

Supporting Information for

Theoretical Design and Mechanism Study on the Metal-free Reduction of CO₂ to CO

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Section 1: Computational details for the extrapolation to the CCSD(T)/CBS limit

In order to verify the reliability of the M06-2X method used in this work, we used the CCSD(T)/CBS results as the standard. Considering the size of reaction systems, we computed the CCSD(T) energy at the complete basis set (CBS) limit as: ¹

$$E_{total}^{(CCSD(T)/CBS)} = E_{HF}^{CBS} + E_{corr}^{(CCSD(T)/CBS)} \quad (1)$$

Here, E_{HF}^{CBS} is the Hartree-Fork (HF) energy at CBS. $E_{corr}^{(CCSD(T)/CBS)}$ is the CCSD(T) correlation energy at CBS and can be approximated as:

$$E_{corr}^{(CCSD(T)/CBS)} \approx E_{corr}^{(MP2/CBS)} + E_{corr}^{(CCSD(T)/SB)} - E_{corr}^{(MP2/SB)} \quad (2)$$

In equation 2 $E_{corr}^{(MP2/CBS)}$ is the MP2 correlation energy at CBS, $E_{corr}^{(CCSD(T)/SB)}$ is the CCSD(T) correlation energy at a small basis set (SB), and $E_{corr}^{(MP2/SB)}$ is the MP2 correlation energy at SB.

The extrapolation of the HF energy to CBS is assumed to be given by: ²

$$E_{HF}^{CBS} = \frac{E_{HF}^Y \exp(-\alpha\sqrt{Y}) - E_{HF}^X \exp(-\alpha\sqrt{X})}{\exp(-\alpha\sqrt{X}) - \exp(-\alpha\sqrt{Y})} \quad (3)$$

Here, X or Y is cardinal number of basis set and α is constant. The extrapolation of the correlation energy to CBS is assumed to be given by:

$$E_{corr}^{CBS} = \frac{X^\beta E_{corr}^X - Y^\beta E_{corr}^Y}{X^\beta - Y^\beta} \quad (4)$$

where β is a constant and X or Y is the cardinal number of the basis set.

In this paper, the CCSD(T) and MP2 energies were computed by CFOUR.³ We used the aug-cc-pVDZ and aug-cc-pVTZ basis sets for extrapolation (X is 2 and Y is 3). The values of α (4.42) and β (2.46) for the extrapolation using the aug-cc-pVDZ and aug-cc-pVTZ basis sets were taken from the manual of the ORCA software.⁴ The silylborane M6 was selected as the testing case. The results in Table S1 show that the M06-2X/LB//MB is quite accurate for the systems we studied because the energy difference between M06-2X/LB//MB and CCSD(T)/CBS is very small.

Table S1. Relative potential energies (all in kcal/mol) of the CO₂ reduction reaction by silylborane M6 with different methods. The sum of the single point energies of silylborane and CO₂ is used as the reference.

	$\Delta E^\ddagger_1$	I	$\Delta E^\ddagger_2$	P
M062X/LB//MB	17.1	-24.7	-6.9	-54.3
CCSD(T)/CBS	16.6	-24.1	-7.3	-54.8
Absolute Difference	0.5	0.6	0.4	0.5

1 P. Jurečka and P. Hobza, *Chem. Phys. Lett.*, 2002, **365**, 89–94.

2 D. G. Truhlar, *Chem. Phys. Lett.*, 1998, **294**, 45–48.

3 M. E. Harding, T. Metzroth, J. Gauss and A. A. Auer, *J. Chem. Theory Comput.*, 2008, **4**, 64–74.

4 F. Neese, *WIREs Comput Mol Sci*, 2011, **2**, 73–78.

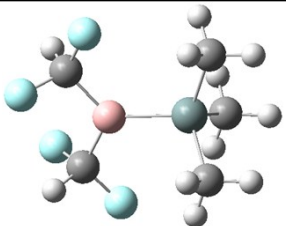
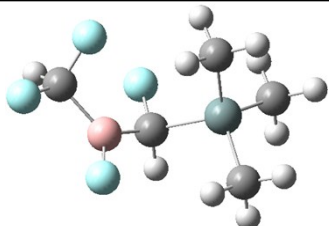
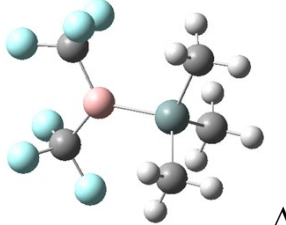
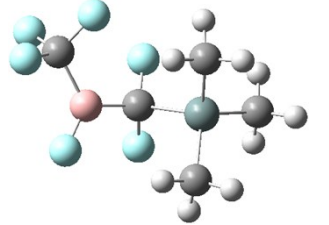
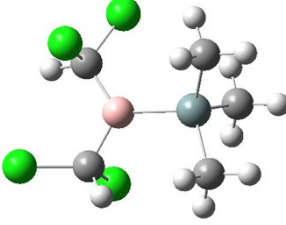
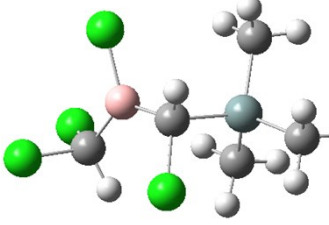
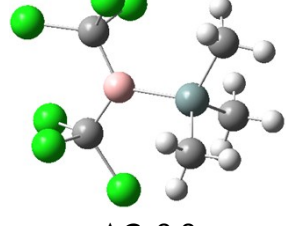
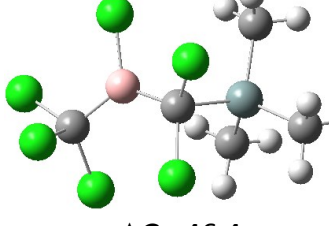
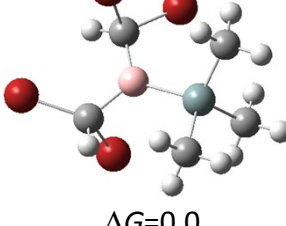
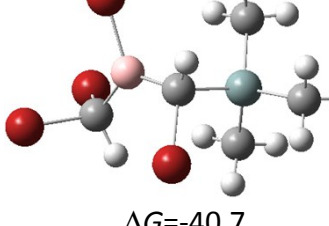
Section 2: Solvent effect

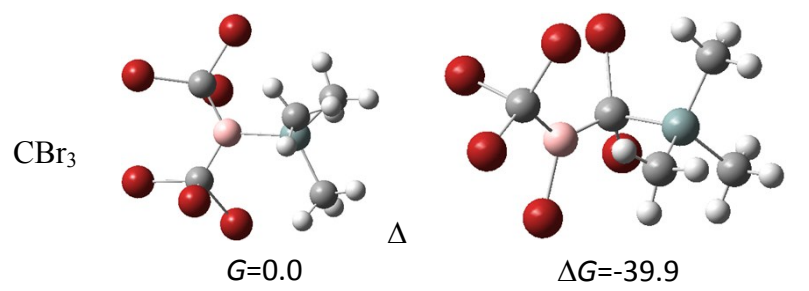
Table S2. Free-energy barriers (in kcal mol⁻¹) for the reduction of CO₂ by M2 (Me₂BSiEt₃), M7 (Et₂BSiMe₃), M8 (Et₂BSiEt₃), and M39 (PFP₂BSi(CHF₂)₃) at 298.15 K in four solvents.

Silylborane	Solvent	Dielectric constant	$\Delta G_1^\ddagger$	$\Delta G_2^\ddagger$	$\Delta G_{Tot}^\ddagger$
M2	CarbonTetraChloride	2.23	29.7	30.6	30.6
	Chloroform	4.71	30.4	31.5	31.5
	1,1,1-TriChloroEthane	7.08	29.4	31.3	31.3
	DiChloroMethane	8.93	30.0	31.6	31.6
M7	CarbonTetraChloride	2.23	27.4	31.4	31.4
	Chloroform	4.71	28.2	32.3	32.3
	1,1,1-TriChloroEthane	7.08	27.2	32.0	32.0
	DiChloroMethane	8.93	27.8	32.4	32.4
M8	CarbonTetraChloride	2.23	29.5	30.7	30.7
	Chloroform	4.71	30.3	31.5	31.5
	1,1,1-TriChloroEthane	7.08	29.4	31.2	31.2
	DiChloroMethane	8.93	30.0	31.5	31.5
M39	CarbonTetraChloride	2.23	30.8	15.4	30.8
	Chloroform	4.71	32.6	16.2	32.6
	1,1,1-TriChloroEthane	7.08	32.2	15.5	32.2
	DiChloroMethane	8.93	32.7	15.9	32.7

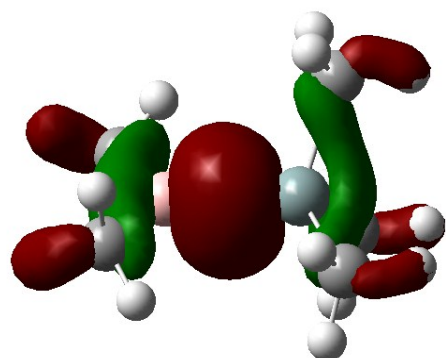
Section 3: Stability of the silylboranes (R₁)₂BSiMe₃ with R₁ = CH_xX_{3-x} (x = 0 to 1, X = F or Cl)

Table S3. Relative Gibbs free energy (in kcal mol⁻¹) at 298.15 K in gas phase computed at the M06-2x/LB//MB level for the silylboranes (R₁)₂BSiMe₃ with R₁ = CH_xX_{3-x} (x = 0 to 1, X = F, Cl or Br). Green, blue, and red balls are fluorine chlorine, and bromine atoms. A ΔG of 0.0 implies that the free-energy of that compound is used as reference.

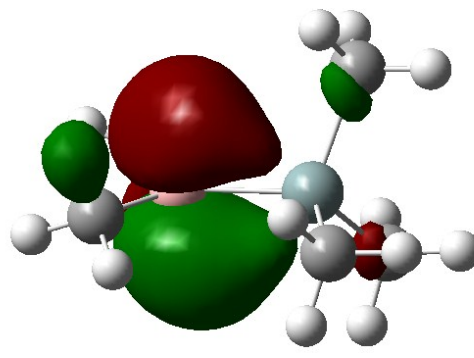
R1	Compound 1	Compound
CHF ₂	 $\Delta G=0.0$	 $G=-54.9$ Δ
CF ₃	 $G=0.0$ Δ	 $G=-40.6$ Δ
CHCl ₂	 $\Delta G=0.0$	 $\Delta G=-45.8$
CCl ₃	 $\Delta G=0.0$	 $\Delta G=-46.4$
CHBr ₂	 $\Delta G=0.0$	 $\Delta G=-40.7$



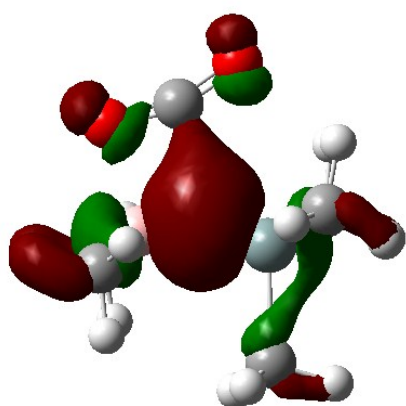
Section 4: The HOMO and LUMO of M1, M1-TS1, M1-TS2



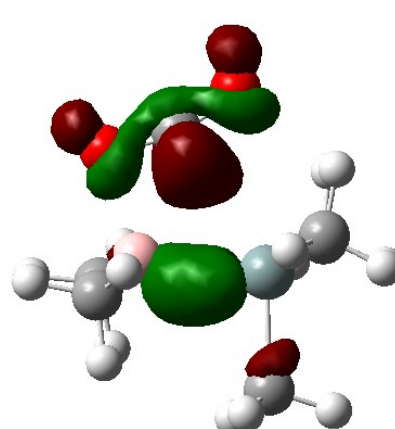
HOMO of M1



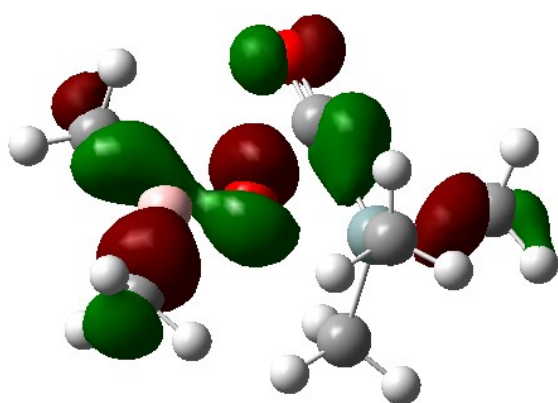
LUMO of M1



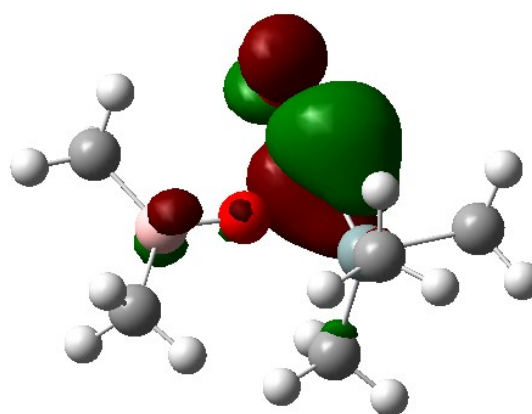
HOMO of M1-TS1



LUMO of M1-TS1



HOMO of M1-TS2



LUMO of M1-TS2

Figure S1. The HOMO and LUMO orbitals of M1, M1-TS1, M1-TS2. Other silylboranes and their transition states have similar HOMO and LUMO with M1 and the transition states of M1.

Section 5: Cartesian coordinates of the 36 silylboranes and the transition states for the E1 and E2 steps of the CO₂ reduction by the 36 silylboranes

M1

B	-1.5673586917	3.3654460141	-2.0146442172
Si	-2.2493678011	2.4084932602	-0.3569397219
C	-0.0133500852	3.4966041436	-2.2298843957
H	0.2690470670	2.5973994945	-2.8052158411
H	0.2821053031	4.3564680693	-2.8430381604
H	0.5936966608	3.4741184215	-1.3185773799
C	-2.5459957118	3.9908775052	-3.0750709795
H	-2.0976037364	4.1615360575	-4.0610769101
H	-3.4985845396	3.4636232272	-3.1915250196
H	-2.8036360224	4.9875286950	-2.6752085356
C	-1.3227206195	0.7715041815	-0.1281468400
H	-0.2415480549	0.9390742630	-0.0687152186
H	-1.6370985238	0.2783826437	0.7988587433
H	-1.5101039119	0.0783768322	-0.9553634559
C	-1.8919564260	3.4818268343	1.1651626782
H	-2.4258262964	4.4373103707	1.1241552953
H	-2.2064128338	2.9620511214	2.0775588918
H	-0.8216453800	3.6975835223	1.2543290063
C	-4.1068239218	2.0566760150	-0.4169952542
H	-4.6811236336	2.9837968314	-0.5242583961
H	-4.3631373989	1.4067934508	-1.2610986525
H	-4.4414520568	1.5601171393	0.5009089575

M2

B	-1.4982407332	3.3510278535	-2.0138775921
Si	-2.2144242378	2.4102277411	-0.3573662613
C	0.0075510589	3.1307500355	-2.4172822444
H	0.6848708721	2.8793736438	-1.5938811525
H	-0.0046023656	2.2463034092	-3.0788263793
H	0.4386012940	3.9484502077	-3.0073142660
C	-2.3965104978	4.3041315827	-2.8841266507
H	-2.0249870563	4.4758741154	-3.9015109347
H	-3.4567712398	4.0327279696	-2.9214742981
H	-2.3577962936	5.2808888607	-2.3695712676
C	-1.6442788386	0.5975921556	-0.3498014844
H	-1.8804490441	0.1519609204	0.6258088624
H	-0.5489279865	0.5815169202	-0.4323127648
C	-2.2677661046	-0.2410720870	-1.4720551401
H	-2.0439208018	0.1835368122	-2.4585403947
H	-1.9005810993	-1.2722491185	-1.4697147067
H	-3.3586502027	-0.2800205956	-1.3765931142
C	-1.4968803813	3.2602299511	1.1862056969

H	-0.4012509201	3.2516618383	1.1102496336
H	-1.7431574345	2.6523570945	2.0672478894
C	-2.0001205659	4.6950723016	1.3838905335
H	-3.0883143858	4.7180921793	1.5103183005
H	-1.5568620291	5.1695786524	2.2650774837
H	-1.7615946411	5.3250932896	0.5182312819
C	-4.1091987751	2.4648311962	-0.2533388265
H	-4.5276238573	1.9950327800	-1.1539098746
H	-4.4321364519	3.5143340935	-0.2902589918
C	-4.6697714436	1.7853238533	1.0018985585
H	-4.2888779008	2.2617014090	1.9126093148
H	-5.7629609239	1.8281197741	1.0412331233
H	-4.3802223356	0.7288928078	1.0418284343

M3

B	-1.5465215788	3.4181107167	-1.9917935109
Si	-2.1541438470	2.3900338567	-0.3424602454
C	-1.3553154774	4.9778799147	-1.9295174440
H	-2.3658412619	5.4178871616	-1.8833825571
H	-0.8449768945	5.3195154878	-1.0217939559
H	-0.8596559477	5.4058486223	-2.8086705724
C	-1.3268433152	2.6659902870	-3.3551461133
H	-0.2311571723	2.5761456330	-3.4591556542
H	-1.7283545645	1.6502404417	-3.4198819416
H	-1.6566468409	3.2537218444	-4.2211726758
C	-1.6403820125	0.5778446892	-0.4299857925
C	-2.5274182835	-0.4546173925	-0.0954462715
C	-2.1300453449	-1.7897086527	-0.1440874331
C	-0.8323569295	-2.1166975419	-0.5287547900
C	0.0662347405	-1.1064058334	-0.8664063902
C	-0.3390257732	0.2248970903	-0.8190978130
H	-3.5449447007	-0.2105627726	0.2024817988
H	-2.8334255258	-2.5744793815	0.1178847577
H	-0.5214400177	-3.1562915950	-0.5683928769
H	1.0783717410	-1.3566883123	-1.1699670073
H	0.3741406596	1.0036051527	-1.0881716867
C	-1.5164365222	3.1360863694	1.2676252598
C	-1.8294646067	4.4648837249	1.5992227344
C	-1.3589554193	5.0468470606	2.7727172880
C	-0.5576543359	4.3075483788	3.6414593606
C	-0.2355586204	2.9891517514	3.3327316607
C	-0.7130908511	2.4102951932	2.1573438077
H	-2.4610655608	5.0522528585	0.9339970301
H	-1.6160368836	6.0747019134	3.0107338218
H	-0.1877947626	4.7588998712	4.5571436310
H	0.3851742626	2.4085773966	4.0086515381
H	-0.4592566565	1.3773463444	1.9295327507
C	-4.0435337771	2.4732615050	-0.3451790768
C	-4.7881998432	2.7935160358	0.7980294601
C	-6.1816832162	2.8234559015	0.7635765343

C	-6.8570666144	2.5330658067	-0.4187663242
C	-6.1362175650	2.2104941967	-1.5671010822
C	-4.7448674943	2.1830795615	-1.5270771411
H	-4.2723321862	3.0220098164	1.7279049314
H	-6.7398398529	3.0712752587	1.6615611410
H	-7.9422464777	2.5567003062	-0.4464032720
H	-6.6579372255	1.9813269663	-2.4914624931
H	-4.1961507290	1.9193513669	-2.4304261913

M4

B	-1.5182315739	3.2610346579	-1.9424240071
Si	-2.2546646215	2.3943407724	-0.2654837054
C	-0.0457857751	3.7999378677	-1.8674393998
H	0.6014958382	3.3125253827	-1.1307398981
H	0.4545337986	3.8043790430	-2.8421817753
H	-0.1337453133	4.8554690925	-1.5593644932
C	-2.3922299369	3.4436555278	-3.2291034474
H	-2.3395524495	2.4902409889	-3.7781994311
H	-3.4554391101	3.6194360638	-3.0331815897
H	-2.0130850668	4.2214334205	-3.9007578174
C	-1.7082063072	0.5918726701	-0.2005295291
C	-2.1020342530	-0.2622795915	0.8224486443
C	-1.7501503608	-1.6029246722	0.8492901401
C	-0.9817704631	-2.1175186959	-0.1905178558
C	-0.5784066610	-1.2994620320	-1.2383745700
C	-0.9530845572	0.0369435132	-1.2237255884
F	-0.6375891544	-3.3972098199	-0.1834155889
F	0.1469604748	-1.8000734892	-2.2325072217
F	-0.5690750177	0.8018498069	-2.2604318763
F	-2.1349749685	-2.3973822181	1.8416500278
F	-2.8497400546	0.2150586038	1.8219918405
C	-1.5674142797	3.3481231968	1.2121952144
C	-0.8406707936	2.8521435008	2.2859729315
C	-0.3414438962	3.6787232750	3.2872591650
C	-0.5652307162	5.0468661267	3.2181926531
C	-1.2801842528	5.5852536963	2.1529608641
C	-1.7562671634	4.7255449402	1.1790271749
F	-0.0924474903	5.8441122499	4.1655363556
F	-1.4903496596	6.8951104427	2.0843008746
F	-2.4489776808	5.2514651181	0.1519700246
F	0.3521809860	3.1731163911	4.3014199791
F	-0.5756542235	1.5472440259	2.3911085569
C	-4.1435434673	2.3605977150	-0.1824734905
C	-4.8077174154	1.6884966618	-1.2038881358
C	-6.1886305350	1.5976417476	-1.2818467947
C	-6.9527792261	2.2088094775	-0.2944722219
C	-6.3322172342	2.8898197189	0.7447302675
C	-4.9446768762	2.9546213770	0.7853000273
F	-8.2754569396	2.1390941881	-0.3442492216
F	-7.0677745327	3.4692935561	1.6871579983

F	-4.3990317962	3.6165872258	1.8096591054
F	-6.7814179759	0.9413517543	-2.2733544805
F	-4.0854316361	1.0838758177	-2.1610701182

M5

B	-1.5335381484	3.3852277716	-2.0089987932
Si	-2.2245741550	2.4326504115	-0.3627910105
C	-0.2001674944	4.1906001165	-1.9185795723
H	-0.0638189309	4.7342201401	-0.9781377549
H	0.6062497853	3.4369811956	-1.9414113512
H	-0.0317184977	4.8626558567	-2.7659467621
C	-2.3676087723	3.2182918600	-3.3191405127
H	-2.9111025803	2.2718309483	-3.4062934242
H	-3.1420663411	4.0035248815	-3.2743372850
H	-1.7879371213	3.3978284542	-4.2302423566
Cl	-1.7138948311	0.4367048990	-0.5068831790
Cl	-1.4480491183	3.1436023060	1.4080616315
Cl	-4.2789331609	2.5366829219	-0.2212013608

M6

B	-1.3169430109	-0.0004608737	-0.0112724944
Si	0.6960321692	0.0047129056	0.0058089352
C	-2.0783509537	1.3380720072	0.2621392151
H	-3.1115199032	1.3428853623	-0.1010107821
H	-2.1348039689	1.4169726515	1.3622729881
H	-1.5598086337	2.2401404819	-0.0758539724
C	-2.0737386192	-1.3438725764	-0.2739758689
H	-1.5503368755	-2.2501057045	0.0447093362
H	-3.0989903512	-1.3522040064	0.1108215255
H	-2.1531811254	-1.4168424540	-1.3730738287
F	1.3256040835	-1.1194365275	-0.9392936235
F	1.3177784551	1.3939020242	-0.4810649554
F	1.2793237339	-0.2596232902	1.4704505252

M7

B	-1.5484258896	3.3764261499	-1.9999061681
Si	-2.2205128530	2.4181808420	-0.3287369968
C	-0.0786355029	3.9233590794	-2.1488827729
H	-0.0876506451	4.8722418295	-2.7062682068
H	0.3922239868	3.2142843218	-2.8565338889
C	0.7883137428	4.0480064584	-0.8941920403
H	0.8539667428	3.0925240177	-0.3618166373
H	1.8089179168	4.3660343538	-1.1287433788
H	0.3655105081	4.7792510551	-0.1974199924
C	-2.5354805012	3.4364989470	-3.2326861706
H	-3.4921423465	3.8581071616	-2.8836549499
H	-2.8011106380	2.3896264935	-3.4643715950
C	-2.0731303377	4.1501825946	-4.5055808355
H	-1.1416699108	3.7183885241	-4.8873789687
H	-2.8189282022	4.0859269575	-5.3037595755

H	-1.8843467894	5.2123689438	-4.3169390933
C	-1.3532866697	0.7348375482	-0.1945652562
H	-1.5473317949	0.1125149331	-1.0751847507
H	-0.2683632689	0.8441834238	-0.0923480565
H	-1.7204131796	0.1922836457	0.6845609423
C	-1.9160547952	3.3571311050	1.2890999422
H	-0.8492246874	3.4201362997	1.5246754339
H	-2.3142509725	4.3770434497	1.2530872833
H	-2.4134503839	2.8353208998	2.1152877589
C	-4.0819196130	2.0893326652	-0.4520604246
H	-4.6550028643	3.0232650910	-0.4710587885
H	-4.3324024414	1.5266666013	-1.3583545744
H	-4.4262389622	1.5054499304	0.4094267322

M8

B	-1.5262840342	3.3699025032	-2.0158563756
Si	-2.3097721376	2.4733277731	-0.3541454781
C	-0.2265365711	4.2491314465	-1.8358653975
H	0.5442982514	3.5220246681	-1.5154730247
H	-0.3317801207	4.8986227366	-0.9545249323
C	0.2916458170	5.0529318889	-3.0318631071
H	-0.4653882412	5.7578489374	-3.3928971801
H	1.1852631028	5.6305637631	-2.7764933359
H	0.5521684564	4.3991451368	-3.8702861589
C	-2.1597513173	3.1771983783	-3.4454801362
H	-1.3973542177	3.2493368021	-4.2334302355
H	-2.7559733314	4.1039424899	-3.5661677440
C	-3.0603188310	1.9626862425	-3.6896079066
H	-3.8776357586	1.9184077021	-2.9625259158
H	-3.5065624294	1.9778997632	-4.6887566907
H	-2.4925686255	1.0303295289	-3.5974498019
C	-2.0836776026	0.5921525010	-0.5410433726
H	-2.8506543836	0.2006143044	-1.2217691861
H	-2.2627278125	0.1170436849	0.4326686478
C	-0.6863680469	0.2167399452	-1.0524484192
H	0.0971855616	0.6097855659	-0.3938020349
H	-0.5452553219	-0.8667949100	-1.1186271911
H	-0.5067830528	0.6306306143	-2.0533947160
C	-1.3739990597	3.0217205841	1.2116749894
H	-0.2948559538	3.0007949781	1.0073682939
H	-1.5436828198	2.2809514149	2.0050901290
C	-1.7795831387	4.4143190146	1.7127262769
H	-2.8296888918	4.4307211284	2.0244489865
H	-1.1775897859	4.7341935935	2.5691945144
H	-1.6661036336	5.1744567218	0.9307394844
C	-4.1519446815	2.8538155565	-0.0669698019
H	-4.7293435579	2.5644411046	-0.9537817575
H	-4.2828658584	3.9391433560	0.0374796473
C	-4.7098892339	2.1384858685	1.1710689500
H	-4.1543984594	2.4141863680	2.0748952794

H	-5.7629189353	2.3825618054	1.3448926070
H	-4.6368332050	1.0507491028	1.0633474801

M9

B	-1.6799732343	3.2853372505	-1.9689704570
Si	-2.2568834881	2.3449375509	-0.2537922961
C	-0.1528723293	3.2917453981	-2.3683812838
H	0.4298344339	2.5366239108	-1.8259289165
H	0.1898471430	4.2669479912	-1.9692461035
C	0.1818830679	3.2289900334	-3.8652361346
H	-0.3763371782	3.9772407923	-4.4367690177
H	1.2475160042	3.3979023395	-4.0461949918
H	-0.0665949892	2.2456560912	-4.2782242771
C	-2.7669335902	3.9212251585	-2.9116801445
H	-2.3653960124	4.6709303257	-3.6045166857
H	-3.5978732722	4.3800083126	-2.3638602027
C	-3.3408387952	2.7345315212	-3.7258079533
H	-3.8333743498	2.0074863166	-3.0695568020
H	-4.0852806332	3.0835798003	-4.4469951207
H	-2.5585504499	2.2113005971	-4.2879166008
C	-1.4819309796	0.6248773894	-0.2236248042
C	-1.4373237389	-0.1415081856	-1.3987100297
C	-0.8868581094	-1.4205899393	-1.4082048493
C	-0.3597682557	-1.9558707591	-0.2343712826
C	-0.3884502497	-1.2105455900	0.9416160583
C	-0.9454450049	0.0673425488	0.9445420329
H	-1.8441796801	0.2654406063	-2.3253136297
H	-0.8641076217	-1.9968777959	-2.3283089750
H	0.0749541018	-2.9508601452	-0.2379878461
H	0.0233990815	-1.6243307676	1.8572772176
H	-0.9580596574	0.6435963049	1.8673897768
C	-1.6493116704	3.3048864022	1.2564585577
C	-2.4814535542	3.5930386710	2.3470436350
C	-1.9970441457	4.2773059897	3.4611378217
C	-0.6667437155	4.6847642033	3.5056086312
C	0.1794583648	4.4040668124	2.4342448552
C	-0.3104051498	3.7232010558	1.3234336246
H	-3.5222299311	3.2782352313	2.3264885756
H	-2.6591502803	4.4897216338	4.2953036788
H	-0.2886202088	5.2180982437	4.3725218611
H	1.2189375437	4.7166996852	2.4648254014
H	0.3655264334	3.5042815131	0.4983595904
C	-4.1338093029	2.1769852483	-0.1542872995
C	-4.7742876433	0.9307123941	-0.1896864021
C	-6.1652799552	0.8342408769	-0.1731701204
C	-6.9437403339	1.9869884876	-0.1181667187
C	-6.3282184655	3.2369334082	-0.0768793461
C	-4.9392774495	3.3264949827	-0.0964545629
H	-4.1768115986	0.0224117603	-0.2299238673
H	-6.6404939393	-0.1418460232	-0.2005363231

H	-8.0269528644	1.9131750491	-0.1048978145
H	-6.9305435110	4.1392817122	-0.0294591883
H	-4.4729495211	4.3101713380	-0.0549129024

M10

B	-1.4644388352	3.1109624439	-2.0703151780
Si	-2.1520311075	2.3041877310	-0.3346793963
C	0.0598677394	3.0391105453	-2.4499963751
H	0.3466728074	4.0657680728	-2.7289608106
H	0.1217813700	2.4879725695	-3.4033577652
C	1.0645703450	2.4685378262	-1.4449522433
H	0.9408085866	1.3879927224	-1.3229044670
H	2.0966221872	2.6449049288	-1.7612524297
H	0.9436283526	2.9291935078	-0.4569914089
C	-2.5241888334	3.7334338210	-3.0494423896
H	-3.1636770657	4.4289843667	-2.4864992693
H	-3.2091756081	2.9049163661	-3.3057457520
C	-2.0058045345	4.4008169900	-4.3257082849
H	-1.4111968388	3.7051725989	-4.9267233992
H	-2.8257739846	4.7623308034	-4.9527647857
H	-1.3680417953	5.2590977306	-4.0899218298
C	-1.4109404139	0.5782692088	-0.1397703351
C	-0.6236975598	0.1047169326	0.9008139912
C	-0.0245281950	-1.1500586606	0.8641197322
C	-0.2079837931	-1.9626855429	-0.2462643291
C	-0.9817803414	-1.5209077655	-1.3149955934
C	-1.5572319850	-0.2652595839	-1.2352668427
F	0.3593571992	-3.1596783618	-0.2924179670
F	-1.1509544828	-2.2947850700	-2.3813380638
F	-2.2894029083	0.1650468479	-2.2788906376
F	0.7273204010	-1.5726250509	1.8747606533
F	-0.3764392974	0.8600582169	1.9744044987
C	-1.6951709252	3.3914660151	1.1356472374
C	-2.0750511174	3.0721975847	2.4334018603
C	-1.7958349977	3.8942719866	3.5141846651
C	-1.1200102981	5.0902270285	3.2927422584
C	-0.7377264942	5.4540295111	2.0075102585
C	-1.0373023651	4.5996452341	0.9557098518
F	-0.8461568201	5.8900642777	4.3133702276
F	-0.1047505631	6.6038898658	1.8014289859
F	-0.6832020416	4.9878201258	-0.2817493994
F	-2.1644568670	3.5623140804	4.7463351872
F	-2.7388193997	1.9343362207	2.6598693169
C	-4.0442987007	2.1918195207	-0.2922872211
C	-4.7607848213	3.3853058740	-0.2986292791
C	-6.1455261331	3.4441593549	-0.2924327579
C	-6.8637881313	2.2544708500	-0.2799230489
C	-6.1926625838	1.0392685241	-0.2724009983
C	-4.8028369391	1.0266581201	-0.2776203781
F	-8.1889679518	2.2808879212	-0.2741955711

F	-6.8819464214	-0.0964388400	-0.2578402755
F	-4.2136611938	-0.1724097345	-0.2619006722
F	-6.7846885568	4.6090211422	-0.2965538034
F	-4.0924299819	4.5515119708	-0.3038603784

M11

B	-1.5674865169	3.4781551333	-1.9632977053
Si	-2.2723210362	2.5582123507	-0.2990342857
C	-0.1826827955	4.1938011372	-1.8583313556
H	-0.0245715896	4.7246823676	-0.9133538470
H	-0.0165412570	4.8969913020	-2.6830559425
C	0.8568532863	3.0447875622	-1.9524359953
H	0.7319349593	2.4594875912	-2.8701874687
H	1.8715305993	3.4509552255	-1.9541532574
H	0.7792007973	2.3583628976	-1.1020465079
C	-2.3649659448	3.3908886869	-3.3054997596
H	-1.6718796739	3.5012148997	-4.1515909735
H	-2.9347642128	4.3412520921	-3.2970887650
C	-3.3300225397	2.2229892472	-3.5359002960
H	-4.0810569279	2.1595929614	-2.7415006192
H	-3.8635244994	2.3292141069	-4.4843248897
H	-2.7947188016	1.2690536403	-3.5586075790
Cl	-2.2244569593	0.5045299761	-0.5077278319
Cl	-1.1581419730	3.0094374691	1.3787691099
Cl	-4.2193345172	3.1056379134	0.1153568163

M12

B	0.8426904271	0.0284007900	0.0053580065
Si	-1.1324202318	-0.3752444110	-0.0230274602
C	1.3124933297	1.5231217901	0.0354098339
H	2.0557360261	1.6574918321	-0.7671875322
H	1.9093368722	1.6373474069	0.9571244899
C	0.2270081859	2.6017376485	-0.0381461083
H	-0.4797348754	2.4996758959	0.7923300150
H	0.6447393121	3.6113024640	0.0027174804
H	-0.3469829452	2.5150691334	-0.9665493664
C	1.8378737613	-1.1833611839	0.0172372485
H	1.5700107718	-1.8502086364	-0.8186820104
H	1.5831630772	-1.7933528493	0.9011795243
C	3.3354685180	-0.8705997185	-0.0020433172
H	3.6221447592	-0.2517003740	0.8544170836
H	3.9390439196	-1.7818087071	0.0312160665
H	3.6130865050	-0.3231196576	-0.9085456567
F	-1.8979728487	0.2209112737	1.2490048438
F	-1.8608104340	0.2241457416	-1.3147460787
F	-1.4452101300	-1.9429604382	-0.0293060626

M13

B	-1.4763301285	3.3550651055	-1.9877237439
Si	-2.1951703048	2.3432364857	-0.3666201913

C	-0.1884622055	4.2359471851	-1.9037559972
C	0.9357168500	3.8482552728	-1.1518390275
C	2.0761004394	4.6422842641	-1.0854180536
C	2.1024573749	5.8750449098	-1.7344767741
C	0.9950959544	6.2978091538	-2.4673276973
C	-0.1248706435	5.4777623693	-2.5661436165
H	0.9214667105	2.8987455420	-0.6246915936
H	2.9380038860	4.3091086040	-0.5154359171
H	2.9834041978	6.5064147690	-1.6672567770
H	1.0107297931	7.2597025682	-2.9707986910
H	-0.9759929224	5.8065046256	-3.1575433828
C	-2.2749701763	3.3096568481	-3.3322534516
C	-1.6113627237	3.4531002723	-4.5664935272
C	-2.2943423772	3.3619431916	-5.7758291966
C	-3.6724053265	3.1582175897	-5.7806424204
C	-4.3598111847	3.0261020692	-4.5751853728
C	-3.6635398693	3.0807900681	-3.3729637594
H	-0.5380357769	3.6252143143	-4.5725410871
H	-1.7553130858	3.4581367144	-6.7134389386
H	-4.2102414351	3.0985583729	-6.7221314187
H	-5.4337069158	2.8667645277	-4.5758357623
H	-4.2122498006	2.9589586310	-2.4425405741
C	-2.9192548150	0.6591408281	-0.8408057475
H	-3.6803916787	0.7414362251	-1.6227356668
H	-2.1364114641	-0.0120214300	-1.2114122160
H	-3.3784932808	0.1851160770	0.0346679772
C	-0.9476857220	2.0303831083	1.0242510117
H	-1.4752332358	1.5854555268	1.8766833746
H	-0.1568664673	1.3325036472	0.7279749710
H	-0.4763054424	2.9567996522	1.3683259500
C	-3.5678139278	3.4036281530	0.4092456531
H	-3.1698703925	4.3674066094	0.7455438447
H	-4.3960557499	3.6060189468	-0.2769441585
H	-3.9769486008	2.8870288187	1.2857432988

M14

B	-1.4037907111	3.3915815084	-1.9372206503
Si	-2.1603240113	2.4430469193	-0.2885217068
C	0.0230892644	4.0254472476	-1.9788327873
C	0.6973341340	4.1976072650	-3.2051823362
C	1.9898589213	4.7088465616	-3.2611590588
C	2.6383115196	5.0847144373	-2.0863313316
C	1.9979042949	4.9311336948	-0.8581769214
C	0.7159241574	4.3945645385	-0.8095173106
H	0.1990914399	3.9092672994	-4.1268266983
H	2.4913783540	4.8175624338	-4.2179923839
H	3.6444664165	5.4914812794	-2.1271455379
H	2.5029748955	5.2192754684	0.0586065174
H	0.2358514862	4.2668521504	0.1555581847
C	-2.2787423310	3.4070937091	-3.2361050867

C	-2.4148630117	4.5808056220	-4.0000970749
C	-3.2504132085	4.6296536291	-5.1130753905
C	-3.9381989803	3.4874541091	-5.5169111565
C	-3.7999580422	2.3037217915	-4.7942373229
C	-2.9991473771	2.2751433419	-3.6571839096
H	-1.8661223520	5.4727116009	-3.7057419146
H	-3.3554125660	5.5543074708	-5.6726111942
H	-4.5803762901	3.5191861865	-6.3918086622
H	-4.3299786493	1.4096358712	-5.1081416563
H	-2.9171919699	1.3490813853	-3.0919900441
C	-1.3488621344	0.7202353117	-0.2215674668
H	-0.2603071308	0.8505129247	-0.2893624231
H	-1.6417808198	0.1646552342	-1.1232162631
C	-1.6965902052	-0.0969308369	1.0289914491
H	-2.7799881645	-0.2211977699	1.1376398652
H	-1.2514574504	-1.0969228640	0.9978644646
H	-1.3288920936	0.3974231246	1.9346147518
C	-1.8189328940	3.3428138053	1.3670640055
H	-1.7920620004	4.4276107927	1.2007374907
H	-0.8104840301	3.0637237993	1.7034116529
C	-2.8313500184	3.0317297785	2.4789246613
H	-2.9046241986	1.9567335551	2.6728242137
H	-2.5536862055	3.5190027164	3.4193848417
H	-3.8335971531	3.3809035869	2.2109240298
C	-4.0465893928	2.2486987946	-0.4167450903
H	-4.4094608009	1.7710508939	0.5032385490
H	-4.2994601651	1.5619503941	-1.2335205158
C	-4.7640667651	3.5889200266	-0.6285290664
H	-4.4930703916	4.0268320307	-1.5956047612
H	-5.8530421148	3.4789280635	-0.6086327162
H	-4.4936477973	4.3157621876	0.1474003501

M15

B	-1.5730178291	3.4081022533	-2.0193355887
Si	-2.2536478165	2.4031451060	-0.3772262788
C	-0.1124720924	3.2150486861	-2.5320199307
C	0.5330911053	1.9633413705	-2.5405923984
C	1.8443770076	1.8290458841	-2.9855662989
C	2.5615872959	2.9532128818	-3.3899730898
C	1.9567558186	4.2089412890	-3.3700614259
C	0.6313166687	4.3317098856	-2.9651874473
H	-0.0017933401	1.0804030938	-2.2033858898
H	2.3129842003	0.8498940796	-2.9977247718
H	3.5922242741	2.8518636207	-3.7170318664
H	2.5146417845	5.0874376996	-3.6798598030
H	0.1606821258	5.3120105731	-2.9681213052
C	-2.4787624214	4.4984372680	-2.6773378223
C	-3.4599570099	5.2024633565	-1.9515857595
C	-4.2748028261	6.1475904674	-2.5647348008
C	-4.1549784855	6.3869668614	-3.9332359772

C	-3.2070791028	5.6918343036	-4.6808089548
C	-2.3689941874	4.7735294538	-4.0540889208
H	-3.5771261407	5.0143382128	-0.8863579725
H	-5.0126458236	6.6883098524	-1.9802525128
H	-4.8020611381	7.1131743622	-4.4162551318
H	-3.1155447864	5.8720400913	-5.7476119155
H	-1.6224624228	4.2444716619	-4.6413998001
C	-1.1778519650	0.9278737615	0.1115824517
C	-1.4747899743	-0.3611810271	-0.3576556009
C	-0.6235718315	-1.4347858321	-0.1054003624
C	0.5444942030	-1.2391706365	0.6284708912
C	0.8513324795	0.0297419930	1.1138869859
C	-0.0033695613	1.0995511732	0.8575662902
H	-2.3853125343	-0.5291154711	-0.9298812874
H	-0.8725787336	-2.4236894312	-0.4789912436
H	1.2100493956	-2.0741143209	0.8260813958
H	1.7565616369	0.1863970586	1.6929240978
H	0.2498352237	2.0839921528	1.2449470630
C	-2.1385836336	3.7035636883	0.9958540897
C	-1.0161731005	4.5459314524	1.0626000934
C	-0.8998014302	5.5183136122	2.0532457703
C	-1.9143843681	5.6745464702	2.9948343156
C	-3.0406959371	4.8571418171	2.9401617272
C	-3.1502565822	3.8830204404	1.9494957318
H	-0.2169304267	4.4447150645	0.3279878568
H	-0.0221990212	6.1569592781	2.0860408585
H	-1.8295211281	6.4344433458	3.7657140258
H	-3.8362185844	4.9790432154	3.6693434725
H	-4.0399310235	3.2581345512	1.9131815709
C	-4.0246916597	1.7613170630	-0.5051536322
C	-4.8834594476	2.0840823547	-1.5652094762
C	-6.1866207983	1.5907497943	-1.6132714621
C	-6.6577752641	0.7633217561	-0.5983719736
C	-5.8199132151	0.4236201778	0.4624830818
C	-4.5179809214	0.9142903284	0.5023536149
H	-4.5366682503	2.7322058699	-2.3657576533
H	-6.8326707651	1.8526527364	-2.4458459763
H	-7.6728308995	0.3792662688	-0.6348699356
H	-6.1793370655	-0.2272003674	1.2540071666
H	-3.8672843798	0.6244278917	1.3260878973

M16

B	-1.5511693146	3.3986725286	-1.9351018836
Si	-2.1556090761	2.3841368918	-0.2805270330
C	-0.6080581726	4.6259658387	-1.7981428789
C	-0.8870841059	5.8065043339	-2.5101398950
C	-0.0986113409	6.9430862429	-2.3573586633
C	1.0136190009	6.9095413774	-1.5186252640
C	1.3264958544	5.7426065653	-0.8236188629
C	0.5119983696	4.6216569188	-0.9469491613

H	-1.7474965633	5.8357018338	-3.1747059151
H	-0.3451914650	7.8513721965	-2.8983696374
H	1.6363877948	7.7917225139	-1.4064464864
H	2.1972594440	5.7118187990	-0.1759610282
H	0.7612278737	3.7208968895	-0.3904633390
C	-2.0360277376	2.8802950082	-3.3179532043
C	-3.1513432691	2.0294499589	-3.4524316701
C	-3.5610593207	1.5605675547	-4.6937756034
C	-2.8433102315	1.9117636335	-5.8373414007
C	-1.7251802310	2.7357305907	-5.7349326306
C	-1.3343665545	3.2201515370	-4.4900846727
H	-3.7221010131	1.7360017413	-2.5724178187
H	-4.4312928188	0.9168622144	-4.7733879637
H	-3.1548065883	1.5375042356	-6.8078931865
H	-1.1619235894	3.0022452473	-6.6237331499
H	-0.4616844038	3.8634209500	-4.4157151868
C	-1.8555884459	0.5418846309	-0.5654700215
C	-2.8181249447	-0.4420918418	-0.7456663965
C	-2.4877421632	-1.7607721527	-1.0347133679
C	-1.1516615813	-2.1152879222	-1.1634436094
C	-0.1569126453	-1.1551196642	-1.0126095656
C	-0.5330936840	0.1464009164	-0.7284060292
F	-0.8231115693	-3.3694358631	-1.4410235215
F	1.1208364705	-1.4923664273	-1.1479684786
F	0.4329333963	1.0725135760	-0.6037126412
F	-3.4351789767	-2.6782011780	-1.2001388888
F	-4.1211538686	-0.1442435909	-0.6771377028
C	-1.2949736851	2.9499648503	1.3050895269
C	-0.5327129451	2.1776954868	2.1729398472
C	0.1207530906	2.7213554826	3.2726736196
C	0.0068233274	4.0812061577	3.5294870166
C	-0.7605622210	4.8867725709	2.6960738116
C	-1.3969180753	4.3045132513	1.6116375845
F	0.6238161200	4.6111151040	4.5768149825
F	-0.8773194780	6.1857196228	2.9488869190
F	-2.1423793565	5.0940602155	0.8255691645
F	0.8441253639	1.9539895514	4.0816588802
F	-0.4016351809	0.8618241398	1.9828859110
C	-3.9844409715	2.7139236968	0.0494226644
C	-4.6710310253	2.0296716068	1.0450519981
C	-5.9964627944	2.2924212371	1.3533884352
C	-6.6636969145	3.2900562279	0.6493696010
C	-6.0078894798	4.0097266090	-0.3413648920
C	-4.6804461679	3.7117057524	-0.6192458615
F	-7.9309732507	3.5588511759	0.9305864357
F	-6.6489746365	4.9692991355	-1.0000403221
F	-4.0660746885	4.4368447509	-1.5648664411
F	-6.6317439362	1.6156982049	2.3040720480
F	-4.0364177686	1.0777725190	1.7380592020

M17

B	-1.6182292693	3.3930917255	-1.9990122320
Si	-2.2687784807	2.6101943914	-0.2400228272
C	-0.2160661491	4.0565858306	-2.0059619757
C	0.7848217763	3.7637720258	-1.0574184289
C	2.0190784430	4.3999775398	-1.0894709972
C	2.2732065755	5.3761347678	-2.0519855266
C	1.2961120433	5.7039162028	-2.9894558612
C	0.0735554325	5.0416960783	-2.9729946657
H	0.6086564529	3.0121047156	-0.2924631204
H	2.7790093551	4.1453898338	-0.3578942494
H	3.2322279657	5.8851303289	-2.0672844531
H	1.4890353708	6.4708888520	-3.7328299545
H	-0.6831475122	5.3012247333	-3.7081987325
C	-2.4695125523	3.2638665577	-3.2883228168
C	-3.8687615117	3.4168320931	-3.3046139926
C	-4.5915877795	3.3055194130	-4.4870376533
C	-3.9366758669	2.9906474487	-5.6760181532
C	-2.5545421530	2.8107080502	-5.6851271781
C	-1.8293634187	2.9665950463	-4.5091256108
H	-4.3980261456	3.6458000330	-2.3849347111
H	-5.6674634785	3.4476246852	-4.4791710202
H	-4.5039048920	2.8822190058	-6.5954639774
H	-2.0435694811	2.5595323756	-6.6092298878
H	-0.7499179857	2.8403135092	-4.5254427531
Cl	-1.2265581503	0.8534331432	0.0966117114
Cl	-1.9018420789	3.8583133761	1.3622707729
Cl	-4.2653523699	2.1060263025	-0.1212112030

M18

B	-1.5778614530	3.4855250764	-2.0065554027
Si	-2.3490081017	2.7672639301	-0.2904340034
C	-0.1589741929	4.1023481559	-2.0557730930
C	0.8072773816	3.8010536314	-1.0746248717
C	2.0872973354	4.3398966703	-1.1323458536
C	2.4187919149	5.2310345723	-2.1511284465
C	1.4723453000	5.5774080233	-3.1149096902
C	0.2044956595	5.0103732523	-3.0722823914
H	0.5499606526	3.1356945158	-0.2558966521
H	2.8204805518	4.0812165649	-0.3751666109
H	3.4130476133	5.6662026964	-2.1876970668
H	1.7263999024	6.2862550390	-3.8967085242
H	-0.5302794308	5.2880740909	-3.8229452969
C	-2.4948518971	3.3550281911	-3.2541956314
C	-1.9564191749	3.1316002229	-4.5369528811
C	-2.7787542679	2.9738721356	-5.6471947465
C	-4.1623021764	3.0664419836	-5.5048871993
C	-4.7217950547	3.2910759577	-4.2484320265
C	-3.8977087969	3.4104104127	-3.1355238358
H	-0.8787231506	3.0559741433	-4.6555304385

H	-2.3437760095	2.7829425731	-6.6232476283
H	-4.8052546770	2.9533776958	-6.3725130831
H	-5.7992642693	3.3551311329	-4.1352324553
H	-4.3486381417	3.5675460696	-2.1586059389
F	-2.7768306429	1.2308854354	-0.4030972733
F	-1.3890350878	2.8446091343	0.9891011888
F	-3.6746460404	3.5680610892	0.1258710001

M19

B	-1.4235964314	3.4672588594	-1.9986013271
Si	-2.3191776401	2.5762035097	-0.3873890996
C	-0.2961985712	4.5458367976	-1.9415014095
C	0.2895926636	5.1280255307	-3.0794088075
C	1.2883333270	6.0873717090	-3.0125698313
C	1.7517930431	6.5030832829	-1.7706015602
C	1.2193383295	5.9538996953	-0.6115538563
C	0.2233900018	4.9960109158	-0.7178876243
F	2.7045576425	7.4156876588	-1.6924621178
F	1.6698420595	6.3436550330	0.5755009573
F	-0.2314117986	4.4983981526	0.4327483464
F	1.8098682382	6.6063096088	-4.1180238078
F	-0.0810292726	4.7657017621	-4.3044874271
C	-2.0302564038	3.0273602437	-3.3828279104
C	-2.6938061022	3.9065363630	-4.2316030568
C	-3.3408474579	3.4885054599	-5.3842375998
C	-3.3122150847	2.1407061723	-5.7252858680
C	-2.6485950923	1.2299666368	-4.9121058809
C	-2.0314444187	1.6889627394	-3.7581709525
F	-3.9156674949	1.7250415203	-6.8313270289
F	-2.6117751954	-0.0564661037	-5.2446849082
F	-1.3898081363	0.7971766171	-2.9872153574
F	-3.9764971597	4.3559723055	-6.1656170799
F	-2.7302859430	5.2095598234	-3.9255938148
C	-3.6990260383	1.4361772742	-1.0008199854
H	-3.3125744265	0.5594766631	-1.5283046913
H	-4.2803741604	1.0798385261	-0.1422844612
H	-4.3892331542	1.9624188534	-1.6702721087
C	-1.1213122718	1.5372866388	0.6375541148
H	-1.6644044483	1.0654210613	1.4645053305
H	-0.6866422891	0.7389631614	0.0267217102
H	-0.3082034279	2.1331670007	1.0588721143
C	-3.1850449051	3.8877347606	0.6687729647
H	-3.9455275571	4.4161604867	0.0830504556
H	-3.7001812766	3.3909861794	1.4994693840
H	-2.4980018793	4.6258172263	1.0870854059

M20

B	-1.4847978734	3.5452282919	-1.8872281181
Si	-2.2109327892	2.3992154873	-0.3505775579
C	-0.0500351598	4.1547323227	-1.9650213689

C	0.4300777942	4.8913858300	-3.0614763578
C	1.7117964700	5.4172958519	-3.1183471872
C	2.5760471902	5.2234761776	-2.0478642508
C	2.1525209187	4.5126688541	-0.9322036264
C	0.8639540850	4.0036581609	-0.9113030070
F	3.8000288392	5.7205868504	-2.0891690581
F	2.9759581054	4.3357926436	0.0947397974
F	0.5118372210	3.3458490583	0.1945279575
F	2.1196747239	6.1061877976	-4.1778542058
F	-0.3440074365	5.1369679295	-4.1149291091
C	-2.4630711780	3.6680156266	-3.1135785187
C	-2.1808661696	3.0724779167	-4.3384114100
C	-3.1104008384	2.9932456290	-5.3638578869
C	-4.3686953947	3.5564881451	-5.1801756440
C	-4.6820490000	4.1858741490	-3.9814125232
C	-3.7280382336	4.2258463058	-2.9755283934
F	-5.2671072114	3.5012953242	-6.1547397215
F	-5.8789699041	4.7386253726	-3.8134767279
F	-4.0497797972	4.8393121965	-1.8259957369
F	-2.8127988572	2.3976481503	-6.5140766261
F	-0.9770880809	2.5185087286	-4.5336975691
C	-1.1948056066	0.7928965234	-0.2772857144
H	-0.1511237474	1.0347087354	-0.0496140678
H	-1.1940312325	0.3151119720	-1.2660014363
C	-1.7488306854	-0.1819189308	0.7715543358
H	-2.7758163413	-0.4811112148	0.5353339688
H	-1.1465848183	-1.0937142542	0.8339949000
H	-1.7610098820	0.2741958746	1.7680231480
C	-2.1844354399	3.3013074214	1.3225571970
H	-1.2979997027	2.9903930064	1.8876479644
H	-3.0541341932	2.9563068323	1.8967890434
C	-2.2178688574	4.8306963648	1.2028491830
H	-3.0856552392	5.1688589024	0.6267846017
H	-2.2611371281	5.3157562564	2.1829700521
H	-1.3205805294	5.2019636073	0.6939626520
C	-4.0053405395	1.8773979853	-0.7069879623
H	-4.6294240327	2.7677203903	-0.8468889403
H	-4.3751251681	1.4046121496	0.2138504949
C	-4.1908387320	0.9049673665	-1.8795372060
H	-3.6223777491	-0.0185890463	-1.7229734164
H	-5.2410956964	0.6243469268	-2.0074500118
H	-3.8515524250	1.3364624140	-2.8280212916

M21

B	-1.7842573771	3.3964976835	-2.1995798421
Si	-2.3789834452	2.5194243938	-0.4405116412
C	-0.3741409063	2.8849151857	-2.6660399564
C	-0.1669178854	1.5371708857	-2.9337859958
C	1.0926808089	0.9785343448	-3.0648489395
C	2.2043077103	1.8034582033	-2.9324186640

C	2.0422122704	3.1613392775	-2.6851451437
C	0.7602510666	3.6794527677	-2.5703795130
F	3.4244240127	1.2937956235	-3.0500406909
F	3.1099654514	3.9447924253	-2.5609031057
F	0.6241612950	4.9848918026	-2.2987452569
F	1.2500209941	-0.3176387802	-3.3103394132
F	-1.2374103619	0.7356896546	-3.0549262020
C	-2.5509661777	4.5072814327	-2.9676384132
C	-3.8197348365	4.9411325757	-2.5500456011
C	-4.5530631196	5.9055868431	-3.2226456625
C	-4.0161137075	6.4801585780	-4.3684626753
C	-2.7633652543	6.0904493044	-4.8276207733
C	-2.0579236582	5.1215710805	-4.1311811896
F	-4.6991314786	7.4022954093	-5.0242852593
F	-2.2616796542	6.6466568800	-5.9242644813
F	-0.8705243619	4.7884445211	-4.6268730981
F	-5.7498304842	6.2846956399	-2.7908013822
F	-4.3763637866	4.4271181814	-1.4556626789
C	-1.0111939978	1.2901113241	-0.0122963846
C	-1.1324312420	-0.0864635586	-0.2359078816
C	-0.0326808659	-0.9354148272	-0.1118916090
C	1.2098093846	-0.4192952012	0.2453256070
C	1.3471409147	0.9457571341	0.4990541316
C	0.2457163171	1.7869916283	0.3732911791
H	-2.0936724629	-0.5003123503	-0.5326125181
H	-0.1452761830	-1.9984987346	-0.3014383621
H	2.0688338374	-1.0776981787	0.3311053538
H	2.3117297776	1.3519194207	0.7894173336
H	0.3676213705	2.8520659474	0.5686491493
C	-2.3741703286	3.8102201170	0.9352903959
C	-2.3892889821	5.1922028345	0.7054131722
C	-2.3642979791	6.1008164385	1.7614285696
C	-2.3285394761	5.6401773746	3.0743700682
C	-2.3062629894	4.2700280425	3.3274148220
C	-2.3202853005	3.3677504075	2.2673272676
H	-2.4157812911	5.5758465872	-0.3119028990
H	-2.3712339795	7.1673627308	1.5584839701
H	-2.3114836500	6.3464387889	3.8987617204
H	-2.2707723288	3.9051754590	4.3493887883
H	-2.2786280724	2.3004715852	2.4778147417
C	-4.0360622307	1.6401181976	-0.5719854987
C	-4.3105190334	0.7937371928	-1.6576002237
C	-5.5330432207	0.1346123484	-1.7630212014
C	-6.5071245718	0.3156425037	-0.7840056392
C	-6.2554194009	1.1574286630	0.2965568209
C	-5.0311757229	1.8143677373	0.3992312936
H	-3.5585617699	0.6402577906	-2.4288980542
H	-5.7258856917	-0.5173576651	-2.6096530662
H	-7.4614852230	-0.1956356624	-0.8650595260
H	-7.0142477698	1.3053028651	1.0589928558

H -4.8509995719 2.4783790904 1.2417513841

M22

B -1.4946687983 3.1696632908 -2.0517818354
Si -2.3673057292 2.3162956883 -0.4203035823
C -1.3921789811 4.7324440801 -1.8149242785
C -0.3554045035 5.4733268118 -1.2599422104
C -0.4947088570 6.8192490274 -0.9449414029
C -1.7020915026 7.4639506634 -1.1823749123
C -2.7557150129 6.7624523349 -1.7534112098
C -2.5699741073 5.4271158714 -2.0722331357
F -1.8449044421 8.7438168340 -0.8704549081
F -3.9253298902 7.3556476328 -1.9680560467
F -3.5992724721 4.7561286557 -2.6217223534
F 0.5185366473 7.4925915820 -0.4124142094
F 0.8257868941 4.9060903156 -1.0003483093
C -1.1246903629 2.5416351821 -3.4124612193
C -0.0897374613 3.0551413484 -4.2010558216
C 0.2575876599 2.5026714629 -5.4241310611
C -0.4628504060 1.4131567330 -5.9013453000
C -1.5118627532 0.8799142501 -5.1591340112
C -1.8171188217 1.4452636993 -3.9329372516
F -0.1524585799 0.8831630595 -7.0718032448
F -2.2031943974 -0.1488920746 -5.6337212478
F -2.8467926325 0.9314986374 -3.2565078161
F 1.2569401672 2.9997238562 -6.1422000529
F 0.6244935369 4.0918238905 -3.7684786778
C -2.7272037366 0.4693859269 -0.3231843823
C -3.7561579703 -0.0724937023 0.4396203845
C -3.9791944153 -1.4404855495 0.5243957229
C -3.1403025334 -2.3087976078 -0.1625004855
C -2.0881923072 -1.8082901895 -0.9204805987
C -1.9016417378 -0.4364118659 -0.9784630336
F -3.3367289272 -3.6166559421 -0.0875813363
F -1.2780686152 -2.6392077358 -1.5670738069
F -0.8656156912 0.0211451387 -1.6972508353
F -4.9742068234 -1.9239409387 1.2590021517
F -4.5689184591 0.7249672589 1.1376643782
C -1.0555514526 2.6455114595 0.8974878161
C -1.3161189947 2.8974373243 2.2383516550
C -0.3026752612 3.1432444653 3.1534299656
C 1.0200242653 3.1307948571 2.7207256462
C 1.3224951320 2.8753428480 1.3884312499
C 0.2774613727 2.6281339713 0.5125726487
F 1.9961239806 3.3646775428 3.5851319285
F 2.5838616230 2.8673255637 0.9772117021
F 0.5778561465 2.3704437543 -0.7761866821
F -0.5760159936 3.3885970970 4.4293648163
F -2.5778050668 2.9164005763 2.6756640339
C -3.9224164066 3.3239682573 -0.0903205183

C	-3.8752470117	4.5937545013	0.4748451751
C	-4.9742546170	5.4397067478	0.5118968926
C	-6.1840634868	4.9998023959	-0.0092377731
C	-6.2773928643	3.7337335178	-0.5751197063
C	-5.1476124094	2.9311319803	-0.6185266649
F	-7.2454464792	5.7909029286	0.0207541177
F	-7.4298906090	3.3199355247	-1.0884133669
F	-5.2518085209	1.7501106997	-1.2387588520
F	-4.8686939687	6.6628732192	1.0187013149
F	-2.7233323491	5.0742532078	0.9640977992

M23

B	-1.6305597174	3.5274560787	-2.0905111353
Si	-2.3248104957	2.9456172307	-0.2652546258
C	-0.2048318064	4.1630457022	-2.0459941635
C	0.0596831961	5.4699574586	-2.4454220629
C	1.3139324214	6.0437467280	-2.3124753242
C	2.3527977139	5.2853633808	-1.7817375360
C	2.1330043465	3.9714865583	-1.3830506111
C	0.8593295951	3.4417450549	-1.5128351662
F	3.5597174160	5.8168912363	-1.6625458900
F	3.1318279385	3.2486851062	-0.8923860517
F	0.6503930897	2.1727196419	-1.1410041584
F	1.5357965223	7.2973593873	-2.6895731521
F	-0.9255725709	6.2123049633	-2.9577929205
C	-2.4554715336	3.4068054244	-3.3919993640
C	-3.7541065416	2.8684179852	-3.4060716602
C	-4.5165278431	2.7422882710	-4.5551018284
C	-3.9774390885	3.1542040218	-5.7679799989
C	-2.6901633460	3.6774439443	-5.8200702078
C	-1.9555419438	3.7910298581	-4.6514931311
F	-4.6848892069	3.0391867453	-6.8752694880
F	-2.1780794560	4.0517181618	-6.9849556951
F	-0.7235162597	4.2690305936	-4.7829404235
F	-5.7384701894	2.2300994804	-4.5124220080
F	-4.3096609785	2.4372968956	-2.2777778613
Cl	-2.6968646285	0.9335424510	-0.1173413183
Cl	-0.9641792023	3.4174898306	1.2078330872
Cl	-4.0116736145	4.0203134489	0.2240550570

M24

B	-1.4791654797	3.3411474455	-2.1778670136
Si	-1.9015525051	2.2335129262	-0.5496475646
C	-0.1892934755	4.2055471112	-2.0493236290
C	0.0051686714	4.9815076440	-0.9069516743
C	1.1610131762	5.7124907193	-0.6851304679
C	2.1812439053	5.6500832492	-1.6280657549
C	2.0348198117	4.8774959956	-2.7759740708
C	0.8547944506	4.1784582014	-2.9729432909
F	3.2977549232	6.3345106622	-1.4357980744

F	3.0208160782	4.8203456880	-3.6635869454
F	0.7458932096	3.4298028673	-4.0726702430
F	1.3017299027	6.4669839066	0.3974143899
F	-0.9838322604	5.0680423123	-0.0116225519
C	-2.3418714550	3.2754059355	-3.4567792912
C	-2.1735391693	4.1255948692	-4.5632369544
C	-2.9789471212	4.0577051996	-5.6879135258
C	-4.0045121743	3.1186389947	-5.7343718536
C	-4.2268616237	2.2640496805	-4.6603942043
C	-3.4061788073	2.3637192557	-3.5498832382
F	-4.7775886792	3.0456746130	-6.8015075731
F	-5.2145102938	1.3806837782	-4.7095388789
F	-3.6646246031	1.5421464791	-2.5335286866
F	-2.7927447335	4.8794488475	-6.7126690180
F	-1.2360700562	5.0668286886	-4.5602737407
F	-1.8208520704	0.6723807548	-0.8649051608
F	-0.7903366305	2.4784958430	0.5694313490
F	-3.3159127872	2.5357613400	0.1154196360

M25

B	-1.5503588353	3.4017749389	-2.0318569264
Si	-2.2322268362	2.4143970397	-0.3977108293
Cl	0.1820634246	3.6336161167	-2.2510219550
Cl	-2.6200063973	4.0521968764	-3.2663450408
C	-1.4758454922	0.6860686233	-0.4096158419
H	-0.3823864166	0.7402436936	-0.4257213285
H	-1.7742862492	0.1358972722	0.4897475911
H	-1.8004731225	0.1079057072	-1.2807259901
C	-1.6362340066	3.3460591939	1.1307413705
H	-1.9354774747	2.8127347822	2.0399325466
H	-0.5446919576	3.4319577011	1.1327514242
H	-2.0568117904	4.3556384403	1.1792504905
C	-4.1116348936	2.3209280469	-0.4319696289
H	-4.5563565689	3.3214790369	-0.4392450628
H	-4.4642046572	1.7926949407	-1.3239319749
H	-4.4892153831	1.7888642163	0.4481348593

M26

B	-1.6054442709	3.3898305855	-2.1202300036
Si	-2.2374647395	2.4206335314	-0.4505818730
Cl	0.0892729757	3.3454903805	-2.6039684963
Cl	-2.7106022863	4.2672416914	-3.1740811454
C	-1.6834539302	0.6147845096	-0.5948683567
H	-0.6102127383	0.5942649191	-0.8236362578
H	-2.1870210984	0.1539968483	-1.4544835959
C	-1.9673780040	-0.1960405121	0.6770787509
H	-3.0377427881	-0.2145350978	0.9085738747
H	-1.6359688866	-1.2339946152	0.5755731673
H	-1.4516955425	0.2308926238	1.5444810154
C	-1.4353193063	3.1968372675	1.0827511874

H	-1.9492445556	2.7801707721	1.9609482530
H	-1.6469321438	4.2735392178	1.0965623437
C	0.0752669779	2.9555068732	1.1945499594
H	0.6132921467	3.3934155777	0.3480261778
H	0.4845258179	3.3939372428	2.1098100834
H	0.3080242148	1.8851084960	1.2090568100
C	-4.1191504667	2.5487447507	-0.3193824444
H	-4.4698315731	1.8048954531	0.4084233547
H	-4.5596638773	2.2645643785	-1.2838861497
C	-4.6068179313	3.9448348083	0.0914607524
H	-4.2584759632	4.7117898373	-0.6087277385
H	-5.6992899478	3.9982389527	0.1189591912
H	-4.2385023606	4.2138074357	1.0871496524

M27

B	0.0277220979	-0.4489422764	2.1240423563
Si	0.0151485449	0.0279576627	0.1478461184
Cl	-1.4031643116	-0.2952755066	3.1307609454
Cl	1.4779451816	-1.1037636521	2.8750622149
C	-0.4253756705	-1.5581915937	-0.7650571037
C	-1.4386592575	-1.5998747681	-1.7321254758
C	-1.7279700216	-2.7802858612	-2.4148570612
C	-1.0069755925	-3.9389456657	-2.1403758971
C	0.0067273896	-3.9166021503	-1.1837601398
C	0.2923418263	-2.7366035208	-0.5032596177
H	-2.0077875107	-0.7005797372	-1.9554700270
H	-2.5156873965	-2.7937267576	-3.1620064576
H	-1.2330342964	-4.8589171879	-2.6708001598
H	0.5722499606	-4.8178032801	-0.9677111309
H	1.0922793840	-2.7318223260	0.2355834142
C	-1.2571198237	1.3620641655	-0.2084496079
C	-2.6151057449	1.1516947742	0.0825135082
C	-3.5659023216	2.1321181041	-0.1839409773
C	-3.1744156254	3.3463502871	-0.7458554381
C	-1.8336775353	3.5736985866	-1.0419276047
C	-0.8841884279	2.5881560340	-0.7760642169
H	-2.9363898765	0.2078829871	0.5187671094
H	-4.6110370746	1.9509538409	0.0475253690
H	-3.9150765776	4.1128337306	-0.9528816409
H	-1.5254980018	4.5171527586	-1.4820947166
H	0.1603536802	2.7749430416	-1.0146235145
C	1.7279496853	0.6048491983	-0.3586870533
C	2.4216728047	1.5461338909	0.4171464195
C	3.6765233779	2.0094038649	0.0333618658
C	4.2633987790	1.5324605897	-1.1375644621
C	3.5925972587	0.5961686927	-1.9195509280
C	2.3347993041	0.1374192309	-1.5318475683
H	1.9771022136	1.9255532852	1.3364580960
H	4.1986090251	2.7365107483	0.6476995942
H	5.2440978920	1.8890372063	-1.4373737102

H	4.0485644016	0.2215929928	-2.8309111838
H	1.8206082596	-0.5979023893	-2.1469143178

M28

B	-1.9686816175	3.2367937228	-2.1892248180
Si	-2.3584088349	2.3195884095	-0.4285178394
Cl	-0.7194855890	4.4452055654	-2.3379150020
Cl	-2.9761980095	2.8682500326	-3.5731813803
C	-1.5579716613	0.6234970991	-0.3949916051
C	-0.7677814954	0.1513516577	-1.4339757105
C	-0.1317687929	-1.0813590293	-1.3838508074
C	-0.2845435324	-1.8693239719	-0.2495797664
C	-1.0582170320	-1.4254286117	0.8186749515
C	-1.6744677774	-0.1876883314	0.7277384362
F	0.3145818011	-3.0482074981	-0.1815954437
F	-1.1904237207	-2.1834465974	1.9003469748
F	-2.4037902175	0.2379619024	1.7644726453
F	0.6166869694	-1.5079345311	-2.3936627405
F	-0.5847426618	0.9022729145	-2.5294914721
C	-1.6324954485	3.3056631105	1.0011029063
C	-2.3541467890	3.9521658448	1.9984574388
C	-1.7368595664	4.6840087370	3.0049920358
C	-0.3513109458	4.7795288210	3.0254164396
C	0.4073193247	4.1455821607	2.0479634103
C	-0.2466809813	3.4249693832	1.0613253670
F	0.2491010601	5.4741843774	3.9798381738
F	1.7316918968	4.2347945929	2.0700121897
F	0.5018050842	2.8144608238	0.1316318573
F	-2.4558981410	5.2885718242	3.9434237615
F	-3.6876448478	3.8854618195	2.0255206774
C	-4.2298760754	2.2083791506	-0.3118661748
C	-4.9980341557	1.0652523315	-0.1345297036
C	-6.3881575447	1.1052346200	-0.1295657720
C	-7.0370742245	2.3183861759	-0.3153055551
C	-6.3024886188	3.4849734143	-0.5073980234
C	-4.9221714378	3.3996127677	-0.5048968002
F	-8.3604535700	2.3663315716	-0.3148230112
F	-6.9247843014	4.6428797409	-0.6900619009
F	-4.2115917081	4.5248989957	-0.6916031219
F	-7.0971378583	-0.0043651882	0.0423271139
F	-4.4237320166	-0.1295685453	0.0211785252

M29

B	1.3253490907	0.0301762384	-0.0053858839
Si	-0.6936083494	0.0138876932	-0.0037255647
Cl	2.2097260803	1.5242039677	-0.0145258414
Cl	2.1557119583	-1.4980700344	0.0026228788
Cl	-1.4681321931	1.9049142147	-0.0138804552
Cl	-1.3592040468	-0.9847249210	-1.6630019276
Cl	-1.3566075400	-0.9657751587	1.6678417940

M30

B	-1.5505354282	3.3727882143	-2.0147044091
Si	-2.2176609777	2.4222605785	-0.3765808428
Cl	-0.0195520014	4.2011324501	-1.9749884878
Cl	-2.4922064158	3.3445769705	-3.4789803950
F	-1.7111260676	0.9164205878	-0.3519544702
F	-1.7026778349	3.1287471967	0.9487153643
F	-3.8045066619	2.4008264525	-0.3296399177

M31

B	-1.5437851853	3.3749605344	-2.0560280527
Si	-2.2184962257	2.4201831634	-0.3913747906
F	-2.1642346078	4.4337581199	-2.5655989652
F	-0.4396171542	3.0000118371	-2.6928749198
C	-1.6646204000	0.6190196747	-0.4271289545
H	-2.0855985153	0.0831580447	-1.2839799356
H	-0.5738950443	0.5467902123	-0.4893135867
H	-1.9859001568	0.1014052738	0.4835248407
C	-1.4771599682	3.2733268894	1.1224225673
H	-1.7743766731	4.3256441835	1.1760566332
H	-1.8256287508	2.7797325014	2.0366539260
H	-0.3832988091	3.2292362687	1.1145003605
C	-4.0980287091	2.5413554694	-0.3141781324
H	-4.4219892278	3.5872154309	-0.3116566307
H	-4.5717336957	2.0452296987	-1.1673915737
H	-4.4744037372	2.0691887031	0.6000723998

M32

B	-1.2592489542	1.2539464349	-0.0486206692
Si	0.3924274700	0.0669366769	0.0613884828
F	-1.1973941626	2.5623798933	-0.2718585877
F	-2.4866712037	0.7611321814	0.0980906281
C	0.3426496838	-1.1428080869	-1.4035163632
H	0.8818867181	-2.0537613546	-1.1091525667
H	0.9167234528	-0.7080579810	-2.2326429097
C	-1.0700512765	-1.5012917648	-1.8875109742
H	-1.5926461011	-0.6175223735	-2.2694269373
H	-1.0441730724	-2.2411219421	-2.6933641467
H	-1.6845265265	-1.9104536194	-1.0792933530
C	1.9584714954	1.1221583595	-0.0186976539
H	1.9734463459	1.8084729977	0.8377445225
H	1.9045410987	1.7559813138	-0.9133606485
C	3.2446903352	0.2853923385	-0.0462148187
H	3.2550645922	-0.3980634320	-0.9026810419
H	4.1365784028	0.9153815413	-0.1179233985
H	3.3444887626	-0.3218400508	0.8597618342
C	0.3307734117	-0.9014706112	1.6894670872
H	0.2836275138	-0.1923057550	2.5262763680
H	1.2812942464	-1.4400735488	1.8021658682

C	-0.8382140531	-1.8923268819	1.7687837548
H	-0.7537954057	-2.6599324080	0.9919040915
H	-0.8681631923	-2.4057517769	2.7346779601
H	-1.8003125811	-1.3878631505	1.6295484721

M33

B	-0.0077593337	-0.2679403052	2.5058932629
Si	0.0068644604	-0.0389990255	0.4851375135
F	-0.0834674340	0.7429380987	3.3617241876
F	0.0670557723	-1.4787058967	3.0493171441
C	-1.4610929855	-0.9614048602	-0.2443405675
C	-2.7684112808	-0.5422540666	0.0502123064
C	-3.8712528594	-1.2088888479	-0.4743964089
C	-3.6843746914	-2.3118231299	-1.3065195241
C	-2.3960319246	-2.7420200215	-1.6102795665
C	-1.2937106510	-2.0710513353	-1.0825469850
H	-2.9283150954	0.3233899275	0.6917021232
H	-4.8748765904	-0.8701912176	-0.2359783337
H	-4.5433159916	-2.8336923627	-1.7172794511
H	-2.2477838733	-3.5993555144	-2.2597906688
H	-0.2908021066	-2.4136480360	-1.3271764734
C	-0.0959547311	1.7793997774	0.0364262178
C	0.5927961018	2.7361596041	0.7971044335
C	0.5758994799	4.0819813585	0.4422427419
C	-0.1364482539	4.4951841861	-0.6819581787
C	-0.8302140987	3.5613378860	-1.4473215675
C	-0.8092383501	2.2147172654	-1.0893253466
H	1.1454352217	2.4280775644	1.6821393912
H	1.1126068182	4.8088204545	1.0441965496
H	-0.1533720406	5.5450049677	-0.9585486612
H	-1.3885348639	3.8812331700	-2.3218815332
H	-1.3604096088	1.4932761397	-1.6890323945
C	1.6105481356	-0.7843342119	-0.1503669942
C	2.0955904637	-1.9897093729	0.3805691520
C	3.2578510071	-2.5734621236	-0.1165869788
C	3.9586428331	-1.9554233528	-1.1504857095
C	3.4959862260	-0.7551737578	-1.6843133084
C	2.3309074508	-0.1749352331	-1.1867265046
H	1.5596685361	-2.4770245013	1.1927879997
H	3.6197220211	-3.5060992546	0.3053535293
H	4.8671895100	-2.4074773956	-1.5365938740
H	4.0432608826	-0.2698787422	-2.4867040407
H	1.9791631841	0.7660579255	-1.6045179015

M34

B	-1.3843166887	3.3699665895	-1.8624415029
Si	-2.1836940168	2.4018229395	-0.2769053277
F	-0.1838313602	3.9126139428	-1.7508748298
F	-2.0282636414	3.5282713269	-3.0030942697
C	-1.6219331073	0.6125530069	-0.3002026584

C	-2.1460053214	-0.3255296220	0.5815568582
C	-1.7785013954	-1.6615567970	0.5481553407
C	-0.8581103462	-2.0816383018	-0.4074563301
C	-0.3182945503	-1.1759530903	-1.3127714677
C	-0.7123745125	0.1529284147	-1.2435784538
F	-0.4963120254	-3.3544594306	-0.4555362420
F	0.5546198869	-1.5872761339	-2.2241293363
F	-0.1872934048	1.0076894450	-2.1347255957
F	-2.2896884150	-2.5380618380	1.4039341073
F	-3.0363626516	0.0652756514	1.4976852987
C	-1.5611083691	3.3081697497	1.2444147986
C	-1.6114020660	4.6972815022	1.1979025395
C	-1.1605972617	5.5060177113	2.2266489200
C	-0.6245149560	4.9004734472	3.3586894094
C	-0.5497080159	3.5162133014	3.4444784480
C	-1.0161734955	2.7415244036	2.3891664647
F	-0.1838264127	5.6485218225	4.3585990159
F	-0.0319741635	2.9483345387	4.5272679411
F	-0.9162229937	1.4159868453	2.5110151423
F	-1.2327500694	6.8289084418	2.1494821224
F	-2.1431674704	5.2850405702	0.1122974210
C	-4.0608658844	2.4204419225	-0.3683504462
C	-4.9223881326	2.9292850340	0.5960082303
C	-6.3020414648	2.9125478260	0.4359030379
C	-6.8459218816	2.3708362767	-0.7222722953
C	-6.0170708729	1.8485954724	-1.7092543491
C	-4.6457329448	1.8864899219	-1.5122862390
F	-8.1600890482	2.3476923391	-0.8851246913
F	-6.5412726065	1.3251772565	-2.8107579610
F	-3.8540312386	1.3672144848	-2.4603143238
F	-7.1022133721	3.4053349526	1.3740704921
F	-4.4417174752	3.4544051861	1.7259596160

M35

B	-1.5363943194	3.3963548301	-2.0514768977
Si	-2.2090690350	2.4371233297	-0.3991964972
F	-0.3860803858	4.0322190645	-2.0322266430
F	-2.2335084518	3.3752937534	-3.1657059141
Cl	-1.5175680149	0.5091727462	-0.4097075961
Cl	-1.5355259228	3.3676219543	1.2916043800
Cl	-4.2527174370	2.4021248185	-0.3751491347

M36

B	-1.5435865372	3.3776779924	-2.0288870846
Si	-2.2149780053	2.4235728513	-0.3817763304
F	-0.3862559080	4.0053062667	-2.0236096478
F	-2.2470993453	3.3845189385	-3.1417136772
F	-1.7247583350	0.9124889424	-0.3589903188
F	-1.6882659487	3.1225789580	0.9428468030
F	-3.8016771278	2.4178067941	-0.3268631564

M1-TS1

B	0.7838700231	-0.2305405989	-0.0048597866
Si	-0.3525324383	1.5508637303	0.0122207792
C	-1.2200581021	-1.0208949866	0.0404962466
O	-2.3370699017	-0.6936235692	-0.0095443644
O	-0.2483105817	-1.7224258158	0.0995341315
C	1.6324633985	-0.3555637973	1.3378061245
H	2.1439443075	-1.3267563878	1.3694692306
H	2.4107377784	0.4168239082	1.3606648555
H	1.0476097561	-0.2546877577	2.2597183267
C	1.4955149639	-0.4479441272	-1.4137831235
H	2.0883997593	-1.3722743126	-1.4029380216
H	0.8029762894	-0.5032138231	-2.2622095019
H	2.1907137398	0.3746980054	-1.6217627305
C	1.1006810430	2.7673396902	0.0828442064
H	1.6221456515	2.7117959356	1.0435582257
H	1.8300153006	2.5990243599	-0.7153723145
H	0.7093323836	3.7859077289	-0.0289682175
C	-1.4127425232	1.9006113040	1.5370712472
H	-0.8857949983	1.6183813945	2.4555504278
H	-1.6147061723	2.9768363785	1.5932563811
H	-2.3741655168	1.3803283980	1.5163136181
C	-1.3196539740	1.9256587157	-1.5657766734
H	-0.6945410482	1.7634703111	-2.4510454246
H	-2.2228347535	1.3168000559	-1.6649510465
H	-1.6242787017	2.9788424058	-1.5652383804

M2-TS1

B	0.7888478986	-0.2368826404	-0.0456975455
Si	-0.3294095847	1.5523997757	0.0661643224
C	-1.2082414169	-1.0296098932	0.1083112279
O	-2.3101416557	-0.7141040277	0.3172145472
O	-0.2520618598	-1.7244246093	-0.1018753436
C	1.6454338227	-0.4944141927	1.2718529326
H	2.1551251801	-1.4655404777	1.2135325731
H	2.4262628012	0.2712168893	1.3607857572
H	1.0681171075	-0.4731446883	2.2044561861
C	1.4945104626	-0.3200091835	-1.4736444181
H	0.8018422544	-0.2746052603	-2.3219891185
H	2.2089761443	0.5028414829	-1.5973123192
H	2.0650106685	-1.2550245630	-1.5549881060
C	1.1363739266	2.7487783375	0.2991007049
H	1.9391452494	2.5258112462	-0.4137826574
H	1.5536713170	2.5849861538	1.3011289013
C	0.6979675334	4.2126562679	0.1497427652
H	-0.1260227302	4.4560418953	0.8312841939
H	1.5180096700	4.9039777060	0.3689354394
H	0.3543261270	4.4216686008	-0.8686373706
C	-1.4863533469	1.8764491621	1.5515893242

H	-0.9689510086	2.5930921080	2.2037652448
H	-1.6071096387	0.9659506926	2.1495197156
C	-2.8679266095	2.4307812040	1.1810620285
H	-3.4192851309	1.7299281484	0.5460551123
H	-3.4762315209	2.6198924252	2.0711782164
H	-2.7841951161	3.3758001259	0.6332018907
C	-1.1191288055	2.0077891902	-1.6035501540
H	-0.2736718948	2.1882571924	-2.2834052890
H	-1.6201134244	2.9783636648	-1.4910023782
C	-2.0838260164	1.0087518882	-2.2523133905
H	-2.9788749945	0.8543157186	-1.6430316974
H	-2.4094046934	1.3527170492	-3.2391387607
H	-1.6109839945	0.0284107126	-2.3962519345

M3-TS1

B	0.8454528721	-0.2133043967	0.0053501166
Si	-0.3401215844	1.5671070745	-0.0255044574
C	-1.1221730871	-0.9742502897	0.0341284080
O	-2.2553906736	-0.7202473176	-0.0460888482
O	-0.1312315392	-1.6569062652	0.1516240452
C	1.7152945284	-0.2279568770	1.3424880729
H	1.1723229015	-0.0178084169	2.2706188133
H	2.1811794409	-1.2180741061	1.4429984639
H	2.5262754309	0.5043577932	1.2629242563
C	1.5893551698	-0.4273010641	-1.3888294574
H	2.1590287503	0.4660958324	-1.6734490596
H	2.3089316613	-1.2521499046	-1.2929305434
H	0.9174981994	-0.6722763068	-2.2194317516
C	1.0755160867	2.8207135172	-0.1073595939
C	1.4829370364	3.4278335335	-1.3030942383
C	2.5412282388	4.3347233801	-1.3264339137
C	3.2114694498	4.6549003455	-0.1492811875
C	2.8141266663	4.0723166295	1.0528397688
C	1.7567202161	3.1676218617	1.0706189189
H	0.9601013352	3.2065856289	-2.2295932403
H	2.8372918164	4.7951213534	-2.2642224644
H	4.0354974339	5.3616936956	-0.1659958196
H	3.3253775262	4.3260545989	1.9765441042
H	1.4509032542	2.7284436308	2.0181975374
C	-1.2657208921	1.9422698892	1.5764689675
C	-1.6894690375	3.2617458937	1.8062948214
C	-2.3688393598	3.6121646393	2.9697817724
C	-2.6293900172	2.6469006696	3.9406973100
C	-2.2060688565	1.3361778672	3.7424854263
C	-1.5326304705	0.9931603457	2.5712987610
H	-1.4809558535	4.0298419046	1.0630965942
H	-2.6901784147	4.6381004882	3.1216181521
H	-3.1558192921	2.9176618320	4.8507698655
H	-2.3980331890	0.5803263419	4.4977708473
H	-1.2043751998	-0.0378837305	2.4496302534

C	-1.4764616074	1.8099641703	-1.5116376145
C	-2.8168539406	2.1872540475	-1.3453240813
C	-3.6646800156	2.3408496951	-2.4402296089
C	-3.1890786684	2.1155136047	-3.7292594463
C	-1.8637868601	1.7318717933	-3.9183422200
C	-1.0204175725	1.5791759023	-2.8202072025
H	-3.2092429591	2.3493258180	-0.3442885708
H	-4.6992835946	2.6315363013	-2.2851203404
H	-3.8492636708	2.2334461537	-4.5830713713
H	-1.4866824814	1.5483024572	-4.9199257594
H	0.0086100236	1.2713098801	-2.9912199379

M4-TS1

B	0.6757622810	-0.2483996758	-0.0587174238
Si	-0.3727431346	1.6808855487	0.0338849047
C	-1.3017313839	-0.6790157620	0.2560439517
O	-2.4185731953	-0.4156655197	0.4712251368
O	-0.3929432207	-1.4758209115	0.0691766608
C	1.6877491066	-0.3679468545	1.1624864522
H	2.0412670549	-1.4087206539	1.1772905356
H	2.5668585917	0.2655741432	1.0029973032
H	1.2800757697	-0.1468649420	2.1516172082
C	1.2513699056	-0.2720780718	-1.5445561679
H	0.4941381630	-0.3452318711	-2.3291388542
H	1.8918660725	0.5858422999	-1.7700695344
H	1.8838369204	-1.1688972129	-1.6145165912
C	1.2144627208	2.6782393476	0.3281733282
C	1.6633597687	2.9027262613	1.6274763127
C	2.8289539470	3.5964146486	1.9186763351
C	3.6020906432	4.0841789523	0.8734574325
C	3.2054313261	3.8661779887	-0.4395899351
C	2.0317396196	3.1680086206	-0.6870446749
F	4.7209164080	4.7457596071	1.1276013241
F	3.9496043954	4.3203652293	-1.4413587474
F	1.7151789436	2.9654652872	-1.9715845947
F	3.2139040924	3.7842888528	3.1756547984
F	0.9755397988	2.4126610030	2.6664268433
C	-1.5944210374	2.1960877283	1.3964458350
C	-2.4524856349	3.2858966497	1.3007947453
C	-3.3557858631	3.6251646624	2.3024315858
C	-3.4176783090	2.8541146147	3.4530357396
C	-2.5811063480	1.7519620875	3.5913519446
C	-1.6962143313	1.4546380819	2.5705535482
F	-4.2721709305	3.1627167145	4.4167993734
F	-2.6400583964	1.0029177787	4.6863731210
F	-0.9175287096	0.3725421712	2.7349145997
F	-4.1553994665	4.6767362763	2.1630685143
F	-2.4471675008	4.0655123596	0.2160350251
C	-1.1001993548	2.1770402847	-1.6443664658
C	-1.0290741774	3.4909980825	-2.1068296846

C	-1.5419835494	3.8915471237	-3.3301957334
C	-2.1570569440	2.9517955073	-4.1487474028
C	-2.2462097353	1.6304717170	-3.7358172242
C	-1.7187670144	1.2735061767	-2.5023376359
F	-2.6530503939	3.3165478005	-5.3209440957
F	-2.8259605392	0.7238903922	-4.5142516496
F	-1.8269893327	-0.0244062981	-2.1684273007
F	-1.4500738919	5.1553375575	-3.7267518547
F	-0.4375390987	4.4295924341	-1.3638895939

M5-TS1

B	0.8064791121	-0.3939194363	0.0001516836
Si	-0.3816702816	1.4729434310	-0.0000818939
C	-1.1594640853	-0.8468603429	-0.0001489244
O	-2.3118990823	-0.6490830526	-0.0003400912
O	-0.2135958123	-1.6355704856	0.0000260236
C	1.5525829836	-0.3607808098	1.3993418062
H	2.2829493629	0.4493946747	1.4679805932
H	0.8895248163	-0.3003349080	2.2692799480
H	2.1032359295	-1.3096225520	1.4766145358
C	1.5530267630	-0.3608609791	-1.3988034040
H	2.2834039942	0.4493198345	-1.4672614773
H	2.1037174411	-1.3097000503	-1.4758405317
H	0.8902448302	-0.3004796433	-2.2689565730
Cl	1.2269468385	2.7614623493	0.0001280471
Cl	-1.4660156472	1.9468344563	1.6809737093
Cl	-1.4655141508	1.9467611689	-1.6814799194

M6-TS1

B	0.7549755775	-0.3495022005	0.0000383022
Si	-0.3024995946	1.4509250663	0.0000763777
C	-1.2023333215	-0.8544130855	-0.0003807026
O	-2.3202070190	-0.5221696640	-0.0005434761
O	-0.2792762247	-1.6500159216	-0.0003109439
C	1.5346197333	-0.3646396995	1.3879316751
H	2.1530613558	-1.2716573803	1.4227464928
H	2.2097823357	0.4931385983	1.4731966931
H	0.8874875948	-0.3688217949	2.2718672432
C	1.5351187966	-0.3642904905	-1.3875782748
H	2.1535992971	-1.2712819011	-1.4223855179
H	0.8883021202	-0.3682820827	-2.2717454930
H	2.2102890511	0.4935258394	-1.4724005066
F	0.9486146759	2.4404301911	0.0004375342
F	-1.1642950580	1.8168962207	1.2902088456
F	-1.1638149269	1.8172287183	-1.2902821205

M7-TS1

B	0.8031970930	-0.3151299246	-0.0362040335
Si	-0.3008960391	1.5054197918	-0.0746040268
C	-1.2080066270	-1.0409660886	-0.0246096354

O	-2.3055566047	-0.7085526373	0.1819740067
O	-0.2664417839	-1.7600418441	-0.2264165211
C	1.4403724150	-0.6144910009	1.4018361011
H	1.8936535945	-1.6168023196	1.3509382921
H	0.6675409681	-0.6716012591	2.1825662178
C	2.5159073299	0.3853356475	1.8489998518
H	2.0928044128	1.3772998922	2.0392965446
H	3.0038952080	0.0581904900	2.7720203246
H	3.2947922231	0.5004542726	1.0867956009
C	1.7219339640	-0.4519732264	-1.3355199543
H	2.2260307898	-1.4286070536	-1.2655605973
H	2.5223229918	0.2979460833	-1.2635466062
C	1.0383874039	-0.3299040632	-2.6996337430
H	0.6594448604	0.6839499479	-2.8682809880
H	1.7246918282	-0.5613384034	-3.5201710958
H	0.1881003235	-1.0176995252	-2.7833815509
C	1.1135910007	2.6892071735	-0.5182831928
H	2.0050157596	2.5548395573	0.1000458204
H	1.4060618031	2.5684398681	-1.5669370405
H	0.7590875820	3.7187319829	-0.3845846576
C	-0.9683416583	1.9640346931	1.6320803746
H	-1.3004373241	3.0090070851	1.6290356569
H	-1.8267910594	1.3434887637	1.9095375550
H	-0.2045162586	1.8575176904	2.4095414410
C	-1.6689219434	1.8320099567	-1.3454770093
H	-1.6961842990	2.9085098223	-1.5533713326
H	-1.5026072271	1.3178086102	-2.2972504099
H	-2.6515424244	1.5381146312	-0.9668179795

M8-TS1

B	0.8667976422	-0.3047108841	-0.0824764843
Si	-0.4244688847	1.3879112814	0.0359899530
C	-1.0520392107	-1.2477104296	0.0698536436
O	-2.1918061668	-1.0468683814	-0.0678829625
O	-0.0271207850	-1.8467217560	0.2561764312
C	1.8648818978	-0.2542436607	1.1690179160
H	1.3537822749	0.0048065948	2.1067709368
H	2.5668151264	0.5697037864	0.9743861059
C	2.6667571210	-1.5464863634	1.3771379107
H	3.2386452021	-1.8120660201	0.4822801456
H	3.3765626225	-1.4448163797	2.2040675808
H	2.0079743893	-2.3892150506	1.6090263352
C	1.4445738475	-0.5468077573	-1.5555308428
H	2.3633658928	-1.1479393188	-1.5006025752
H	1.7623047559	0.4286738492	-1.9533703008
C	0.4839517665	-1.2102755696	-2.5513469563
H	-0.4983603148	-0.7188906930	-2.5620962042
H	0.8693117011	-1.1810279042	-3.5752733783
H	0.3213708319	-2.2627840240	-2.2966498103
C	0.8843595917	2.7849856251	0.0994108621

H	0.4158028037	3.6553056088	-0.3822994496
H	1.7375868727	2.5220804818	-0.5398081871
C	1.3753728587	3.1977604950	1.4930070715
H	1.8391704340	2.3661392384	2.0303109581
H	2.1160590543	4.0013538430	1.4279565757
H	0.5498675068	3.5635897047	2.1118986177
C	-1.4423142420	1.5469650218	1.6360128566
H	-0.7348155887	1.5150239222	2.4758475896
H	-2.1190293633	0.6968493139	1.7730162438
C	-2.2551678782	2.8493805848	1.6923353323
H	-3.0763686405	2.8297449020	0.9691931976
H	-2.6937058901	3.0081644570	2.6825729622
H	-1.6389754068	3.7264303509	1.4610384360
C	-1.5069208545	1.7636871475	-1.4832736408
H	-2.1734467240	2.5874310454	-1.1910049527
H	-2.1663964423	0.9172140523	-1.7084708645
C	-0.7306967578	2.1842876841	-2.7404147914
H	-0.0571747430	1.3964857184	-3.0909074632
H	-1.4101408965	2.4233123347	-3.5647277423
H	-0.1200914397	3.0734722324	-2.5530379983

M9-TS1

B	0.8088159000	-0.1980485412	-0.0228055802
Si	-0.3372231796	1.6502184036	0.0094573813
C	-1.1512681197	-0.9092723084	0.0681737741
O	-2.2721088009	-0.6826638243	-0.1525270834
O	-0.1809269133	-1.5830983744	0.3325437301
C	1.8544157595	-0.2105727788	1.1861171209
H	2.6364448978	0.5262317933	0.9654587093
H	2.3467893709	-1.1946028608	1.1293701685
C	1.3372326563	0.0091518174	2.6068431291
H	0.5721373322	-0.7316278360	2.8690491782
H	2.1407578715	-0.0820653304	3.3443916469
H	0.8986508387	1.0074105254	2.7242723156
C	1.3573452602	-0.4709201812	-1.5057407304
H	2.2221051302	-1.1473743481	-1.4205245298
H	1.7609657063	0.4614965751	-1.9238831384
C	0.3616901843	-1.0548131855	-2.5167591240
H	-0.5221715365	-0.4153629858	-2.6323380497
H	0.8142597572	-1.1578260982	-3.5075955578
H	0.0237629411	-2.0519631506	-2.2134132738
C	1.0526177886	2.8661192864	0.4563164778
C	0.8492675275	3.7992700094	1.4846860943
C	1.8342162396	4.7234352242	1.8319180624
C	3.0501816621	4.7363442485	1.1568839479
C	3.2787092876	3.8154623534	0.1367052304
C	2.2935749245	2.8927580903	-0.2022769645
H	-0.0918212837	3.8071885269	2.0281009330
H	1.6476750096	5.4323441366	2.6329846195
H	3.8181494767	5.4551826955	1.4255645897

H	4.2272598697	3.8107237495	-0.3917614738
H	2.5120877679	2.1718573462	-0.9861220786
C	-1.7509356281	1.9782420747	1.2226235425
C	-2.0120647938	1.2011693963	2.3589683315
C	-3.0372854948	1.5286391527	3.2437788808
C	-3.8262242926	2.6516279519	3.0090943570
C	-3.5848593153	3.4416284743	1.8878729235
C	-2.5596475799	3.1054924815	1.0064774887
H	-1.4073411626	0.3214614851	2.5685339489
H	-3.2199170455	0.9057251664	4.1140701349
H	-4.6266371299	2.9088591354	3.6959982793
H	-4.1962212082	4.3184131941	1.6969911469
H	-2.3877287789	3.7306225908	0.1322428562
C	-0.9792880907	2.0561211806	-1.7202680563
C	-0.1248997030	2.5574842397	-2.7134275209
C	-0.5693922369	2.7569090023	-4.0186760630
C	-1.8878742670	2.4647931201	-4.3578020975
C	-2.7607650102	1.9879634153	-3.3827478578
C	-2.3109100500	1.7888406367	-2.0795418920
H	0.9038440061	2.8076085603	-2.4675082783
H	0.1129006185	3.1455636703	-4.7686719417
H	-2.2362918050	2.6177221677	-5.3746877209
H	-3.7941786251	1.7708689686	-3.6356620316
H	-3.0082476052	1.4214819516	-1.3312708032

M10-TS1

B	0.6983803520	-0.2987420715	-0.0288749649
Si	-0.3948536986	1.6587551135	-0.0072706802
C	-1.3187855008	-0.6730769630	0.0507052577
O	-2.4404013770	-0.4040554071	0.2456835866
O	-0.4332232215	-1.4827107564	-0.1854207042
C	1.4674911461	-0.7132768526	1.3080676651
H	2.0460316363	-1.5926217746	0.9762772850
H	0.7569116972	-1.1043767812	2.0440465279
C	2.4129045235	0.2625246007	2.0150133450
H	1.8475413268	1.0001226915	2.5888317406
H	3.0557987554	-0.2697741849	2.7223476567
H	3.0631208074	0.7986556464	1.3163935353
C	1.4686465973	-0.2248811365	-1.4440073789
H	1.0490086309	0.4752034476	-2.1728992053
H	1.3000305606	-1.2211265800	-1.8812623234
C	2.9817315175	0.0102078151	-1.3472510555
H	3.4616896285	-0.7333446188	-0.7032076210
H	3.4444883272	-0.0573113340	-2.3362279983
H	3.2256004344	0.9956427136	-0.9416266884
C	1.1051809882	2.7859273734	0.2905040847
C	1.9517272053	3.1916075291	-0.7393879125
C	3.0374255270	4.0325756832	-0.5441439193
C	3.3039935021	4.5105293843	0.7320058443
C	2.4830521677	4.1427361241	1.7890510830

C	1.4076719746	3.2989424442	1.5498583715
F	4.3374490597	5.3117549852	0.9393557161
F	2.7325573832	4.5929353497	3.0130869382
F	0.6689208624	2.9647376096	2.6150341477
F	3.8157581433	4.3822906774	-1.5617768778
F	1.7402437611	2.7757632237	-1.9941489200
C	-1.7079980519	2.1458282936	1.2773035306
C	-2.7046022224	3.0973666548	1.0938291430
C	-3.6710742405	3.3681410620	2.0572844913
C	-3.6576624183	2.6691158998	3.2544602226
C	-2.6821890968	1.7039197122	3.4788957722
C	-1.7402965438	1.4707891751	2.4937270693
F	-4.5721388452	2.9161328737	4.1804275051
F	-2.6660182588	1.0225568961	4.6189939330
F	-0.8237260463	0.5184249115	2.7313575760
F	-4.6045140189	4.2871889622	1.8356668173
F	-2.7885192123	3.7997342062	-0.0394053229
C	-1.0558060424	2.1132347230	-1.7313716185
C	-1.5057390181	1.1844681027	-2.6632768183
C	-1.9664324072	1.5288746644	-3.9267925221
C	-1.9759099795	2.8649328145	-4.2990521475
C	-1.5217478656	3.8311019616	-3.4094802481
C	-1.0713647541	3.4405478959	-2.1586380073
F	-2.4107025975	3.2184852688	-5.4987472530
F	-1.5193048489	5.1104320713	-3.7651522536
F	-0.6269300780	4.4072120021	-1.3495672665
F	-2.3853255789	0.5950571169	-4.7731620735
F	-1.4928135190	-0.1292330262	-2.3796133426

M11-TS1

B	-1.2788714606	-0.3320213490	0.2164390941
Si	0.8600243673	0.1801760953	-0.1584593415
C	-0.0662321324	-1.8263803010	0.8413782379
O	0.9277677945	-2.3575263089	1.1564202981
O	-1.2980387773	-1.8358170277	0.7838335083
C	-1.9031928157	-0.3575726440	-1.2477368318
H	-1.3640375754	-1.0419917745	-1.9162621064
H	-1.8576799680	0.6325382135	-1.7108850158
C	-3.3739044655	-0.8025957950	-1.1399471839
H	-3.9612097355	-0.0832315484	-0.5598135647
H	-3.8286393032	-0.8808505361	-2.1313853398
H	-3.4651273873	-1.7799769745	-0.6546233374
C	-1.7902410185	0.6039589651	1.3985120883
H	-1.1616052320	0.5105638145	2.2942377707
H	-2.7460420110	0.1243740348	1.6719431871
C	-2.0459295754	2.0821285974	1.0902656799
H	-2.5753523477	2.2061087317	0.1389142797
H	-2.6543001386	2.5419541739	1.8739304651
H	-1.1140206150	2.6488642569	1.0219432825
Cl	0.5385591538	1.9567306640	-1.1529600146

Cl	1.9846130882	-0.9440652316	-1.4664587820
Cl	1.9844931553	0.6725119439	1.4909806263

M12-TS1

B	0.7769621351	-0.3095116764	-0.0070544502
Si	-0.2380250674	1.5196804570	0.0608627219
C	-1.1947993601	-0.7553337948	-0.1466315094
O	-2.3002963447	-0.3968622811	-0.2473390578
O	-0.2992039790	-1.5779801626	-0.0616736346
C	1.4813985881	-0.3695406615	1.4280020877
H	0.7408354719	-0.3606893734	2.2388672368
H	2.1021756694	0.5233429594	1.5732557722
C	2.3583996710	-1.6258142145	1.5512100700
H	3.1891631151	-1.5987965940	0.8398263129
H	2.7829668300	-1.7123990722	2.5555443469
H	1.7796776767	-2.5354515157	1.3563233393
C	1.6046183816	-0.3412601730	-1.3687635132
H	2.2136925734	-1.2571646782	-1.3385357058
H	2.3190769915	0.4920624759	-1.3692245410
C	0.7801354910	-0.3283828873	-2.6611429529
H	0.1843476732	0.5862723644	-2.7545973516
H	1.4176761395	-0.3958443440	-3.5469949586
H	0.0889211231	-1.1789396391	-2.6990570165
F	1.0395935991	2.4759228906	0.1044282337
F	-1.0677482322	1.8004003663	1.3937435296
F	-1.1163344780	2.0322363741	-1.1683018564

M13-TS1

B	0.8205537607	-0.2678103079	0.0510381118
Si	-0.1568715863	1.6289702267	-0.0452753210
C	-1.2308656149	-0.8516016166	0.3275812260
O	-2.2852949114	-0.4270276872	0.5763513602
O	-0.3531504958	-1.6342346026	0.0809611677
C	1.6445771219	-0.5165022264	1.3838166607
C	2.8694953301	-1.2033799590	1.3575061029
C	3.5733780355	-1.4801960880	2.5269462535
C	3.0625042907	-1.0830052065	3.7607879334
C	1.8425537696	-0.4146085814	3.8176983274
C	1.1501156488	-0.1355104471	2.6416974399
H	3.2731113523	-1.5358276665	0.4049775626
H	4.5185745248	-2.0124512923	2.4760315272
H	3.6103238129	-1.2976380695	4.6733457399
H	1.4322301241	-0.1078998585	4.7750715843
H	0.1980606341	0.3873328095	2.7075618765
C	1.4801748764	-0.4234950762	-1.3862349989
C	0.8165513107	-1.0020225252	-2.4789990114
C	1.4075140441	-1.0762091401	-3.7379510311
C	2.6834568502	-0.5581432324	-3.9427649503
C	3.3608189796	0.0304800738	-2.8777790461
C	2.7654280746	0.0940394353	-1.6206570870

H	-0.1836111737	-1.4100938763	-2.3511755307
H	0.8683913705	-1.5369736981	-4.5603060419
H	3.1455522031	-0.6123150186	-4.9235569387
H	4.3566561613	0.4382405584	-3.0237464275
H	3.3100575572	0.5592802505	-0.8020825551
C	1.3577885200	2.7405716291	-0.2655296890
H	2.1202225634	2.5453904555	0.4965234942
H	1.8118584774	2.6222465635	-1.2528306684
H	1.0313917465	3.7822140864	-0.1556770330
C	-1.0739720142	2.3327374337	1.4551951926
H	-1.8632055405	1.6880359721	1.8503499681
H	-0.3736258495	2.5694156178	2.2629226005
H	-1.5427059548	3.2747598989	1.1438676250
C	-1.2500109274	1.8146636901	-1.5745606367
H	-1.4161002084	2.8818656404	-1.7642339937
H	-0.7628801997	1.3904924450	-2.4589644729
H	-2.2309162760	1.3437609091	-1.4542185286

M14-TS1

B	1.0061554632	-0.3647461463	0.2950958989
Si	-0.4131856710	1.2149353676	0.0589589168
C	-0.8532580538	-1.4337511814	0.4923501119
O	-2.0070612111	-1.2777834357	0.4820518156
O	0.2172591886	-1.9765019137	0.5312534895
C	1.8900869357	-0.2432279535	1.6073823952
C	3.2032374375	-0.7423842362	1.6105928169
C	3.9967868803	-0.6959301997	2.7541126458
C	3.4920191526	-0.1476772732	3.9313916390
C	2.1912134058	0.3479497055	3.9577549800
C	1.4065030129	0.2988997868	2.8078887563
H	3.6082185793	-1.1770505730	0.7000326532
H	5.0087070335	-1.0891682913	2.7275209628
H	4.1093817809	-0.1077721044	4.8237338316
H	1.7887451510	0.7751023538	4.8713361119
H	0.3938587185	0.6930294199	2.8504255068
C	1.6793512261	-0.5219982323	-1.1340060871
C	1.1810070169	-1.3650653120	-2.1392966363
C	1.7416334866	-1.3932731992	-3.4135931479
C	2.8153783016	-0.5620241198	-3.7234641780
C	3.3318960941	0.2820154357	-2.7431583653
C	2.7735382150	0.2941970934	-1.4672047411
H	0.3361744411	-2.0191645980	-1.9339905039
H	1.3333827986	-2.0590746944	-4.1680643137
H	3.2476914184	-0.5745817775	-4.7190844119
H	4.1736700994	0.9294464109	-2.9700198908
H	3.1924653794	0.9556745681	-0.7116604368
C	0.7722329070	2.7002229316	0.0053406678
H	1.4072838591	2.6198105513	-0.8841681401
H	1.4404339096	2.6653876664	0.8752051691
C	0.0062505213	4.0319253435	-0.0166796627

H	-0.5782386402	4.1735740508	0.8986490864
H	0.6885761330	4.8835784227	-0.1044896785
H	-0.6920455985	4.0826216652	-0.8604291631
C	-1.6429574082	1.5641550942	1.4872340306
H	-1.1544671215	2.2906381221	2.1512133891
H	-1.8127109383	0.6691887126	2.0954428520
C	-2.9994620291	2.1196118925	1.0348762562
H	-3.5432152344	1.3839162242	0.4332763249
H	-3.6292470766	2.3784371945	1.8919880319
H	-2.8834947611	3.0229043993	0.4252044590
C	-1.3088960811	1.1193295756	-1.6226123211
H	-2.2540592289	1.6708656274	-1.5402609757
H	-1.5956739394	0.0805898193	-1.8320330746
C	-0.5030058212	1.6742961734	-2.8076290309
H	0.4527189148	1.1559579120	-2.9322194327
H	-1.0620885141	1.5690882182	-3.7431362530
H	-0.2849824286	2.7391554587	-2.6752553805

M15-TS1

B	0.9294906069	-0.3201385474	-0.0484654877
Si	-0.3328395819	1.4545582955	0.0376596655
C	-1.0306636361	-1.1613880883	-0.1424476152
O	-2.1617640026	-0.9585720351	-0.3042221494
O	-0.0039136811	-1.7788188223	0.0078349354
C	1.7189530722	-0.3697919476	1.3294336750
C	1.0519697972	-0.4811018674	2.5594548215
C	1.7445488588	-0.4781865669	3.7673905997
C	3.1333868941	-0.3643235631	3.7706480412
C	3.8192882314	-0.2766100325	2.5612593981
C	3.1188031060	-0.2839292649	1.3571243724
H	-0.0342062892	-0.5511281391	2.5819345137
H	1.1992340657	-0.5557553265	4.7032925148
H	3.6776419703	-0.3516233617	4.7101081504
H	4.9027923057	-0.2037500252	2.5546734315
H	3.6684523901	-0.2152956916	0.4226999127
C	1.6944551169	-0.3963001376	-1.4426755440
C	1.5116972062	-1.4565285646	-2.3459737965
C	2.1709026467	-1.4965980389	-3.5734016395
C	3.0375280056	-0.4703135225	-3.9367276613
C	3.2497189445	0.5844949512	-3.0526680504
C	2.5917173525	0.6174825126	-1.8258173826
H	0.8432335506	-2.2758047643	-2.0962390395
H	2.0045405454	-2.3334489023	-4.2453292789
H	3.5474067640	-0.4955642487	-4.8947796689
H	3.9295327610	1.3892363206	-3.3161283324
H	2.7811587069	1.4522497170	-1.1570395259
C	1.0177028485	2.7832744691	0.1169818832
C	1.0960683880	3.7267635436	-0.9202307009
C	2.0898245573	4.7036826354	-0.9372360688
C	3.0315180193	4.7596977774	0.0859411003

C	2.9688066239	3.8384394924	1.1290822454
C	1.9752772580	2.8624996210	1.1430616532
H	0.3790195328	3.6924913919	-1.7358824369
H	2.1290675204	5.4174524758	-1.7545760279
H	3.8103431354	5.5161641651	0.0717625831
H	3.6988375101	3.8717337929	1.9322285328
H	1.9733023001	2.1428240433	1.9564638807
C	-1.4713325410	1.6546880819	1.5426040857
C	-2.8453615348	1.3700626953	1.4648351243
C	-3.6799696675	1.5106105361	2.5717307403
C	-3.1605597544	1.9462623771	3.7877865603
C	-1.8059485634	2.2531361959	3.8848183445
C	-0.9770358949	2.1132312554	2.7744476712
H	-3.2777147969	1.0451125645	0.5228581981
H	-4.7378120679	1.2834771446	2.4801074371
H	-3.8093613633	2.0561158142	4.6514689052
H	-1.3928292016	2.6090111539	4.8238808354
H	0.0724743131	2.3705350652	2.8759076330
C	-1.3634613458	1.7996987170	-1.5060443424
C	-2.3226799891	2.8244813484	-1.4734486350
C	-3.0649217527	3.1565022662	-2.6043536477
C	-2.8620452283	2.4661385265	-3.7971894950
C	-1.9110236174	1.4510627553	-3.8536078710
C	-1.1679193232	1.1252616364	-2.7199389370
H	-2.4944013364	3.3720926956	-0.5486878042
H	-3.8017811312	3.9524662675	-2.5535225462
H	-3.4411470052	2.7208679858	-4.6796540048
H	-1.7424911596	0.9123082859	-4.7810996577
H	-0.4170102928	0.3418648291	-2.7942187056

M16-TS1

B	0.8211589811	-0.2905790040	0.1895769780
Si	-0.3643701532	1.6931783125	0.2208009569
C	-1.1834048738	-0.7631431669	0.5867115286
O	-2.3329543305	-0.6005123210	0.5434371007
O	-0.1770153962	-1.4403940556	0.7470531942
C	1.9572783364	-0.0547312790	1.2644736028
C	3.2083653406	0.4395582053	0.8555575006
C	4.2112976545	0.7209221735	1.7769694865
C	3.9915435273	0.5002430869	3.1367733812
C	2.7739567859	-0.0249821184	3.5592785732
C	1.7708331362	-0.3005118758	2.6315714662
H	3.4014030126	0.6051054863	-0.2010150549
H	5.1668159801	1.1077664380	1.4347498708
H	4.7687355859	0.7271587642	3.8599370523
H	2.5989781357	-0.2144243879	4.6136843864
H	0.8261327087	-0.6996376604	2.9865103027
C	1.1663474657	-0.6492500598	-1.3155270895
C	0.9297202547	-1.9468053931	-1.7970909900
C	1.2506346168	-2.3070714407	-3.1030933062

C	1.8131290457	-1.3729649021	-3.9691338291
C	2.0645723477	-0.0820861508	-3.5126952110
C	1.7480285599	0.2686234570	-2.2023116648
H	0.4817909242	-2.6935563152	-1.1471523525
H	1.0542426915	-3.3183199598	-3.4458274599
H	2.0552393541	-1.6495111595	-4.9904297477
H	2.5065226581	0.6559642084	-4.1751898589
H	1.9484614911	1.2850424659	-1.8799030668
C	1.0709602766	2.8246958813	0.7502599123
C	1.9962239658	3.4282027207	-0.0971580001
C	3.1250415530	4.0929583005	0.3628685692
C	3.3676982891	4.1642365921	1.7267714701
C	2.4764897478	3.5758362653	2.6128070267
C	1.3566537930	2.9311984364	2.1118401683
F	4.4499018711	4.7807068648	2.1800106270
F	2.7099487858	3.6164372256	3.9192262568
F	0.5480081495	2.3571480756	3.0112498156
F	3.9785874326	4.6451007821	-0.4934310685
F	1.8621044435	3.3624577064	-1.4294096421
C	-1.8061131494	2.1314099885	1.3991502489
C	-2.0326952607	1.4164539195	2.5715164004
C	-3.0669164590	1.6793779729	3.4510064665
C	-3.9372714114	2.7253522987	3.1664321059
C	-3.7556480715	3.4729062558	2.0134170307
C	-2.7027160753	3.1674265807	1.1566733986
F	-4.9358949240	3.0020346112	3.9914814745
F	-4.5838519590	4.4728915419	1.7329841990
F	-2.5899751292	3.9300877436	0.0669275839
F	-3.2355481737	0.9478727148	4.5470827366
F	-1.2271151445	0.3831323387	2.8781624745
C	-0.9202031488	2.1321638865	-1.5344610721
C	-0.8402669726	3.4293206186	-2.0404668449
C	-1.1708892457	3.7481612850	-3.3483110452
C	-1.6153567112	2.7446801077	-4.2008067830
C	-1.7339898395	1.4434287188	-3.7348476022
C	-1.3957168677	1.1670884677	-2.4178882428
F	-1.9372151605	3.0338608195	-5.4531647753
F	-2.1688528732	0.4817645726	-4.5415089629
F	-1.5519306678	-0.1018407145	-2.0181529327
F	-1.0751734216	4.9975547655	-3.7904646336
F	-0.4359264778	4.4331176502	-1.2592444763

M17-TS1

B	-0.0521520420	0.4676407151	-0.7378554401
Si	0.0623133166	-1.4010565210	0.4629008274
C	-0.0171276272	-1.1487098140	-2.0493281415
O	0.0147135027	-2.2719455185	-2.3518868993
O	-0.0314377613	0.0501092797	-2.3027290648
C	1.3416972336	1.1217694264	-0.3854237602
C	1.5495799459	1.8084092769	0.8233409469

C	2.7815194987	2.3785853848	1.1283924212
C	3.8416500693	2.2735739502	0.2314772473
C	3.6614634271	1.5956879241	-0.9712513868
C	2.4292349626	1.0229061321	-1.2694501603
H	0.7399391614	1.8920675048	1.5415661122
H	2.9130809611	2.9027747342	2.0696563589
H	4.8042374225	2.7150727327	0.4698040855
H	4.4822051742	1.5069809744	-1.6759620211
H	2.3189561354	0.4970365683	-2.2142001201
C	-1.4735098315	1.0721865952	-0.4128908790
C	-1.5992924653	2.3994500573	0.0230691312
C	-2.8514663846	2.9656907904	0.2502655176
C	-4.0061477016	2.2150140713	0.0464581104
C	-3.9055492829	0.8982189976	-0.3969635606
C	-2.6522244151	0.3389976990	-0.6224350183
H	-0.7096084272	3.0051092612	0.1657886790
H	-2.9243194333	3.9965002101	0.5829090337
H	-4.9816816179	2.6545632126	0.2294630523
H	-4.8001286091	0.3060428735	-0.5609576567
H	-2.5988486198	-0.6958707098	-0.9588623788
Cl	-0.2161611000	-0.6025368961	2.3403674747
Cl	1.9297438201	-2.2702433291	0.4463207000
Cl	-1.3325953123	-2.9260285832	0.3721327894

M18-TS1

B	0.8351582528	-0.3685834531	-0.0472267568
Si	0.0055423020	1.5526281148	0.0300672719
C	-1.1805137524	-0.6501700180	0.1395939021
O	-2.2357169965	-0.2062655764	0.3496895113
O	-0.3604550037	-1.5215049218	-0.0915331385
C	1.6532305918	-0.5723851628	1.2927070160
C	1.1122994146	-0.2643874219	2.5512285332
C	1.8118102170	-0.5304721004	3.7251537045
C	3.0782087063	-1.1055616080	3.6613097050
C	3.6378583373	-1.4139178343	2.4230139010
C	2.9323465453	-1.1482701802	1.2526050061
H	0.1338661898	0.2088185677	2.6231243916
H	1.3728784547	-0.2800872786	4.6857558911
H	3.6296803087	-1.3093200247	4.5739642927
H	4.6244770172	-1.8637841805	2.3690799493
H	3.3748216581	-1.3991162119	0.2922711575
C	1.5122917206	-0.3324763929	-1.4809990064
C	2.7046534975	0.3848093437	-1.6762598595
C	3.3200462030	0.4307101210	-2.9232553344
C	2.7543187205	-0.2378267662	-4.0067232070
C	1.5693853627	-0.9484239767	-3.8359566764
C	0.9528132330	-0.9870228299	-2.5881715885
H	3.1536305870	0.9161627488	-0.8412970608
H	4.2418868141	0.9899902368	-3.0488284969
H	3.2332296143	-0.2022571135	-4.9802151766

H	1.1213597698	-1.4707181462	-4.6755515523
H	0.0276240828	-1.5470724047	-2.4790441367
F	1.3301208962	2.4374733688	0.0507805450
F	-0.8312446094	2.0202473877	1.3091909221
F	-0.8364518002	1.9778407543	-1.2554440711

M19-TS1

B	0.7740622674	-0.4160718761	-0.0040885690
Si	-0.2906119347	1.4461815020	0.0012402214
C	-1.1684259115	-1.1015099846	-0.0199202901
O	-2.2836669894	-0.7844604575	-0.0672325999
O	-0.1936189427	-1.8186545367	0.0301435636
C	1.4974545852	-0.4024426890	1.4213065792
C	2.8361826563	-0.0547366870	1.5878691390
C	3.4554172507	-0.0051634733	2.8303626643
C	2.7258713352	-0.3112569111	3.9708920608
C	1.3854510795	-0.6566888894	3.8559821093
C	0.8061521099	-0.6861740918	2.5968851833
F	3.3038226271	-0.2715433577	5.1641745850
F	0.6743536701	-0.9427719785	4.9419067511
F	-0.5035766037	-0.9967404194	2.5378486245
F	4.7372819499	0.3299292947	2.9346971153
F	3.5919437113	0.2611338595	0.5286098340
C	1.6743867330	-0.6920331381	-1.2970828247
C	1.7603446418	0.0757542113	-2.4515111605
C	2.5867680074	-0.2502965665	-3.5215318090
C	3.3605229377	-1.3986901006	-3.4583093105
C	3.3013787771	-2.2071718598	-2.3287138081
C	2.4707460454	-1.8388150982	-1.2835234786
F	4.1482853612	-1.7294681591	-4.4724589078
F	4.0389673645	-3.3107883672	-2.2634577068
F	2.4437617714	-2.6374871863	-0.2087486686
F	2.6294327677	0.5230452413	-4.6024073316
F	1.0321032297	1.1943070204	-2.5873211675
C	1.2387214113	2.5641027988	0.0128548514
H	1.5758040890	2.7089341129	1.0448672932
H	2.0788370766	2.1785980598	-0.5692081879
H	0.9676937364	3.5443861959	-0.3958728012
C	-1.2042255957	1.7820857090	1.6171188359
H	-2.0988467669	1.1669735267	1.7461639986
H	-0.5627841799	1.6585664379	2.4949790285
H	-1.5243396823	2.8316159876	1.5917368511
C	-1.4846117273	1.8167218742	-1.4170616556
H	-1.4185136252	1.0995946713	-2.2389050322
H	-2.5148667820	1.8234180906	-1.0490729096
H	-1.2625014062	2.8062606361	-1.8311573056

M20-TS1

B	0.8113328516	-0.5179601791	0.0279261676
Si	-0.4697060244	1.2429071653	0.0530602231

C	-1.0537866323	-1.4180865406	-0.0832186646
O	-2.1999460095	-1.2421759322	-0.1037399572
O	0.0013921690	-2.0126965470	-0.0644366110
C	1.4051273452	-0.4468533429	1.5119110741
C	0.7550926311	-0.9713308970	2.6265879556
C	1.2269272238	-0.8378679683	3.9247488537
C	2.4017612828	-0.1339106395	4.1491887221
C	3.0814970619	0.4211029025	3.0721762334
C	2.5758381708	0.2563096171	1.7908890632
F	2.8697503600	0.0108557586	5.3817227621
F	4.2054542519	1.1001295390	3.2757152350
F	3.2671345091	0.8222164394	0.7913612497
F	0.5560017585	-1.3590783517	4.9467086427
F	-0.4162011426	-1.6240651378	2.4833470812
C	1.8171811245	-0.6573332638	-1.2095241602
C	1.5062849521	-0.2576840723	-2.5045302108
C	2.3572696644	-0.4153730997	-3.5887866346
C	3.5854901614	-1.0310129831	-3.3957538548
C	3.9334538016	-1.4803869175	-2.1290318186
C	3.0482529160	-1.3019889480	-1.0749576976
F	4.4161178134	-1.1990831561	-4.4152629052
F	5.0982173131	-2.0925641930	-1.9407016244
F	3.4294227407	-1.7959121511	0.1077530054
F	2.0034379132	0.0078730510	-4.7988023562
F	0.3268168909	0.3323549250	-2.7535986753
C	0.8324585733	2.6224436057	-0.0812563816
H	1.5176033887	2.5548325984	0.7710565653
H	0.2345745190	3.5285264898	0.0990695646
C	1.6289027536	2.7884887307	-1.3783794672
H	0.9884702507	2.7347935503	-2.2648484625
H	2.1421829420	3.7546980027	-1.3965567119
H	2.3943308360	2.0129781935	-1.4667758625
C	-1.2724524721	1.4176196385	1.7761237056
H	-1.5276689645	0.4310652450	2.1790767037
H	-2.2368452102	1.9171809638	1.6091236151
C	-0.4710925838	2.2141089060	2.8155275717
H	-0.3333424845	3.2531837293	2.4998899422
H	-0.9829228492	2.2296175330	3.7827713674
H	0.5267808568	1.7928330507	2.9775521397
C	-1.8719281168	1.5608417379	-1.1913274253
H	-2.7724392072	1.0729389820	-0.8015614743
H	-1.6776812133	1.1217079573	-2.1718471506
C	-2.1406941404	3.0668547906	-1.3405232231
H	-1.2966845808	3.5812767793	-1.8110409187
H	-3.0248917042	3.2481001995	-1.9591021970
H	-2.3190074070	3.5459389184	-0.3698984187

M21-TS1

B	0.9737484171	-0.4328349462	0.1868053612
Si	-0.3691256822	1.4276682332	0.3237717638

C	-0.7649037201	-1.1981394934	0.8317601513
O	-1.8995279948	-1.1221624888	1.0766573742
O	0.2799639342	-1.8230500097	0.6865703491
C	2.2424737164	-0.2865963686	1.1481610146
C	2.2684668829	0.4214857115	2.3446393178
C	3.3861136325	0.5035583801	3.1635605169
C	4.5333785306	-0.1913715005	2.8103518422
C	4.5393489076	-0.9648868512	1.6569791858
C	3.4003541514	-1.0139540374	0.8673595496
F	5.6098716073	-0.1396178565	3.5834814797
F	5.6225435957	-1.6653090375	1.3346521661
F	3.4405991770	-1.8229770514	-0.1969309825
F	3.3534474878	1.2107110561	4.2890885880
F	1.1653519907	1.0482639929	2.7828759101
C	1.1646038735	-0.5706567014	-1.4017293573
C	0.1433321176	-1.0991505973	-2.1968916271
C	0.1614280638	-1.1216437279	-3.5809757034
C	1.2648619997	-0.6081957496	-4.2473922418
C	2.3244248202	-0.1016381810	-3.5112412053
C	2.2624631703	-0.1028817649	-2.1232505204
F	1.3072249576	-0.6075671278	-5.5729962337
F	3.3979810662	0.3757108389	-4.1346754808
F	3.3383427507	0.4010929455	-1.4999024393
F	-0.8643490618	-1.6142536049	-4.2667277618
F	-0.9661018782	-1.5961811820	-1.6181601535
C	0.9054152665	2.7970706568	0.5901439662
C	2.1097064464	2.8932781092	-0.1205809109
C	2.9982792822	3.9438377767	0.0968809569
C	2.6987021136	4.9259584194	1.0366989046
C	1.5086958841	4.8495522433	1.7550750473
C	0.6237949662	3.7964952383	1.5361952224
H	2.3771226956	2.1378467457	-0.8485004728
H	3.9245949135	3.9897850380	-0.4674548624
H	3.3901608597	5.7446257852	1.2104936529
H	1.2677838225	5.6083756065	2.4931613960
H	-0.2921926124	3.7503617261	2.1182366773
C	-1.7584066298	1.7161909046	1.5667483250
C	-1.7849296596	1.2301562214	2.8823013884
C	-2.8006208469	1.5881999038	3.7629185139
C	-3.8146512322	2.4498743224	3.3486732393
C	-3.8054607062	2.9488450776	2.0505958373
C	-2.7878617196	2.5834731042	1.1697990009
H	-1.0066506812	0.5592021163	3.2331250130
H	-2.8007269992	1.1925543864	4.7738017537
H	-4.6073749301	2.7290075704	4.0358391906
H	-4.5902455071	3.6210539753	1.7176923620
H	-2.7992015649	2.9847849558	0.1593343694
C	-1.1002614415	1.5638602018	-1.4065188788
C	-0.4074785475	2.2165092542	-2.4375352553
C	-0.8805254688	2.1942589009	-3.7480349504

C	-2.0614171858	1.5195879793	-4.0506478560
C	-2.7788513361	0.8897261462	-3.0355294302
C	-2.3044879692	0.9176892746	-1.7263991934
H	0.5149787918	2.7482403176	-2.2181238400
H	-0.3260330247	2.7012937478	-4.5321532198
H	-2.4251366626	1.4894656837	-5.0730564156
H	-3.7044561185	0.3707260297	-3.2639632046
H	-2.8746651346	0.4170978475	-0.9462865411

M22-TS1

B	-1.2839745522	0.2095723058	-1.2654911712
Si	0.9250113682	0.1209451704	0.0137890751
C	0.3674658314	0.2439850727	-2.3425127236
O	1.4630797844	0.1312936157	-2.7515464204
O	-0.8173990440	0.3678129186	-2.7206660509
C	-2.0501649563	1.5453494509	-0.8567376943
C	-1.6640377585	2.6083131526	-0.0537822028
C	-2.4454635987	3.7424070817	0.1293350061
C	-3.6662815590	3.8431807334	-0.5205673478
C	-4.0875881341	2.8132394152	-1.3528303799
C	-3.2747497306	1.7026640285	-1.5072394518
F	-4.4216053942	4.9192270436	-0.3569373623
F	-5.2490359336	2.9033005313	-1.9892231489
F	-3.6976000584	0.7334589906	-2.3289714498
F	-2.0237585453	4.7287500107	0.9136678213
F	-0.4835793088	2.5992495362	0.5877571241
C	-1.8926495803	-1.2450096749	-1.0695690061
C	-1.2757091255	-2.3718711009	-1.6160204170
C	-1.7189988353	-3.6697571455	-1.4160726856
C	-2.8823138098	-3.8794110733	-0.6909097153
C	-3.5810497024	-2.7867677372	-0.1933141868
C	-3.0884990492	-1.5052683741	-0.3930083167
F	-3.3331442628	-5.1067443761	-0.4908218558
F	-4.7174472987	-2.9759732015	0.4663420925
F	-3.8284552548	-0.5103602267	0.0952234053
F	-1.0287983446	-4.6988636525	-1.8992714534
F	-0.1550159339	-2.2392035173	-2.3481543577
C	0.4212846969	0.3955563329	1.8405971451
C	-0.8670020891	0.2171427163	2.3354742426
C	-1.2281151109	0.4173414864	3.6578312660
C	-0.2643200263	0.8289853072	4.5676808778
C	1.0339225997	1.0310141582	4.1291120360
C	1.3509685743	0.8199274157	2.7915899652
C	2.2891414073	1.3637650374	-0.3886364255
C	2.0322615016	2.5130577033	-1.1299576819
C	3.0118502530	3.4304671679	-1.4733666868
C	4.3202218670	3.1973068943	-1.0696475173
C	4.6287037771	2.0502627644	-0.3502041571
C	3.6183964434	1.1546670359	-0.0297001493
C	1.5313381295	-1.6580884541	-0.1187961197

C	0.7632306046	-2.6653697937	0.4644702301
C	0.9901966544	-4.0157136787	0.2539459680
C	2.0580258561	-4.4024733572	-0.5439300593
C	2.8748877749	-3.4357060729	-1.1159318171
C	2.6000927765	-2.0906855737	-0.9062124455
F	-0.3013521877	-2.3454929544	1.2168262543
F	0.1722226642	-4.9248841369	0.7728116945
F	2.2942811920	-5.6852063458	-0.7611910954
F	3.9019577718	-3.8032488146	-1.8711728547
F	3.4045063923	-1.2237865720	-1.5179801251
F	3.9734998167	0.0548146269	0.6358756244
F	5.8824332572	1.8168537480	0.0178231365
F	5.2743426907	4.0588818126	-1.3852020855
F	2.7148004199	4.5050945698	-2.1943063973
F	0.7978677309	2.7350022379	-1.6159676784
F	-1.8471194554	-0.1558338269	1.5112936042
F	-2.4813577885	0.2249669221	4.0512990104
F	-0.5825988507	1.0264534944	5.8366816301
F	1.9716826307	1.4265804455	4.9817444354
F	2.6237598132	1.0462837260	2.4656180492

M23-TS1

B	0.8402922084	-0.5087309856	-0.0368658959
Si	0.0542567317	1.6734824531	0.0545396650
C	-1.1786248421	-0.4627871214	-0.0565994533
O	-2.2681773722	-0.0520079410	-0.0265687174
O	-0.4133962163	-1.4375577913	-0.0892328044
C	1.5213462615	-0.5094574796	1.3892588534
C	0.8009178407	-0.7908552954	2.5535255446
C	1.3619778459	-0.7766842830	3.8194298016
C	2.7055427646	-0.4513788307	3.9570631279
C	3.4616895286	-0.1462153791	2.8327034364
C	2.8649189414	-0.1724737347	1.5807851162
F	3.2627384471	-0.4312827403	5.1564910619
F	4.7448200485	0.1658281372	2.9631474226
F	3.6409837009	0.1387161715	0.5434833232
F	0.6296237784	-1.0522157933	4.8911363286
F	-0.5127135586	-1.0503824487	2.4806989737
C	1.6690963127	-0.7219180695	-1.3730968501
C	2.7257438027	-1.6317061687	-1.3974066442
C	3.4437879048	-1.9168900650	-2.5498792963
C	3.0939592717	-1.2968715654	-3.7424730263
C	2.0280443670	-0.4070222020	-3.7717333390
C	1.3363574921	-0.1549634248	-2.5973191565
F	3.7664777696	-1.5639047150	-4.8512706095
F	1.6741738505	0.1760103306	-4.9101899215
F	0.2922830282	0.6869796432	-2.6669114059
F	4.4463771585	-2.7867131014	-2.5250087868
F	3.0760686433	-2.2867986536	-0.2869459958
Cl	1.8835483889	2.5018310481	-0.3691233527

Cl	-0.4158377565	2.1571041436	1.9970345150
Cl	-1.3129357774	2.6524968394	-1.1133633532

M24-TS1

B	0.8458160498	-0.5974672287	0.0068911663
Si	0.0505785858	1.4232089781	-0.1170938293
C	-1.0910806071	-0.6791519697	0.0858609938
O	-2.1769355313	-0.2512958110	0.1409389635
O	-0.3260407118	-1.6522236462	0.0368921469
C	1.6996127450	-0.7443909114	1.3369480817
C	2.6591303708	-1.7516865207	1.4072010099
C	3.4238311097	-1.9798609448	2.5398709219
C	3.2276097958	-1.1812998515	3.6616662359
C	2.2737716392	-0.1727098563	3.6388336070
C	1.5300023090	0.0174459434	2.4831189230
F	3.9471682059	-1.3882766525	4.7540627405
F	2.0756978935	0.5847871747	4.7105308900
F	0.5987128561	0.9868916129	2.4970784634
F	4.3320378905	-2.9476999083	2.5672785976
F	2.8656717884	-2.5351470288	0.3440456580
C	1.5400524585	-0.5489998536	-1.4214783309
C	0.7992519487	-0.7251417164	-2.5919386626
C	1.3562085467	-0.6901414688	-3.8588019161
C	2.7190473574	-0.4478136330	-3.9848475539
C	3.4945578850	-0.2411690125	-2.8514592682
C	2.8988385844	-0.2832238074	-1.5985541063
F	3.2757382672	-0.4099412665	-5.1845956897
F	4.7942469209	-0.0013663049	-2.9740520231
F	3.6888674918	-0.0555576458	-0.5494393392
F	0.6084082064	-0.8715541071	-4.9397618865
F	-0.5260862366	-0.9126460162	-2.5085457080
F	1.4609278471	2.1130940935	0.1316257188
F	-1.0192248308	2.1318813650	0.8106283665
F	-0.3866283237	1.7178791553	-1.6165176004

M25-TS1

B	-0.8910093682	0.1284461909	0.0003745125
Si	1.1256616479	-0.5642752622	-0.0001920054
C	0.0920707938	1.9470445844	0.0003485712
O	1.1241528880	2.4709413671	0.0001610597
O	-1.1114068388	1.7936168703	0.0006203277
Cl	-1.6711985592	-0.4086156108	1.5421300810
Cl	-1.6719412067	-0.4082585887	-1.5411294500
C	0.7633632701	-2.4125102765	-0.0003212821
H	0.1983528438	-2.7103584686	-0.8879461721
H	1.7179399479	-2.9525921908	-0.0006093499
H	0.1987717390	-2.7105652570	0.8875007110
C	2.0800640617	-0.1311116316	1.5637985669
H	2.4685675245	0.8908860669	1.5640612743
H	1.4495952064	-0.2676415828	2.4489294202

H	2.9334620068	-0.8125454932	1.6578483913
C	2.0793111406	-0.1307452571	-1.5645403901
H	2.4678243796	0.8912487391	-1.5647452705
H	2.9326567067	-0.8121648346	-1.6591670539
H	1.4484128160	-0.2670563648	-2.4493989416

M26-TS1

B	-1.2296238821	0.1174852118	-0.2611624491
Si	0.8611707362	-0.0429599795	0.1952549719
C	-0.7998337489	-1.6595498592	-1.2065702643
O	0.0357531323	-2.3786630378	-1.5608461332
O	-1.9096717178	-1.1862285530	-1.0642243579
Cl	-1.4708612550	1.5009500954	-1.4085184214
Cl	-2.1539947292	0.1954203280	1.2911328472
C	1.0378936661	1.3345258677	1.4826816951
H	2.1051092561	1.3097070313	1.7496834135
H	0.4923077821	1.0320659902	2.3846964811
C	0.6387464159	2.7529735299	1.0669089329
H	-0.4438362853	2.8385447823	0.9403858443
H	0.9449671130	3.4825104632	1.8228363918
H	1.1035696018	3.0409753806	0.1171440273
C	1.9326684005	0.3350225877	-1.3135888907
H	1.5109243976	1.1966720776	-1.8446696515
H	1.8945714770	-0.5107673282	-2.0112530377
C	3.3912256230	0.6194072532	-0.9226962792
H	3.8301545804	-0.2180325968	-0.3682354902
H	4.0146095981	0.7906716766	-1.8052608030
H	3.4657017341	1.5105657127	-0.2904958235
C	1.4191613422	-1.6486515223	1.0357916654
H	2.2843995387	-1.3759386736	1.6558625143
H	1.7964065661	-2.3502219942	0.2827901321
C	0.3635849833	-2.3294932998	1.9174097694
H	-0.5046606999	-2.6616435211	1.3340234468
H	0.7716139322	-3.2122673911	2.4184439663
H	-0.0165525589	-1.6507092314	2.6870775023

M27-TS1

B	0.2207580360	0.6366536189	2.0090183976
Si	-0.0511642592	-0.0370554469	-0.0354170410
C	-0.8900792295	-1.0371949467	2.2766695251
O	-1.4244013598	-1.9665583126	1.8397369555
O	-0.4896263420	-0.2762737804	3.1491329624
Cl	-0.5597446672	2.2648964193	2.1469288197
Cl	1.9928815140	0.5761353075	2.3696242497
C	0.7743400903	1.3940830972	-0.9272426718
C	0.0303496569	2.4216917126	-1.5223434168
C	0.6643867814	3.4673493725	-2.1888057932
C	2.0539603448	3.5001577225	-2.2700965636
C	2.8087682497	2.4824159990	-1.6904647657
C	2.1734305855	1.4376643544	-1.0260577829

H	-1.0550895574	2.4047024738	-1.4751284669
H	0.0728285197	4.2546675568	-2.6456505594
H	2.5489056783	4.3158452349	-2.7883432538
H	3.8921308207	2.5019959912	-1.7562637171
H	2.7719100691	0.6468787286	-0.5801375368
C	-1.8512782920	-0.2099606189	-0.5574128871
C	-2.8032847886	0.7834610314	-0.2712740329
C	-4.1355008163	0.6313545625	-0.6492724747
C	-4.5438875985	-0.5186413865	-1.3203052054
C	-3.6171741688	-1.5177451358	-1.6056714169
C	-2.2860483544	-1.3651045280	-1.2242695688
H	-2.5083610950	1.6840631292	0.2611068549
H	-4.8540638375	1.4112081346	-0.4165164591
H	-5.5820232184	-0.6377772801	-1.6147643509
H	-3.9307457530	-2.4207223299	-2.1204049212
H	-1.5798903283	-2.1640437420	-1.4363794267
C	0.9247477065	-1.5969017399	-0.4192555541
C	1.4883229972	-2.4437798163	0.5430643904
C	2.2062355173	-3.5795684071	0.1746300088
C	2.3755282114	-3.8886202541	-1.1719194092
C	1.8352040133	-3.0536520827	-2.1476652831
C	1.1234679388	-1.9175494711	-1.7724429217
H	1.3952123834	-2.2131510167	1.6025699162
H	2.6365714205	-4.2181215722	0.9396425085
H	2.9344590634	-4.7732116205	-1.4610872155
H	1.9732232627	-3.2833194429	-3.1996542286
H	0.7201938049	-1.2666325157	-2.5467566642

M28-TS1

B	0.0432526986	0.6058528363	2.6024662357
Si	0.0299500603	-0.0770409374	0.4632967295
C	0.2966928805	-1.3629444371	2.6386922803
O	0.4903205867	-2.4314228100	2.2243369947
O	0.1340971275	-0.5844179018	3.5887033467
Cl	-1.5854194390	1.3655645619	2.7021691794
Cl	1.4476756846	1.6897673347	2.8570532468
C	0.2809884430	1.6499527596	-0.2435091253
C	-0.7623471013	2.5210992328	-0.5527256039
C	-0.5452167871	3.7953649465	-1.0572553376
C	0.7567681475	4.2357195034	-1.2573650908
C	1.8261865383	3.4040353581	-0.9509859500
C	1.5706028431	2.1372680390	-0.4490015631
F	0.9783623785	5.4494608461	-1.7362903961
F	3.0716730277	3.8266870556	-1.1314533016
F	2.6276278881	1.3805561037	-0.1375380115
F	-1.5664129713	4.5921515091	-1.3479769442
F	-2.0322724107	2.1546068507	-0.3719501545
C	-1.6765977058	-0.7242791253	-0.0124534074
C	-2.5175418601	-1.4200693823	0.8497618035
C	-3.7788265262	-1.8668489588	0.4833948328

C	-4.2395816248	-1.6063066465	-0.7996474253
C	-3.4407313613	-0.9028025010	-1.6931765351
C	-2.1872907896	-0.4751077915	-1.2859152683
F	-5.4393559868	-2.0234566077	-1.1704603747
F	-3.8844120488	-0.6426051337	-2.9164227574
F	-1.4654510475	0.2219538136	-2.1665407677
F	-4.5393733446	-2.5307705282	1.3449126048
F	-2.1367465425	-1.6858256711	2.1100528164
C	1.3748383261	-1.2098959701	-0.2341500912
C	1.2431595810	-1.9073603936	-1.4298896398
C	2.2368746108	-2.7453033107	-1.9231954504
C	3.4113269865	-2.9050038224	-1.2024800382
C	3.5822271035	-2.2328597999	0.0032700266
C	2.5695903941	-1.4051860723	0.4540437294
F	4.3659716322	-3.7012523059	-1.6565848255
F	4.6976484433	-2.3941183961	0.7036531244
F	2.7522388709	-0.7899485886	1.6312929800
F	2.0673154522	-3.3910023059	-3.0707221366
F	0.1308518425	-1.7988533530	-2.1603837346

M29-TS1

B	0.7392802386	-0.4955243365	0.0008658820
Si	-0.4160522199	1.4552714853	0.0001158538
C	-1.1994320358	-0.8778671478	-0.0017919847
O	-2.3493743382	-0.7040513673	-0.0032227908
O	-0.2411692332	-1.6743908422	-0.0008429903
Cl	1.6261620937	-0.4169997858	1.5453799131
Cl	1.6301386719	-0.4158413351	-1.5413021589
Cl	1.1984724228	2.7014106951	0.0026985345
Cl	-1.5033109438	1.8694474057	1.6806424307
Cl	-1.4989306721	1.8707482855	-1.6829153972

M30-TS1

B	-0.9384360834	0.3041125912	-0.0001230831
Si	1.0119387615	-0.6170565388	0.0003211118
C	0.4008379376	1.7134209114	-0.0003037920
O	1.4803930277	2.1464202358	-0.0002823337
O	-0.8322749203	1.8543347526	-0.0004789632
Cl	-1.6456855546	-0.2710843541	1.5416992357
Cl	-1.6453298947	-0.2718165984	-1.5418351250
F	0.5425751798	-2.1266895275	0.0006254684
F	1.8948564635	-0.3763588640	1.2944853578
F	1.8951560828	-0.3769736081	-1.2937528765

M31-TS1

B	0.7837052452	-0.2409571867	-0.0001626484
Si	-0.3947941642	1.5426918285	-0.0001299106
C	-1.1116535574	-1.0306599694	-0.0003411428
O	-2.2485294140	-0.7905870830	-0.0004659653
O	-0.1050667517	-1.7079421050	-0.0002442905

F	1.4821638357	-0.3040881468	1.1567987125
F	1.4822665321	-0.3040137872	-1.1570651020
C	1.1225305987	2.6662598858	0.0001525141
H	1.7407520659	2.4976751135	0.8867439691
H	1.7410370345	2.4977534683	-0.8862556088
H	0.7969427472	3.7132835232	0.0001437566
C	-1.3932087740	1.8557510287	1.5632379771
H	-2.3413158697	1.3112393360	1.5764864307
H	-0.8177254716	1.5761319709	2.4522307811
H	-1.6185022144	2.9257994551	1.6385886169
C	-1.3928313870	1.8560036977	-1.5636869112
H	-2.3408867122	1.3114105228	-1.5773012588
H	-1.6182016109	2.9260478393	-1.6388693407
H	-0.8170892199	1.5766228266	-2.4525867785

M32-TS1

B	0.9402823113	-0.2016934008	0.0452522204
Si	-0.4134081984	1.4534178846	0.0015759092
C	-0.8666826656	-1.1768909069	0.0805016742
O	-2.0212326494	-1.0477528893	0.0371393354
O	0.1984097926	-1.7550576618	0.1350301787
F	1.6708898594	-0.1504393208	1.1820036666
F	1.6160227685	-0.2520884766	-1.1269655768
C	0.9900965463	2.7263021919	0.1346954096
H	1.7965068879	2.4414602832	-0.5516384415
H	1.4124727737	2.6705194475	1.1452427156
C	0.5233170230	4.1558862899	-0.1735555405
H	-0.2937406559	4.4674483163	0.4870121546
H	1.3386654197	4.8747965866	-0.0459223628
H	0.1674430770	4.2434292423	-1.2056173033
C	-1.5560597565	1.6364251104	1.4973095517
H	-2.5247252090	1.1675816465	1.2905394262
H	-1.7586587910	2.7098921370	1.6167190221
C	-0.9617610281	1.0753361719	2.7964727720
H	0.0124348568	1.5219079273	3.0202107012
H	-1.6190742876	1.2614995814	3.6508374502
H	-0.8070082226	-0.0083784402	2.7328533790
C	-1.3325529059	1.6709515840	-1.6395602857
H	-1.6989363046	0.7051469517	-2.0060052387
H	-0.6037345295	2.0209999816	-2.3823805652
C	-2.5092567159	2.6545659949	-1.5442104689
H	-2.1892598707	3.6379979469	-1.1838379752
H	-2.9866994190	2.7999441362	-2.5178890834
H	-3.2737698785	2.2856786787	-0.8528337815

M33-TS1

B	0.9536530311	-0.1096302667	0.0892188007
Si	-0.3555282832	1.6140035995	-0.0028676370
C	-0.8820361052	-0.9596174828	-0.0904780431
O	-2.0347038601	-0.8456465012	-0.1467281669

O	0.1809654910	-1.5637842887	-0.0503255371
F	1.5368288999	-0.1478352384	1.3139093978
F	1.7639206889	-0.0435839504	-0.9932798246
C	1.0239742223	2.8936303567	0.0374840256
C	1.1879321518	3.8306637263	-0.9916265176
C	2.1841351245	4.8028987702	-0.9196618018
C	3.0325203061	4.8509502111	0.1823646558
C	2.8803861510	3.9288856656	1.2167511901
C	1.8848263728	2.9600108401	1.1448573993
H	0.5289506974	3.8091808649	-1.8556054530
H	2.2950579701	5.5228145823	-1.7248254069
H	3.8100029451	5.6067593279	0.2379343498
H	3.5384324933	3.9647463470	2.0794485697
H	1.7796319093	2.2452604137	1.9569176238
C	-1.4306349300	1.8193847758	1.5208638123
C	-2.2123265104	2.9761578182	1.6628054231
C	-2.9915791419	3.1813916413	2.7981236428
C	-2.9930910481	2.2349417484	3.8208395830
C	-2.2091264790	1.0900546963	3.7079907660
C	-1.4348143740	0.8878304176	2.5675084239
H	-2.2112082646	3.7299356767	0.8769704738
H	-3.5935371015	4.0804557804	2.8872463536
H	-3.5990339675	2.3938003248	4.7074693896
H	-2.1974931494	0.3557938396	4.5074426417
H	-0.8112758794	-0.0029891294	2.5079178463
C	-1.3121480883	1.7451883876	-1.6110996040
C	-0.6286340004	1.6010422921	-2.8304018786
C	-1.3109853670	1.6477718607	-4.0434371439
C	-2.6912907767	1.8380839010	-4.0581389210
C	-3.3863363864	1.9726898451	-2.8589928952
C	-2.7017802880	1.9224323508	-1.6462718073
H	0.4485475229	1.4443443371	-2.8318868301
H	-0.7663933029	1.5334174480	-4.9755995978
H	-3.2246521422	1.8753913271	-5.0030413318
H	-4.4631165837	2.1109803858	-2.8665372874
H	-3.2588374539	2.0058906606	-0.7159847520

M34-TS1

B	1.2018387030	0.2380102937	-0.2705555801
Si	-0.3873993493	1.7278099639	0.0036655391
C	-0.3791695963	-0.8321542849	0.3865717310
O	-1.4537106588	-0.9685399294	0.7991617446
O	0.7273219726	-1.2348248451	0.0277632520
F	2.1877836576	0.5467125104	0.5924912893
F	1.4457255615	0.3604388938	-1.5942068355
C	0.8585564779	3.1402382937	-0.0891986538
C	1.5502346622	3.5256180209	1.0567404255
C	2.5159130623	4.5204581709	1.0559786742
C	2.8276837516	5.1539108175	-0.1404019588
C	2.1802961533	4.7839410497	-1.3123141022

C	1.2197606908	3.7832365101	-1.2709559270
F	3.7479901443	6.1054268961	-0.1650276546
F	2.4891449522	5.3813313441	-2.4572235500
F	0.6499900125	3.4452736858	-2.4302157231
F	3.1438465935	4.8634118899	2.1744005700
F	1.2979346228	2.9166005038	2.2197990826
C	-1.3565955639	1.8606791361	1.6184193137
C	-0.9045708168	1.1899417823	2.7523651340
C	-1.5658684770	1.2196390025	3.9673682750
C	-2.7406683181	1.9571762527	4.0715688950
C	-3.2342195906	2.6365695781	2.9667889595
C	-2.5396444287	2.5756369581	1.7641671661
F	-3.3913225094	2.0030893111	5.2233791742
F	-4.3604562408	3.3328604465	3.0638068587
F	-3.0635280138	3.2341360021	0.7280156330
F	-1.1014544215	0.5544775715	5.0176438805
F	0.2103360669	0.4464602086	2.6722567424
C	-1.5316386300	1.7914841624	-1.4895044841
C	-1.8521541911	0.6737237225	-2.2511830835
C	-2.6751955858	0.7292821860	-3.3670439856
C	-3.1952367740	1.9555074885	-3.7577835220
C	-2.8831581031	3.1049229570	-3.0399715287
C	-2.0576915161	3.0038499193	-1.9320718513
F	-3.9816670408	2.0327543818	-4.8194895851
F	-3.3648980134	4.2789443251	-3.4283227417
F	-1.7410465983	4.1329626775	-1.2946102459
F	-2.9598716478	-0.3680729044	-4.0575616865
F	-1.3549206885	-0.5337335568	-1.9331799464

M35-TS1

B	-1.5467605613	0.7128486981	-0.0003283080
Si	0.5892573474	0.0462875493	0.0001360598
C	-1.5476873041	-1.3140676245	-0.0002967789
O	-1.0856574384	-2.3753726402	-0.0001817143
O	-2.4980778847	-0.5242539353	-0.0005112467
F	-1.6626100199	1.3665985787	-1.1632087719
F	-1.6631022104	1.3666334531	1.1624834983
Cl	1.3442999217	1.9477729973	0.0002598090
Cl	1.2947135124	-0.8990654438	-1.6749144309
Cl	1.2939956372	-0.8989996326	1.6755258819

M36-TS1

B	0.7727973163	-0.3736078154	-0.0000367494
Si	-0.3863244125	1.4648467176	0.0001491932
C	-1.1636752375	-0.8654113148	-0.0003888324
O	-2.2965652744	-0.6180305614	-0.0004961063
O	-0.1924483370	-1.6249300183	-0.0004000558
F	1.4468149013	-0.3410359032	1.1611124033
F	1.4471246552	-0.3406016698	-1.1609940287
F	0.8682701363	2.4356863196	0.0005114773

F	-1.2552898518	1.7874027381	1.2901198980
F	-1.2549199117	1.7878845647	-1.2899499074

M1-TS2

B	0.8061860396	0.2215829163	-0.0158938840
Si	-1.0715382420	2.8873219619	0.0082170309
C	0.4330302424	2.8027073091	1.3808107792
O	1.2739384794	2.7822081583	2.1660271195
O	0.2405949146	1.4330109038	0.2690341383
C	0.2112784048	-0.6653569474	-1.1833657467
H	0.9901672793	-0.8724089933	-1.9291221061
H	-0.0905218825	-1.6455531426	-0.7911824435
H	-0.6469310576	-0.2211934990	-1.6966602688
C	2.0483035956	-0.2450441068	0.8476566945
H	2.4393190833	-1.2239277081	0.5547187096
H	2.8639868989	0.4852327510	0.7730629743
H	1.7822361216	-0.2875341552	1.9114284839
C	-1.7282731519	4.5915133339	0.5398991085
H	-0.9649757032	5.3718374821	0.4331131410
H	-2.5866566898	4.8804114931	-0.0800092043
H	-2.0600716470	4.5903633452	1.5852893122
C	-0.5053860434	3.1511423850	-1.7621993017
H	0.4799453065	3.6315977612	-1.7746649971
H	-0.4168632975	2.2009040097	-2.2959933579
H	-1.2003755909	3.8075187725	-2.2962293049
C	-2.5060920571	1.7234256659	0.3427245962
H	-3.4573907587	2.1969383878	0.0784445248
H	-2.3962186826	0.7884963807	-0.2136567869
H	-2.5460948233	1.4720394448	1.4090607089

M2-TS2

B	0.7863439372	0.3332679547	-0.1125596879
Si	-1.0883738659	2.9523045217	-0.0356211602
C	0.4418940626	2.8273026818	1.3135590861
O	1.2665038372	2.7575093558	2.1145230136
O	0.4207517211	1.6493881408	-0.0075737554
C	0.0636275092	-0.5977961377	-1.1682871341
H	-0.5950187318	-0.0669736683	-1.8623127354
H	0.7975864412	-1.1698661562	-1.7489448092
H	-0.5394216373	-1.3453586650	-0.6325812253
C	1.9083738564	-0.2137851334	0.8614609722
H	1.6023744436	-0.0896073657	1.9089539457
H	2.1470611084	-1.2692105557	0.7005553740
H	2.8314437136	0.3687570675	0.7522977782
C	-1.7657934563	4.6011403327	0.6551988148
H	-0.9500309679	5.3331024925	0.7358941899
H	-2.0914269055	4.4105126787	1.6890433031
C	-2.9187389913	5.2036352156	-0.1566666204
H	-3.7192263317	4.4735515092	-0.3279713323
H	-3.3685464453	6.0649671969	0.3474132360

H	-2.5734934390	5.5438979411	-1.1387503464
C	-0.7899143221	3.2941993859	-1.8645106571
H	-1.7177108760	3.6916042235	-2.2966180222
H	-0.5720848404	2.3484596919	-2.3715623335
C	0.3552656767	4.2914997650	-2.0939312772
H	1.2997324962	3.9024484297	-1.6977647408
H	0.5050588405	4.4971829582	-3.1581068124
H	0.1544213141	5.2489205484	-1.5993882466
C	-2.3673729870	1.6442019665	0.4158188409
H	-2.3131789290	0.8361801581	-0.3236697489
H	-3.3631543808	2.0969950533	0.3240261282
C	-2.1918269162	1.0690150577	1.8284608469
H	-2.2414212419	1.8543152172	2.5916532534
H	-2.9681468925	0.3347085727	2.0634920124
H	-1.2234801112	0.5653515684	1.9366158603

M3-TS2

B	0.5841768535	0.0932219850	-0.2165860187
Si	-0.9917574492	2.9052450122	0.1106797447
C	0.7455747694	2.6321125095	1.0767872503
O	1.7700619177	2.5541888305	1.6089220751
O	0.0759927559	1.2588557395	0.3252794056
C	-0.3322962008	-0.7922786246	-1.1436324697
H	0.1006347573	-0.8247168389	-2.1530796960
H	-0.3372219649	-1.8304494646	-0.7863303998
H	-1.3622793181	-0.4360063946	-1.2338011939
C	2.0738245495	-0.2964442499	0.1362671804
H	2.1972170781	-0.4079831179	1.2207065146
H	2.3977984108	-1.2244443292	-0.3434710945
H	2.7658529065	0.5033388437	-0.1580072914
C	-0.8904629964	4.7973981802	-0.0048467835
C	-1.4497825067	5.4999857038	-1.0818805493
C	-1.4420882020	6.8941683928	-1.1160243737
C	-0.8737388958	7.6135990107	-0.0686404176
C	-0.3122060477	6.9364450098	1.0126761089
C	-0.3189647957	5.5447534888	1.0363729238
H	-1.8954795642	4.9510572295	-1.9080345457
H	-1.8773799672	7.4173646607	-1.9621363471
H	-0.8637483589	8.6990473706	-0.0952337830
H	0.1357074889	7.4922256129	1.8308384577
H	0.1261375763	5.0325337924	1.8889639148
C	-1.4318470425	2.3828546023	-1.6472339482
C	-2.7484610941	2.0387460846	-1.9761475058
C	-3.0797613159	1.6184120714	-3.2649057669
C	-2.0968266027	1.5398539331	-4.2468428805
C	-0.7822578126	1.8910628071	-3.9407753964
C	-0.4577328467	2.3095632841	-2.6536050385
H	-3.5249804752	2.0859603974	-1.2151541708
H	-4.1052630714	1.3487446340	-3.4989274115
H	-2.3522680410	1.2091346517	-5.2488200773

H	-0.0124870341	1.8376946379	-4.7049361073
H	0.5750649753	2.5786340075	-2.4322485549
C	-2.3285796162	2.4741080558	1.3497691049
C	-3.1522191042	3.4765377473	1.8829060914
C	-4.1953208642	3.1599861682	2.7512998214
C	-4.4339980203	1.8331273905	3.0982214155
C	-3.6287227125	0.8231996820	2.5750396931
C	-2.5856337734	1.1425965492	1.7106825624
H	-2.9763597863	4.5161554562	1.6180972656
H	-4.8203637136	3.9500403437	3.1560726317
H	-5.2455681617	1.5852920900	3.7756702072
H	-3.8117227036	-0.2127507881	2.8436368208
H	-1.9591513439	0.3494165407	1.3117551868

M4-TS2

B	0.9866801207	0.4332785336	-0.4704809942
Si	-1.1323041087	2.7011758263	0.2169566550
C	0.3448449856	2.4287290602	1.4576574505
O	1.2241654299	2.3592861186	2.1958959923
O	0.0926105250	1.2308120879	0.2370330963
C	0.5928410705	-0.1031408083	-1.8972394074
H	-0.3714473878	0.2453707288	-2.2740675953
H	1.3767191538	0.1564573807	-2.6215963002
H	0.5719148464	-1.2008757763	-1.8674008337
C	2.3583478330	0.0930374036	0.2237010180
H	2.2221109491	-0.2471859135	1.2562589485
H	2.9365517558	-0.6583964373	-0.3209446866
H	2.9694898906	1.0047400429	0.2825609387
C	-1.6082471187	4.4909775892	0.7248703583
C	-0.5762036053	5.4227964399	0.7403987672
C	-0.7444496634	6.7565495486	1.0752019150
C	-2.0205349203	7.1982695245	1.4051507319
C	-3.0879507560	6.3104123287	1.3886237961
C	-2.8676317130	4.9812023888	1.0464336873
F	-2.2191775640	8.4689890606	1.7271216299
F	-4.3076806897	6.7395646458	1.6949420301
F	-3.9390030919	4.1804136915	1.0307699496
F	0.2784188801	7.6043512345	1.0762038495
F	0.6621590258	5.0129976556	0.3981976254
C	-0.8553267786	3.0207577705	-1.6199535634
C	-1.9518686782	3.2528627579	-2.4393926069
C	-1.8363773382	3.4770377412	-3.8031677014
C	-0.5686504190	3.4918238578	-4.3740889534
C	0.5563283279	3.2850667148	-3.5844574958
C	0.3928186351	3.0608956329	-2.2252989848
F	-0.4323990522	3.7066848320	-5.6743227650
F	1.7659700232	3.2985412101	-4.1329493011
F	1.5038276289	2.8640648808	-1.4949691750
F	-2.9080793521	3.6783639149	-4.5600516628
F	-3.1777317606	3.2452867892	-1.8988446845

C	-2.5805365426	1.6300971380	0.7257796818
C	-3.1197557035	1.7081686146	2.0028533959
C	-4.1685317732	0.9046057590	2.4228050256
C	-4.7044505068	-0.0183236067	1.5320696183
C	-4.1869541209	-0.1338168288	0.2473312299
C	-3.1320584262	0.6849907943	-0.1286115896
F	-5.7083748393	-0.7950770800	1.9111103974
F	-4.6983351565	-1.0217310943	-0.5977025395
F	-2.6441504520	0.5436820929	-1.3668945638
F	-4.6617384486	1.0071530286	3.6512813273
F	-2.6150581147	2.5901375554	2.8757982997

M5-TS2

B	0.8498518416	0.1840751407	0.0287057722
Si	-0.9465220324	2.8084964601	-0.1129650312
C	0.4654887515	2.7920145328	1.2070759484
O	1.2671596379	2.8906779493	2.0328998461
O	0.3340059683	1.4715822124	0.2358752977
C	0.1444001366	-0.7005582951	-1.0539449111
H	0.8448210810	-1.3862375475	-1.5412126405
H	-0.6005091865	-1.3268013224	-0.5409892189
H	-0.3907963050	-0.1246649240	-1.8146016252
C	2.0770815576	-0.2448477602	0.9050390164
H	2.9860192884	0.1872812524	0.4618472004
H	2.0247623986	0.1341959462	1.9305231868
H	2.2169827984	-1.3289642931	0.9279306590
Cl	-1.8359789015	4.6491836792	0.3057504570
Cl	-0.3615609276	3.0619630008	-2.0634180110
Cl	-2.5346365634	1.5299548248	0.1441424533

M6-TS2

B	0.8369733871	0.1990987867	0.0055622286
Si	-0.8835654417	2.8539376335	-0.2339086776
C	0.5141807288	2.7835299118	1.0721533993
O	1.2867272248	2.8317590169	1.9349406417
O	0.4430088277	1.5449895663	0.0269646457
C	0.1467745203	-0.7290265720	-1.0496527646
H	-0.0771883790	-1.7153070790	-0.6287960319
H	-0.7650808220	-0.3033150048	-1.4765577422
H	0.8545589471	-0.9037122353	-1.8724171765
C	1.9380683827	-0.2392177504	1.0329846501
H	1.5194118137	-0.2065945105	2.0488807078
H	2.3036362887	-1.2539565720	0.8570950416
H	2.7890885983	0.4506486003	1.0387320518
F	-1.6191428914	4.2298849303	0.1348292804
F	-0.4527221285	3.1123782579	-1.7427137001
F	-2.0694083095	1.8053956435	-0.0592161813

M7-TS2

B	0.6984339636	0.0149263852	0.2726283016
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Si	-1.0129236201	2.7529668324	0.0442968866
C	0.3438987970	2.6572773209	1.5591283841
O	1.1152615239	2.6425831160	2.4128419031
O	0.0772120600	1.1925712080	0.5886515514
C	0.1129485468	-0.8971215760	-0.8856505577
H	-0.7899347563	-0.4620833482	-1.3315876943
H	-0.1928877189	-1.8534142988	-0.4343568560
C	1.1532241332	-1.1899521829	-1.9804954084
H	2.0514358756	-1.6529050335	-1.5575704833
H	0.7588874380	-1.8674619602	-2.7434737757
H	1.4671696341	-0.2701339829	-2.4874850162
C	2.0358900069	-0.3536813755	1.0396102980
H	2.2912654000	-1.4139066171	0.9207838427
H	1.9260599702	-0.1639576767	2.1148088241
C	3.1930239922	0.5118226651	0.5018162521
H	2.9855362968	1.5778131595	0.6452103503
H	4.1346362021	0.2888564437	1.0119893454
H	3.3511733970	0.3475159561	-0.5703222866
C	-1.5051588617	4.5679822926	0.3296897001
H	-2.2570009246	4.8789631195	-0.4069889058
H	-1.9362257435	4.7195360023	1.3267573263
H	-0.6459647416	5.2425582159	0.2313813468
C	-0.2273902273	2.7535471911	-1.6630633866
H	-0.2591896898	1.7558681895	-2.1112113255
H	-0.7289555293	3.4655404981	-2.3264374951
H	0.8262519812	3.0497849324	-1.5909669565
C	-2.6054366852	1.8002334499	0.3235533106
H	-2.7743542378	1.6605729281	1.3976593067
H	-3.4629278491	2.3490263789	-0.0794117355
H	-2.5565446375	0.8080725067	-0.1332548005

M8-TS2

B	1.9649428654	-0.0360062325	-0.4465058109
Si	-1.2096569181	-0.2055324791	0.0884680259
C	-0.2788372227	1.5665389341	0.4874476820
O	0.2422646831	2.5470312533	0.7918227473
O	0.6446218619	0.3262090664	-0.3912670838
C	2.3665858354	-1.5285832350	-0.8013639731
H	3.0834343580	-1.4992883018	-1.6353901455
H	1.5078658717	-2.1194740010	-1.1430483206
C	3.0441841838	-2.2290126065	0.3914015097
H	2.3539779088	-2.3389729840	1.2355504769
H	3.3981569338	-3.2291224479	0.1245686210
H	3.9065345566	-1.6553435827	0.7477517161
C	3.0565623606	1.0792686986	-0.1616792047
H	4.0657303961	0.6500606340	-0.1341403250
H	2.8767133649	1.5284878345	0.8261035058
C	3.0008508518	2.1939903584	-1.2223984889
H	2.0160908897	2.6704051492	-1.2364726636
H	3.7464320125	2.9709500518	-1.0297710202

H	3.1906332402	1.7961202393	-2.2259193830
C	-0.6100627316	-1.5513595150	1.2644847521
H	0.0565165805	-2.2272043135	0.7148893592
H	-1.4813975053	-2.1407585854	1.5784741847
C	0.1104878099	-1.0003661249	2.5039377065
H	-0.5395080978	-0.3327534518	3.0814155909
H	0.4331195545	-1.8033423522	3.1741353344
H	1.0052025659	-0.4290656709	2.2264356665
C	-2.9011424945	0.3323454778	0.7911690997
H	-2.7840276399	0.5477396773	1.8632576184
H	-3.5905124297	-0.5218622535	0.7293676016
C	-3.5086396200	1.5477353035	0.0832155306
H	-3.6517657913	1.3577866697	-0.9873104581
H	-4.4812764678	1.8280945993	0.4992870774
H	-2.8567143498	2.4260393344	0.1705186122
C	-1.5494971174	-0.6820599433	-1.7044423720
H	-0.6788591124	-1.2503706461	-2.0523214849
H	-1.5686520747	0.2300876379	-2.3160904036
C	-2.8399525065	-1.4855705450	-1.9029822136
H	-3.7255181684	-0.8973783705	-1.6431610880
H	-2.9519540144	-1.8083553081	-2.9425932937
H	-2.8511804232	-2.3861009686	-1.2777316856

M9-TS2

B	0.8698510208	0.3205425503	-0.0958862807
Si	-0.6803630514	2.9656752522	-0.2542107825
C	1.1756653212	3.0547749019	0.4668438534
O	2.2269240869	3.1112817912	0.9435456032
O	0.7895030117	1.6550480558	-0.4854169693
C	0.4148699683	-0.7889438338	-1.1225330902
H	-0.5751570324	-1.1328004736	-0.7738416688
H	1.0640370015	-1.6700390133	-1.0225454002
C	0.3276130820	-0.3533401360	-2.5859234013
H	1.3098368132	-0.0476181709	-2.9641143649
H	-0.0403974952	-1.1596035018	-3.2280750702
H	-0.3442455971	0.5019090070	-2.7030519061
C	1.4084171073	-0.0285766714	1.3537926560
H	1.1328335526	0.7614675976	2.0669845753
H	2.5088766416	0.0167547944	1.3086968620
C	0.9728770811	-1.3944507985	1.8949157929
H	1.3218743821	-2.2084436267	1.2518108986
H	1.3643158550	-1.5762576614	2.9002132166
H	-0.1197700074	-1.4657753130	1.9427654352
C	-1.4364287764	4.2490655992	0.9239726590
C	-0.6802765270	5.3468312355	1.3619087356
C	-1.2437975491	6.3524413424	2.1418898652
C	-2.5866771869	6.2761073453	2.5072634291
C	-3.3579187203	5.1966146630	2.0856420117
C	-2.7861798566	4.1944936475	1.3023046809
H	0.3705742395	5.4249105462	1.0857063081

H	-0.6367725182	7.1910338204	2.4691346357
H	-3.0285744999	7.0548872852	3.1214095307
H	-4.4043383608	5.1320066718	2.3684280791
H	-3.4010389442	3.3565818513	0.9823232255
C	-0.5879103188	3.7352788635	-1.9559860052
C	0.3264617797	3.3096999082	-2.9303747859
C	0.3326556667	3.8819717835	-4.2004447522
C	-0.5813307887	4.8832900018	-4.5193523038
C	-1.4973878005	5.3178247451	-3.5639190064
C	-1.4945353134	4.7530099547	-2.2909064945
H	1.0359058057	2.5242191819	-2.6873706815
H	1.0519614354	3.5460906034	-4.9411308726
H	-0.5775266559	5.3276891751	-5.5100873096
H	-2.2087642437	6.1010188409	-3.8071380994
H	-2.2034174181	5.1109916831	-1.5473983561
C	-1.8934274198	1.5191782120	-0.1374997423
C	-2.0509526532	0.8102192009	1.0643385629
C	-2.8624773296	-0.3197566801	1.1327736052
C	-3.5433518982	-0.7562312998	-0.0036137079
C	-3.4157632383	-0.0533622496	-1.1988074128
C	-2.5971188871	1.0747471435	-1.2627948099
H	-1.5343906618	1.1429959371	1.9647178211
H	-2.9671882211	-0.8564869196	2.0711544670
H	-4.1758681689	-1.6371578669	0.0458743491
H	-3.9497617550	-0.3848746259	-2.0842187803
H	-2.4977866127	1.6086604303	-2.2058686262

M10-TS2

B	0.5488274187	0.1939800451	0.2265790595
Si	-0.6828264568	3.0301862117	-0.5239367072
C	1.2366156491	2.9429628540	-0.2317179188
O	2.3685025046	2.9959032904	-0.0320065148
O	0.3942343427	1.4470516522	-0.3610916725
C	-0.6974362537	-0.7772783146	0.2817853955
H	-0.5532398527	-1.4954060888	-0.5426809233
H	-1.6313478894	-0.2558500321	0.0474640399
C	-0.8336991802	-1.5622173050	1.5959664539
H	-0.9902439906	-0.8945111371	2.4496043710
H	-1.6782576969	-2.2561984270	1.5603899468
H	0.0674024243	-2.1466544070	1.8078451994
C	1.9717967759	-0.2495061069	0.7452460761
H	1.8889421227	-0.4270147630	1.8281387851
H	2.7217307207	0.5365768534	0.6151617529
C	2.4579487103	-1.5457032778	0.0702201968
H	2.5823135153	-1.4074399055	-1.0091217770
H	3.4224971021	-1.8660146675	0.4734256762
H	1.7475750307	-2.3661877417	0.2157932760
C	-1.9357833162	2.4214876600	0.7471771998
C	-3.2880832472	2.6021248833	0.4869016700
C	-4.2856680419	2.1672216100	1.3467445379

C	-3.9207555033	1.5385085885	2.5319957009
C	-2.5776999393	1.3596117277	2.8410031169
C	-1.6137413012	1.8066655909	1.9492352395
F	-4.8544995109	1.1143813895	3.3704251042
F	-2.2280747827	0.7565601985	3.9724655979
F	-0.3283537407	1.6073938288	2.2873556928
F	-5.5686782536	2.3412670225	1.0546551492
F	-3.6526640821	3.2049661841	-0.6526747788
C	-0.9301005326	4.9154040270	-0.2563830059
C	-0.4288773029	5.4374308845	0.9308532353
C	-0.5205415158	6.7730455926	1.2870537410
C	-1.1591580985	7.6461787605	0.4140396135
C	-1.6896822072	7.1713896637	-0.7781286944
C	-1.5713757844	5.8220248113	-1.0908381396
F	-1.2678404798	8.9307897185	0.7237096291
F	-2.3072432189	8.0085942056	-1.6049040704
F	-2.1162754379	5.4233897960	-2.2456629434
F	-0.0216151174	7.2198525688	2.4344299750
F	0.1753820127	4.5968195483	1.7952521388
C	-1.0475340930	2.7281487440	-2.3353782205
C	-0.4228157100	3.4829962276	-3.3190776831
C	-0.6358786080	3.2739455411	-4.6727691499
C	-1.5114458394	2.2680136435	-5.0653591527
C	-2.1518989388	1.4858478047	-4.1117899070
C	-1.9035342514	1.7245177124	-2.7675516455
F	-1.7329202591	2.0512724213	-6.3534117938
F	-2.9841092060	0.5232162988	-4.4922905607
F	-2.5267190109	0.9486474454	-1.8725968804
F	-0.0234338790	4.0170135557	-5.5868316424
F	0.4217229546	4.4588305553	-2.9579051383

M11-TS2

B	0.7628562567	0.1689251750	0.1293512577
Si	-0.8831526808	2.8688772016	-0.2249257263
C	0.4180197052	2.8255917466	1.2048771968
O	1.1660836489	2.9088691712	2.0813263217
O	0.2232007071	1.4516594864	0.3199204231
C	0.0644051319	-0.7533162091	-0.9290083802
H	0.8066125782	-1.3563574199	-1.4658313400
H	-0.4954755788	-0.1746543029	-1.6723867349
C	-0.9041666666	-1.6992402611	-0.1817623464
H	-1.6872438100	-1.1341100007	0.3331849031
H	-1.3930997859	-2.3849444017	-0.8785338254
H	-0.3788074364	-2.3031730528	0.5659799959
C	1.9432214948	-0.2434736294	1.0827647004
H	1.5123254624	-0.3462581078	2.0922639054
H	2.6462977196	0.5958882523	1.1749109464
C	2.6859909575	-1.5260826309	0.6971984630
H	3.1720878550	-1.4224081955	-0.2781512724
H	3.4602282033	-1.7768924795	1.4271550852

H	2.0028875861	-2.3792733167	0.6323477353
Cl	-1.6688828231	4.7842186611	0.0433395660
Cl	-0.0679923518	2.9975258400	-2.1039680039
Cl	-2.5968614547	1.7360950838	-0.1240252666

M12-TS2

B	0.9515712799	0.2076531654	-0.0275302041
Si	-0.9732827577	2.7213301937	-0.1178925107
C	0.3155372777	2.6299375576	1.2951413692
O	1.0248549620	2.6612876401	2.2120243161
O	0.4287019291	1.5031610977	0.1376043534
C	0.4525236462	-0.5525354352	-1.3069256765
H	0.6778451813	0.0895146147	-2.1724424814
H	-0.6470176718	-0.5798981692	-1.2704947771
C	1.0231443791	-1.9566006244	-1.5183941513
H	0.7472977190	-2.6244015887	-0.6960478162
H	0.6571290785	-2.4053718403	-2.4457223312
H	2.1171344802	-1.9355803517	-1.5699461581
C	2.0201402238	-0.2661021972	1.0185597018
H	2.1589161703	-1.3514311759	0.9810640286
H	1.7134836305	-0.0057834030	2.0391325134
C	3.3632660067	0.4341883164	0.7130581845
H	3.2686841405	1.5212557823	0.7981306570
H	4.1401823885	0.1117852463	1.4108725943
H	3.7122392076	0.2061383955	-0.3001740133
F	-1.8297450403	4.0138348076	0.2909919152
F	-0.4718129364	3.1254673288	-1.5734193521
F	-2.0855692489	1.5808138576	-0.1041280762

M13-TS2

B	0.9591905901	0.2994658252	-0.0626972414
Si	-1.1028203019	2.7681433398	-0.0506100629
C	0.6860037906	3.1230714882	0.8208925393
O	1.6925430455	3.3647878473	1.3155224785
O	0.5298605096	1.5952016592	-0.1454392715
C	0.7155847488	-0.6314467842	-1.3069539798
C	0.4819502503	-2.0085162970	-1.1722484898
C	0.2119225405	-2.8059707037	-2.2822140495
C	0.1935111217	-2.2403293913	-3.5551999246
C	0.4361016294	-0.8766626350	-3.7151610611
C	0.6832064748	-0.0832436180	-2.5991876229
H	0.5008008108	-2.4576160503	-0.1817511938
H	0.0193240561	-3.8671365143	-2.1562222367
H	-0.0083420312	-2.8616435177	-4.4226860867
H	0.4286528042	-0.4362846826	-4.7077368050
H	0.8690341028	0.9811579483	-2.7207485930
C	1.6433651145	-0.2263842271	1.2530385750
C	1.2886323683	0.2912609958	2.5081022500
C	1.8773253562	-0.1732293733	3.6800226571
C	2.8589944937	-1.1606040922	3.6155769969

C	3.2357778457	-1.6859579973	2.3819768007
C	2.6231643465	-1.2303815594	1.2171030142
H	0.5273054840	1.0667543010	2.5719911760
H	1.5787292730	0.2361692601	4.6401617615
H	3.3287040235	-1.5196547298	4.5263369697
H	4.0021994561	-2.4531954472	2.3289634469
H	2.9166951525	-1.6517757401	0.2584378429
C	-2.0017369902	4.2370075690	0.7555047642
H	-2.0464558215	4.1414001268	1.8474387233
H	-1.5109978863	5.1899096664	0.5233875903
H	-3.0345821362	4.2950391704	0.3890127910
C	-1.0380590880	3.1565665326	-1.8823298356
H	-0.1086554253	3.6744131817	-2.1428391672
H	-1.0707560666	2.2259869639	-2.4564167258
H	-1.8787248838	3.7931556583	-2.1758109212
C	-2.1050592174	1.2740423248	0.4955239145
H	-3.1721643501	1.5159394331	0.5381074560
H	-1.9480643000	0.4360059137	-0.1917121788
H	-1.7986359866	0.9449623759	1.4956580225

M14-TS2

B	0.8942954167	0.1721198614	-0.1351362043
Si	-1.0241852766	2.8255790848	-0.2905080396
C	0.8433886830	3.0562806174	0.4525779064
O	1.8423831744	3.2370076332	0.9814568403
O	0.5207781499	1.4546190973	-0.4051460946
C	-1.5463116591	4.6092017361	0.1959620262
H	-1.0890373128	5.3025597828	-0.5266247798
H	-1.0851226086	4.8560377778	1.1631609059
C	-3.0550905451	4.8741870225	0.2944587253
H	-3.4921084690	4.3302179224	1.1382777707
H	-3.2690176437	5.9369090051	0.4480728664
H	-3.5911516687	4.5604571076	-0.6072064295
C	-1.1265788131	2.7226551822	-2.1692437018
H	-1.1955836482	1.6582757080	-2.4195598445
H	-0.1567024487	3.0527134432	-2.5651511737
C	-2.2631987304	3.5126708840	-2.8246698967
H	-2.2049034066	4.5794669513	-2.5856017904
H	-2.2310498174	3.4172914218	-3.9144616826
H	-3.2438001706	3.1529102030	-2.4948537145
C	-2.0747480343	1.6966026710	0.7834896210
H	-2.1303153356	0.7051954535	0.3252336079
H	-3.0928788719	2.1050826507	0.7994840105
C	-1.5409977605	1.5814909419	2.2183284135
H	-1.4994889570	2.5593384662	2.7136106789
H	-2.1714753404	0.9271282804	2.8279180178
H	-0.5293616980	1.1574479959	2.2318961758
C	-0.2295446455	-0.9419316170	-0.1023316358
C	-0.5405437336	-1.6459962821	1.0697109927
C	-1.0103903096	-1.1928723612	-1.2405685449

C	-1.6052647447	-2.5445764584	1.1133127282
H	0.0458475793	-1.4764236160	1.9711368226
C	-2.0632045343	-2.1040653021	-1.2109708513
H	-0.7916350130	-0.6626916012	-2.1651266947
C	-2.3686889616	-2.7754673668	-0.0282582529
H	-1.8371532483	-3.0664250595	2.0370381719
H	-2.6501412576	-2.2858321186	-2.1064026149
H	-3.1955817088	-3.4783694863	0.0017052011
C	2.4089803976	-0.1668347988	0.1157465504
C	3.4117907741	0.7767777894	-0.1626237094
C	2.8136832734	-1.4253345392	0.5895659745
C	4.7569527079	0.4882237909	0.0435173758
H	3.1287829549	1.7453718598	-0.5634835467
C	4.1566439593	-1.7184989335	0.8112262398
H	2.0641253373	-2.1884451879	0.7820862563
C	5.1298345765	-0.7595119799	0.5400119134
H	5.5145998178	1.2322793133	-0.1827328703
H	4.4456822893	-2.6958799289	1.1856722476
H	6.1786504417	-0.9871741276	0.7061859717

M15-TS2

B	0.8616181919	0.2527459676	0.0400618976
Si	-0.8541495085	2.9423751051	-0.1456899879
C	0.7847359132	3.0341062855	0.9638772502
O	1.6942114907	3.1570451762	1.6499831213
O	0.6505273903	1.5986155521	-0.1458643105
C	0.3117126262	-0.7774361735	-1.0118415020
C	-0.4980442469	-0.3644538409	-2.0830558866
C	-0.9864028959	-1.2727404510	-3.0154261974
C	-0.6642816469	-2.6243691381	-2.9028462468
C	0.1534072323	-3.0582901117	-1.8626547338
C	0.6351646580	-2.1419736252	-0.9314473594
H	-0.7463867992	0.6870924512	-2.1894396741
H	-1.6163691586	-0.9286484305	-3.8302232978
H	-1.0443066131	-3.3366068054	-3.6294996151
H	0.4176768060	-4.1082037946	-1.7792526635
H	1.2804746890	-2.4903971350	-0.1296522471
C	1.6692541485	-0.2126630969	1.3139490337
C	2.9024393713	0.3649141817	1.6518272374
C	3.6004364860	-0.0335773602	2.7890344624
C	3.0652069519	-1.0083061152	3.6284118472
C	1.8380023757	-1.5901064779	3.3192862761
C	1.1568792431	-1.2027402530	2.1673234505
H	3.3237844858	1.1369642373	1.0128640529
H	4.5572895594	0.4219782459	3.0250732479
H	3.6033651517	-1.3138473239	4.5205884945
H	1.4160643201	-2.3495508254	3.9707187689
H	0.2046718198	-1.6729065463	1.9265365402
C	-1.7133596304	4.4288996278	0.6887200236
C	-1.0197839538	5.6459778370	0.7990230518

C	-1.5979501526	6.7635040539	1.3918433105
C	-2.8966381871	6.6861787168	1.8954484500
C	-3.6035675246	5.4923396485	1.7997882663
C	-3.0150725222	4.3757856196	1.2025416194
H	-0.0061822993	5.7280074196	0.4043106958
H	-1.0394343761	7.6918988216	1.4641806941
H	-3.3518204974	7.5543275390	2.3624325865
H	-4.6138373960	5.4255537446	2.1924644477
H	-3.5815182453	3.4497720200	1.1392461773
C	-0.5000757945	3.5335600535	-1.8917870657
C	-1.3431043831	4.5079781735	-2.4518229003
C	-1.1692267404	4.9405937795	-3.7641718587
C	-0.1319215380	4.4220794418	-4.5354838646
C	0.7232558271	3.4658619904	-3.9934560533
C	0.5365073170	3.0213797531	-2.6869413469
H	-2.1424544170	4.9393182328	-1.8538448899
H	-1.8374407951	5.6884319680	-4.1798855677
H	0.0116316252	4.7652958083	-5.5556056477
H	1.5364585439	3.0624977283	-4.5889514574
H	1.1989119866	2.2662568572	-2.2755943377
C	-2.1026954269	1.5568970606	0.0809322220
C	-3.1642396557	1.4466111137	-0.8250319643
C	-4.1039695821	0.4243382045	-0.7058594330
C	-4.0049261426	-0.4941129981	0.3358738880
C	-2.9678633479	-0.3843785329	1.2602452313
C	-2.0250944200	0.6326499006	1.1302665910
H	-3.2480141320	2.1523715648	-1.6504547658
H	-4.9089890119	0.3418678650	-1.4297029715
H	-4.7336199232	-1.2933330060	0.4284404145
H	-2.8897256299	-1.0932536447	2.0792463350
H	-1.2133386566	0.6923577719	1.8554151745

M16-TS2

B	0.8195284584	0.2177918593	-0.0799647756
Si	-0.7391327499	2.9204742541	-0.2433336848
C	0.9957031711	2.9824050705	0.6299333815
O	1.9757689574	3.0965782985	1.2136943605
O	0.6766437863	1.5668078539	-0.3706966486
C	0.0420620478	-0.7955531278	-0.9834905670
C	-0.2382943809	-2.1050007130	-0.5643370888
C	-1.0310878990	-2.9531779119	-1.3349986083
C	-1.5255393967	-2.5166528590	-2.5622627669
C	-1.2202874497	-1.2357977924	-3.0223318883
C	-0.4498413999	-0.3871880559	-2.2349451269
H	0.1611225991	-2.4628448935	0.3806243563
H	-1.2578687659	-3.9544463521	-0.9823250818
H	-2.1456157716	-3.1749293234	-3.1629301806
H	-1.5994428264	-0.8961989903	-3.9809900651
H	-0.2364313025	0.6214746843	-2.5848986537
C	1.7213131850	-0.1841674266	1.1398658747

C	3.0716021319	0.1966811169	1.1764094702
C	3.8838357296	-0.1348251932	2.2568906404
C	3.3521632149	-0.8347602892	3.3381141585
C	2.0097171483	-1.2036461469	3.3320526011
C	1.2063382108	-0.8895251977	2.2382087578
H	3.4918742122	0.7625453968	0.3479963850
H	4.9279964457	0.1620105422	2.2604509033
H	3.9815278559	-1.0864836464	4.1860964476
H	1.5869133415	-1.7371732531	4.1776619112
H	0.1566255526	-1.1756877798	2.2595671253
C	-1.5022422669	4.4445058121	0.6370650300
C	-2.7353058921	4.5190463021	1.2767182621
C	-3.1969768445	5.6809878493	1.8847115480
C	-2.4104597651	6.8243122785	1.8612154434
C	-1.1729973145	6.8006712143	1.2291520656
C	-0.7547946618	5.6201470841	0.6364967953
F	-2.8396496939	7.9380383692	2.4375092972
F	-0.4175484395	7.8931117769	1.1976159487
F	0.4440966473	5.6302948338	0.0238647385
F	-4.3812385411	5.7062342720	2.4870210372
F	-3.5484473618	3.4588219869	1.3315925240
C	-0.5930259003	3.5343603043	-2.0056930722
C	-1.7378245314	3.9927534676	-2.6510897471
C	-1.7226353370	4.4784285760	-3.9494210198
C	-0.5112737387	4.5361118411	-4.6289562710
C	0.6601349721	4.1198472050	-4.0086717989
C	0.6029838669	3.6349515220	-2.7086002982
F	-0.4721941366	5.0021888574	-5.8681140795
F	1.8173407780	4.2024097613	-4.6545172819
F	1.7594255077	3.2940738776	-2.1330191395
F	-2.8369125341	4.8926423516	-4.5408239379
F	-2.9078898366	3.9711285241	-2.0036717658
C	-1.9602194350	1.5273459536	0.1017257913
C	-2.7451668444	0.8840744614	-0.8397269408
C	-3.3982619533	-0.3132872228	-0.5648683680
C	-3.2621740629	-0.8910373347	0.6880222715
C	-2.4950019571	-0.2636829333	1.6659329057
C	-1.8719059335	0.9303177247	1.3525483524
F	-3.8469243463	-2.0505312162	0.9524940155
F	-2.3458104414	-0.8293883767	2.8607079821
F	-1.0913092060	1.5150401276	2.2824650125
F	-4.1081112294	-0.9250901185	-1.5049627512
F	-2.8436140766	1.3564655096	-2.0859233246

M17-TS2

B	0.8720002355	0.1695482901	0.0097594689
Si	-1.2168400101	2.5366047950	-0.2262044160
C	0.3226668394	2.8254247952	0.8810371586
O	1.1942907942	3.0992902233	1.5871744143
O	0.3461169216	1.4790053046	-0.0767787070

C	0.9259175916	-0.6596928459	-1.2984250653
C	0.9241986953	-0.0252205486	-2.5524302175
C	0.9585662400	-0.7649953702	-3.7290618322
C	0.9761920326	-2.1577689370	-3.6713003327
C	0.9660108398	-2.8088586367	-2.4390229785
C	0.9489664966	-2.0644498561	-1.2639716418
H	0.9041829389	1.0598630059	-2.5992000131
H	0.9654555389	-0.2599579305	-4.6896776079
H	0.9944392104	-2.7373596487	-4.5893557175
H	0.9700238023	-3.8934358349	-2.3965591693
H	0.9339760240	-2.5753525489	-0.3046976528
C	1.3273290830	-0.3321425753	1.4111827412
C	0.6266147399	0.0392268550	2.5699721984
C	1.0118504883	-0.4212689783	3.8240610485
C	2.1287331418	-1.2469576716	3.9436783063
C	2.8450874818	-1.6220722184	2.8094105905
C	2.4378806547	-1.1788777652	1.5543460505
H	-0.2503327954	0.6800347923	2.4903601430
H	0.4490180834	-0.1336600403	4.7061916607
H	2.4394523908	-1.5988117796	4.9225888284
H	3.7164214700	-2.2624301835	2.9031417175
H	2.9966906760	-1.4796964683	0.6715095199
Cl	-2.4988591657	3.9952809710	0.5460184667
Cl	-0.9135258542	3.1678188571	-2.1491960191
Cl	-2.4316332861	0.8793729184	-0.0669225225

M18-TS2

B	0.8026897837	0.1207492012	0.0720785861
Si	-1.2677766311	2.5581105850	-0.2882220033
C	0.1516429631	2.7358071206	0.9641262568
O	0.9664935044	2.9964012876	1.7441835571
O	0.1694375326	1.3769447471	0.0705112542
C	0.7329338131	-0.7170347422	-1.2335093626
C	0.4538048036	-0.1116279853	-2.4709806183
C	0.3847802027	-0.8658408016	-3.6370582778
C	0.5753257644	-2.2456996785	-3.5840433425
C	0.8375942257	-2.8697064949	-2.3660998379
C	0.9217883020	-2.1095204337	-1.2040788204
H	0.2918086384	0.9610002365	-2.5173119400
H	0.1766707461	-0.3814384568	-4.5857760409
H	0.5143443943	-2.8364285068	-4.4931444251
H	0.9745460056	-3.9456546951	-2.3238816270
H	1.1196417819	-2.6015512422	-0.2553799360
C	1.5037742536	-0.3346717625	1.3870065937
C	2.7039299844	-1.0621175427	1.3539949302
C	3.3340914546	-1.4615098572	2.5293531981
C	2.7576313073	-1.1623639256	3.7615815608
C	1.5579104661	-0.4546269773	3.8180557708
C	0.9473871345	-0.0362975196	2.6409632914
H	3.1555327445	-1.3042681641	0.3949952637

H	4.2703229964	-2.0089509680	2.4848490880
H	3.2426810264	-1.4805104515	4.6793057201
H	1.1058817744	-0.2238182782	4.7773475373
H	0.0138087589	0.5195891961	2.6968371225
F	-2.1710710055	3.8444232655	0.0327744311
F	-0.8424537037	2.8239752812	-1.7996231157
F	-2.3331932142	1.3907588765	-0.0964797220

M19-TS2

B	0.9170280214	0.1449367432	-0.1827184053
Si	-0.8559077676	2.9191201175	-0.1311589111
C	0.8813308221	2.8721480240	0.8760698751
O	1.8733116700	2.9309636012	1.4383031866
O	0.6424959439	1.4393600938	-0.3455888818
C	0.5134926004	-0.9071251442	-1.3002333594
C	0.5327819699	-2.2894847106	-1.0998862124
C	0.1994899975	-3.2054028072	-2.0877610448
C	-0.1772585376	-2.7439419203	-3.3414135077
C	-0.2224719957	-1.3787414864	-3.5891054093
C	0.1161442884	-0.4935834283	-2.5752168072
F	-0.5007624989	-3.6031970864	-4.2967762844
F	-0.5890419010	-0.9338882732	-4.7875972159
F	0.0420684548	0.8043854355	-2.8835134688
F	0.2286329368	-4.5118131420	-1.8440948943
F	0.8578020459	-2.8024192222	0.0901457672
C	1.6400480795	-0.3150228009	1.1607811562
C	1.1745657637	0.1221179913	2.3932053009
C	1.7929213392	-0.1912661345	3.5937767177
C	2.9342684678	-0.9829847043	3.5693289107
C	3.4344354796	-1.4472068523	2.3582576645
C	2.7791447463	-1.1090240768	1.1830209058
F	3.5476918003	-1.2955770633	4.7031813744
F	4.5288520702	-2.2009627399	2.3411133965
F	3.2855745407	-1.5664224871	0.0327949783
F	1.3123941666	0.2537617727	4.7511069560
F	0.0666073438	0.8915007010	2.4528683072
C	-1.6870565458	4.1906402341	1.0001167333
H	-1.0774884221	5.0925873804	1.1267622839
H	-2.6530950862	4.4940473273	0.5782511625
H	-1.8840222435	3.7748707710	1.9956654542
C	-0.3921454818	3.7875727728	-1.7180381561
H	0.1495765668	3.1248284037	-2.3936753116
H	-1.3107778472	4.1271788549	-2.2107503609
H	0.2184475524	4.6741926533	-1.5170601805
C	-2.0802272133	1.5005636676	-0.2086266629
H	-1.9874382905	0.8725414959	0.6842548476
H	-3.1034005698	1.8901590064	-0.2417201369
H	-1.8975834750	0.8774843097	-1.0878353571

M20-TS2

B	0.7887899655	0.1664501073	0.2522683539
Si	-1.2293862564	2.8626419470	-0.1258028202
C	0.5045702900	3.1111831323	0.8796361277
O	1.5056108837	3.3704752652	1.3571647127
O	0.1256617891	1.2996832817	0.4521167122
C	1.9475959792	-0.2900293955	1.2323761870
C	2.0800908644	0.2593234052	2.5106947556
C	3.0816943595	-0.1132958641	3.3952199883
C	4.0030709092	-1.0779971071	3.0091318725
C	3.9082359967	-1.6605057086	1.7529597874
C	2.8893100503	-1.2648156839	0.8971902926
F	4.9670824904	-1.4453567938	3.8409326596
F	4.7871218902	-2.5871011999	1.3840078534
F	2.8482658082	-1.8685138389	-0.2929098122
F	3.1622334078	0.4341235029	4.6043446019
F	1.2100591887	1.1711477217	2.9592485357
C	0.3412349643	-0.7165441357	-0.9994650381
C	1.0630753157	-0.7439043740	-2.1828579118
C	0.5954017990	-1.3700648349	-3.3293458571
C	-0.6417712595	-2.0035383191	-3.2938759634
C	-1.3942514967	-1.9993418288	-2.1257824819
C	-0.8892566413	-1.3546756259	-1.0042920181
F	-1.1066285406	-2.6106904022	-4.3795915111
F	-2.5793072177	-2.6031549896	-2.0965689576
F	-1.6426217083	-1.3426566334	0.1067991555
F	1.3061009982	-1.3674125032	-4.4534762214
F	2.2462006499	-0.1170787806	-2.2451028322
C	-2.5018329264	2.0278325300	0.9694684532
H	-2.6302005857	1.0052166239	0.5964849324
H	-3.4543923747	2.5554167190	0.8235560425
C	-2.1465568325	1.9831329765	2.4638715306
H	-1.9929291000	2.9860589552	2.8774223079
H	-2.9473476469	1.5108600219	3.0404154157
H	-1.2312826667	1.4083704886	2.6252672463
C	-1.6562466963	4.7146127180	-0.2062045020
H	-2.5863874405	4.8035885260	-0.7867967847
H	-0.8896088593	5.2377997675	-0.7960455008
C	-1.8322567935	5.4003823518	1.1531257999
H	-0.9338981882	5.3058171153	1.7770188961
H	-2.0366399834	6.4700111791	1.0479687732
H	-2.6644042038	4.9600766151	1.7128995061
C	-1.0034983781	2.3458449857	-1.9182591955
H	-1.7694715648	2.8715109927	-2.5038367837
H	-1.2031922670	1.2722283950	-2.0070415792
C	0.3869164524	2.6698316286	-2.4841278501
H	1.1738872758	2.1361785785	-1.9418537944
H	0.4646419204	2.3789848044	-3.5362038524
H	0.6046969294	3.7426033288	-2.4248887323

M21-TS2

B	0.9920779627	0.1943801312	-0.0935480955
Si	-1.1260617202	2.7906614839	0.1625411723
C	0.1556066130	2.2181495118	1.5793193778
O	0.7914863067	1.9418771079	2.4944757960
O	0.5137066673	1.4499807445	0.0147886884
C	-0.0057099180	-0.9035542727	-0.6402164820
C	-1.2826493420	-0.9780210971	-0.0996707745
C	-2.2797496186	-1.7765043526	-0.6341311292
C	-1.9890901105	-2.5414375694	-1.7576248274
C	-0.7160429312	-2.5159876587	-2.3143594436
C	0.2525449207	-1.7035949097	-1.7428290394
F	-2.9359326356	-3.2935201197	-2.3053399483
F	-0.4503432982	-3.2484085549	-3.3926390925
F	1.4613258208	-1.6631957445	-2.3161915336
F	-3.4992142788	-1.8068983455	-0.1051956453
F	-1.5837018597	-0.2411326087	0.9882089529
C	2.4585722048	-0.1283637683	0.3797917580
C	3.3568597488	0.8852062933	0.7326767279
C	4.6511660345	0.6294048497	1.1619554050
C	5.0892199296	-0.6851031590	1.2532679311
C	4.2341478320	-1.7261414629	0.9170680907
C	2.9471316270	-1.4335755504	0.4904672584
F	6.3213766054	-0.9456461824	1.6635021704
F	4.6523516973	-2.9841721120	1.0129908012
F	2.1683743718	-2.4783403864	0.2021853174
F	5.4717766193	1.6248322076	1.4835338094
F	3.0073144296	2.1712159690	0.6589896290
C	-2.4541242185	3.4476413074	1.3354430917
C	-3.1727073605	4.6066066262	1.0067865743
C	-4.1888637738	5.0811082585	1.8324926731
C	-4.5105079447	4.3988935916	3.0040069710
C	-3.8112418297	3.2450505784	3.3481434626
C	-2.7916847199	2.7786332155	2.5203557443
H	-2.9278630180	5.1544243527	0.0986966651
H	-4.7272275071	5.9850269335	1.5642586460
H	-5.3019763552	4.7680108429	3.6488799528
H	-4.0559714433	2.7105986850	4.2608746658
H	-2.2587269416	1.8729513172	2.8083108636
C	-0.1937553201	4.2094314006	-0.6154947310
C	0.9736495348	4.7549758847	-0.0642236168
C	1.5996183951	5.8498156236	-0.6525010209
C	1.0650923319	6.4223951029	-1.8047365402
C	-0.0934338812	5.8947619023	-2.3678346805
C	-0.7152610518	4.7956679796	-1.7785456715
H	1.4150766901	4.3208229289	0.8299534262
H	2.5064598854	6.2535704981	-0.2134068550
H	1.5539602541	7.2756032758	-2.2647463037
H	-0.5112898928	6.3339942993	-3.2683990651
H	-1.6123696218	4.3845197544	-2.2374621547
C	-2.0720271450	1.7987647998	-1.1210855741

C	-1.4487320867	1.4030422847	-2.3160166686
C	-2.1390761513	0.6694712664	-3.2747980157
C	-3.4698459514	0.3092247872	-3.0500254137
C	-4.1061151993	0.6996022111	-1.8761236853
C	-3.4122430697	1.4458416313	-0.9220095144
H	-0.4067661143	1.6668395347	-2.4884183751
H	-1.6413810401	0.3705877014	-4.1927236218
H	-4.0054157971	-0.2778672030	-3.7902519406
H	-5.1381451315	0.4166041112	-1.6949419084
H	-3.9186143013	1.7436696780	-0.0073675783

M22-TS2

B	0.7817324155	0.1316676278	-0.0271291374
Si	-1.4981260503	2.5119186022	0.4262099999
C	-1.0521377102	1.3289071281	1.8777760886
O	-0.9369176327	0.6638402387	2.7982743484
O	0.0963164144	1.1700192199	0.5115536315
C	0.0124609869	-0.9676635161	-0.8673064585
C	0.5545426754	-1.5313811748	-2.0212908893
C	-0.1642440801	-2.3789731274	-2.8538736859
C	-1.4757609049	-2.7003855408	-2.5239679018
C	-2.0451047211	-2.1873104009	-1.3638197473
C	-1.2947583346	-1.3386538989	-0.5664118164
F	-2.1875009907	-3.4849411667	-3.3170171192
F	-3.3116295855	-2.4608568336	-1.0656145152
F	-1.8963694179	-0.8521245500	0.5334521297
F	0.3786998669	-2.8693560278	-3.9602419885
F	1.8001225413	-1.2275282826	-2.3917518173
C	2.3407945284	0.0436483552	0.1727640190
C	3.0173822581	-1.1751786586	0.2296664788
C	4.3855164413	-1.2691851303	0.4308509979
C	5.1295614128	-0.1032115604	0.5665361852
C	4.5022768088	1.1342228277	0.5003376078
C	3.1289217160	1.1858281564	0.3087894324
F	6.4387078426	-0.1723250296	0.7532352632
F	5.2184272968	2.2482319322	0.6096494520
F	2.5807921387	2.4001053031	0.2115857436
F	4.9884756958	-2.4513332236	0.4945570157
F	2.3423360108	-2.3220864228	0.1041550058
C	-2.9910654390	3.4555770713	1.1534775682
C	-4.0754191062	3.9261913239	0.4184939790
C	-5.1141956476	4.6493506013	0.9887457769
C	-5.0806030228	4.9333850157	2.3483117127
C	-4.0089331662	4.5025903005	3.1197997299
C	-2.9932077020	3.7858558510	2.5054651980
F	-6.0633681798	5.6245509362	2.9054483248
F	-3.9621897014	4.7845389601	4.4163723796
F	-1.9535234661	3.4134376760	3.2732649258
F	-6.1319909266	5.0749669137	0.2497027492
F	-4.1505981488	3.7025142489	-0.8981295349

C	-0.2391267285	3.8809994996	0.2765769005
C	-0.3002681743	4.7629708718	-0.7933293719
C	0.5947655469	5.8107394643	-0.9449447252
C	1.5792916577	5.9942778452	0.0201187956
C	1.6620074563	5.1389409931	1.1125490116
C	0.7502397681	4.1002378928	1.2240195009
F	2.4428692934	6.9911114867	-0.1029838494
F	2.6082774975	5.3169073542	2.0255956458
F	0.8549352239	3.2835601223	2.2782149641
F	0.5193791637	6.6336817663	-1.9840755629
F	-1.2547082732	4.5966496178	-1.7194247624
C	-2.1210475392	1.6514290409	-1.1096593019
C	-3.3701098571	1.0405933368	-1.1697755325
C	-3.7854083754	0.2965723396	-2.2636602542
C	-2.9194553487	0.1450369783	-3.3415443713
C	-1.6619739350	0.7344965142	-3.3183931744
C	-1.2894731231	1.4806996324	-2.2100148860
F	-3.2688818568	-0.6173592040	-4.3660058237
F	-0.8149553107	0.5363529111	-4.3224394851
F	-0.0512822784	1.9872323838	-2.1925744248
F	-4.9678505432	-0.3024462678	-2.2745128636
F	-4.1942945968	1.1099239474	-0.1208140803

M23-TS2

B	0.9695069021	0.2033619936	-0.0631993901
Si	-0.9671774948	2.7502931506	-0.1960593200
C	0.4630382525	2.6871586890	1.0773983596
O	1.2625636278	2.8089965139	1.9006127070
O	0.5924340581	1.5308082797	-0.1030858656
C	0.8920185468	-0.6456002918	-1.3679793287
C	0.7337718403	-0.0509561128	-2.6258650023
C	0.6598383963	-0.7842893761	-3.8000826538
C	0.7384432920	-2.1701874624	-3.7389337640
C	0.8884842673	-2.8071278391	-2.5131975480
C	0.9624759724	-2.0436185518	-1.3588791953
F	0.6668600416	-2.8847398968	-4.8486208047
F	0.9516389446	-4.1319929786	-2.4588140828
F	1.0790353602	-2.7117140663	-0.2110925788
F	0.5176602637	-0.1799762573	-4.9729475047
F	0.6587275644	1.2722703935	-2.7426570084
C	1.4211949013	-0.3635254264	1.3305456791
C	0.6614010137	-0.1176226369	2.4690863101
C	1.0237827349	-0.5692282503	3.7275972653
C	2.1989543899	-1.3006136883	3.8604251482
C	2.9862670748	-1.5737597679	2.7469883684
C	2.5824746050	-1.1080803242	1.5049377922
F	2.5687920675	-1.7409883881	5.0525651480
F	4.1070589669	-2.2709121676	2.8847817798
F	3.3537430378	-1.3801889865	0.4497553239
F	0.2708709173	-0.3176529816	4.7906332572

F	-0.4867084370	0.5756516911	2.3598640573
Cl	-2.3675783418	3.8371041202	0.8789461858
Cl	-0.3111388973	3.9660228864	-1.6890501373
Cl	-2.1406356790	1.2061939755	-0.8851356176

M24-TS2

B	0.6336008445	-0.0271247018	0.1855583514
Si	-0.4491062691	2.9445312039	-0.2454693882
C	0.1783448298	2.4108056302	1.4664832543
O	0.5220116542	2.2342780021	2.5542403294
O	-0.0348563578	1.1541360652	0.4076849815
C	0.0132951680	-1.0427721384	-0.8232011778
C	0.7795569263	-2.0133276304	-1.4752608576
C	0.2369751801	-2.9188346816	-2.3721799788
C	-1.1274226283	-2.8741337204	-2.6354904435
C	-1.9306005817	-1.9303757797	-2.0077728559
C	-1.3535775235	-1.0320515430	-1.1213543377
F	-1.6617007253	-3.7328697623	-3.4877081075
F	-3.2340437652	-1.8995396102	-2.2572786487
F	-2.1666132071	-0.1591231967	-0.5330561164
F	1.0001455129	-3.8181833763	-2.9817034629
F	2.0955220563	-2.0837032681	-1.2667026703
C	1.9780602074	-0.2684228071	0.9577071099
C	2.8930080122	0.7632226802	1.1538870007
C	4.0820838042	0.5944732712	1.8448212083
C	4.3790874951	-0.6580072330	2.3698825705
C	3.4968287717	-1.7183724106	2.1954994425
C	2.3211066899	-1.5084538298	1.4912760659
F	5.5073941345	-0.8420333433	3.0360608399
F	3.7863796843	-2.9100392930	2.7026351679
F	1.4918874837	-2.5440960941	1.3463395136
F	4.9305786902	1.6020883301	2.0045661330
F	2.6479293145	1.9801399948	0.6401245699
F	-0.3977379907	4.5393972772	-0.1476350036
F	0.4560459003	2.6740857109	-1.5243945782
F	-1.9846729722	2.6223162562	-0.4502376742

M25-TS2

B	0.9308188375	0.2673409597	-0.3753508569
Si	-1.1286529704	2.9305217717	0.0147580522
C	0.4606549303	2.8202309915	1.2476137013
O	1.3372659589	2.8688064887	1.9689085790
O	0.2422998085	1.2563096014	0.1380155550
Cl	0.3146741437	-0.6441994049	-1.7878174192
Cl	2.5096355164	-0.2347164635	0.2836393542
C	-1.7234796408	4.6264313776	0.6090637804
H	-0.9712804675	5.4084202831	0.4532189308
H	-2.6189553284	4.9175629657	0.0457810155
H	-1.9941395389	4.6222383608	1.6712897865
C	-0.5658742920	3.1473049610	-1.7525783903

H	-0.5856800250	2.1913390252	-2.2820093676
H	-1.2091955189	3.8693636847	-2.2661834229
H	0.4604827052	3.5288235879	-1.7887450510
C	-2.4575761228	1.7008381658	0.4671590689
H	-3.4478091091	2.1605299737	0.3853835134
H	-2.3951628234	0.8253734100	-0.1840953822
H	-2.3274239329	1.3554123928	1.4981380211

M26-TS2

B	0.6813315523	0.1388468209	-0.1021030676
Si	-1.0765606486	2.9970276197	-0.1091440946
C	0.5400122330	2.8657677062	1.1030509798
O	1.3966264203	2.8438280552	1.8461999139
O	0.4222588324	1.4119277873	-0.2517657835
Cl	-0.2150924870	-1.1234820137	-1.0065554786
Cl	1.9294992509	-0.4490068182	1.0376420258
C	-1.7173125830	4.5996353036	0.6856914240
H	-2.0221748513	4.4086129205	1.7241549541
H	-2.6392322070	4.8696790622	0.1495840195
C	-0.7289330213	5.7708831532	0.6337367239
H	-0.4257994102	5.9936011656	-0.3954203365
H	-1.1560473955	6.6854059445	1.0551806608
H	0.1841464432	5.5550173889	1.2026678175
C	-0.6169200859	3.4229269936	-1.8779883255
H	0.4433414152	3.7048145486	-1.9048433309
H	-1.1840483253	4.3242662753	-2.1463961432
C	-0.8828650953	2.2968259131	-2.8834321784
H	-1.9404134414	2.0118123514	-2.8951592108
H	-0.6144966781	2.6103821078	-3.8964415728
H	-0.3006397529	1.4070404668	-2.6337705405
C	-2.3210520203	1.6595271838	0.3059992676
H	-2.2392704667	0.8582108024	-0.4355722479
H	-3.3188468671	2.1078966834	0.2066490682
C	-2.1544014647	1.0854824842	1.7212393521
H	-2.2242947212	1.8668186468	2.4871492999
H	-2.9282301338	0.3442072534	1.9381969812
H	-1.1866079355	0.5846013487	1.8407873554

M27-TS2

B	0.4356617524	0.0665586213	-0.2126446616
Si	-1.0181017259	2.9538795956	-0.1339102526
C	0.6956358883	2.7595076120	0.8752913593
O	1.6482921484	2.6842791428	1.4883926549
O	0.4134848265	1.3520271100	-0.4828157688
Cl	0.4649323535	-1.1507117864	-1.5209371804
Cl	0.4382207429	-0.5650455874	1.4615225105
C	-1.6047373224	4.4775762792	0.8278102533
C	-2.9725703475	4.7171450103	1.0315308617
C	-3.4162589776	5.8789163452	1.6601942306
C	-2.4970011395	6.8286560437	2.0994425182

C	-1.1347184000	6.6162636399	1.9023732429
C	-0.7000170646	5.4530566813	1.2717146728
H	-3.7034958161	3.9844146686	0.6966745018
H	-4.4793626862	6.0411344491	1.8091925932
H	-2.8409748135	7.7320204641	2.5935056436
H	-0.4129066164	7.3537011607	2.2393468927
H	0.3705181966	5.3195306348	1.1153631233
C	-0.7514818539	3.5134982408	-1.8987989585
C	-1.2259916394	4.7863007078	-2.2606654003
C	-1.1595651933	5.2284953863	-3.5797140201
C	-0.6201264485	4.4046795262	-4.5629457643
C	-0.1447698551	3.1401358055	-4.2228951351
C	-0.2049567866	2.6982712532	-2.9049225799
H	-1.6515855995	5.4435699488	-1.5080345162
H	-1.5284144885	6.2166834603	-3.8359207398
H	-0.5665806766	4.7481126909	-5.5916326500
H	0.2814749477	2.4955408025	-4.9851826788
H	0.1875546873	1.7210278921	-2.6474821365
C	-2.2424744653	1.5996161819	0.2566271421
C	-2.5984814686	0.6705086685	-0.7323875163
C	-3.4691917932	-0.3751710544	-0.4432596471
C	-3.9839523548	-0.5152245821	0.8453809369
C	-3.6368094481	0.3965967915	1.8380671287
C	-2.7777536666	1.4535252809	1.5423100083
H	-2.1798574159	0.7588350748	-1.7331673897
H	-3.7378305272	-1.0854988208	-1.2186226113
H	-4.6534380248	-1.3383500463	1.0748081434
H	-4.0309674485	0.2846915795	2.8431611810
H	-2.5186575309	2.1651047795	2.3233732742

M28-TS2

B	0.7272048294	0.2840068895	-0.8733631475
Si	-1.1262627541	2.8619212594	-0.0062547670
C	0.6081799767	2.5853783117	0.8150847665
O	1.6158505207	2.5748430554	1.3475588770
O	0.0264962485	1.1318519792	-0.1187448529
Cl	0.0449564541	-0.3681357110	-2.3728454857
Cl	2.3492537839	-0.2275040839	-0.3972557750
C	-2.4219166714	1.8324448078	0.8454988019
C	-3.1182577100	0.8377465547	0.1693626115
C	-4.0717903145	0.0487225924	0.7960449346
C	-4.3293705218	0.2474220185	2.1479889307
C	-3.6383954599	1.2210740534	2.8608187236
C	-2.6990857375	1.9936570155	2.1964454904
F	-5.2327173649	-0.4997395131	2.7623182900
F	-3.8814799914	1.3984286928	4.1533103263
F	-2.0321806882	2.9211695183	2.8966031530
F	-4.7304327390	-0.8882565183	0.1264082997
F	-2.8713570776	0.6209215478	-1.1233001397
C	-1.4241011060	4.6738080800	0.5024993443

C	-0.3858841090	5.5726845130	0.2769802720
C	-0.4584889959	6.9229504502	0.5780532148
C	-1.6374158914	7.4150364737	1.1263065771
C	-2.7082755546	6.5605477498	1.3565202171
C	-2.5876450136	5.2131367773	1.0399641825
F	-1.7419278871	8.7012692076	1.4225267391
F	-3.8349988382	7.0386521188	1.8704681908
F	-3.6557339186	4.4424578489	1.2654549337
F	0.5633456714	7.7378610630	0.3472662403
F	0.7549662182	5.1120094641	-0.2709115208
C	-1.0708239908	3.0018567701	-1.8667475462
C	-2.2612459487	3.1892283251	-2.5552147244
C	-2.3145187268	3.2881028012	-3.9367554558
C	-1.1272776675	3.2178414677	-4.6580528760
C	0.0871403474	3.0510018961	-4.0017094863
C	0.0935937989	2.9489696349	-2.6190660767
F	-1.1539100035	3.3136956181	-5.9779692093
F	1.2143250939	2.9814188728	-4.6964857481
F	1.2752834954	2.7745561004	-2.0076777398
F	-3.4685282277	3.4528639183	-4.5699717038
F	-3.4032880515	3.2660240538	-1.8588387123

M29-TS2

B	0.8859151121	0.1844639307	-0.1126955007
Si	-0.9885059216	2.8937774216	-0.0563713651
C	0.5043248367	2.7435570975	1.1480574026
O	1.3352074670	2.8450209196	1.9341444122
O	0.3369795061	1.3915259326	0.1590822114
Cl	0.1661030778	-0.8128255378	-1.3583333262
Cl	2.2951019496	-0.3560541945	0.7779284720
Cl	-1.7212387019	4.7583609890	0.4688892190
Cl	-0.4879300303	3.1139465902	-2.0172855391
Cl	-2.5418654367	1.6409721157	0.3459825541

M30-TS2

B	0.8617212134	0.2227894515	-0.1000794752
Si	-0.9886060004	2.9070274223	-0.1083253248
C	0.5083676922	2.7436785004	1.0488772407
O	1.3184959388	2.8179954339	1.8640048712
O	0.4662935606	1.5209273490	-0.0726785960
Cl	0.1523410381	-0.8556659047	-1.2806802225
Cl	2.0689907967	-0.3549609697	1.0308830020
F	-1.7014125124	4.2352043609	0.4118294236
F	-0.6394256577	3.2351588659	-1.6142357398
F	-2.0777694763	1.7824648392	0.1211777485

M31-TS2

B	0.7237631281	0.1950809726	-0.1809251517
Si	-1.0182933893	2.9628882451	-0.0826669640
C	0.6467935277	2.8738445222	1.0435551245

O	1.5446480259	2.8757184343	1.7494471798
O	0.4810237780	1.5096715309	-0.1948972648
F	-0.0684352765	-0.6699077007	-0.8236737981
F	1.7625318827	-0.3281790967	0.4712274289
C	-1.7033287358	4.5642873847	0.6686967416
H	-2.6590202159	4.8201649011	0.1940922858
H	-1.8866829687	4.4697624378	1.7455685445
H	-1.0245988594	5.4117564405	0.5158347498
C	-0.6671993034	3.3532305439	-1.8770149613
H	-0.6673220342	2.4375315961	-2.4733231540
H	-1.4079151356	4.0560546110	-2.2713323067
H	0.3222922103	3.8118755044	-1.9791552021
C	-2.2517555920	1.6326104369	0.3810525685
H	-2.1266389117	1.3446542906	1.4315875837
H	-3.2724066130	2.0129003942	0.2674499499
H	-2.1208893101	0.7384744625	-0.2328164685

M32-TS2

B	2.3914973817	0.6235933223	-0.0054843141
Si	-0.8011516794	0.0526681599	-0.1882014439
C	0.3549905390	-1.2984489946	0.7629724366
O	0.9661253690	-2.1369719083	1.2408351558
O	1.1734387338	0.3424507276	0.4676446866
F	2.5993284464	1.6217326150	-0.8719773386
F	3.4690791999	-0.0808998257	0.3466903846
C	-2.3368485634	-1.0661417959	-0.3087786854
H	-2.1192449286	-1.9103983271	-0.9783559654
H	-3.1327803155	-0.4919504456	-0.8043303495
C	-2.8336541166	-1.5902187085	1.0434929408
H	-3.0542336897	-0.7701336257	1.7369331937
H	-3.7437730072	-2.1893192915	0.9442264056
H	-2.0826322103	-2.2277618732	1.5263036055
C	-1.2870328657	1.5225534061	0.8765634158
H	-0.5252733912	2.2925079222	0.7148774375
H	-1.2046927690	1.2422013789	1.9347144341
C	-2.6903007110	2.0599281608	0.5697349941
H	-3.4665249341	1.3231071278	0.7983882615
H	-2.9044665067	2.9577381491	1.1569134592
H	-2.7948892850	2.3292529480	-0.4876918844
C	-0.2357985257	0.3296973704	-1.9589293344
H	0.3554935696	1.2502771563	-2.0005206862
H	-1.1345673755	0.4809544112	-2.5712689945
C	0.5794005231	-0.8407673079	-2.5298821891
H	0.0173028439	-1.7809649793	-2.4944410480
H	0.8557542996	-0.6625871275	-3.5728262612
H	1.5121098433	-0.9941475747	-1.9739166620

M33-TS2

B	0.3440995054	0.1520456426	-0.1586331494
Si	-0.9702100246	2.9419335689	-0.1433795433

C	0.7675667701	2.7273169344	0.7918646087
O	1.7482907465	2.6216143866	1.3683090492
O	0.4333976924	1.4411859949	-0.5309068374
F	0.3121261879	-0.8368045872	-1.0498243802
F	0.3096090486	-0.2037280085	1.1306487803
C	-1.6124092446	4.3796133324	0.9169980739
C	-2.9896399862	4.6239701785	1.0415745502
C	-3.4681708882	5.7335336603	1.7348410320
C	-2.5746670820	6.6266891561	2.3222406612
C	-1.2043348444	6.4085418827	2.2083168221
C	-0.7351730036	5.2970486953	1.5115041567
H	-3.7013950485	3.9353686795	0.5907742626
H	-4.5378592245	5.8998649349	1.8186844294
H	-2.9455268073	7.4894240046	2.8670180834
H	-0.5021010034	7.1010922901	2.6620077546
H	0.3420894578	5.1565996844	1.4283301497
C	-0.7158192583	3.6428228479	-1.8625895737
C	-0.0577847064	2.9492647314	-2.8919877411
C	0.0197962679	3.4830498071	-4.1751630918
C	-0.5542841779	4.7204864868	-4.4561505174
C	-1.2058571354	5.4254659738	-3.4481709247
C	-1.2839047667	4.8922203331	-2.1639719631
H	0.4073015787	1.9940375643	-2.6756116247
H	0.5353808940	2.9326619354	-4.9560932317
H	-0.4898063787	5.1363517535	-5.4571420073
H	-1.6513417885	6.3928513114	-3.6582197723
H	-1.7924173303	5.4592058219	-1.3893505959
C	-2.2271664844	1.5690089283	0.1033538181
C	-2.5171106965	0.6934766920	-0.9552990946
C	-3.4153553592	-0.3561765741	-0.7872144964
C	-4.0236441744	-0.5587500843	0.4509717367
C	-3.7400907150	0.2945653269	1.5137334000
C	-2.8549425686	1.3566026629	1.3373468811
H	-2.0309663179	0.8336172308	-1.9191143987
H	-3.6352735504	-1.0189589392	-1.6181208241
H	-4.7161552528	-1.3837010295	0.5865246401
H	-4.2070559646	0.1343076185	2.4804841231
H	-2.6489146540	2.0234268639	2.1714742555

M34-TS2

B	0.4787220875	0.0458452556	-0.1624125833
Si	-1.0100499832	2.9209497188	-0.0978182801
C	0.7251232655	2.7352017900	0.7488691214
O	1.6949138155	2.7195517701	1.3537953802
O	0.2877571268	1.3741763542	-0.3096627991
F	-0.4508970707	-0.8266745540	-0.5376815873
F	1.5923644957	-0.4300114578	0.3762434661
C	-2.2956676750	1.6981841731	0.4841697734
C	-2.8523572425	0.7705050543	-0.3880941467
C	-3.7797084197	-0.1720745386	0.0311343056

C	-4.1508989613	-0.2044261185	1.3703089203
C	-3.5986310585	0.6949171416	2.2765911515
C	-2.6817701957	1.6262972900	1.8158929352
F	-5.0294131349	-1.1021784344	1.7883631339
F	-3.9506044569	0.6519626613	3.5556926649
F	-2.1464897587	2.4815117180	2.6985555112
F	-4.3004521994	-1.0441252012	-0.8223109642
F	-2.4884913188	0.7675919166	-1.6719998233
C	-1.5321441950	4.6196361197	0.6026281212
C	-2.7794087165	4.9724484784	1.1074843126
C	-3.0646780949	6.2500283506	1.5735045997
C	-2.0797000929	7.2281732194	1.5333051155
C	-0.8222624949	6.9269681507	1.0236325761
C	-0.5852998889	5.6398968850	0.5686084543
F	-2.3406808826	8.4499930061	1.9726642191
F	0.1200615760	7.8607575406	0.9720539204
F	0.6326802029	5.3758069689	0.0589158443
F	-4.2684037570	6.5447420809	2.0503725871
F	-3.7761454578	4.0831798115	1.1535111561
C	-0.8405466664	3.3086873166	-1.9158157098
C	0.3784420365	3.4354967711	-2.5676168477
C	0.4619086378	3.7429981630	-3.9185235555
C	-0.7102457018	3.9361979325	-4.6410549953
C	-1.9487630474	3.8303573203	-4.0172555543
C	-1.9880748329	3.5284475346	-2.6649902361
F	-0.6468276939	4.2306200614	-5.9307148320
F	-3.0626595120	4.0202217423	-4.7133564416
F	-3.1801984136	3.4357624844	-2.0609662145
F	1.6385157279	3.8632481979	-4.5206540615
F	1.5198261765	3.2818007145	-1.8878286137

M35-TS2

B	0.8561807563	0.1895354051	-0.1489035239
Si	-0.9661325666	2.8947262497	-0.0487161826
C	0.5627809415	2.7474871362	1.1080475248
O	1.4149364639	2.8189922923	1.8774207646
O	0.3820648588	1.4531616376	0.0769649988
F	0.2620403282	-0.5856566191	-1.0311386134
F	1.9077320113	-0.2477501001	0.5133141357
Cl	-1.7317668296	4.7290813447	0.5451551046
Cl	-0.5631783405	3.1840422016	-2.0262429086
Cl	-2.4886710093	1.6025906394	0.3722353523

M36-TS2

B	0.8380155145	0.2212261601	-0.1241467533
Si	-0.9828717930	2.9112070010	-0.0981526415
C	0.5271335180	2.7207764214	1.0411291490
O	1.3604478013	2.7457735756	1.8380081664
O	0.4122072965	1.5216521488	-0.0847858339
F	0.3006071610	-0.6267630821	-0.9742274253

F	1.7947455322	-0.1794832785	0.6890689981
F	-1.6552857175	4.2603321561	0.4286494767
F	-0.6669951024	3.2375874660	-1.6138945820
F	-2.1103581724	1.8265042808	0.1524662263