.34080300	2.62391500	C	-2.75409000	-1.00273000	0.34050800
C	-3.02283800	3.42855100	2.14203000	C	-3.79407500	-1.94571400	0.31475300
H	-1.59290100	4.09944000	0.68170900	C	-1.50494500	-1.35237100	-0.22730100
H	-4.17057200	0.24762700	2.40956200	C	-3.61969200	-3.21732200	-0.23874800
H	-4.40589500	2.45555600	3.48152500	H	-4.77644600	-1.69800700	0.70370500
H	-3.11181500	4.40570800	2.60812800	C	-1.34318600	-2.62856300	-0.77157400
C	-2.70308900	-0.45220200	0.26030600	C	-2.37994600	-3.56800300	-0.78085000
C	-3.88134000	-1.22210200	0.20799900	H	-0.37967000	-2.91437900	-1.18428100
C	-1.50919700	-0.98584400	-0.26805300	H	-2.20640000	-4.54908200	-1.20894400
C	-3.91783100	-2.51671600	-0.34309600	S	-1.40641400	1.43907900	-0.95103000
H	-4.79440700	-0.77580400	0.58059200	C	-0.59575300	3.04672600	-0.99769600
C	-1.53703800	-2.28022000	-0.79839200	C	0.51927100	3.33889700	-0.20378900
C	-2.70204800	-3.04211900	-0.83056200	C	-1.10048600	3.99194700	-1.89923800
H	-0.61845400	-2.72210500	-1.17444700	C	1.11805800	4.59491300	-0.30822200
H	-2.65415500	-4.04465600	-1.23919800	H	0.92664800	2.58733600	0.46310500
S	-0.94958900	1.75327500	-0.97202000	C	-0.49332300	5.24541200	-1.99371300
C	0.10792200	3.21231900	-0.97438000	H	-1.95811500	3.74693600	-2.51887000
C	1.23942500	3.30809000	-0.15661000	C	0.61358200	5.54694100	-1.19774500
C	-0.22008000	4.24084100	-1.86630600	H	1.98728500	4.82413000	0.30147600
C	2.03446400	4.45276100	-0.22673300	H	-0.88317600	5.98089600	-2.69159200
H	1.50690200	2.48966200	0.50233200	H	1.08836600	6.52102500	-1.27625700
C	0.58226500	5.38166000	-1.92636800	Pd	0.11123400	-0.18257800	-0.31841700
H	-1.09331600	4.14676000	-2.50516800	C	5.85295800	-2.54325000	0.01270900
C	1.70718900	5.48803900	-1.10595100	C	4.50556800	-2.24097000	-0.21433200
H	2.91711800	4.52908500	0.40169900	C	3.98840400	-1.03073800	0.30553000
H	0.32973700	6.18145900	-2.61672000	C	4.80966300	-0.15140000	1.05000800
H	2.33374300	6.37416700	-1.15771600	C	6.14394900	-0.50961400	1.27158800
Pd	0.27426500	-0.09174500	-0.32093200	C	6.66749800	-1.69137900	0.75383300
C	5.52784800	-3.40120400	-0.00201200	H	6.26227300	-3.46352800	-0.39650700
C	4.25395000	-2.86713000	-0.22729200	H	6.77727600	0.15303000	1.85623100
C	3.94705100	-1.59956100	0.32092800	H	7.70923800	-1.94843600	0.92823300
C	4.90026600	-0.89167900	1.09013900	C	4.30288900	1.15100700	1.63124400
C	6.15155100	-1.47826000	1.30902700	H	4.14493500	1.89960900	0.84840500
C	6.46952600	-2.71960900	0.76415500	H	3.34372000	1.02695500	2.14443600
H	5.77760300	-4.36763000	-0.43283400	H	5.02605100	1.54908900	2.35052900
H	6.88411400	-0.94776700	1.91237000	C	3.66952400	-3.21288200	-1.01860600
H	7.45049400	-3.15523800	0.93657600	H	2.94987100	-3.73775200	-0.38283400
C	4.61815700	0.46546500	1.69784400	H	3.08779400	-2.70894200	-1.79734400
H	4.59259700	1.24510800	0.92997500	H	4.31381000	-3.95576300	-1.49992400
H	3.64894200	0.49502900	2.20640600	C	2.55820300	-0.67181900	0.06325800
H	5.39440700	0.72122700	2.42642900	O	2.21868800	0.51534900	-0.24841200
C	3.27073100	-3.66064500	-1.06039600	O	1.64395000	-1.56631200	0.16894500
H	2.47462900	-4.08352900	-0.43952400	O	-4.71796700	-4.03225300	-0.20329100
H	2.77924700	-3.04179900	-1.81798500	C	-4.60523100	-5.32592200	-0.77034800
H	3.78504600	-4.48159500	-1.57053200	H	-5.58355900	-5.79469000	-0.64665900
C	2.60143300	-0.99471600	0.07912200	H	-4.35890300	-5.27944000	-1.83989800
O	2.47541900	0.23693100	-0.21649900	H	-3.84719700	-5.93079900	-0.25446100
O	1.54701900	-1.72067300	0.16724700	37 (Y=Me, W=X=Z=H)			
N	-5.10948400	-3.24152700	-0.41796100	C	-3.41011800	1.93234100	1.08383900
C	-5.04687000	-4.65439300	-0.75188800	C	-2.84355200	0.81540500	0.46900500
H	-4.46600800	-5.24739100	-0.02554700	C	-3.13961700	-0.49752500	0.89340500
H	-6.06170400	-5.05681800	-0.78923200	C	-4.00087100	-0.62358200	1.99803100
H	-4.60038100	-4.80163100	-1.74186900	C	-4.56037800	0.48442000	2.63045200
C	-6.25640000	-2.78524000	0.34755900	C	-4.27145400	1.76750900	2.16890300
H	-7.08902100	-3.47382400	0.18765500	H	-3.18004100	2.92876900	0.72373100
H	-6.05760900	-2.72883100	1.43126600	H	-4.20964800	-1.61752300	2.38053500
H	-6.58390600	-1.79374800	0.01265100	H	-5.21356100	0.34303000	3.48689500
37 (Y=OMe, W=X=Z=H)							
C	-2.77868000	2.74976900	1.11044400	H	-4.70253800	2.64055600	2.65043500
C	-2.47237800	1.52596000	0.51469700	C	-2.59666000	-1.71285700	0.22678700
C	-3.01974800	0.31348900	0.98462100	C	-3.42094000	-2.85616200	0.15026800
				C	-1.29698400	-1.78747400	-0.31797100
				C	-2.99514200	-4.05541300	-0.41974700

H	-4.43927600	-2.79222400	0.52576800	H	-1.90273400	3.74574500	-2.51519700
C	-0.86262900	-2.99112000	-0.88856300	C	0.61118400	5.54422000	-1.08519100
C	-1.69306600	-4.10978800	-0.93460100	H	1.93792000	4.81140400	0.45116900
H	0.14627900	-3.06020400	-1.28544500	H	-0.83664900	5.98799600	-2.62354100
H	-1.32553400	-5.03219900	-1.38041200	H	1.08193000	6.52206400	-1.13539600
S	-1.74758500	0.99418700	-0.96602600	Pd	0.13167700	-0.20196700	-0.33335100
C	-1.26921900	2.73040900	-0.93628800	C	5.88168900	-2.52108700	0.00454600
C	-0.26045800	3.20680700	-0.09112900	C	4.53276100	-2.22737800	-0.22414400
C	-1.92070800	3.58959400	-1.82960900	C	4.00620100	-1.02330900	0.30151800
C	0.08211800	4.55864100	-0.13605900	C	4.81954100	-0.14184500	1.05276000
H	0.26336100	2.52621400	0.57064200	C	6.15561700	-0.49216000	1.27522300
C	-1.56950800	4.94024100	-1.86470000	C	6.68833500	-1.66751700	0.75221700
H	-2.69252300	3.20306200	-2.48862000	H	6.29856500	-3.43604700	-0.40872200
C	-0.57054600	5.42414400	-1.01760200	H	6.78310700	0.17142600	1.86493500
H	0.86821500	4.93229900	0.51371100	H	7.73136800	-1.91831100	0.92767500
H	-2.07340300	5.60945800	-2.55619100	C	4.30296300	1.15346400	1.64112300
H	-0.29482600	6.47455100	-1.04971100	H	4.14030800	1.90583200	0.86287900
Pd	0.05081000	-0.31633000	-0.34800600	H	3.34458900	1.01938300	2.15334500
C	6.13416400	-1.54291900	-0.00180800	H	5.02281500	1.55221900	2.36322900
C	4.75525300	-1.49715800	-0.23695000	C	3.70694300	-3.20120800	-1.03663300
C	4.01350100	-0.42118100	0.30567800	H	2.99317400	-3.73963700	-0.40548200
C	4.64776700	0.58003000	1.07903400	H	3.12043800	-2.69736300	-1.81178200
C	6.02420900	0.47666400	1.30733600	H	4.35911900	-3.93329000	-1.52357300
C	6.76656500	-0.57081600	0.76841400	C	2.57532900	-0.67374500	0.05872100
H	6.71397700	-2.35766000	-0.42827500	O	2.22304200	0.51431900	-0.23746400
H	6.51611100	1.23323800	1.91362400	O	1.66643100	-1.57705600	0.14697100
H	7.83705200	-0.62917800	0.94835300	Cl	-4.86855200	-4.42726100	-0.39316400
C	3.89911100	1.74848100	1.68347300	37 (Y=CF ₃ , W=X=Z=H)			
H	3.59338600	2.46373900	0.91356300	C	-1.57465300	3.56667300	1.07847900
H	2.98537100	1.43051900	2.19633300	C	-1.60679200	2.30180400	0.49054600
H	4.53423100	2.26827400	2.40814500	C	-2.47711400	1.29166700	0.95143100
C	4.12702100	-2.59036600	-1.07416400	C	-3.28006200	1.60571600	2.06192600
H	3.52966700	-3.26935700	-0.45757600	C	-3.24505200	2.85990600	2.66748500
H	3.45318500	-2.18918400	-1.83802700	C	-2.39570000	3.84718900	2.17093000
H	4.90526000	-3.17380600	-1.57674400	H	-0.91045800	4.33124300	0.69148300
C	2.54286800	-0.33522400	0.05634900	H	-3.92510200	0.83468800	2.47109600
O	1.98305100	0.77381700	-0.22348900	H	-3.87520800	3.05954000	3.52931700
O	1.81690300	-1.39206700	0.12251500	H	-2.36006600	4.83045700	2.63102600
C	-3.90462500	-5.26154700	-0.47624900	C	-2.58034700	-0.05105600	0.31475300
H	-3.55788600	-6.05575700	0.19796000	C	-3.84542000	-0.66555600	0.26781300
H	-4.92836200	-5.00522100	-0.18451900	C	-1.47514700	-0.74468300	-0.23203300
H	-3.94067800	-5.69050700	-1.48487700	C	-4.01806900	-1.93574900	-0.27706900
37 (Y=Cl, W=X=Z=H)				H	-4.71476200	-0.12873900	0.63234000
C	-2.81447200	2.68233600	1.09687100	C	-1.66214600	-2.02501800	-0.77044400
C	-2.48033000	1.47142200	0.48993900	C	-2.91903000	-2.62721400	-0.79057600
C	-3.01926800	0.24573900	0.93481700	H	-0.80853000	-2.56736200	-1.16599500
C	-3.87569400	0.29743100	2.04845600	H	-3.04558000	-3.61872000	-1.21347900
C	-4.20381100	1.49888700	2.67274000	S	-0.57911600	1.91831700	-0.95373000
C	-3.67860100	2.69704300	2.19207100	C	0.66099900	3.22293000	-0.97049900
H	-2.40132100	3.61210600	0.72243600	C	1.77093300	3.20430100	-0.11782700
H	-4.26775300	-0.63349100	2.44554100	C	0.49454500	4.24822000	-1.90930300
H	-4.86221500	1.49467400	3.53659100	C	2.70980000	4.23270500	-0.20252300
H	-3.92800000	3.64166600	2.66669300	H	1.90906300	2.38726400	0.58137400
C	-2.72831100	-1.05882300	0.27742800	C	1.44137000	5.27137200	-1.98443200
C	-3.76433200	-2.01391000	0.22452600	H	-0.36553100	4.24302400	-2.57229900
C	-1.47043700	-1.39065900	-0.27500100	C	2.54636700	5.26409900	-1.13105200
C	-3.54599900	-3.26508200	-0.33815100	H	3.57586900	4.22039000	0.45279800
H	-4.75119900	-1.76750200	0.60040700	H	1.31556800	6.06850300	-2.71142000
C	-1.27892900	-2.66251400	-0.83042900	H	3.28485900	6.05841700	-1.19403900
C	-2.30318000	-3.60996800	-0.86376200	Pd	0.40119900	-0.07372100	-0.31162800
H	-0.30469100	-2.93071500	-1.22884100	C	5.24359300	-3.94629000	-0.00913700
H	-2.13960000	-4.59330500	-1.29233400	C	4.03440600	-3.27730900	-0.22945400
S	-1.38915900	1.42280000	-0.95840300	C	3.87943000	-1.97366100	0.29890100
C	-0.58735100	3.03494200	-0.95769200	C	4.91659500	-1.36307900	1.04352100
C	0.49814100	3.32350300	-0.12247900	C	6.09682100	-2.08273100	1.25826500
C	-1.06811600	3.98799700	-1.86395700	C	6.26585100	-3.36123400	0.73302000
C	1.09158100	4.58436300	-0.19060900	H	5.37754600	-4.94191800	-0.42443300
H	0.88709200	2.56647800	0.54920300	H	6.89230500	-1.62792500	1.84315800
C	-0.46599500	5.24614800	-1.92205500	H	7.19388900	-3.90133700	0.90213200

C	4.79710500	0.02617800	1.63227400	O	-4.93631100	-4.64129100	-0.81867400
H	4.84478700	0.79295800	0.85260400	O	-6.05199700	-3.03264200	0.14081000
H	3.84670400	0.17023900	2.15672800	37 (Z=NMec, W=X=Y=H)			
H	5.60954800	0.20479500	2.34402100	C	3.52794500	-2.19288900	1.04017600
C	2.95859700	-3.97236700	-1.103568000	C	2.91858200	-1.04627000	0.53053900
H	2.13463900	-4.30392500	-0.39579600	C	3.13348200	0.23032000	1.09510500
H	2.52079800	-3.31455900	-1.79325100	C	3.97252100	0.28086700	2.22447800
H	3.37510200	-4.84848100	-1.54302100	C	4.58108000	-0.85735700	2.74743700
C	2.60728200	-1.22892200	0.06590500	C	4.36398000	-2.10005900	2.15320500
O	2.60770200	0.00922100	-0.23524500	H	3.35399500	-3.15625400	0.57389900
O	1.47788000	-1.83245500	0.16777200	H	4.12175700	1.23753200	2.71501700
C	-5.37793400	-2.57455000	-0.25850200	H	5.21477800	-0.77295200	3.62598500
F	-6.36886500	-1.66096300	-0.38412600	H	4.83138200	-2.99589600	2.55182000
F	-5.52834900	-3.47478700	-1.25561600	C	2.53506100	1.47115600	0.54802600
F	-5.60798000	-3.23587400	0.90193000	C	3.26441900	2.67538900	0.62238000
37 (Y=NO ₂ , W=X=Z=H)				C	1.24830900	1.54641000	-0.03363800
C	-2.32519700	3.12460100	1.07361300	C	2.76950000	3.88589600	0.16248800
C	-2.14871900	1.87413100	0.48076100	H	4.27159100	2.65657100	1.03065500
C	-2.84206700	0.73376900	0.93785200	C	0.73853900	2.75951900	-0.49130000
C	-3.68740800	0.90664200	2.04748600	C	1.48109700	3.96228400	-0.41384400
C	-3.85874300	2.14718700	2.65770800	H	3.39404100	4.76735000	0.24451200
C	-3.18203300	3.26196000	2.16600900	H	-0.27044900	2.77497000	-0.88450700
H	-1.79520000	3.98924500	0.69045200	S	1.87181000	-1.11695200	-0.94894100
H	-4.19964200	0.03941300	2.45191300	C	1.50095700	-2.86914600	-1.14196100
H	-4.51451600	2.23757200	3.51865500	C	0.47748300	-3.49698500	-0.42282800
H	-3.30867900	4.23592800	2.62968300	C	2.25540100	-3.58180200	-2.08231700
C	-2.72257600	-0.60687100	0.29844800	C	0.22537600	-4.85221400	-0.64099600
C	-3.86740800	-1.41978700	0.25412100	H	-0.12932300	-2.92891300	0.27323800
C	-1.51516700	-1.10860600	-0.24841100	C	1.99478900	-4.93725700	-2.29031500
C	-3.80176400	-2.69678900	-0.29097900	H	3.03715400	-3.07872800	-2.64384200
H	-4.82260700	-1.06358700	0.61889500	C	0.98188900	-5.57229000	-1.56887700
C	-1.48239100	-2.40595100	-0.78441500	H	-0.57180100	-5.34204600	-0.08916100
C	-2.61588000	-3.21359600	-0.80858800	H	2.57978300	-5.49210400	-3.01828900
H	-0.54735200	-2.79756600	-1.17288200	H	0.77639900	-6.62608400	-1.73550200
H	-2.59585700	-4.21639000	-1.21773300	Pd	-0.01333100	0.01196100	-0.23724300
S	-1.07171900	1.67217600	-0.96504700	C	-6.17731000	0.76947600	0.18769500
C	-0.06192600	3.16274200	-0.97585400	C	-4.80068200	0.83995700	-0.05388600
C	1.04283400	3.31701300	-0.13059600	C	-3.97914300	-0.21563500	0.40623700
C	-0.40361800	4.15698100	-1.90078300	C	-4.53268900	-1.31271400	1.10694600
C	1.79830300	4.48735000	-0.20787200	C	-5.91116500	-1.32586700	1.34698200
H	1.32008900	2.52562900	0.55651600	C	-6.73165000	-0.29889300	0.88761400
C	0.36042400	5.32342800	-1.96782900	H	-6.81784000	1.56885900	-0.17668600
H	-1.25632000	4.01755100	-2.55862500	H	-6.34202100	-2.15753400	1.89901300
C	1.45838900	5.48872300	-1.12127400	H	-7.80196100	-0.33111600	1.07508100
H	2.66003100	4.61067600	0.44159200	C	-3.69486400	-2.46343800	1.62132000
H	0.09853300	6.09736100	-2.68344400	H	-3.35716500	-3.10480200	0.80104200
H	2.05458200	6.39507300	-1.17843900	H	-2.79454400	-2.11764500	2.13962000
Pd	0.22091300	-0.13599200	-0.32158700	H	-4.27835000	-3.07231400	2.31960600
C	5.61131000	-3.18505300	0.03169500	C	-4.25595600	2.03307300	-0.80913000
C	4.31078400	-2.72105300	-0.19503100	H	-3.70304600	2.70398300	-0.14398900
C	3.95139700	-1.44875500	0.31102600	H	-3.56060900	1.73668500	-1.60115100
C	4.87977600	-0.66776200	1.04081100	H	-5.07591000	2.59646800	-1.26642200
C	6.15961800	-1.18709400	1.26232100	C	-2.50687500	-0.17485300	0.14813500
C	6.52875600	-2.43163700	0.75876900	O	-1.87622900	-1.21129800	-0.23675100
H	5.90139400	-4.15376300	-0.36698200	O	-1.85757600	0.91868800	0.31640300
H	6.87397200	-0.60156400	1.83550000	N	0.96931500	5.15954100	-0.89032200
H	7.53117200	-2.81407400	0.93310200	C	1.65670100	6.40142200	-0.57983100
C	4.54397800	0.69490300	1.60766500	H	1.11310100	7.23365900	-1.03151000
H	4.47008700	1.44688200	0.81575300	H	1.73267600	6.58664200	0.50359300
H	3.58352900	0.69677700	2.13347900	H	2.67185300	6.40627100	-0.99560100
H	5.31944000	1.00990800	2.31323300	C	-0.41749200	5.22531200	-1.32150800
C	3.36010100	-3.59335500	-0.98617100	H	-1.12806000	5.00312600	-0.50970100
H	2.59138600	-4.03095000	-0.34142300	H	-0.62649200	6.22930400	-1.69670300
H	2.83349000	-3.03069100	-1.76379000	H	-0.60715800	4.51963300	-2.13876000
H	3.91023300	-4.40770900	-1.46809700	37 (Z=OMe, W=X=Y=H)			
C	2.57861800	-0.91867000	0.07009000	C	3.42329900	-2.11082700	1.10398400
O	2.37934000	0.30310400	-0.23429500	C	2.85858000	-0.96317600	0.54729200
O	1.55793300	-1.69427700	0.16743600	C	3.10986700	0.32246500	1.07350700
N	-5.01862400	-3.51582300	-0.32561100	C	3.93169700	0.38522200	2.21356600

C	4.49428200	-0.75413900	2.78426300	C	0.55621600	3.12040300	-0.74865700
C	4.24518500	-2.00733200	2.22665300	C	1.21641400	4.35752400	-0.75604700
H	3.22435400	-3.08337200	0.66795000	H	3.06086100	5.34980600	-0.23746400
H	4.10477000	1.35308100	2.67346000	H	-0.45152700	3.06157700	-1.15304000
H	5.11672200	-0.66144100	3.66984700	S	1.95022900	-0.70368600	-0.96301500
H	4.67654300	-2.90420000	2.66189200	C	1.70359600	-2.48685100	-1.01861500
C	2.56174800	1.56704300	0.47573800	C	0.74775700	-3.12915500	-0.22333200
C	3.34593300	2.73419300	0.50304600	C	2.48230300	-3.21211100	-1.92893200
C	1.27425400	1.65798700	-0.11211700	C	0.58762400	-4.51082800	-0.33532000
C	2.89863800	3.95212800	-0.00424300	H	0.12229000	-2.55390500	0.44996300
H	4.35287800	2.68450300	0.90858500	C	2.31378600	-4.59410900	-2.03048600
C	0.81940300	2.87303800	-0.61601000	H	3.21064000	-2.69880600	-2.54985200
C	1.61805800	4.02644200	-0.56339000	C	1.36866300	-5.24280200	-1.23325100
H	3.55114500	4.81669600	0.03323000	H	-0.15725700	-5.01290200	0.27531600
H	-0.17635100	2.96352400	-1.03903600	H	2.91714500	-5.15927500	-2.73511000
S	1.82422400	-1.05127900	-0.94113600	H	1.23476800	-6.31769900	-1.31732800
C	1.40916800	-2.79800700	-1.08577200	Pd	-0.00439700	0.33657000	-0.30389700
C	0.35082200	-3.37195500	-0.37227700	C	-6.20123600	0.68762700	0.06276100
C	2.16577000	-3.56212400	-1.98316100	C	-4.83051400	0.84020600	-0.17439000
C	0.06527500	-4.72617700	-0.55228000	C	-3.94288100	-0.12808300	0.35113100
H	-0.25599200	-2.76408800	0.28926900	C	-4.42611600	-1.21967700	1.11035500
C	1.87186100	-4.91613100	-2.15224600	C	-5.80262400	-1.31474800	1.34249200
H	2.97432700	3.09987100	-2.54184000	C	-6.68727800	-0.37500800	0.81969300
C	0.82362300	-5.49779400	-1.43607100	H	-6.89179900	1.41836200	-0.35081600
H	-0.75888800	-5.17482600	-0.00519100	H	-6.18067500	-2.14150300	1.93879000
H	2.45810900	-5.51142600	-2.84646000	H	-7.75462600	-0.47088500	1.00213900
H	0.59221800	-6.55047800	-1.57298600	C	-3.51635300	-2.27874800	1.69466300
Pd	-0.03029100	0.15636200	-0.27181900	H	-3.12933100	-2.94254200	0.91497800
C	-6.15099200	1.15990700	0.10534800	H	-2.64589600	-1.84290500	2.19583800
C	-4.77040400	1.17342800	-0.12394100	H	-4.06292000	-2.88428500	2.42499800
C	-3.99701700	0.08875400	0.35309900	C	-4.36291600	2.02313400	-0.99445700
C	-4.60125400	-0.97922100	1.05779200	H	-3.86457100	2.76870500	-0.36694700
C	-5.98116600	-0.93454600	1.28429900	H	-3.64134200	1.73150500	-1.76439900
C	-6.75472100	0.12093800	0.80837100	H	-5.21566000	2.50042500	-1.48805800
H	-6.75496900	1.98143300	-0.27178600	C	-2.47548900	-0.00034500	0.09928600
H	-6.45073800	-1.74327600	1.83875100	O	-1.76923300	-1.01126500	-0.21820500
H	-7.82719700	0.13368700	0.98550200	O	-1.90346600	1.14370000	0.20193200
C	-3.81677500	-2.15877600	1.59092800	C	0.53864500	5.59220300	-1.30196300
H	-3.49636600	-2.82026000	0.77979000	H	-0.10058700	5.35341500	-2.15899700
H	-2.90908000	-1.84568700	2.11709300	H	-0.10089300	6.06070900	-0.54173400
H	-4.43272600	-2.73743900	2.28701200	H	1.27008200	6.34254400	-1.62098400
C	-4.17365400	2.33755500	-0.88500000	37 (Z=Cl, W=X=Y=H)			
H	-3.59788700	2.99206300	-0.22315500	C	3.62815100	-1.83130100	1.04982600
H	-3.48645200	2.00843500	-1.67111800	C	2.96498100	-0.72850500	0.51123200
H	-4.96808500	2.92925800	-1.35116500	C	3.12854300	0.56871700	1.04204800
C	-2.52354000	0.06689800	0.10832000	C	3.96152100	0.69019500	2.16839600
O	-1.92649300	-1.00142800	-0.24549600	C	4.61774000	-0.40595500	2.72397100
O	-1.83253000	1.13838900	0.25445100	C	4.45758000	-1.67051800	2.16011600
O	1.06139900	5.15713400	-1.08297800	H	3.49783200	-2.81398300	0.61076800
C	1.81378300	6.35817500	-1.03782000	H	4.06932500	1.66617400	2.63095400
H	2.74426900	6.27448400	-1.61530500	H	5.24500300	-0.27077300	3.60041500
H	1.18034800	7.12593300	-1.48604100	H	4.96447600	-2.53379200	2.58152900
H	2.05551100	6.64449700	-0.00555100	C	2.47864100	1.77554500	0.46242100
37 (Z=Me, W=X=Y=H)				C	3.18777600	2.99381400	0.48395900
C	3.70149500	-1.50953400	1.07090000	C	1.17834600	1.77085900	-0.09331700
C	3.00407500	-0.44911500	0.49172000	C	2.64060500	4.17673900	-0.00047000
C	3.12837500	0.87299500	0.96944900	H	4.20467500	3.00962900	0.86537400
C	3.96195700	1.06376200	2.08605600	C	0.61986500	2.96083200	-0.57586600
C	4.65326400	0.01110400	2.68155100	C	1.34843400	4.14812200	-0.52103200
C	4.52928500	-1.27977200	2.17016000	H	3.20715600	5.10122600	0.01840100
H	3.59969800	-2.51243400	0.67170700	H	-0.38918500	2.97033700	-0.97394700
H	4.04204200	2.06068700	2.50769300	S	1.90857300	-0.89580400	-0.95426600
H	5.27970500	0.20022700	3.54870400	C	1.60973400	-2.66682300	-1.08172100
H	5.06328400	-2.10987500	2.62369200	C	0.63707600	-3.31357800	-0.31073000
C	2.43922200	2.03351000	0.34461400	C	2.36625500	-3.37546300	-2.02333900
C	3.10356600	3.27631000	0.31472100	C	0.43788700	-4.68441900	-0.47874100
C	1.14225600	1.96883300	-0.21439700	H	0.02884000	-2.74977300	0.38751600
C	2.50975700	4.41230200	-0.22393300	C	2.15829900	-4.74677900	-2.18084400
H	4.11966200	3.34216800	0.69399000	H	3.10763800	-2.85798200	-2.62500500

C	1.19651800	-5.40060600	-1.40808700	H	-4.22889200	-2.15919400	0.55276300
H	-0.31979200	-5.18992500	0.11295900	H	-3.47997600	-1.49598500	1.99590400
H	2.74410500	-5.29930800	-2.90979200	H	-5.18915600	-1.96757600	2.03506200
H	1.03207500	-6.46688600	-1.53573100	C	-3.47556900	3.12289600	-0.62469700
Pd	-0.01550800	0.17848900	-0.25256200	H	-2.77976600	3.54829000	0.10522500
C	-6.18629600	0.72294900	0.13208100	H	-2.86418300	2.69382900	-1.42488700
C	-4.81062900	0.84146500	-0.09555400	H	-4.07087900	3.93763900	-1.04903300
C	-3.95952600	-0.18928400	0.36978600	C	-2.51680200	0.41763300	0.17875900
C	-4.48303000	-1.30830700	1.06015800	O	-2.19875500	-0.74456700	-0.23688000
C	-5.86248200	-1.36807900	1.28538800	O	-1.57485400	1.26089300	0.40888300
C	-6.71144200	-0.36644900	0.82173400	C	2.34285800	4.62524000	-0.72351100
H	-6.84956700	1.50188000	-0.23531300	F	3.19525500	5.47869500	-0.11139100
H	-6.27135500	-2.21578700	1.82953500	F	2.59406300	4.70887200	-2.05269400
H	-7.78189500	-0.43495000	0.99800400	F	1.09131600	5.09737700	-0.53429400
C	-3.61445500	-2.43316400	1.58103000	37 (Z=NO ₂ , W=X=Y=H)			
H	-3.24670300	-3.06161000	0.76363000	C	3.48887700	-2.15144600	1.06271100
H	-2.73227300	-2.06038600	2.11171200	C	2.88943000	-1.00719800	0.53668600
H	-4.18683400	-3.06214700	2.27048100	C	3.11159200	0.26825800	1.09877800
C	-4.30154900	2.05534500	-0.84237400	C	3.93029500	0.32696600	2.24002800
H	-3.78090800	2.74562800	-0.17126300	C	4.51905000	-0.81218200	2.78458900
H	-3.58832900	1.78712900	-1.62834100	C	4.30514500	-2.05445100	2.19032400
H	-5.13659300	2.58949300	-1.30678900	H	3.31786700	-3.11740100	0.60126100
C	-2.48962000	-0.09776100	0.12881500	H	4.08020500	1.28705500	2.72343200
O	-1.80932600	-1.11405400	-0.22983400	H	5.13656200	-0.72712300	3.67394200
O	-1.87955200	1.02198000	0.28234800	H	4.76055100	-2.95067800	2.60152300
Cl	0.62800000	5.63524900	-1.12602400	C	2.53191200	1.51906700	0.53707600
37 (Z=CF ₃ , W=X=Y=H)				C	3.30833400	2.69744700	0.59275800
C	2.70706500	-3.26956500	0.98494800	C	1.23773700	1.58435800	-0.03260100
C	2.43642000	-1.98269700	0.51906500	C	2.82904600	3.91414600	0.12813900
C	3.00518400	-0.84123500	1.12312600	H	4.31931300	2.64931000	0.98553600
C	3.82132800	-1.05918500	2.24699800	C	0.74998100	2.81060200	-0.49571800
C	4.08362400	-2.33846000	2.73232500	C	1.54326300	3.95243900	-0.40615400
C	3.53230100	-3.44885500	2.09555500	H	3.42708200	4.81577000	0.16490900
H	2.27336800	-4.13098100	0.48968100	H	-0.24817400	2.89590900	-0.90838100
H	4.23359800	-0.19852800	2.76397700	S	1.84889700	-1.09384300	-0.94737200
H	4.71134200	-2.46364000	3.60986000	C	1.47810800	-2.84654900	-1.12694000
H	3.73105600	-4.45242200	2.46041300	C	0.45072500	-3.46603800	-0.40610100
C	2.78696800	0.54313000	0.61980600	C	2.23496900	-3.56535400	-2.06079800
C	3.85412400	1.46104400	0.70575700	C	0.19730600	-4.82222300	-0.61590900
C	1.56019600	0.98938000	0.07652100	H	-0.15782200	-2.89237700	0.28382400
C	3.72041000	2.78081600	0.29241400	C	1.97225600	-4.92168900	-2.25962000
H	4.81534000	1.12353500	1.08178800	H	3.01823000	-3.06745200	-2.62474900
C	1.42962000	2.32172500	-0.32914900	C	0.95589700	-5.54949200	-1.53653500
C	2.49720800	3.21666400	-0.21957000	H	-0.60258000	-5.30696900	-0.06377400
H	4.55808800	3.46580300	0.36783000	H	2.55774200	-5.48253000	-2.98237600
H	0.47734200	2.67549700	-0.71092400	H	0.74885300	-6.60383300	-1.69682900
S	1.39310600	-1.72009700	-0.94171100	Pd	-0.02806600	0.05419400	-0.22932400
C	0.52841300	-3.28528900	-1.15169200	C	-6.15183200	0.91353800	0.19184800
C	-0.58423800	-3.62797600	-0.37490300	C	-4.77169600	0.96700200	-0.03375400
C	0.98852100	-4.13886000	-2.16173800	C	-3.97811400	-0.12624400	0.39019100
C	-1.22704300	-4.84404900	-0.60786600	C	-4.56165000	-1.24176700	1.03769100
H	-0.95446600	-2.94399500	0.38034400	C	-5.94221200	-1.23550300	1.26245700
C	0.33670400	-5.35305800	-2.38495400	C	-6.73526600	-0.17189700	0.83939500
H	1.84519100	-3.85391400	-2.76528900	H	-6.77184300	1.74071000	-0.14410700
C	-0.76837000	-5.70562800	-1.60777200	H	-6.39687600	-2.08023200	1.77378900
H	-2.09451100	-5.11225500	-0.01183400	H	-7.80792000	-0.18917700	1.01458500
H	0.69094300	-6.01773000	-3.16757400	C	-3.75629800	-2.43155000	1.51399100
H	-1.27755400	-6.64859000	-1.78614300	H	-3.42394000	-3.04810000	0.67269000
Pd	-0.08258000	-0.11486900	-0.17308400	H	-2.85499600	-2.12844300	2.05674900
C	-5.72795700	2.42465300	0.21759300	H	-4.36264600	-3.05371600	2.18013400
C	-4.38344700	2.09400300	0.01369700	C	-4.19993100	2.17966800	-0.73563900
C	-3.94087200	0.80521000	0.39772500	H	-3.64622600	2.81879200	-0.04078200
C	-4.83280700	-0.12467400	0.98419300	H	-3.50003300	1.90563600	-1.53136500
C	-6.16137400	0.26249600	1.18897200	H	-5.00593100	2.77220500	-1.17969100
C	-6.61102500	1.52328600	0.80539800	C	-2.50692800	-0.10551500	0.15064600
H	-6.08025300	3.40647400	-0.08824400	O	-1.87687600	-1.14542000	-0.23509700
H	-6.84938100	-0.43955900	1.65323300	O	-1.83712800	0.97621500	0.33206900
H	-7.64941500	1.80288700	0.96419700	N	1.01362500	5.23401700	-0.89783000
C	-4.40905700	-1.51183700	1.41670800	O	1.73754700	6.22581200	-0.79737600

O	-0.11780400	5.24173100	-1.38133000	C	5.50930000	0.55886200	-1.57742000
38-ts (W=NMe ₂ , X=Y=Z=H)				H	3.82959200	1.14893700	-2.77986200
C	4.09911500	-0.07776700	-2.13541700	H	5.32572700	-1.50141800	1.10126500
C	3.14371400	-0.72938600	-1.33188400	H	6.94508400	-0.15129100	-0.12675700
C	3.53251100	-1.41688300	-0.15645800	H	6.21821700	1.17524500	-2.12247600
C	4.90251300	-1.34282300	0.18730000	C	2.73402900	-1.97822800	0.58090400
C	5.84249000	-0.70472200	-0.61093200	C	3.32527100	-3.07453000	1.25672600
C	5.44456700	-0.08135800	-1.79679900	C	1.33295500	-1.83647900	0.70392700
H	3.76332500	0.44235300	-3.02771200	C	2.59892000	-3.93208200	2.07048200
H	5.23240000	-1.77979300	1.12275200	H	4.38169000	-3.27236200	1.11098900
H	6.88310600	-0.68110500	-0.29948100	C	0.60638000	-2.68269200	1.55712000
H	6.16796200	0.42398000	-2.43009200	C	1.23136400	-3.72145800	2.24525400
C	2.60694600	-2.17923100	0.72171200	H	3.09934300	-4.76178700	2.56217000
C	3.16192500	-3.21074300	1.51925500	H	-0.46272400	-2.54021100	1.67289600
C	1.21765900	-1.95177400	0.85238800	H	0.64478400	-4.36939600	2.89127800
C	2.41697400	-3.92074300	2.44992700	S	1.58812700	-0.12686100	-1.86897600
H	4.20313100	-3.47968600	1.37803000	C	0.80898800	1.33767900	-0.22498800
C	0.47453000	-2.64557600	1.82165300	C	1.69367600	1.63201500	0.81327300
C	1.06634400	-3.61955700	2.62416400	C	-0.05011300	2.30592400	-0.73751800
H	2.88941400	-4.70689900	3.03254400	C	1.67423300	2.90463600	1.37808200
H	-0.58316100	-2.43502000	1.93954600	H	2.38604100	0.88945500	1.19048500
H	0.46636700	-4.14974200	3.35920400	C	-0.06225800	3.58365200	-0.16809700
S	1.48796400	-0.59311700	-1.91951800	H	-0.72022300	2.07775800	-1.55754100
C	0.81848700	1.09460600	-0.44702200	C	0.79876800	3.88779400	0.89447600
C	1.72909700	1.47262900	0.53432100	H	2.33580000	3.15399600	2.20198400
C	0.00336300	2.04367600	-1.06308200	H	-0.74237600	4.32541900	-0.57114800
C	1.78432400	2.80452900	0.94602200	Pd	0.03996200	-0.70617800	-0.33146400
H	2.38798300	0.75017900	1.00093800	C	-6.02539700	-0.15729200	1.11319500
C	0.06647300	3.37256700	-0.65190700	C	-4.62817900	-0.21640200	1.06289900
H	-0.69515900	1.75756800	-1.84033100	C	-4.01101700	-0.52231500	-0.17321400
C	0.96224700	3.79307400	0.35982700	C	-4.78506400	-0.77618600	-1.33059500
H	2.47865900	3.06102600	1.73726400	C	-6.17939200	-0.73078300	-1.22280000
H	-0.59119200	4.08370700	-1.13752500	C	-6.79836400	-0.41826100	-0.01519100
Pd	-0.04760300	-0.90267600	-0.29393000	H	-6.50836600	0.09215600	2.05468400
C	-6.06499800	0.10994500	1.11113600	H	-6.78289900	-0.94071500	-2.10232100
C	-4.67309900	-0.02623200	1.06263800	H	-7.88295200	-0.37828300	0.04645000
C	-4.08492200	-0.51564300	-0.12750200	C	-4.16965100	-1.11045100	-2.67235400
C	-4.88273700	-0.87284000	-1.24031100	H	-3.70854600	-0.22947700	-3.12981100
C	-6.27186600	-0.74270800	-1.13373000	H	-3.38051100	-1.86468000	-2.58930500
C	-6.86186000	-0.24995200	0.02740800	H	-4.93644400	-1.49211500	-3.35414400
H	-6.52492800	0.50009600	2.01570000	C	-3.84378700	0.06384100	2.32668600
H	-6.89423000	-1.02982800	-1.97762400	H	-3.41750700	-0.85503800	2.74182700
H	-7.94237500	-0.14676700	0.08768500	H	-3.00359200	0.74329200	2.15188600
C	-4.29821500	-1.40387300	-2.53142600	H	-4.49579900	0.51275500	3.08297200
H	-3.80306800	-0.61050000	-3.10015500	C	-2.52165600	-0.57810600	-0.26089300
H	-3.54276300	-2.17644200	-2.35606300	O	-1.89967500	-0.05853800	-1.24194100
H	-5.08895500	-1.83383100	-3.15466500	O	-1.84115700	-1.15673900	0.65972300
C	-3.86092100	0.37087800	2.27647900	O	0.86850500	5.10032100	1.51475800
H	-3.47183000	-0.50837200	2.79981200	C	0.01062200	6.13628600	1.06394000
H	-2.99279500	0.98289900	2.01184600	H	0.22865100	7.00076300	1.69362600
H	-4.48189300	0.94062500	2.97547100	H	0.20574400	6.39416800	0.01447400
C	-2.60039200	-0.65438500	-0.21500600	H	-1.04690100	5.86292300	1.17709800
O	-1.96755200	-0.28537900	-1.25563800	38-ts (W=Me, X=Y=Z=H)			
O	-1.93793900	-1.15053100	0.76422200	C	4.18271000	0.89618400	-1.81386900
N	1.04317900	5.12554000	0.74588200	C	3.24526700	0.03397500	-1.21366600
C	1.81090100	5.47431000	1.92933300	C	3.63768300	-0.86861000	-0.19570800
H	2.86495800	5.19643300	1.80975900	C	4.98714200	-0.79536600	0.22048200
H	1.77176000	6.55572400	2.07451000	C	5.91016900	0.05242500	-0.37744700
H	1.43284300	4.98894200	2.84391100	C	5.51318000	0.89439800	-1.41996100
C	0.03047200	6.06070900	0.28477600	H	3.84526900	1.57656400	-2.59020400
H	0.25279600	7.05231300	0.68394900	H	5.31225000	-1.40638300	1.05471400
H	0.03501300	6.13842100	-0.80899600	H	6.93588600	0.06654000	-0.01968500
H	-0.98722900	5.78082700	0.60177700	H	6.22359300	1.56414400	-1.89575600
38-ts (W=OMe, X=Y=Z=H)				C	2.73347400	-1.85451300	0.45082100
C	4.17304700	0.53836100	-1.94995800	C	3.32383300	-3.01110300	1.01729700
C	3.23686900	-0.25573000	-1.26004800	C	1.33077800	-1.73105700	0.57184800
C	3.63641000	-1.06655100	-0.16962000	C	2.59250400	-3.95258700	1.72754000
C	4.99288200	-0.96787100	0.21851400	H	4.38345200	-3.18630200	0.86536400
C	5.91424700	-0.18804500	-0.46779200	C	0.59853500	-2.66582100	1.32128400

C	1.22152300	-3.76844700	1.90432100	C	0.85964700	3.88394600	0.72466600
H	3.09172900	-4.82662300	2.13669500	H	2.38838100	3.16511600	2.06371500
H	-0.47276300	-2.54154800	1.43806100	H	-0.66718000	4.34293900	-0.72853000
H	0.63074100	-4.48371600	2.47053700	Pd	-0.00282000	-0.70792000	-0.33039100
S	1.60277300	0.20095200	-1.83095400	C	-6.03881000	0.04752500	1.12444100
C	0.80051800	1.52730200	-0.08180600	C	-4.64391100	-0.04862300	1.07072800
C	1.65835000	1.73247400	0.99267000	C	-4.04122300	-0.41395700	-0.15673700
C	-0.05550600	2.53205500	-0.53606700	C	-4.82716000	-0.68890800	-1.30161100
C	1.61905300	2.96551000	1.65513600	C	-6.21915300	-0.60422100	-1.18927500
H	2.34100900	0.96090600	1.32752000	C	-6.82364000	-0.23348000	0.00916300
C	-0.06964700	3.75168700	0.14063900	H	-6.51059800	0.34314500	2.05807900
H	-0.70982800	2.36628100	-1.38327200	H	-6.83241700	-0.82937600	-2.05812900
C	0.76298400	3.99204200	1.24454000	H	-7.90646300	-0.16331900	0.07374600
H	2.27292600	3.11904300	2.51079400	C	-4.22842500	-1.08634000	-2.63363000
H	-0.74126000	4.53363600	-0.20787200	H	-3.75159500	-0.23338000	-3.12677900
Pd	0.04286200	-0.50545000	-0.35770100	H	-3.45592700	-1.85478100	-2.52779400
C	-6.00986700	-0.06748800	1.16613500	H	-5.00832000	-1.47544300	-3.29595400
C	-4.61331600	-0.12795400	1.10188100	C	-3.84700100	0.25877500	2.32023400
C	-4.00506200	-0.32396700	-0.16096200	H	-3.43859400	-0.65364400	2.76644000
C	-4.78764200	-0.46984000	-1.33142900	H	-2.99400600	0.91431000	2.11799800
C	-6.18101000	-0.42812300	-1.21079300	H	-4.48521200	0.74841700	3.06269100
C	-6.79096100	-0.22237000	0.02394000	C	-2.55567600	-0.50917800	-0.24913900
H	-6.48597400	0.09905900	2.12918500	O	-1.92491800	-0.04711400	-1.25407900
H	-6.79086500	-0.55547100	-2.10165700	O	-1.88060300	-1.06459700	0.69081900
H	-7.87492100	-0.18298300	0.09604300	Cl	0.88863200	5.51405600	1.37978900
C	-4.18342800	-0.68563600	-2.70229800	38-ts (W=CF ₃ , X=Y=Z=H)			
H	-3.72583000	0.23210700	-3.08492400	C	4.06641300	-0.41446400	-2.06926100
H	-3.39389400	-1.44382800	-2.69188800	C	3.06682500	-1.03745800	-1.29755500
H	-4.95624900	-1.00634000	-3.40824400	C	3.39707600	-1.75860700	-0.12462100
C	-3.82098500	0.03463800	2.38126300	C	4.76028800	-1.75141400	0.25073800
H	-3.39737900	-0.91964200	2.71033600	C	5.74467800	-1.14211300	-0.51617300
H	-2.97841500	0.72304800	2.26299800	C	5.40206800	-0.48245800	-1.69970300
H	-4.46713600	0.41715600	3.17797800	H	3.77494500	0.13282000	-2.96085200
C	-2.51692500	-0.37606400	-0.26363500	H	5.04916900	-2.21752200	1.18564900
O	-1.89964200	0.21611000	-1.20538800	H	6.77786600	-1.16899700	-0.18165500
O	-1.83062000	-1.02608700	0.60447400	H	6.16133300	0.00077800	-2.30741100
C	0.74444800	5.32881400	1.94876900	C	2.41785400	-2.48973800	0.72048800
H	1.17537500	6.11833200	1.31915700	C	2.90257000	-3.56654100	1.50301900
H	-0.27817900	5.63755900	2.19592200	C	1.04182800	-2.18902300	0.83579400
H	1.31975000	5.29840100	2.87947500	C	2.10250700	-4.25622000	2.40303500
38-ts (W=Cl, X=Y=Z=H)				H	3.93091000	-3.88643500	1.37404200
C	4.14866900	0.40089200	-1.99361900	C	0.24346300	-2.86127100	1.77485100
C	3.19947900	-0.35641800	-1.28044100	C	0.76741400	-3.88620600	2.56170400
C	3.58487700	-1.14515300	-0.16897400	H	2.52086700	-5.07974700	2.97499400
C	4.94478900	-1.06601300	0.21117900	H	-0.80245500	-2.59435600	1.88341900
C	5.87956200	-0.32418300	-0.49890100	H	0.12651300	-4.39970500	3.27342800
C	5.48634600	0.40308900	-1.62563400	S	1.43139400	-0.82212900	-1.91899600
H	3.81510100	0.99652200	-2.83825500	C	0.82056900	0.88940700	-0.46865500
H	5.26992300	-1.58319000	1.10640000	C	1.72846300	1.20613900	0.54084000
H	6.91237800	-0.30109900	-0.16289200	C	0.06313800	1.87523400	-1.10672500
H	6.20596100	0.99028800	-2.18840000	C	1.85197800	2.53754300	0.94399100
C	2.66506800	-2.01189600	0.61306000	H	2.32716800	0.44154800	1.01989200
C	3.23258700	-3.10165800	1.31873600	C	0.20259500	3.20019000	-0.69637800
C	1.26942100	-1.82940300	0.74263500	H	-0.63343000	1.61912900	-1.89543300
C	2.49006100	-3.91267100	2.16513600	C	1.09323600	3.53496900	0.32884300
H	4.28219900	-3.33206800	1.17174200	H	2.53643200	2.79134700	1.74713300
C	0.52744000	-2.62552500	1.62956300	H	-0.38655200	3.97346000	-1.17900700
C	1.13063100	-3.65881700	2.34520900	Pd	-0.14639600	-1.05428900	-0.31776900
H	2.97201600	-4.73966400	2.67917700	C	-6.07497400	0.32402200	1.11687400
H	-0.53588600	-2.44875300	1.75132800	C	-4.69433100	0.10335300	1.06246600
H	0.53300500	-4.26891300	3.01728200	C	-4.14051700	-0.40431100	-0.13750200
S	1.55267400	-0.21269700	-1.89134900	C	-4.96198700	-0.69565500	-1.25345700
C	0.80738700	1.31569900	-0.30215800	C	-6.33989100	-0.48195900	-1.13927700
C	1.69808100	1.62176200	0.72446900	C	-6.89500300	0.02939400	0.03089500
C	-0.03711600	2.28611500	-0.84629700	H	-6.50773300	0.72951700	2.02787800
C	1.71433500	2.91732400	1.25037500	H	-6.98121300	-0.71768000	-1.98469900
H	2.37358500	0.87588400	1.12495000	H	-7.96677200	0.19849000	0.09631000
C	-0.01383300	3.57881800	-0.32036500	C	-4.41861400	-1.24329000	-2.55556900
H	-0.71660100	2.04422100	-1.65442600	H	-3.88199100	-0.47322500	-3.11875900

H	-3.70959600	-2.06201500	-2.39702100	38-ts (X=NMec ₂ , W=Y=Z=H)		
H	-5.23814600	-1.61671900	-3.17783200	C	-3.52078400	-1.42977300
C	-3.85970500	0.43495500	2.28077100	C	-2.58017300	-0.44765500
H	-3.52663100	-0.47255700	2.79448700	C	-3.00410300	0.67421500
H	-2.95566700	0.99617900	2.02449900	C	-4.35701700	0.72128300
H	-4.44515800	1.03351100	2.98588000	C	-5.31161200	-0.23881700
C	-2.67023100	-0.63248200	-0.23275900	C	-4.85681200	-1.33221500
O	-2.01848200	-0.31860500	-1.28080100	H	-3.18139300	-2.29395500
O	-2.02719300	-1.15524800	0.74840800	H	-4.66492500	1.52179000
C	1.28598700	4.97408800	0.71746600	H	-5.53452800	-2.11802000
F	2.25542000	5.56538100	-0.02165300	C	-2.10288900	1.77701100
F	1.65094600	5.10249500	2.01276200	C	-2.68555800	3.04110300
F	0.16088400	5.70077200	0.53674200	C	-0.70786800	1.66544400
38-ts (W=NO ₂ , X=Y=Z=H)				C	-1.96166200	4.10681900
C	4.12268900	0.12949900	-2.03785400	H	-3.73280300	3.19308800
C	3.16480100	-0.59104500	-1.29882800	C	0.01407000	2.73207700
C	3.53965000	-1.34407200	-0.15982400	C	-0.60509800	3.94528000
C	4.90060800	-1.27220700	0.21669200	H	-2.45506400	5.05841300
C	5.84464400	-0.56807300	-0.51928900	H	1.07623400	2.62054900
C	5.46041100	0.12622900	-1.66967300	H	-0.02145200	4.75881700
H	3.79710500	0.69964800	-2.90290800	S	-0.93622700	-0.75893900
H	5.21892100	-1.76295300	1.12910400	C	-0.15393400	-1.65062300
H	6.87800700	-0.54777900	-0.18507800	C	-1.06546000	-1.60857000
H	6.18758800	0.68422800	-2.25191100	C	0.72988200	-2.71726500
C	2.60679500	-2.16491100	0.65483600	C	-1.05557800	-2.64760900
C	3.15428500	-3.24207000	1.39409400	H	-1.76931500	-0.79093600
C	1.21681100	-1.94696200	0.78750600	C	0.71832300	-3.74795300
C	2.39858300	-4.00674600	2.27173400	H	1.42168900	-2.74143700
H	4.19788800	-3.49976000	1.24954500	C	-0.16839000	-3.71603200
C	0.46190900	-2.69306800	1.70584700	H	-1.74958600	-2.61102300
C	1.04676600	-3.71585600	2.45172800	H	1.40558200	-4.58152700
H	2.86498800	-4.82634200	2.81115300	H	-0.17147500	-4.52254800
H	-0.59570700	-2.48635900	1.83039800	Pd	0.59613700	0.26838600
H	0.44032900	-4.28831700	3.14838300	C	6.65130200	0.14582200
S	1.52002300	-0.45190200	-1.91687700	C	5.25475700	0.19168200
C	0.79226600	1.14610600	-0.38864000	C	4.64783200	0.14505800
C	1.69494800	1.48066700	0.62438500	C	5.43037800	0.06721000
C	-0.03242000	2.11055800	-0.98197700	C	6.82375800	0.05027600
C	1.74648000	2.79657000	1.08162800	C	7.43313000	0.08247300
H	2.34834300	0.73623700	1.06148700	H	7.12672500	0.16471200
C	0.02628800	3.42404400	-0.52554200	H	7.43400400	0.00696500
H	-0.71904200	1.84165800	-1.77491500	H	8.51709700	0.05822800
C	0.91288100	3.75096900	0.50205200	C	4.82403000	0.01799900
H	2.42093000	3.08578500	1.87849200	H	4.36736700	-0.95635300
H	-0.59895400	4.19483700	-0.95973000	H	4.03332700	0.76354800
Pd	-0.04017400	-0.84720500	-0.32833500	H	5.59493900	0.20009600
C	-6.04156000	0.09304600	1.14728200	C	4.45757400	0.27218700
C	-4.64959400	-0.03455600	1.08675500	H	4.01974200	1.26636200
C	-4.06528400	-0.45910600	-0.13114300	H	3.62464600	-0.43817200
C	-4.86689200	-0.76100400	-1.25892100	H	5.10331200	0.06082800
C	-6.25557200	-0.64243200	-1.13842100	C	3.15873900	0.17373800
C	-6.84152400	-0.21335600	0.04965500	O	2.54477800	-0.61362200
H	-6.49908800	0.43461100	2.07218700	O	2.47342300	0.99838900
H	-6.88114400	-0.88728600	-1.99294500	N	-6.64051200	-0.12517700
H	-7.92194400	-0.11733200	0.11987400	C	-7.05150600	0.93253600
C	-4.29063800	-1.22264100	-2.58007500	H	-6.80171600	1.91972500
H	-3.80528300	-0.39897000	-3.11315100	H	-8.13479400	0.89260300
H	-3.53074900	-2.00009900	-2.45197800	H	-6.58463800	0.84750900
H	-5.08520700	-1.62376200	-3.21716600	C	-7.55437100	-1.22790400
C	-3.83757600	0.30537200	2.31794600	H	-8.55202900	-0.94924900
H	-3.44431700	-0.59659400	2.79777200	H	-7.62404800	-1.45032500
H	-2.97353300	0.93562700	2.08490600	H	-7.25730600	-2.15107200
H	-4.46075300	0.83645700	3.04432600	38-ts (X=OMe, W=Y=Z=H)		
C	-2.58446400	-0.58724400	-0.23256300	C	-3.77838600	-1.32302300
O	-1.95349700	-0.19500800	-1.26726600	C	-2.82049000	-0.36947100
O	-1.90631500	-1.10210600	0.72986000	C	-3.20473300	0.75153100
N	0.97488000	5.13595600	0.97865500	C	-4.55062400	0.81093700
O	1.76936100	5.39503100	1.88378800	C	-5.50079600	-0.13254300
O	0.22961800	5.95837800	0.44470200	C	-5.11530000	-1.21027800
						-1.08641300

H	-3.45972300	-2.17616000	-2.03685700	H	0.63623200	2.61249200	1.02611400
H	-4.89421200	1.59565900	0.78155400	H	-0.48587500	4.71896000	1.62838600
H	-5.82295100	-1.96578700	-1.40631100	S	-1.38241800	-0.76725400	-1.63945400
C	-2.27830600	1.83164300	0.15007100	C	-0.57869100	-1.66117300	0.36827500
C	-2.84088300	3.09395800	0.46094700	C	-1.45705600	-1.62877900	1.44792800
C	-0.87988900	1.70040300	0.31019900	C	0.30441100	-2.72219000	0.16414200
C	-2.09027000	4.14064500	0.97708600	C	-1.41243500	-2.67473600	2.37735600
H	-3.89417400	3.26084100	0.26353700	H	-2.15848300	-0.81376400	1.57846200
C	-0.12972200	2.74780300	0.86934800	C	0.32835700	-3.75764800	1.10248900
C	-0.72707700	3.96053700	1.20981100	H	0.96894100	-2.73798900	-0.69107900
H	-2.56886700	5.09165400	1.19405700	C	-0.52447500	-3.73727400	2.20897100
H	0.93622500	2.62159500	1.02634600	H	-2.08013400	-2.64660200	3.23463700
H	-0.12236000	4.75927100	1.63124000	H	1.01616600	-4.58626300	0.95462300
S	-1.18688900	-0.70178400	-1.62348800	H	-0.50085500	-4.54841600	2.93114900
C	-0.38752300	-1.61842600	0.38693100	Pd	0.15728200	0.26921700	-0.35501100
C	-1.26237100	-1.56398100	1.46862000	C	6.22937200	0.18690800	1.16312000
C	0.46579400	-2.70295900	0.18020400	C	4.83166600	0.22058900	1.10555200
C	-1.24460200	-2.61180700	2.39687300	C	4.20910900	0.17661100	-0.16426800
H	-1.94110900	-0.73035800	1.60209400	C	4.97717300	0.11360000	-1.35094100
C	0.46270900	-3.74068000	1.11650300	C	6.37206900	0.10871800	-1.24194900
H	1.12835800	-2.73514500	-0.67612000	C	6.99688700	0.13826100	0.00222400
C	-0.38698200	-3.69849400	2.22479600	H	6.71721200	0.20367600	2.13452600
H	-1.90895500	-2.56621700	3.25604900	H	6.97127800	0.07703100	-2.14846500
H	1.12693400	-4.58790000	0.96592900	H	8.08190900	0.12343100	0.06712700
H	-0.38413800	-4.51104200	2.94583400	C	4.35425100	0.06826100	-2.72961300
Pd	0.38777900	0.29106700	-0.34685500	H	3.90743600	-0.91012300	-2.93296200
C	6.46639200	0.05556700	1.13208500	H	3.55294900	0.80504400	-2.84604400
C	5.06959300	0.12403500	1.08334300	H	5.11345500	0.26595600	-3.49312900
C	4.43832900	0.09821900	-0.18253700	C	4.05082700	0.28531200	2.40057100
C	5.19708600	0.01914600	-1.37408100	H	3.60865900	1.27555000	2.54964100
C	6.59210500	-0.02044000	-1.27401700	H	3.22287000	-0.43066700	2.42150300
C	7.22522800	-0.00931000	-0.03372000	H	4.70919900	0.07126800	3.24866900
H	6.96058600	0.05793800	2.10043900	C	2.71933600	0.19236600	-0.25653900
H	7.18469400	-0.06464300	-2.18437100	O	2.10127100	-0.59159900	-1.04567500
H	8.30994500	-0.05103000	0.02433500	O	2.03407900	1.00330800	0.46323900
C	4.56394000	-0.00751300	-2.74856800	C	-7.17416700	-0.22845100	0.13185600
H	4.09063400	-0.97363100	-2.95058800	H	-7.50300800	-1.16625600	0.59578900
H	3.78117100	0.74999100	-2.85816600	H	-7.32627600	0.57713700	0.85670000
H	5.32271700	0.17215900	-3.51695700	H	-7.84099500	-0.04102000	-0.71959200
C	4.29829500	0.20571200	2.38308100	38-ts (X=Cl, W=Y=Z=H)			
H	3.88254400	1.20662500	2.53684300	C	-3.74850700	-1.44123400	-1.50771000
H	3.45239600	-0.48887100	2.40750500	C	-2.81460400	-0.46681700	-1.10729400
H	4.95587000	-0.02695000	3.22689400	C	-3.22186100	0.64530900	-0.33065800
C	2.94862200	0.15078500	-0.26529800	C	-4.57739700	0.67611700	0.06827900
O	2.30642500	-0.62034400	-1.04769100	C	-5.48226700	-0.29046200	-0.34448300
O	2.28901600	0.98096200	0.45612800	C	-5.08662000	-1.35581300	-1.15495500
O	-6.76417400	0.07579300	0.18561800	H	-3.40614000	-2.28323000	-2.10172600
C	-7.77575700	-0.85484300	-0.17000400	H	-4.92540100	1.45584600	0.73304800
H	-8.69149000	-0.49448100	0.30171700	H	-5.79932700	-2.10974800	-1.46983400
H	-7.92080300	-0.89680700	-1.25739600	C	-2.32801300	1.75224900	0.09826600
H	-7.54730400	-1.86146500	0.20389100	C	-2.92669200	3.00207800	0.39309000
38-ts (X=Me, W=Y=Z=H)				C	-0.92734800	1.65883000	0.26642300
C	-3.96281000	-1.44738100	-1.49922400	C	-2.20655200	4.07332300	0.90173900
C	-3.03016400	-0.47247300	-1.09424200	H	-3.98222000	3.14203200	0.18619700
C	-3.44299500	0.62802100	-0.30776800	C	-0.20889300	2.73154000	0.81877000
C	-4.80073900	0.64271100	0.08851100	C	-0.84030600	3.93124500	1.14331700
C	-5.73310200	-0.31014300	-0.31295400	H	-2.71089400	5.01368500	1.10567100
C	-5.29652700	-1.35915200	-1.13790000	H	0.85915600	2.63542400	0.98254500
H	-3.61803300	-2.28444900	-2.09931700	H	-0.25940800	4.75014600	1.55929400
H	-5.13512300	1.42304900	0.76337000	S	-1.16650700	-0.77443800	-1.64504400
H	-5.99670200	-2.12369900	-1.46554300	C	-0.37705500	-1.65199800	0.36747900
C	-2.55071600	1.73205100	0.13247900	C	-1.24792000	-1.59999300	1.45227900
C	-3.14993000	2.97829800	0.44167500	C	0.49580100	-2.72188300	0.16712600
C	-1.14968400	1.64216600	0.29915700	C	-1.20590700	-2.63738000	2.39160900
C	-2.43185000	4.04522300	0.96272900	H	-1.93922000	-0.77641400	1.58219500
H	-4.20593200	3.11704300	0.23692700	C	0.51723900	-3.74771700	1.11593900
C	-0.43210300	2.70896100	0.86410900	H	1.15417500	-2.75193400	-0.69240800
C	-1.06531800	3.90378300	1.20300700	C	-0.32835100	-3.70904600	2.22751100
H	-2.93811200	4.98239800	1.17725800	H	-1.86733200	-2.59459900	3.25299300

H	1.19701700	-4.58348800	0.97183600	H	5.80859200	-0.02169800	-3.43211800
H	-0.30719500	-4.51332100	2.95726400	C	4.62506200	0.41170600	2.42594000
Pd	0.37487700	0.27176800	-0.36831800	H	4.20576900	1.41977800	2.50583300
C	6.43003300	0.20066200	1.19343300	H	3.77904100	-0.28099600	2.47660500
C	5.03307600	0.24003900	1.12409400	H	5.26427400	0.23553400	3.29702500
C	4.42004000	0.16199900	-0.14916900	C	3.34207800	0.16710800	-0.25006800
C	5.19718800	0.05968700	-1.32763800	O	2.72332400	-0.63098700	-1.02526600
C	6.59103900	0.05064400	-1.20707000	O	2.65377700	1.01193300	0.42891100
C	7.20619100	0.11374800	0.04061900	C	-6.50957000	-0.17454400	0.07913800
H	6.91041500	0.24358900	2.16767800	F	-6.72870300	-1.05088900	1.08697900
H	7.19721500	-0.01090000	-2.10732600	F	-7.37697700	-0.49221200	-0.90789400
H	8.29053800	0.09518600	0.11454500	F	-6.84525900	1.05000900	0.53865900
C	4.58660900	-0.02264500	-2.71013800	38-ts (X=NO ₂ , W=Y=Z=H)			
H	4.13554900	-1.00387100	-2.88889000	C	-3.59693400	-1.48957600	-1.47960300
H	3.79144100	0.71541000	-2.85635800	C	-2.65857800	-0.50812700	-1.09824100
H	5.35438700	0.14743400	-3.47165500	C	-3.05722700	0.63768900	-0.36281000
C	4.24447100	0.34663000	2.41165100	C	-4.41094600	0.68614600	0.03027100
H	3.81012100	1.34435100	2.53107100	C	-5.31249100	-0.29181400	-0.35762700
H	3.41029200	-0.36140800	2.44713800	C	-4.93325700	-1.38627300	-1.13462100
H	4.89592200	0.15052700	3.26930800	H	-3.25391900	-2.34944500	-2.04632000
C	2.93216800	0.18378100	-0.25356500	H	-4.77715100	1.48173700	0.66359000
O	2.31364800	-0.60783600	-1.03536000	H	-5.66158500	-2.13423700	-1.42045700
O	2.24395000	1.00863600	0.44874100	C	-2.16169600	1.76087800	0.01816600
Cl	-7.15314400	-0.18346000	0.18529500	C	-2.76466500	3.01812500	0.27019300
38-ts (X=CF ₃ , W=Y=Z=H)				C	-0.75898700	1.68046800	0.17331900
C	-3.34538300	-1.40368600	-1.56184500	C	-2.04359100	4.11363900	0.72197100
C	-2.40485700	-0.43986300	-1.14738300	H	-3.82434900	3.14425100	0.07653100
C	-2.80482200	0.67932600	-0.37833200	C	-0.03880800	2.78058000	0.66569200
C	-4.16303900	0.71811000	0.01023800	C	-0.67257900	3.99001900	0.94609800
C	-5.08454600	-0.23415500	-0.40221100	H	-2.55114000	5.05828100	0.89503100
C	-4.68175600	-1.29890800	-1.21668900	H	1.03196500	2.69748500	0.81791500
H	-3.00526700	-2.24583000	-2.15667300	H	-0.09034400	4.82981400	1.31582600
H	-4.50385600	1.50776200	0.66664500	S	-1.01025000	-0.85562500	-1.60655700
H	-5.39826800	-2.04298900	-1.54828200	C	-0.23581000	-1.62948400	0.42731100
C	-1.90565800	1.78390300	0.04538200	C	-1.08603900	-1.51126800	1.52334600
C	-2.49966800	3.03877200	0.32880200	C	0.62566000	-2.71517800	0.26716800
C	-0.50581400	1.68658200	0.21630800	C	-1.03397500	-2.49868300	2.51473200
C	-1.77532200	4.11204400	0.82700000	H	-1.76558000	-0.67440900	1.62607500
H	-3.55469900	3.18128300	0.12132400	C	0.65733800	-3.68895900	1.26876900
C	0.21723000	2.76200200	0.75702000	H	1.26768000	-2.79570300	-0.60136800
C	-0.40942300	3.96749100	1.06900800	C	-0.16764700	-3.58471600	2.39156800
H	-2.27621400	5.05606300	1.02223000	H	-1.67845000	-2.40441500	3.38469700
H	1.28481600	2.66322100	0.92203400	H	1.32878000	-4.53617900	1.15699500
H	0.17475400	4.78852800	1.47605100	H	-0.13915800	-4.34951800	3.16218100
S	-0.75395800	-0.77232900	-1.66365300	Pd	0.53771200	0.25949100	-0.39528000
C	0.00468200	-1.62858300	0.35758600	C	6.57730700	0.29493400	1.20076200
C	-0.86476200	-1.55038600	1.44198900	C	5.18117600	0.33606000	1.11786200
C	0.86485200	-2.71127000	0.17152700	C	4.57589900	0.14240600	-0.14758000
C	-0.83414000	-2.57513500	2.39557800	C	5.36148000	-0.07532200	-1.30560000
H	-1.54535900	-0.71659600	1.56200300	C	6.75421700	-0.08154500	-1.17337000
C	0.87520300	-3.72334000	1.13497600	C	7.36091300	0.09512800	0.06740100
H	1.52195700	-2.76107700	-0.68799100	H	7.05108300	0.42662900	2.17018800
C	0.03068800	-3.65914500	2.24622100	H	7.36642100	-0.23111400	-2.05901600
H	-1.49446000	-2.51229300	3.25652200	H	8.44452700	0.07707100	0.15102600
H	1.54535600	-4.56868500	1.00245100	C	4.76409800	-0.28283700	-2.68075300
H	0.04283300	-4.45323300	2.98718300	H	4.30504600	-1.27240600	-2.77107200
Pd	0.78811100	0.28021900	-0.39236500	H	3.97817200	0.44515600	-2.90549400
C	6.82143600	0.19413100	1.24087500	H	5.54190900	-0.19292900	-3.44570700
C	5.42606100	0.24805500	1.15205900	C	4.38876200	0.56792800	2.38653300
C	4.82773000	0.13069300	-0.12559000	H	3.97214400	1.57989100	2.41628200
C	5.61884800	-0.02488600	-1.28931400	H	3.54181200	-0.11894800	2.47922900
C	7.01078300	-0.04675500	-1.14992400	H	5.03382300	0.43676900	3.26118000
C	7.61093800	0.05501500	0.10244200	C	3.09025100	0.16433700	-0.26495100
H	7.28989100	0.26728800	2.21908100	O	2.47018400	-0.66676100	-1.00414500
H	7.62747800	-0.14910300	-2.03922200	O	2.39894100	1.03109100	0.38401000
H	8.69393300	0.02585200	0.19116800	N	-6.71209100	-0.17847400	0.08282700
C	5.02692600	-0.15060800	-2.67667400	O	-7.49405400	-1.05365900	-0.28705300
H	4.56285300	-1.13081100	-2.82479400	O	-7.01645000	0.78153000	0.79027000
H	4.24592400	0.59342500	-2.86303500	38-ts (Y=NMMe ₂ , W=X=Z=H)			

C	-3.16571700	-3.13970000	-1.25252300	H	-5.31955700	0.30986700	0.49204000
C	-2.54681900	-1.89483500	-1.02792100	H	-6.61046300	-1.70244000	0.00373400
C	-3.25951200	-0.82686700	-0.43000600	H	-5.53127500	-3.63305500	-1.17064500
C	-4.57971300	-1.11430300	-0.01207000	C	-2.79256300	0.93887200	-0.17140200
C	-5.18833000	-2.34158300	-0.23919000	C	-3.59328600	2.09225800	-0.05352600
C	-4.48507600	-3.36197600	-0.88540200	C	-1.39609500	1.09988400	0.00319400
H	-2.58680000	-3.93540300	-1.71215100	C	-3.07339300	3.33964200	0.29192900
H	-5.13178000	-0.35585700	0.53085500	H	-4.65628000	2.04925400	-0.25905300
H	-6.20644700	-2.50681300	0.10238200	C	-0.88555600	2.34674100	0.38617500
H	-4.94718900	-4.32769100	-1.06844600	C	-1.70403500	3.46696400	0.54045200
C	-2.70665000	0.53591600	-0.20862000	H	0.17949400	2.46186500	0.55743200
C	-3.63211300	1.59987100	-0.12201500	H	-1.26005300	4.41330900	0.82796600
C	-1.33867800	0.83955400	-0.04131000	S	-1.19246900	-1.57720400	-1.53495200
C	-3.26764700	2.92209600	0.18481400	C	-0.31358200	-2.02900500	0.57498200
H	-4.66852000	1.38356600	-0.33883700	C	-1.20848100	-1.97900800	1.64056000
C	-0.97033200	2.14272600	0.32496800	C	0.72751700	-2.95730700	0.52620500
C	-1.90293200	3.16501200	0.45122300	C	-1.02177500	-2.86027500	2.71210900
H	0.07357800	2.37531600	0.50764700	H	-2.03045400	-1.27385600	1.65207400
H	-1.55326900	4.15100000	0.73322800	C	0.89196700	-3.82997100	1.60516800
S	-0.86012300	-1.82213000	-1.53577500	H	1.40367900	-2.99280300	-0.31930000
C	0.07243700	-2.16219400	0.56073900	C	0.02315800	-3.78427700	2.69846200
C	-0.81169200	-2.19818900	1.63660900	H	-1.70387800	-2.81384000	3.55715200
C	1.20650100	-2.97498800	0.51153000	H	1.70271800	-4.55350300	1.57804400
C	-0.52155200	-3.04342300	2.71405400	Pd	0.13074000	-0.12735500	-0.41938300
H	-1.70364000	-1.58369600	1.65272200	C	6.07510100	1.07065300	1.12695000
C	1.47427700	-3.81354300	1.59662400	C	4.69371400	0.85892400	1.05506700
H	1.87549900	-2.94575500	-0.33989900	C	4.13308000	0.48777800	-0.19019600
C	0.61612500	-3.85038100	2.69866800	C	4.94476500	0.34520400	-1.34075900
H	-1.19643400	-3.06093000	3.56605700	C	6.31690900	0.59271600	-1.22298700
H	2.35825500	-4.44553000	1.56775700	C	6.88248900	0.94626700	-0.00066100
Pd	0.30726100	-0.22617200	-0.44221800	H	6.51758300	1.34010900	2.08270900
C	6.07014100	1.61428800	1.16077900	H	6.94609900	0.50136300	-2.10478400
C	4.72149200	1.25139300	1.07271300	H	7.95225900	1.12474700	0.07312000
C	4.22196400	0.81191400	-0.17630400	C	4.39045800	-0.04653900	-2.69352600
C	5.06064600	0.75128300	-1.31475000	H	4.11396400	-1.10528900	-2.71905400
C	6.39560500	1.14877500	-1.18137000	H	3.48653100	0.51556500	-2.94920600
C	6.90193500	1.57154300	0.04497000	H	5.13735500	0.13409900	-3.47324300
H	6.46680000	1.93789500	2.11989300	C	3.86824100	1.01895600	2.31361400
H	7.04326400	1.12034500	-2.05407800	H	3.26457200	1.93150400	2.28080800
H	7.94448800	1.86726300	0.13107000	H	3.16890300	0.18947000	2.45904900
C	4.57136100	0.29147600	-2.67123200	H	4.52331400	1.07101100	3.18923100
H	4.40487300	-0.79010900	-2.68851200	C	2.66512200	0.23740500	-0.29421300
H	3.61855300	0.75534900	-2.94587400	O	2.21104800	-0.75528600	-0.94785200
H	5.30809800	0.54057700	-3.44174400	O	1.83111900	1.02711800	0.27850300
C	3.86625000	1.32914000	2.31911800	H	0.15678400	-4.46949500	3.53071200
H	3.16794000	2.17072300	2.27082100	O	-3.97968400	4.35902600	0.36014000
H	3.25819400	0.43011200	2.46097500	C	-3.50271200	5.65555700	0.68158200
H	4.49958900	1.45716900	3.20295400	H	-4.37704300	6.30897100	0.66520000
C	2.79073100	0.40304100	-0.29804700	H	-3.04914800	5.68397800	1.68140200
O	2.45495300	-0.63200600	-0.95618800	H	-2.77053200	6.01105300	-0.05559000
O	1.87104100	1.09885600	0.26495400	38-ts (Y=Me, W=X=Z=H)			
H	0.83062000	-4.50829600	3.53606000	C	-3.92338300	-2.09147300	-1.37346700
N	-4.20934000	3.94635800	0.21614300	C	-3.08261500	-1.00570200	-1.06150400
C	-5.62210300	3.61514900	0.16492300	C	-3.58557500	0.13040300	-0.38156900
H	-5.94210000	2.96862400	0.99915500	C	-4.94141500	0.07122100	0.01644300
H	-6.20664500	4.53656500	0.20408600	C	-5.76928500	-0.99784000	-0.29949000
H	-5.87442200	3.10600100	-0.77335800	C	-5.26477000	-2.08457100	-1.01915000
C	-3.82846200	5.23999900	0.75739300	H	-3.50105700	-2.94707300	-1.89218100
H	-4.67538400	5.92434900	0.67439400	H	-5.34784400	0.87960600	0.61307800
H	-3.52598400	5.19268400	1.81641700	H	-6.80456000	-0.98975600	0.02988100
H	-2.99859300	5.67406700	0.18757300	H	-5.89985900	-2.92899100	-1.27053500
38-ts (Y=OMe, W=X=Z=H)				C	-2.78684500	1.34023400	-0.05559700
C	-3.62796100	-2.64395600	-1.30099400	C	-3.48808400	2.55803800	0.12945300
C	-2.88261000	-1.47718200	-1.04333900	C	-1.38667000	1.37841400	0.11565000
C	-3.48634500	-0.34974600	-0.43551300	C	-2.88200800	3.74181700	0.53708000
C	-4.83898100	-0.49604000	-0.05022100	H	-4.55140500	2.58197000	-0.08673600
C	-5.57263600	-1.64540700	-0.31237300	C	-0.76890200	2.55612300	0.56806400
C	-4.97062500	-2.72661700	-0.96169200	C	-1.50323300	3.71805700	0.78410300
H	-3.13027400	-3.49009200	-1.76557100	H	0.30220700	2.57050600	0.73925400

H	-0.99227500	4.61652500	1.12407700	Pd	0.15855300	-0.09423200	-0.40992900
S	-1.41098700	-1.21113700	-1.58055900	C	6.09231100	1.13417900	1.13019600
C	-0.55767200	-1.85617200	0.49463100	C	4.71164200	0.91758700	1.06125300
C	-1.44152200	-1.79934200	1.56901400	C	4.15079500	0.54016400	-0.18254700
C	0.40603000	-2.85938000	0.38158300	C	4.96151700	0.39680600	-1.33430000
C	-1.32148900	-2.75567500	2.58438400	C	6.33273900	0.64959000	-1.21867200
H	-2.20477100	-1.03328500	1.63097800	C	6.89845300	1.00895300	0.00185800
C	0.50461700	-3.80567200	1.40521400	H	6.53525000	1.40840300	2.08428500
H	1.07415100	-2.89829800	-0.47011100	H	6.96119000	0.55814700	-2.10089000
C	-0.35343100	-3.75695800	2.50675000	H	7.96760200	1.19159000	0.07362400
H	-1.99437700	-2.70610000	3.43659700	C	4.40859100	0.00034600	-2.68627700
H	1.25494200	-4.58833900	1.32788700	H	4.13892600	-1.06020800	-2.71112400
Pd	0.03202000	0.05707000	-0.39371100	H	3.50142500	0.55682500	-2.94246700
C	6.06563700	0.68668000	1.14653500	H	5.15421300	0.18470900	-3.46621700
C	4.67120800	0.58933900	1.08063600	C	3.88911300	1.07931500	2.32150800
C	4.07248200	0.33426300	-0.17617000	H	3.28671300	1.99277700	2.28973300
C	4.86100200	0.19321300	-1.34324800	H	3.18948200	0.25070800	2.46996500
C	6.24932200	0.32517500	-1.22924400	H	4.54656800	1.13198100	3.19517800
C	6.85122300	0.56311000	0.00362500	C	2.68524400	0.28462200	-0.28378100
H	6.53601400	0.86634400	2.11003300	O	2.23049800	-0.70225300	-0.94787000
H	6.86198500	0.23502400	-2.12271900	O	1.84656500	1.06156000	0.30099700
H	7.93236800	0.65222100	0.07364100	H	0.19847400	-4.49102700	3.48123900
C	4.26731600	-0.07635100	-2.70919600	Cl	-4.13315000	4.70543700	0.50039300
H	3.90599800	-1.10634300	-2.79037600	38-ts (Y=CF ₃ , W=X=Z=H)			
H	3.41008400	0.57000500	-2.92293900	C	-2.77545200	-3.46814300	-1.30409200
H	5.02096300	0.08721200	-3.48620000	C	-2.25255500	-2.18353700	-1.06101700
C	3.87259100	0.74503900	2.35693400	C	-3.05287100	-1.17604400	-0.47046400
H	3.35122900	1.70719700	2.38521500	C	-4.35892900	-1.55591900	-0.08508000
H	3.10403700	-0.02701800	2.46267600	C	-4.87318700	-2.82176000	-0.33300200
H	4.53678200	0.68827200	3.22537200	C	-4.08339500	-3.78514000	-0.96635000
C	2.58857300	0.20825600	-0.27552000	H	-2.13206100	-4.21777900	-1.75515200
O	2.05053400	-0.69920400	-0.98704100	H	-4.97916900	-0.84278800	0.44577000
O	1.82499100	1.02142600	0.35898000	H	-5.88503800	-3.06027500	-0.01812300
H	-0.27165800	-4.49938600	3.29550400	H	-4.47139800	-4.78002700	-1.16402300
C	-3.68018900	5.01400300	0.70443300	C	-2.60410600	0.21953000	-0.22428300
H	-4.74246000	4.85213200	0.49563200	C	-3.60165500	1.21751000	-0.14550100
H	-3.59588500	5.40633600	1.72562600	C	-1.26521100	0.63598300	-0.03941200
H	-3.32341700	5.80093800	0.02821700	C	-3.31186600	2.53671700	0.17870600
38-ts (Y=Cl, W=X=Z=H)				H	-4.62788700	0.96203200	-0.37992400
C	-3.57891400	-2.62192700	-1.34534700	C	-0.98353600	1.96317000	0.32467500
C	-2.84137800	-1.45581900	-1.06364200	C	-1.99426800	2.91245400	0.44373500
C	-3.45361700	-0.34642300	-0.43144100	H	0.04296300	2.26657300	0.49974600
C	-4.80397100	-0.51072000	-0.04543700	H	-1.75320100	3.93670900	0.70862700
C	-5.52924100	-1.65990000	-0.33070000	S	-0.57038600	-1.98133300	-1.54476000
C	-4.92029400	-2.72145200	-1.00541700	C	0.35458600	-2.23397600	0.60165300
H	-3.07610400	-3.45446500	-1.82850300	C	-0.55092400	-2.32663900	1.65442800
H	-5.29030500	0.27759100	0.51750200	C	1.54234100	-2.96521600	0.57639600
H	-6.56548200	-1.73220500	-0.01299000	C	-0.22617000	-3.14615000	2.74233400
H	-5.47465800	-3.62712000	-1.23323400	H	-1.48531800	-1.77860200	1.64857700
C	-2.76922800	0.94166300	-0.14368300	C	1.84273900	-3.78005100	1.67159100
C	-3.58688700	2.08962800	-0.00994600	H	2.22551700	-2.89401100	-0.26109300
C	-1.37756700	1.11460600	0.03451300	C	0.96491700	-3.87173900	2.75457500
C	-3.06126700	3.31764800	0.35894300	H	-0.91704100	-3.20826200	3.57907700
H	-4.64565500	2.02751800	-0.22754900	H	2.76785700	-4.35053200	1.66440000
C	-0.87233800	2.36036500	0.44207900	Pd	0.45944700	-0.30831100	-0.43070900
C	-1.70068200	3.46694200	0.61482800	C	6.06128400	1.98262000	1.13553800
H	0.19198700	2.47911300	0.61552300	C	4.74351500	1.51841800	1.06104100
H	-1.29221000	4.42475200	0.91931900	C	4.27529900	1.01791600	-0.17761500
S	-1.15090600	-1.53331800	-1.55550100	C	5.11246700	0.99738400	-1.31933200
C	-0.27154600	-2.00846100	0.56405200	C	6.41369800	1.49704600	-1.19915000
C	-1.17242500	-1.97896500	1.62446400	C	6.89015300	1.98033500	0.01675900
C	0.77459500	-2.92933300	0.50325100	H	6.43563000	2.35411800	2.08606900
C	-0.98528200	-2.87580400	2.68318300	H	7.05904400	1.50124800	-2.07386900
H	-1.99914900	-1.27954800	1.64324000	H	7.90765700	2.35522100	0.09235000
C	0.93871500	-3.81794500	1.56945200	C	4.65615800	0.47764600	-2.66569300
H	1.45432800	-2.94798200	-0.33982200	H	4.58049600	-0.61435600	-2.66696300
C	0.06482700	-3.79361700	2.65926700	H	3.66739700	0.85717900	-2.94238400
H	-1.67118100	-2.84617200	3.52579600	H	5.36638900	0.77470300	-3.44384800
H	1.75322600	-4.53678400	1.53453200	C	3.88954700	1.55824100	2.31009200

H	3.13979600	2.35403900	2.25434300	C	-4.07294800	-2.44701800	-1.12505200
H	3.34041100	0.62472900	2.46769400	C	-3.19778900	-1.35493700	-0.97029200
H	4.51682000	1.73897400	3.18884400	C	-3.66136100	-0.11067700	-0.47379900
C	2.88004600	0.50443600	-0.28561200	C	-5.02465500	-0.06455900	-0.09477400
O	2.61352700	-0.55958400	-0.93230500	C	-5.88800300	-1.13843200	-0.26328600
O	1.90999000	1.13272100	0.27447000	C	-5.41741200	-2.34069900	-0.79952000
H	1.20561900	-4.51090300	3.59919000	H	-3.67583900	-3.38510600	-1.50198800
C	-4.43010500	3.53520000	0.29814300	H	-5.40939700	0.83650800	0.36884200
F	-4.98492200	3.51839200	1.53427000	H	-6.92648000	-1.04285400	0.04198000
F	-5.42929300	3.28226700	-0.57781700	H	-6.08071600	-3.19060100	-0.93054500
F	-4.00535300	4.79809800	0.07729800	C	-2.82110800	1.09717400	-0.31824300
38-ts (Y=NO ₂ , W=X=Z=H)				C	-3.45931500	2.36072900	-0.28333000
C	-3.28087800	-2.98647400	-1.32369900	C	-1.41602700	1.13056100	-0.16453000
C	-2.62503800	-1.76901900	-1.05756800	C	-2.79812200	3.55277300	-0.05147500
C	-3.31722400	-0.69151800	-0.45414700	H	-4.52520100	2.41358300	-0.47922000
C	-4.65859200	-0.93487600	-0.08044600	C	-0.73787500	2.32037700	0.10803700
C	-5.30324100	-2.13464700	-0.35076500	C	-1.40282800	3.56601600	0.17056000
C	-4.61697000	-3.16672500	-0.99633700	H	-3.37005600	4.47294800	-0.05326900
H	-2.71940400	-3.79334100	-1.78521900	H	0.33283700	2.28459600	0.25793800
H	-5.20422000	-0.16814600	0.45741700	S	-1.53412300	-1.68759100	-1.44616900
H	-6.33684600	-2.26804900	-0.04500300	C	-0.68960400	-2.02222000	0.70778900
H	-5.10800300	-4.11096900	-1.21224100	C	-1.56861700	-1.76142300	1.75603800
C	-2.72440400	0.64588200	-0.18577100	C	0.23644500	-3.06529700	0.76331800
C	-3.61550500	1.73538600	-0.08296700	C	-1.48148100	-2.54387400	2.91351800
C	-1.34642700	0.92166800	-0.00395400	H	-2.30395500	-0.96869800	1.68960900
C	-3.16968600	3.00044700	0.26412300	C	0.30232600	-3.83668000	1.92679400
H	-4.66831000	1.61717100	-0.29906800	H	0.90147000	-3.26478600	-0.06813200
C	-0.92645600	2.20880900	0.38129400	C	-0.55080700	-3.57915100	3.00291300
C	-1.82668600	3.25811900	0.52559600	H	-2.15095700	-2.33301400	3.74357100
H	0.12690300	2.39952200	0.55571900	H	1.02305400	-4.64873400	1.97985400
H	-1.50393600	4.25174300	0.81094800	Pd	-0.04239400	-0.30073200	-0.47440500
S	-0.92901000	-1.74225300	-1.53333200	C	6.02224600	0.20997100	1.01330500
C	-0.04183900	-2.08990700	0.62885700	C	4.62478900	0.18072000	0.94535300
C	-0.96159600	-2.08923800	1.67238600	C	4.01705800	-0.19218200	-0.27663500
C	1.06366100	-2.93932000	0.60891100	C	4.80009800	-0.51796900	-1.40924400
C	-0.73242900	-2.93986300	2.76080400	C	6.19332200	-0.44862300	-1.29881100
H	-1.83405800	-1.44769500	1.65775900	C	6.80366700	-0.09446900	-0.09829400
C	1.26868600	-3.78310200	1.70440900	H	6.49858000	0.47868100	1.95295300
H	1.75686900	-2.93647500	-0.22318700	H	6.80293000	-0.68174500	-2.16824800
C	0.37704400	-3.78497900	2.77987100	H	7.88787600	-0.05678300	-0.02882100
H	-1.43283500	-2.93186000	3.59177700	C	4.19370100	-0.92311600	-2.73541300
H	2.12963900	-4.44641200	1.70326300	H	3.76892100	-1.93066600	-2.68736400
Pd	0.26844500	-0.19148400	-0.41205100	H	3.37833200	-0.25794700	-3.03781400
C	6.09572000	1.49251900	1.08543600	H	4.95687300	-0.90669600	-3.52013700
C	4.73222100	1.18473100	1.02432100	C	3.82938800	0.53006300	2.18492900
C	4.20516200	0.70357800	-0.19898400	H	3.35788600	1.51365100	2.09204400
C	5.03183900	0.54914200	-1.33874100	H	3.02181200	-0.18413700	2.37375500
C	6.38311600	0.89505400	-1.23200900	H	4.48510600	0.54457700	3.06157200
C	6.91597900	1.35686100	-0.03134900	C	2.52722400	-0.25112800	-0.37339100
H	6.51360900	1.84723700	2.02409300	O	1.94601800	-1.22482300	-0.94835100
H	7.02240700	0.79586900	-2.10545700	O	1.80961600	0.68633800	0.12755700
H	7.97068800	1.61144400	0.03387000	H	-0.49457900	-4.18692500	3.90158700
C	4.51668500	0.04675800	-2.67029600	N	-0.71199100	4.74029400	0.40877100
H	4.31279700	-1.02818200	-2.63930700	C	0.69632700	4.68761600	0.76874700
H	3.57988500	0.53203600	-2.96181300	H	1.07330000	5.70605400	0.88113200
H	5.25712700	0.23441500	-3.45423800	H	0.87228100	4.14665500	1.71159700
C	3.89471800	1.36430700	2.27224700	H	1.28569900	4.19736100	-0.01477500
H	3.24313300	2.24038200	2.19202600	C	-1.45067800	5.96959000	0.64178900
H	3.24118400	0.50706100	2.46131800	H	-2.11330400	5.90627200	1.51945300
H	4.54358400	1.49882200	3.14346800	H	-0.74404400	6.78515900	0.80644400
C	2.76072800	0.35188900	-0.29154800	H	-2.06522000	6.23478800	-0.22773000
O	2.36772400	-0.68225000	-0.92485100	38-ts (Z=OMe, W=X=Y=H)			
O	1.87058800	1.08976800	0.26849700	C	-4.02123300	-2.30227700	-1.19705600
H	0.54315700	-4.44732900	3.62452800	C	-3.15734800	-1.20857200	-0.99736300
N	-4.14571900	4.09573400	0.35440300	C	-3.63293200	0.00237300	-0.43693800
O	-5.32484700	3.83898100	0.10771700	C	-4.99031200	0.01333400	-0.03850100
O	-3.72460800	5.20651000	0.67590300	C	-5.84254000	-1.06258700	-0.24856300
38-ts (Z=NMMe ₂ , W=X=Y=H)				C	-5.36274600	-2.22930400	-0.85033300
				H	-3.61733600	-3.21570800	-1.62379700

H	-5.37881200	0.88604700	0.47387600	H	0.38979400	2.58264700	0.57755200
H	-6.87788400	-0.99676200	0.07430300	S	-1.59872800	-1.15727700	-1.54986000
H	-6.01664600	-3.08056100	-1.01547700	C	-0.76082400	-1.77670800	0.54172800
C	-2.80749700	1.21810900	-0.23516100	C	-1.62225500	-1.61861500	1.62408800
C	-3.46896200	2.46394500	-0.16483800	C	0.13099700	-2.84675800	0.45611900
C	-1.39914600	1.25194300	-0.07530000	C	-1.55146000	-2.54120200	2.67473200
C	-2.82445000	3.66211600	0.11775400	H	-2.33056000	-0.80027300	1.66712100
H	-4.53334300	2.50457800	-0.37034200	C	0.18102900	-3.75777500	1.51467700
C	-0.74501800	2.44218200	0.24387400	H	0.78200300	-2.96220900	-0.40179700
C	-1.44558500	3.65125900	0.35220500	C	-0.65471500	-3.60839900	2.62431400
H	-3.39833100	4.58119200	0.14495000	H	-2.20619100	-2.41310000	3.53289000
H	0.32837800	2.46902000	0.39843300	H	0.87548600	-4.59209300	1.45850000
S	-1.49200500	-1.49924000	-1.49730300	Pd	-0.06295200	0.05885500	-0.42559000
C	-0.64280600	-1.93895800	0.63752400	C	6.00137700	0.29403900	1.10070600
C	-1.51948600	-1.73966800	1.70060200	C	4.60374900	0.30039500	1.03155300
C	0.29112800	-2.97602100	0.63285500	C	3.98982700	0.04688500	-0.21833400
C	-1.42133800	-2.58173000	2.81466500	C	4.76797600	-0.19558200	-1.37568300
H	-2.26028000	-0.94957700	1.68010000	C	6.16205200	-0.16551300	-1.25968200
C	0.36773100	-3.80711000	1.75379300	C	6.77775400	0.07035500	-0.03323900
H	0.95392300	-3.12574500	-0.21066600	H	6.48191500	0.47181600	2.05952900
C	-0.48271900	-3.61310600	2.84521100	H	6.76798100	-0.33414900	-2.14635500
H	-2.08807700	-2.41966500	3.65770500	H	7.86239100	0.07965800	0.03878600
H	1.09491500	-4.61499900	1.76107200	C	4.15849300	-0.46853700	-2.73395700
Pd	-0.01299200	-0.14980600	-0.45121500	H	3.71780400	-1.46942800	-2.77912400
C	6.02343400	0.44858700	1.07012200	H	3.35493400	0.23437400	-2.97588600
C	4.62705700	0.39510700	0.99576900	H	4.92455300	-0.39318900	-3.51239600
C	4.03180700	0.02463900	-0.23395200	C	3.81706000	0.56074000	2.29822400
C	4.82643700	-0.27228800	-1.36724600	H	3.37263000	1.56114900	2.29207300
C	6.21746900	-0.17907900	-1.24864600	H	2.99000500	-0.14461400	2.42543100
C	6.81539900	0.17128300	-0.04091200	H	4.47297500	0.48121200	3.17116500
H	6.49039600	0.71604400	2.01471400	C	2.50063000	0.03027100	-0.31960800
H	6.83536300	-0.38938800	-2.11800200	O	1.89629100	-0.85622500	-1.00368000
H	7.89838000	0.22825100	0.03428200	O	1.80055400	0.91782500	0.28749900
C	4.23737900	-0.66854400	-2.70400300	H	-0.61125100	-4.32389800	3.44051800
H	3.83714800	-1.68695100	-2.67736700	C	-0.53612800	5.09754200	1.02900700
H	3.40816200	-0.01805300	-2.99990700	H	0.53228800	4.87829500	1.11590800
H	5.00518600	-0.61971100	-3.48285500	H	-0.65524200	5.90819600	0.29921900
C	3.82280800	0.71849000	2.23658300	H	-0.87987400	5.48377400	1.99712500
H	3.33430200	1.69433800	2.15136200	38-ts (Z=Cl, W=X=Y=H)			
H	3.02765400	-0.01150800	2.41727100	C	-4.11590300	-2.14950000	-1.19855300
H	4.47707900	0.73652000	3.11420800	C	-3.21572800	-1.08554500	-0.99737400
C	2.54551900	-0.06032800	-0.33844500	C	-3.65261700	0.13725400	-0.43208000
O	1.98191500	-1.01742600	-0.96033900	C	-5.00627800	0.19157300	-0.02654800
O	1.80456400	0.83640100	0.20277500	C	-5.89267900	-0.85694000	-0.23374900
H	-0.41792000	-4.26679300	3.71038800	C	-5.45227300	-2.03478700	-0.84362700
O	-0.69668100	4.74485800	0.66234200	H	-3.74422900	-3.07382100	-1.63088100
C	-1.35015300	5.99974600	0.76686800	H	-5.36494500	1.07478400	0.48943600
H	-2.11714500	5.99099200	1.55271200	H	-6.92342700	-0.76045500	0.09542000
H	-0.57355100	6.72041300	1.02895100	H	-6.13359500	-2.86416800	-1.00904600
H	-1.81161600	6.29501500	-0.18481300	C	-2.78981400	1.32945700	-0.23114500
38-ts (Z=Me, W=X=Y=H)				C	-3.42323900	2.59417200	-0.16730300
C	-4.15815200	-1.87292000	-1.28136700	C	-1.38514100	1.31425000	-0.07074700
C	-3.24730700	-0.83171400	-1.01871800	C	-2.74226800	3.76797200	0.11790400
C	-3.66866800	0.35690200	-0.37415400	H	-4.48458500	2.66402100	-0.37867400
C	-5.02007300	0.39808700	0.04072400	C	-0.69087600	2.49060800	0.25433200
C	-5.91725900	-0.62732800	-0.22690300	C	-1.37117100	3.70046100	0.35525600
C	-5.49149400	-1.76889400	-0.91189800	H	-3.26362500	4.71836900	0.15123600
H	-3.79754500	-2.77107800	-1.77411100	H	0.38137700	2.47113200	0.41355800
H	-5.36719800	1.25167500	0.61150000	S	-1.56224800	-1.43119300	-1.49903000
H	-6.94562800	-0.54215600	0.11304300	C	-0.72462600	-1.89936300	0.64137400
H	-6.18165200	-2.57990800	-1.12520900	C	-1.59310300	-1.67176900	1.70485600
C	-2.79193300	1.52379700	-0.10391000	C	0.17438600	-2.96604200	0.63159200
C	-3.40639200	2.79190900	0.04677100	C	-1.52076600	-2.51844700	2.81754700
C	-1.38869500	1.48945000	0.04392900	H	-2.30729200	-0.85751400	1.68745600
C	-2.69910200	3.93144300	0.39313700	C	0.22508700	-3.80087500	1.75142300
H	-4.46951600	2.88636200	-0.14757800	H	0.83021100	-3.13628900	-0.21341800
C	-0.68432500	2.63997600	0.43166600	C	-0.61661200	-3.58021300	2.84447400
C	-1.31785000	3.87220600	0.61957400	H	-2.17991400	-2.33540400	3.66215100
H	-3.22529700	4.87896000	0.48547300	H	0.92505500	-4.63237600	1.75621300

Pd	-0.04340800	-0.12877100	-0.45054300	H	3.34257900	1.53615200	2.01906700
C	6.00741200	0.30707500	1.04373800	H	3.02550800	-0.14831100	2.39227600
C	4.60981000	0.29645500	0.97637400	H	4.48372500	0.63162000	3.03259700
C	3.99770800	-0.07652100	-0.24477800	C	2.53188900	-0.36581900	-0.35760100
C	4.77747800	-0.41814500	-1.37646200	O	1.95685900	-1.34634900	-0.93297600
C	6.17105500	-0.36656800	-1.26465600	O	1.79398100	0.55769900	0.14404600
C	6.78496000	-0.01414500	-0.06557700	H	-0.45333700	-4.38835500	3.86148400
H	6.48701700	0.57610200	1.98141900	C	-0.67509400	4.66685200	0.41055400
H	6.77825300	-0.61097600	-2.13253000	F	-1.48623000	5.66099700	0.83860500
H	7.86946700	0.01027900	0.00418600	F	0.30042800	4.51257100	1.33209600
C	4.17186300	-0.81824600	-2.70462200	F	-0.07719200	5.10655100	-0.72154000
H	3.73893700	-1.82250200	-2.65936400	38-ts (Z=NO ₂ , W=X=Y=H)			
H	3.36390100	-0.14605500	-3.01055900	C	-4.08572300	-2.34439200	-1.14833200
H	4.93883000	-0.80831300	-3.48561300	C	-3.19016000	-1.27088400	-0.97983500
C	3.82349900	0.66595000	2.21578800	C	-3.64027600	-0.02790200	-0.47013300
H	3.36955600	1.65729000	2.11873700	C	-4.99846900	0.03817600	-0.08093200
H	3.00457400	-0.03316000	2.41153100	C	-5.87804100	-1.02211500	-0.25223400
H	4.48270100	0.67448200	3.08970400	C	-5.42580000	-2.22072000	-0.81078900
C	2.51078800	-0.11626900	-0.34212300	H	-3.70716000	-3.28393700	-1.53969500
O	1.91228900	-1.05687100	-0.95828200	H	-5.36635900	0.94000500	0.39444400
O	1.79648600	0.80365400	0.19864000	H	-6.91208700	-0.91772900	0.06330800
H	-0.57186800	-4.23689000	3.70857000	H	-6.10194500	-3.05910500	-0.94975800
Cl	-0.48467900	5.16403700	0.75324400	C	-2.78715600	1.17732500	-0.30831200
38-ts (Z=CF ₃ , W=X=Y=H)				C	-3.43541100	2.43956000	-0.30548300
C	-4.04363800	-2.59049100	-1.13862500	C	-1.38234600	1.17082400	-0.13142400
C	-3.16736800	-1.49985500	-0.97908300	C	-2.76877600	3.62561800	-0.05223100
C	-3.63520900	-0.26424200	-0.46894200	H	-4.49259300	2.49001100	-0.53874400
C	-4.99135200	-0.22171300	-0.07114700	C	-0.70609300	2.36313000	0.16403700
C	-5.85323800	-1.29792900	-0.23521000	C	-1.40268000	3.56528100	0.21063800
C	-5.38366200	-2.49013700	-0.79301700	H	-3.28032200	4.57974000	-0.05755400
H	-3.65031900	-3.52401800	-1.52997300	H	0.36227400	2.37428000	0.34548900
H	-5.37155800	0.67518200	0.40405300	S	-1.53174800	-1.63435400	-1.44999900
H	-6.88723700	-1.21081900	0.08605900	C	-0.70349300	-2.00125800	0.71468900
H	-6.04566000	-3.34084900	-0.92527000	C	-1.58102600	-1.73444200	1.76106300
C	-2.80032500	0.95560000	-0.31663800	C	0.20462400	-3.05902200	0.75554200
C	-3.46279500	2.20724700	-0.31334900	C	-1.50823200	-2.53070100	2.91041300
C	-1.39642000	0.97462100	-0.14692900	H	-2.30229700	-0.92836200	1.70339200
C	-2.80367500	3.40345500	-0.07668400	C	0.25540100	-3.84297100	1.91162600
H	-4.52416300	2.24245000	-0.53167700	H	0.86775400	-3.26022000	-0.07681000
C	-0.73725300	2.17935300	0.13464900	C	-0.59494200	-3.58197900	2.98891400
C	-1.43221700	3.38802500	0.17755500	H	-2.17404300	-2.31650600	3.74228300
H	-3.35059600	4.33997800	-0.08422200	H	0.96289700	-4.66673100	1.95733400
H	0.33242400	2.18166000	0.31463900	Pd	-0.02894600	-0.27465800	-0.45107100
S	-1.50450600	-1.83124500	-1.45922300	C	6.01498600	0.38283000	0.96354400
C	-0.66089500	-2.18871600	0.69719300	C	4.61726600	0.34908900	0.90781700
C	-1.53689800	-1.93849100	1.74937800	C	4.00279500	-0.15669500	-0.26465100
C	0.26499500	-3.23160600	0.73322700	C	4.78182700	-0.60308800	-1.36127600
C	-1.44479900	-2.73467000	2.89731500	C	6.17495500	-0.52375300	-1.26369500
H	-2.27201200	-1.14462800	1.69634300	C	6.79053100	-0.04243400	-0.11135000
C	0.33519500	-4.01603500	1.88786600	H	6.49623500	0.75450300	1.86444100
H	0.92679400	-3.42091300	-0.10303100	H	6.78076800	-0.84834700	-2.10578100
C	-0.51365500	-3.77064000	2.97006400	H	7.87496100	0.00230700	-0.05163200
H	-2.10992900	-2.53276500	3.73286200	C	4.17960400	-1.14186700	-2.64119900
H	1.05644200	-4.82811400	1.92871300	H	3.76170200	-2.14299000	-2.49595800
Pd	-0.02022700	-0.44838200	-0.46557600	H	3.36170000	-0.51525600	-3.01013900
C	6.01632600	0.20565300	1.00475500	H	4.94599400	-1.19834700	-3.42073700
C	4.61942300	0.15773000	0.93926400	C	3.83794600	0.83952900	2.10905900
C	4.01702700	-0.28502900	-0.26335800	H	3.36746100	1.80773200	1.91056800
C	4.80524600	-0.65807000	-1.37930300	H	3.03260000	0.15398200	2.39047300
C	6.19705900	-0.56737200	-1.27102700	H	4.50695000	0.95284400	2.96802200
C	6.80177300	-0.14622000	-0.08957300	C	2.51808000	-0.22357800	-0.34811500
H	6.48897700	0.52863800	1.92880700	O	1.92540000	-1.20463800	-0.90764700
H	6.81034700	-0.83575800	-2.12744400	O	1.78947200	0.71270800	0.14516100
H	7.88532800	-0.09204600	-0.02192200	H	-0.54952000	-4.19941800	3.88134700
C	4.21030800	-1.13180700	-2.68795900	N	-0.67449500	4.80541700	0.51880400
H	3.80094100	-2.14284700	-2.59748200	O	0.52957600	4.72339500	0.75514300
H	3.38723000	-0.49306500	-3.02382100	O	-1.32074700	5.85430900	0.52474500
H	4.97760700	-1.13904200	-3.46863000				
C	3.82419700	0.56354700	2.16156000				