

Supporting Information

Origin of norbornene-mediated selective *meta*-C – H arylation of anisole derivatives overcoming “*ortho* constraint” in Pd/S,O-ligand catalysis

Sheng-Nan Liu, Yang-Yang Xing, Wen-Juan Wang*, Qiong Wang, Chong Yang, Jian-Biao Liu, Fang Huang, De-Zhan Chen*

College of Chemistry, Chemical Engineering and Materials Science, Collaborative Innovation Center of Functionalized Probes for Chemical Imaging in Universities of Shandong, Institute of Molecular and Nano Science, Shandong Normal University, Jinan 250014, P. R. China

Table of Contents

I. Catalytically active species considered by computations.....	S2
II. Free energy profiles for the norbornene insertion.....	S4
III. Free energy profiles for mono- and diarylated pathways.....	S4
IV. Distortion-interaction analysis.....	S9
V. Energy decomposition analysis.....	S9
VI. Calculated energies and imaginary frequencies.....	S10
VII. Cartesian coordinates of all the structures.....	S18

I. Catalytically active species considered by computations.

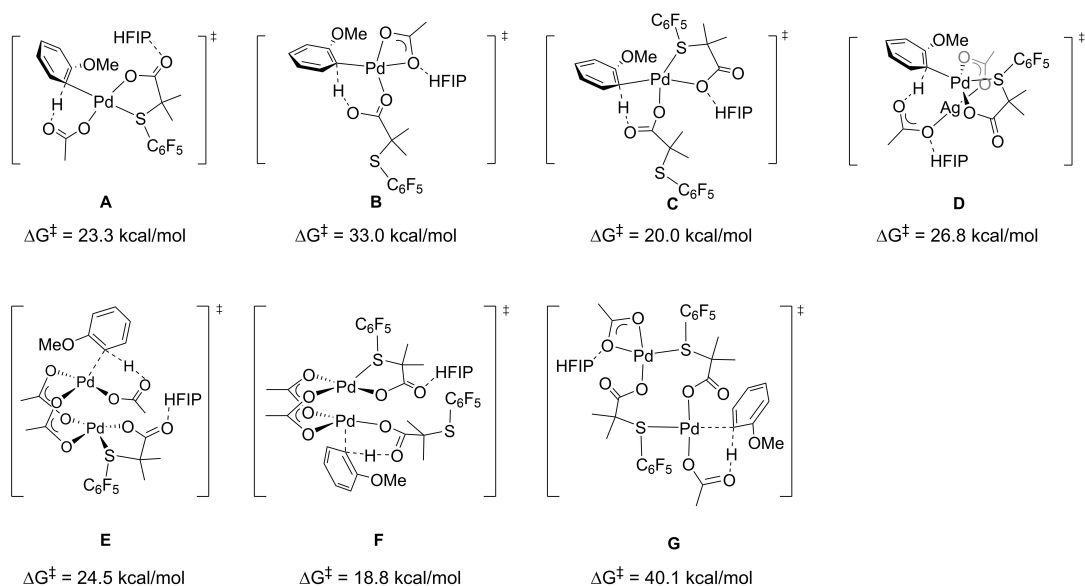


Fig. S1. Reaction free energies for the *ortho*-carbopalladation catalyzed by monomer or dimer palladium (the energies are respect to the $\text{Pd}_3(\text{OAc})_6$ trimer).

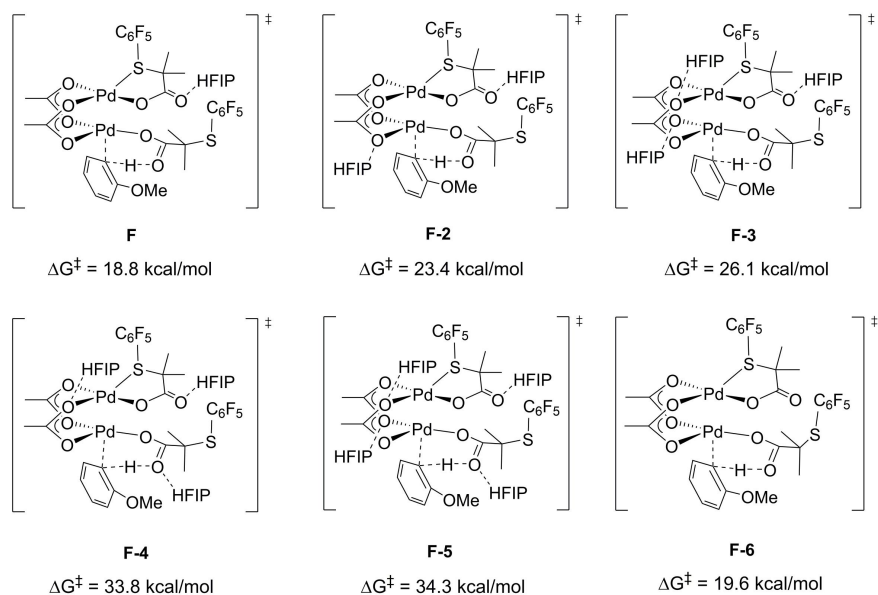


Fig. S2. The effect of noncovalent interactions between the HFIP molecules with both the substrate and the catalyst for Pd catalyzed C–H bond activation.

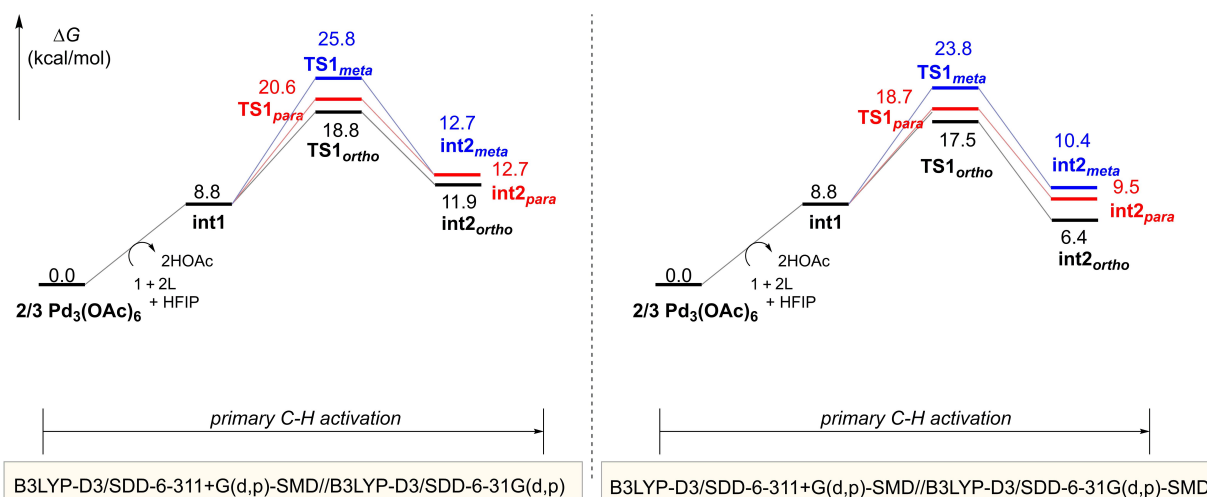


Fig. S3. Free energy profiles for C–H activation based on the structure optimized in the gas-phase and in HFIP solvent, the difference is small and consistent trends.

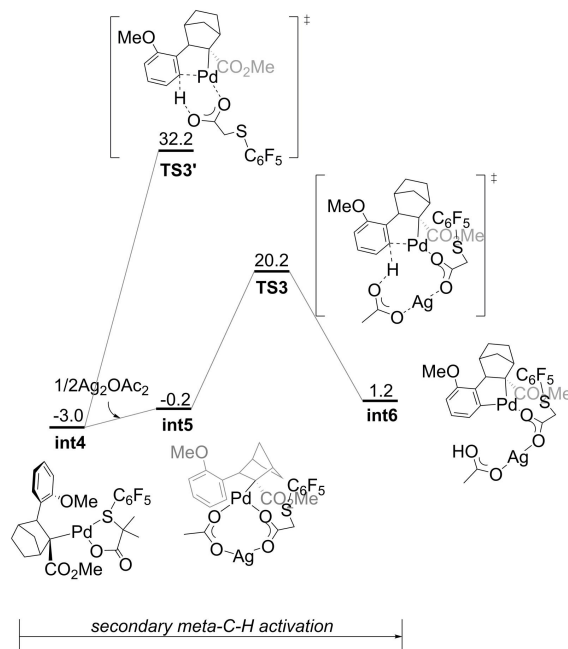


Fig. S4. Free energy profiles for secondary *meta*-C–H activation catalyzed by monomer Pd and heterodimer Pd-Ag.

II. Free energy profiles for norbornene insertion.

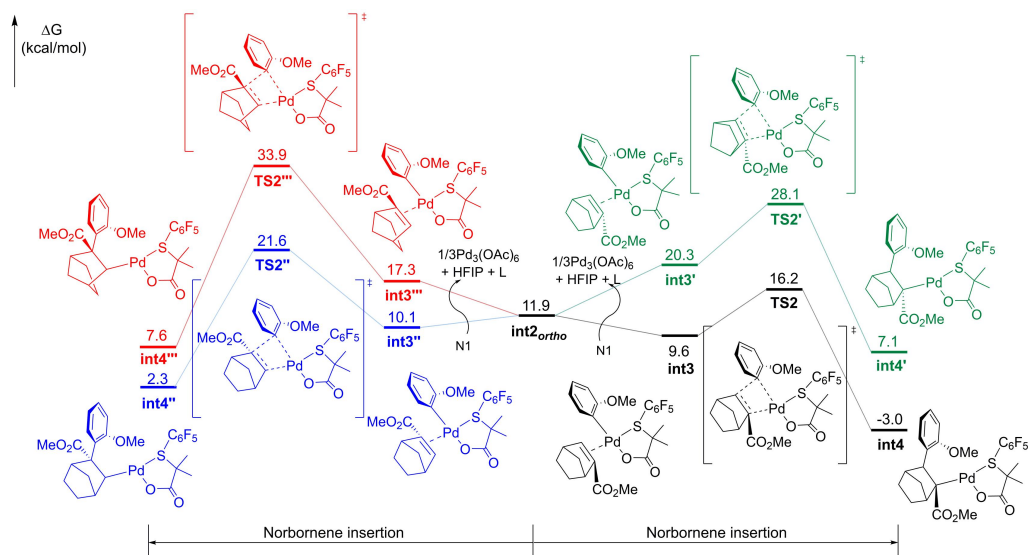


Fig. S5. Free energy profiles for four types of norbornene insertion.

III. Free energy profiles for mono- and diarylated pathways.

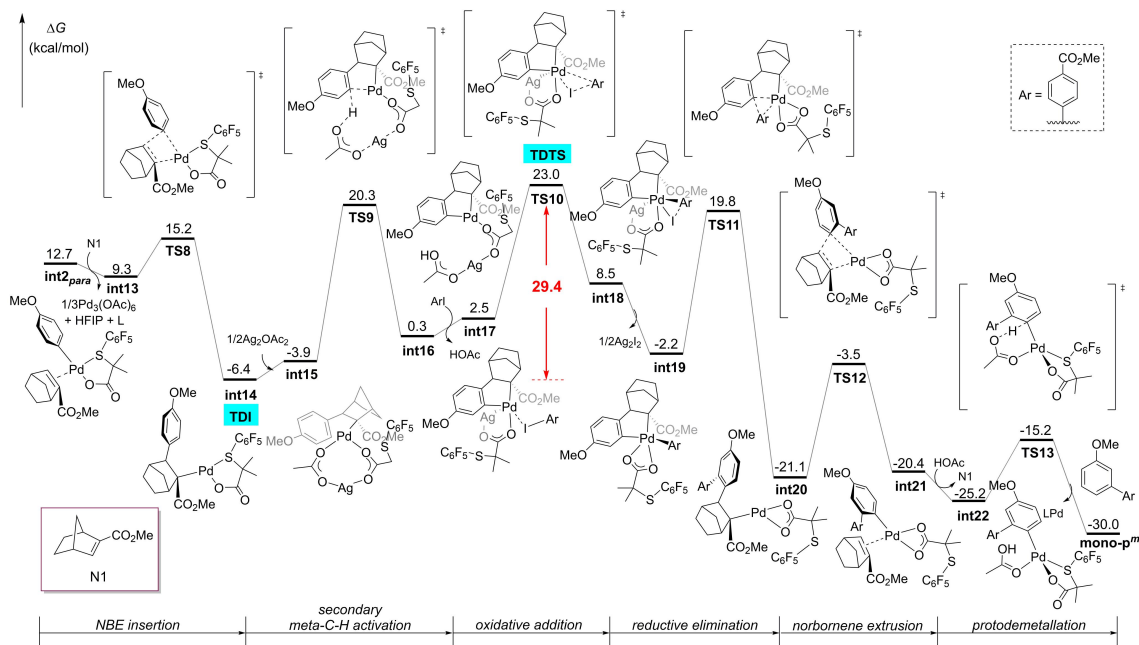


Fig. S6. Free energy profiles for the formation of **mono-p'''** from primary *para*-C–H activation in the **N1** system.

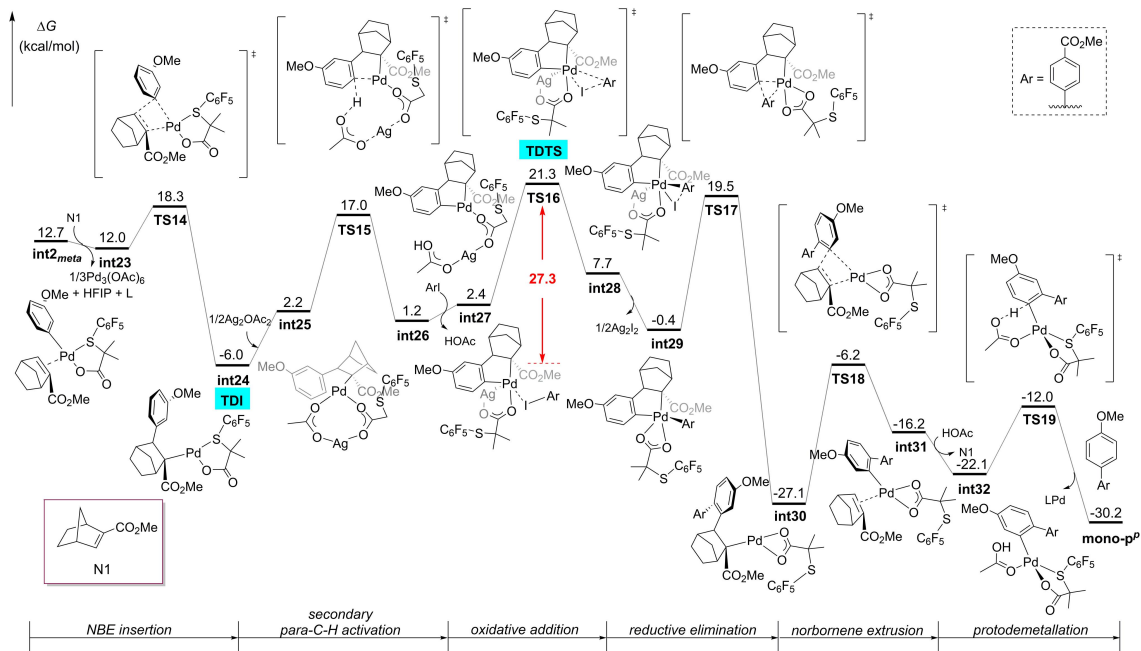


Fig. S7. Free energy profiles for the formation of **mono-p''** from primary *meta*-C–H activation in the **N1** system.

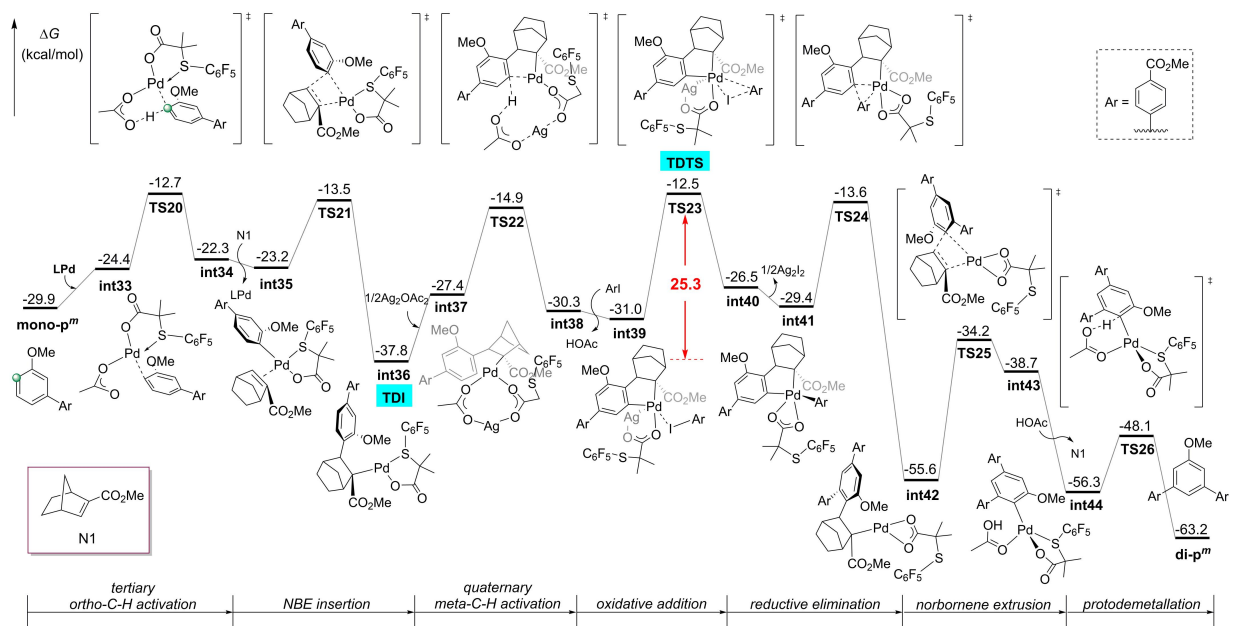


Fig. S8. Free energy profiles for the formation of **di-p'''** from tertiary *ortho*-C–H activation in the **N1** system.

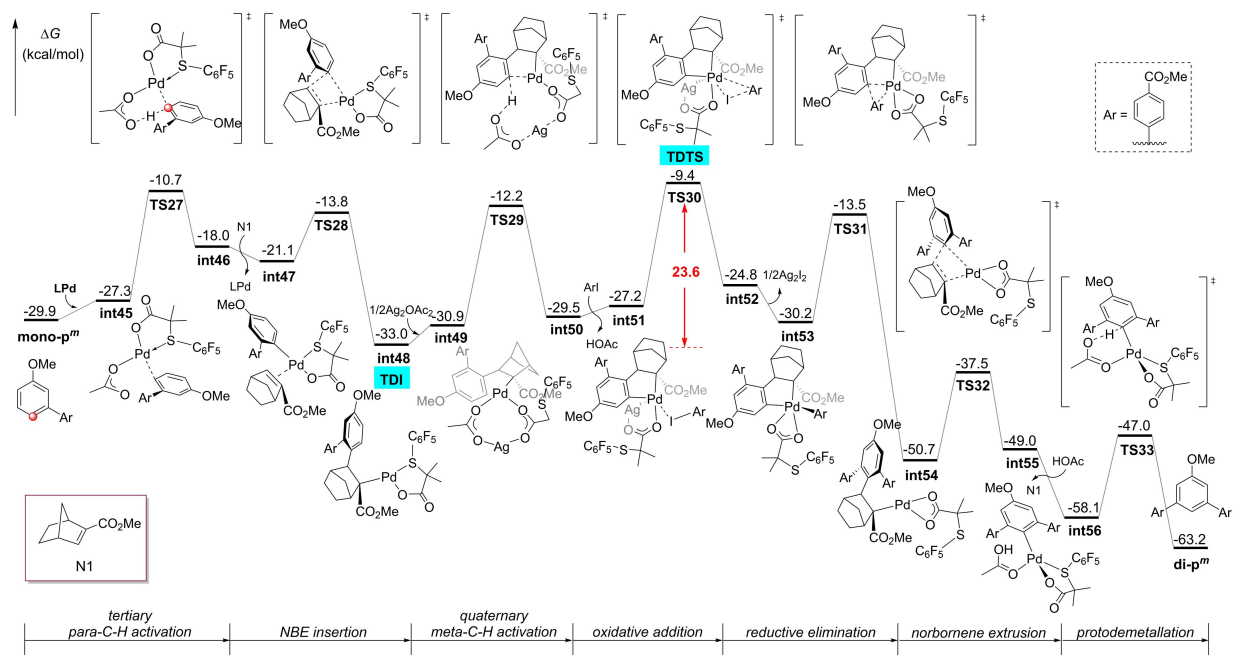


Fig. S9. Free energy profiles for the formation of **di-p^m** from tertiary *para*-C-H activation in the **N1** system.

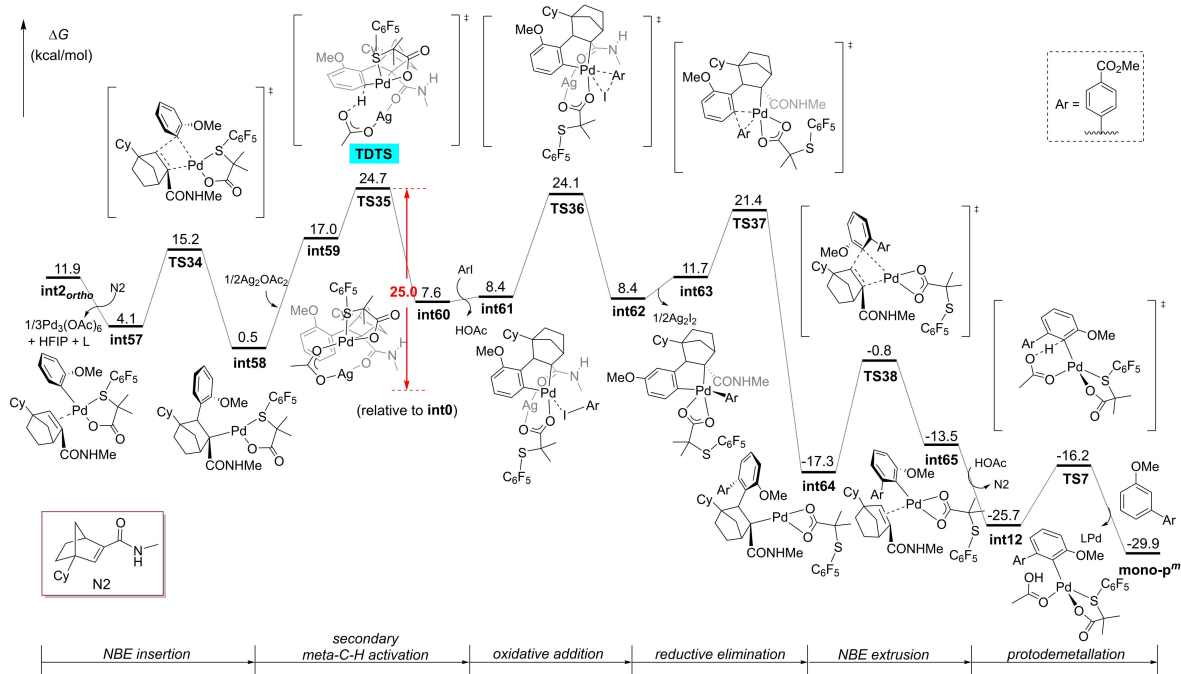


Fig. S10. Free energy profiles for the formation of **mono-p^m** from primary *ortho*-C-H activation in the **N2** system.

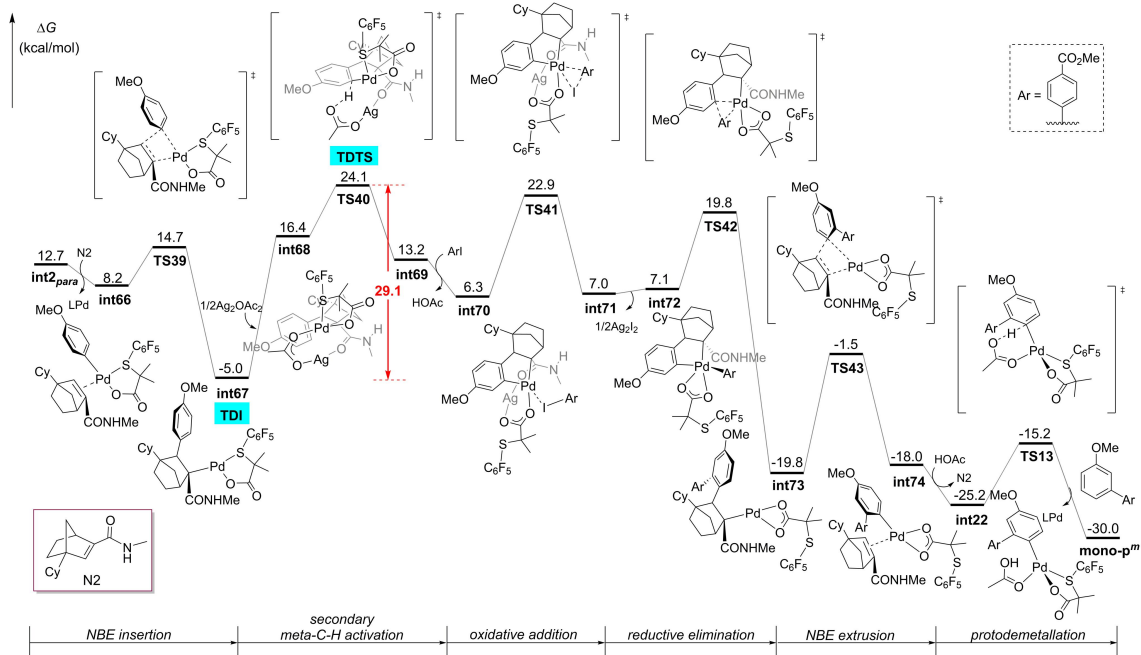


Fig. S11. Free energy profiles for the formation of **mono-p'''** from primary *para*-C-H activation in the **N2** system.

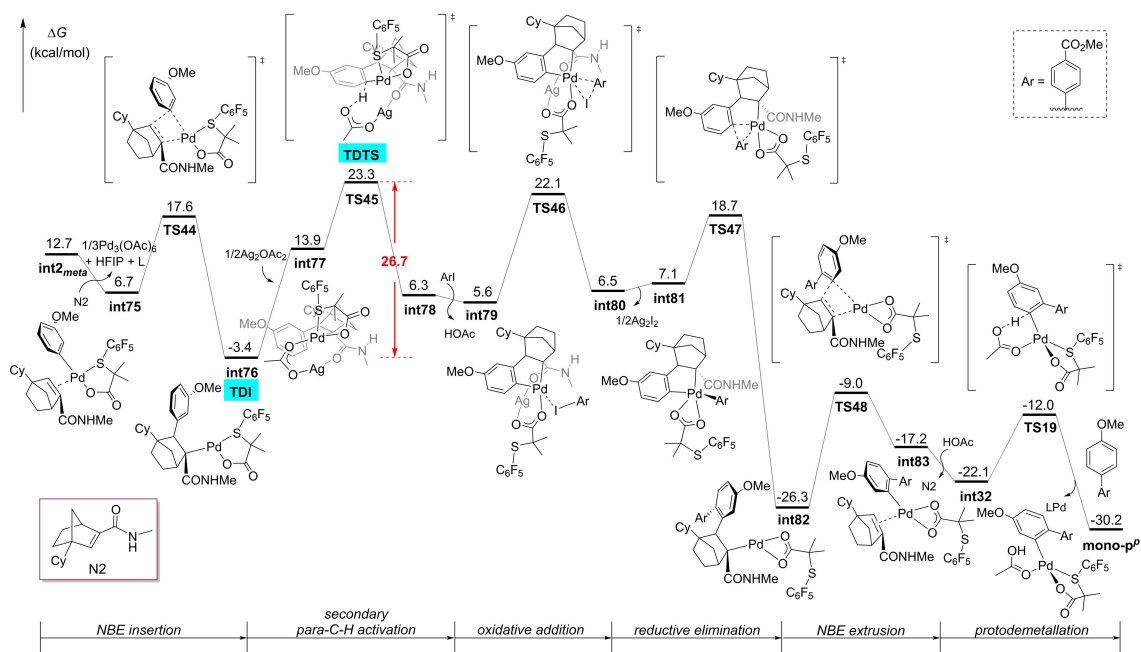


Fig. S12. Free energy profiles for the formation of **mono-p'''** from primary *meta*-C-H activation in the **N2** system.

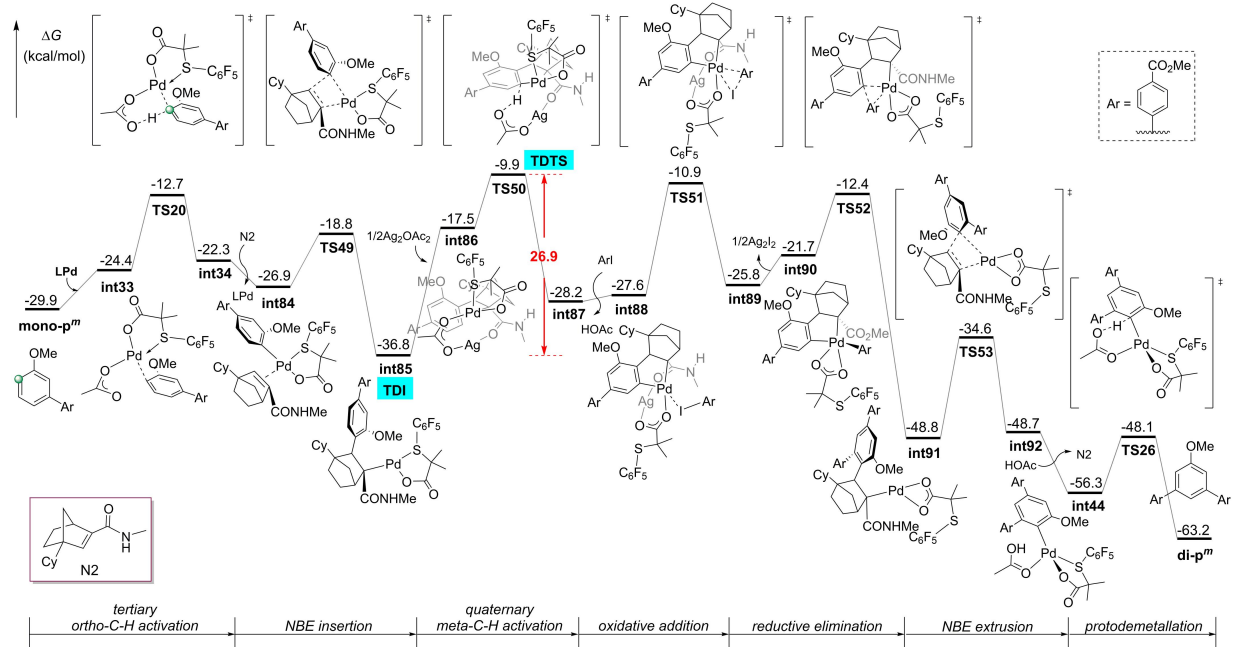


Fig. S13. Free energy profiles for the formation of **di-p^m** from tertiary *ortho*-C-H activation in the **N2** system.

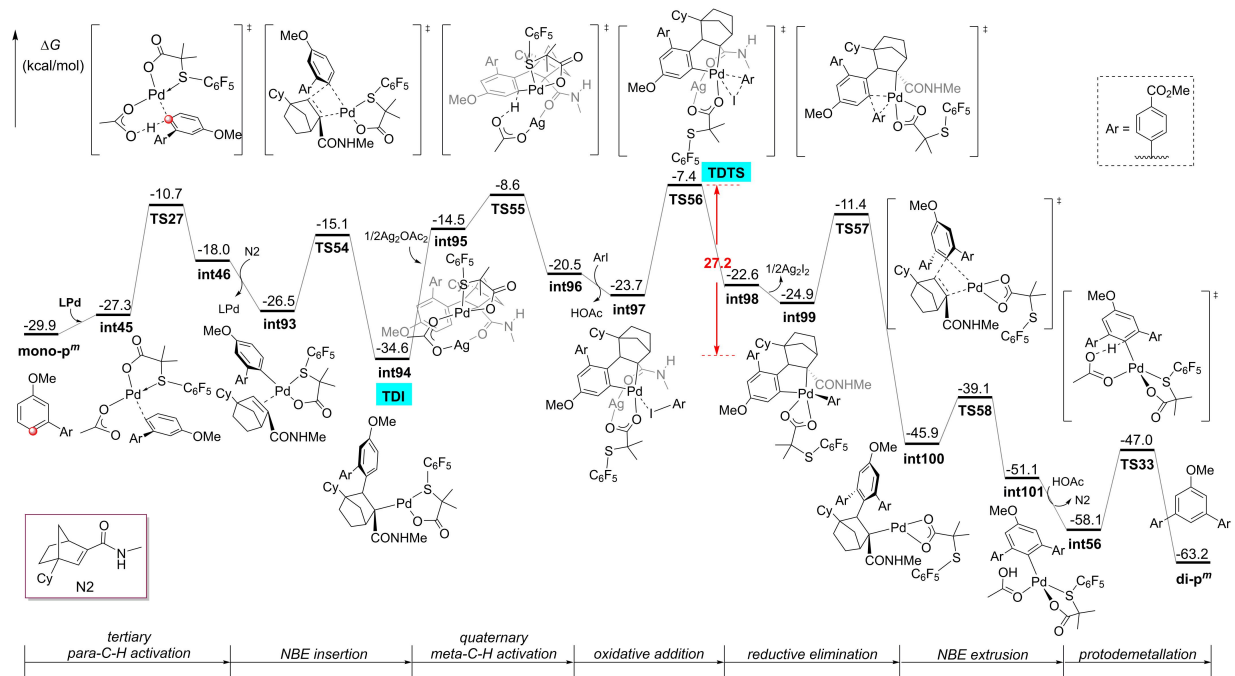


Fig. S14. Free energy profiles for the formation of **di-p^m** from tertiary *para*-C-H activation in the **N2** system.

IV. Distortion-interaction analysis.

Table S1. Distortion of substrate part for TS2, TS2', TS2'' and TS2'''.

Energy (kcal/mol)	E _{dist} (NBE)	E _{dist} (sub)	E _{int}
TS2	9.9	5.8	-47.1
TS2'	22.0	8.7	-51.0
TS2''	15.8	10.8	-48.7
TS2'''	25.9	9.1	-52.4

V. Energy decomposition analysis.

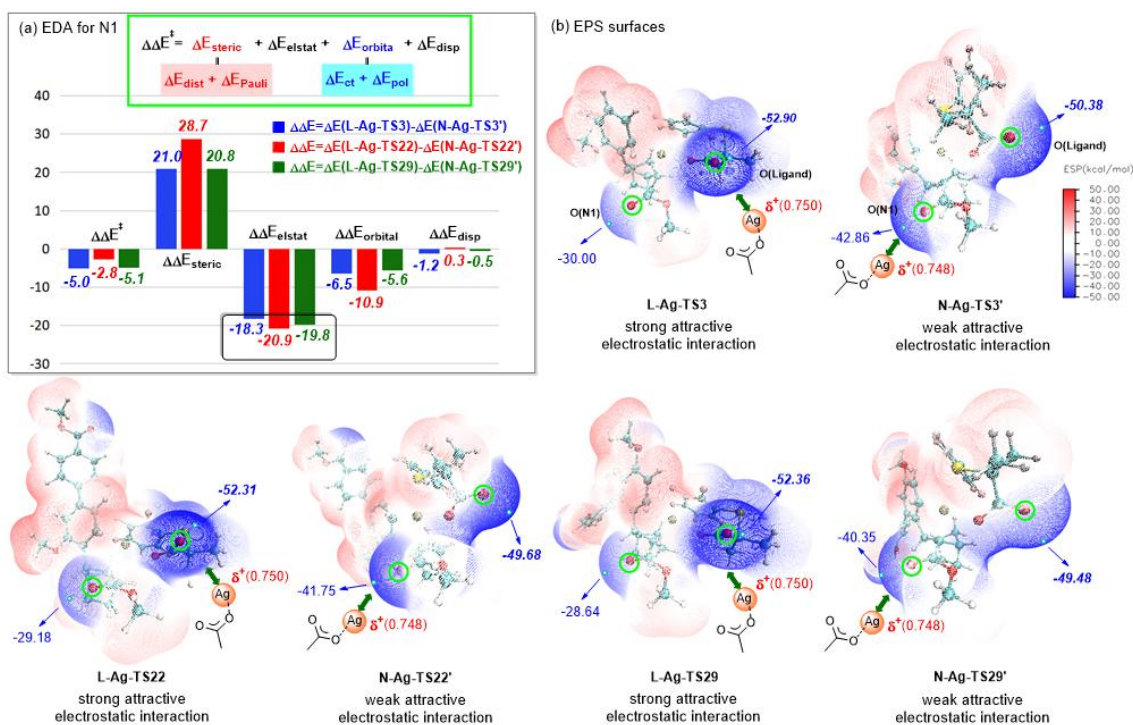


Fig. S15. Energy decomposition analysis in two conformations for secondary and quaternary *meta*-C–H activation in the N1 system.

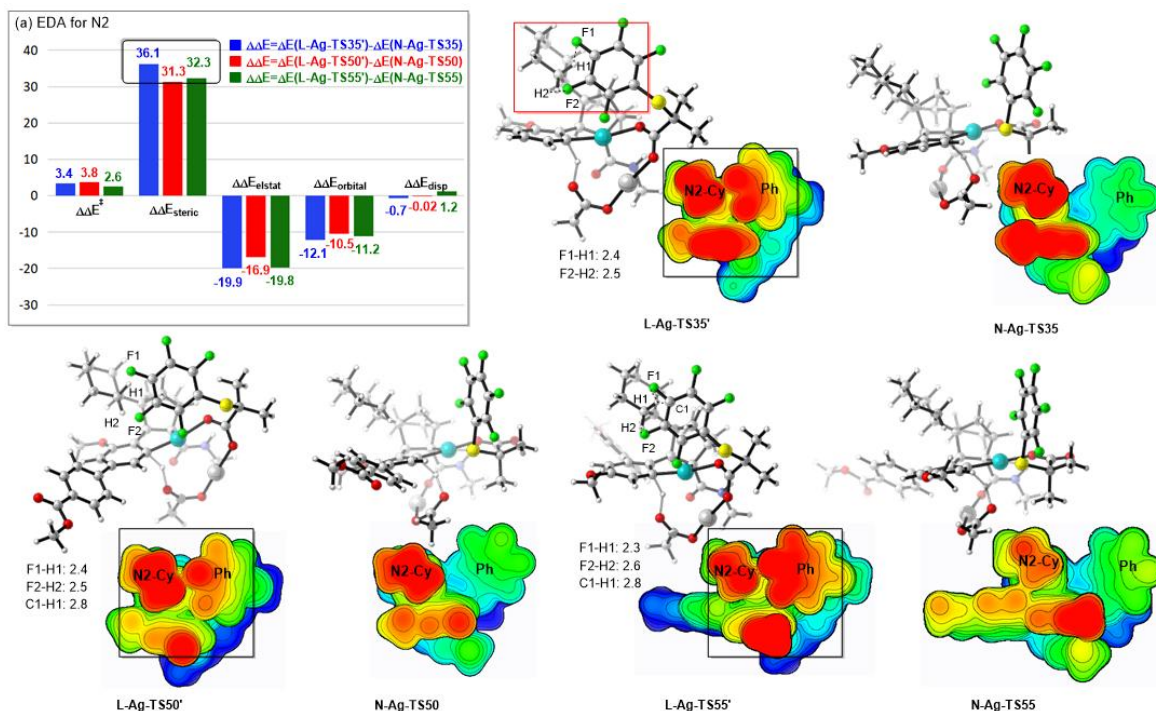


Fig. S16. Energy decomposition analysis in two conformations for secondary and quaternary *meta*-C–H activation in the N2 system.

VI. Calculated energies and imaginary frequencies

Stationary point	Thermal correction to Gibbs free energy at B3LYP-D3/6-31 G(d,p)-SDD (in a.u.) (1)	Single-point energy including solvation energy at B3LYP-D3/6-311++ G(d,p)- SDD (in a.u.) (2)	Gibbs free energies (G) (in a.u.) (3)=(1)+(2)+ $aRT*\ln 31.4$ ($a=3.8088*10^{-7}$)	Imaginary frequencies (in cm-1)
Pd₃(OAc)₆	0.219198	-1755.3950923	-1755.1719907	
1	0.093575	-346.8868957	-346.7894171	
S,O-ligand	0.099624	-1433.4738836	-1433.3703560	
N1	0.150331	-500.7857617	-500.6315271	
N2	0.301535	-715.6862037	-715.3807651	

HOAc	0.0275	-229.178768	-229.1473644	
ArI	0.083513	-471.0969824	-471.0095658	
Ag₂OAc₂	0.045446	-751.2632259	-751.2138763	
Ag₂I₂	-0.048244	-317.0317724	-317.0761128	
int0	0.289644	-3578.8547148	-3578.5611672	
int1	0.453418	-4715.8503677	-4715.3930461	
TS1_{ortho}	0.448602	-4715.8296625	-4715.3771569	-1241.42
int2_{ortho}	0.454523	-4715.8464888	-4715.3880622	
int3	0.374548	-2407.9169979	-2407.5385463	
TS2	0.374075	-2407.9060494	-2407.5280708	-217.38
int4	0.377777	-2407.9403445	-2407.5586639	
int5	0.422668	-2783.5877351	-2783.1611635	
TS3	0.413788	-2783.546362	-2783.1286704	-1056.42
int6	0.421619	-2783.5844469	-2783.1589243	
int7	0.46896	-3025.4908245	-3025.0179609	
TS4	0.472603	-3025.4649316	-3024.9884250	-152.45
int8	0.477582	-3025.4914485	-3025.0099629	
int9	0.486602	-2866.965184	-2866.4746784	
TS5	0.485477	-2866.9426668	-2866.4532862	-241.48
int10	0.486658	-2866.9992431	-2866.5086815	
TS6	0.482139	-2866.972912	-2866.4868694	-198.44
int11	0.484287	-2866.9783283	-2866.4901377	
int12	0.353889	-2595.3995674	-2595.0417748	
TS7	0.350229	-2595.3807955	-2595.0266629	-796.35
mono-p^m	0.198896	-805.9810152	-805.7782156	
TS1_{para}	0.451016	-4715.829167	-4715.3742474	-1396.79
int2_{para}	0.453623	-4715.8443006	-4715.3867740	

int13	0.37101	-2407.9139217	-2407.5390081	
TS8	0.37279	-2407.9064068	-2407.5297132	-208.98
int14	0.380323	-2407.9482536	-2407.5640270	
int15	0.424302	-2783.5952852	-2783.1670796	
TS9	0.415493	-2783.5479637	-2783.1285671	-1171.97
int16	0.421517	-2783.58572	-2783.1602994	
int17	0.467611	-3025.4906183	-3025.0191037	
TS10	0.473971	-3025.4643292	-3024.9864546	-146.67
int18	0.477109	-3025.4905332	-3025.0095206	
int19	0.482226	-2866.9745552	-2866.4884256	
TS11	0.483677	-2866.9410117	-2866.4534311	-268.67
int20	0.486851	-2867.0093792	-2866.5186246	
TS12	0.482561	-2866.977031	-2866.4905664	-187.86
int21	0.47899	-2867.0003392	-2866.5174456	
int22	0.355291	-2595.4001912	-2595.0409966	
TS13	0.350857	-2595.3799102	-2595.0251496	-1275.25
TS1_{meta}	0.447245	-4715.8171771	-4715.3660285	-1233.71
int2_{meta}	0.451405	-4715.8421214	-4715.3868128	
int23	0.37362	-2407.9123281	-2407.5348045	
TS14	0.374801	-2407.9034736	-2407.524769	-216.74
int24	0.376482	-2407.9437715	-2407.5633859	
int25	0.418852	-2783.5801615	-2783.1574059	
TS15	0.412679	-2783.5501137	-2783.1335311	-1230.59
int26	0.420064	-2783.5828731	-2783.1589055	
int27	0.468781	-3025.4918793	-3025.0191947	
TS16	0.472665	-3025.4656951	-3024.9891265	-143.60
int28	0.476601	-3025.4912337	-3025.0107291	

int29	0.483601	-2866.9731402	-2866.4856356	
TS17	0.484062	-2866.9418319	-2866.4538663	-238.90
int30	0.488522	-2867.0206905	-2866.5176255	
TS18	0.485977	-2866.9848136	-2866.4949330	-227.66
int31	0.48296	-2866.997588	-2866.5107244	
int32	0.356576	-2595.3963807	-2595.0359011	
TS19	0.352467	-2595.3762375	-2595.0198669	-1002.92
mono-p^p	0.199132	-805.9816194	-805.7785838	
int33	0.355649	-2595.3992398	-2595.0396872	
TS20	0.352808	-2595.3777472	-2595.0210356	-946.98
int34	0.355663	-2595.3958643	-2595.0362977	
int35	0.479746	-2867.0055702	-2866.5219206	
TS21	0.487038	-2866.9973942	-2866.5064526	-261.46
int36	0.484938	-2867.0340649	-2866.5452233	
int37	0.527976	-3242.6674333	-3242.1355537	
TS22	0.518159	-3242.6377122	-3242.1156496	-1076.72
int38	0.522067	-3242.6661476	-3242.140177	
int39	0.576913	-3484.5843812	-3484.0035646	
TS23	0.580374	-3484.5582511	-3483.9739735	-145.30
int40	0.583	-3484.5832647	-3483.9963611	
int41	0.593278	-3326.0600955	-3325.4629139	
TS24	0.59143	-3326.0330251	-3325.4376915	-287.72
int42	0.587736	-3326.0963702	-3325.5047306	
TS25	0.591051	-3326.0656304	-3325.4706758	-194.47
int43	0.588737	-3326.0704043	-3325.4777637	
int44	0.463484	-3054.4890252	-3054.0216376	
TS26	0.459486	-3054.4719792	-3054.0085896	-877.43

di-p^m	0.304332	-1265.0705635	-1264.7623279	
int45	0.356657	-2595.4049438	-2595.0443832	
TS27	0.353293	-2595.3750673	-2595.0178707	-1074.32
int46	0.357299	-2595.3907159	-2595.0295133	
int47	0.480147	-2867.0026295	-2866.5185789	
TS28	0.481054	-2866.9919035	-2866.5069459	-210.88
int48	0.486391	-2867.0277912	-2866.5374966	
int49	0.531426	-3242.6764492	-3242.1411196	
TS29	0.519806	-3242.6350948	-3242.1113852	-1083.79
int50	0.520368	-3242.6632225	-3242.1389509	
int51	0.578046	-3484.5794267	-3483.9974771	
TS30	0.579163	-3484.5521188	-3483.9690522	-144.05
int52	0.581565	-3484.5791369	-3483.9936683	
int53	0.585055	-3326.0532163	-3325.4642577	
TS31	0.58518	-3326.0265978	-3325.4375142	-159.94
int54	0.594437	-3326.095193	-3325.4968524	
TS32	0.590838	-3326.0706287	-3325.4758871	-239.52
int55	0.587612	-3326.0857064	-3325.4941908	
int56	0.460907	-3054.4892986	-3054.0244880	
TS33	0.458795	-3054.4694457	-3054.0067471	-1296.64
int57	0.52967	-2622.830237	-2622.2966634	
TS34	0.530099	-2622.8129474	-2622.2789448	-247.01
int58	0.531241	-2622.8374274	-2622.3022828	
int59	0.567681	-2998.454529	-2997.8829444	
TS35	0.564242	-2998.4388835	-2997.8707379	-927.69
int60	0.571695	-2998.473549	-2997.8979504	
int61	0.626385	-3240.3892464	-3239.7589578	

TS36	0.629511	-3240.3673117	-3239.7338971	-148.57
int62	0.633136	-3240.3959813	-3239.7589417	
int63	0.639606	-3081.8590779	-3081.2155683	
TS37	0.640393	-3081.8443	-3081.2000034	-259.45
int64	0.64062	-3081.9063761	-3081.2618525	
TS38	0.641444	-3081.8808292	-3081.2354816	-238.45
int65	0.640188	-3081.899793	-3081.2557014	
int66	0.529268	-2622.8232383	-2622.2900667	
TS39	0.527343	-2622.8109827	-2622.2797361	-227.80
int67	0.534006	-2622.8489444	-2622.3110348	
int68	0.568895	-2998.4566906	-2997.8838920	
TS40	0.563594	-2998.4391342	-2997.8716366	-1021.76
int69	0.577798	-2998.4706863	-2997.8889847	
int70	0.623888	-3240.3900247	-3239.7622331	
TS41	0.6284	-3240.3680973	-3239.7357937	-157.37
int71	0.632395	-3240.3974543	-3239.7611557	
int72	0.64381	-3081.8706671	-3081.2229535	
TS42	0.636111	-3081.8426408	-3081.2026262	-265.01
int73	0.641005	-3081.910709	-3081.2658004	
TS43	0.638492	-3081.8790657	-3081.2366701	-244.23
int74	0.637787	-3081.9046569	-3081.2629663	
int75	0.528324	-2622.8247171	-2622.2924895	
TS44	0.530911	-2622.8098937	-2622.2750791	-240.24
int76	0.533867	-2622.8462722	-2622.3085016	
int77	0.567681	-2998.4595157	-2997.8879311	
TS45	0.563675	-2998.4405601	-2997.8729815	-1290.78
int78	0.571965	-2998.475946	-2997.9000774	

int79	0.623103	-3240.3903149	-3239.7633083	
TS46	0.628116	-3240.369089	-3239.7370694	-152.15
int80	0.632429	-3240.3982407	-3239.7619081	
int81	0.643088	-3081.8699686	-3081.222977	
TS47	0.636318	-3081.8445734	-3081.2043518	-238.41
int82	0.642956	-3081.9229398	-3081.2760802	
TS48	0.637392	-3081.889866	-3081.2485704	-234.78
int83	0.639595	-3081.905106	-3081.2616074	
int84	0.638627	-3081.9196022	-3081.2770716	
TS49	0.636511	-3081.9045361	-3081.2641215	-240.51
int85	0.638153	-3081.9349884	-3081.2929318	
int86	0.673496	-3457.5464729	-3456.8690733	
TS50	0.670221	-3457.5311342	-3456.8570096	-965.70
int87	0.675558	-3457.5655733	-3456.8861117	
int88	0.732444	-3699.483744	-3698.7473964	
TS51	0.736267	-3699.4609741	-3698.7208035	-154.97
int89	0.74025	-3699.4885927	-3698.7444391	
int90	0.745972	-3540.9497552	-3540.1998796	
TS52	0.745454	-3540.9344392	-3540.1850816	-265.44
int91	0.74543	-3540.9924571	-3540.2431235	
TS53	0.747307	-3540.9716027	-3540.2203921	-242.85
int92	0.746113	-3540.9929546	-3540.2429380	
int93	0.636054	-3081.9164343	-3081.2764767	
TS54	0.638731	-3081.9008792	-3081.2582446	-198.11
int94	0.641842	-3081.9351001	-3081.2893545	
int95	0.675275	-3457.5435535	-3456.8643749	
TS55	0.670149	-3457.5289027	-3456.8548501	-874.27

int96	0.683516	-3457.5612993	-3456.8738797	
int97	0.73135	-3699.4764788	-3698.7412252	
TS56	0.735437	-3699.4544336	-3698.7150930	-148.78
int98	0.738574	-3699.4818666	-3698.739389	
int99	0.749479	-3540.9584442	-3540.2050616	
TS57	0.742437	-3540.9297792	-3540.1834386	-253.31
int100	0.750617	-3540.9929922	-3540.2384716	
TS58	0.746227	-3540.9777029	-3540.2275723	-240.59
int101	0.743328	-3540.994032	-3540.2468004	
A	0.283538	-2926.3770897	-2926.0896481	-1247.89
B	0.285954	-2926.3639557	-2926.0740981	-870.51
C	0.363113	-4130.684883	-4130.3178664	-843.01
D	0.32707	-3302.021894	-3301.6909204	-1406.07
E	0.373622	-3511.5225451	-3511.1450195	-1056.21
G	0.446355	-4715.793491	-4715.3432324	-1250.66
F-2	0.497596	-5505.9282978	-5505.4267982	-1378.36
F-3	0.542257	-6296.0256516	-6295.4794910	-1329.13
F-4	0.548011	-6296.0191896	-6295.4672750	-1506.93
F-5	0.58809	-7086.11544	-7085.5234464	-1399.54
F-6	0.406614	-3925.729282	-3925.3187644	-1180.82
TS3'	0.370116	-2407.8765534	-2407.5025338	-626.18
int3'	0.374059	-2407.8993682	-2407.5214056	
TS2'	0.37374	-2407.8867781	-2407.5091345	-236.38
int4'	0.377723	-2407.9240987	-2407.5424721	
int3''	0.372878	-2407.914617	-2407.5378354	
TS2''	0.373463	-2407.8969097	-2407.5195431	-241.66
int4''	0.377187	-2407.9313835	-2407.5502929	

int3'''	0.374103	-2407.9043312	-2407.5263246	
TS2'''	0.376003	-2407.8798101	-2407.4999035	-226.17
int4'''	0.377567	-2407.9232942	-2407.5418236	
N-Ag-TS3'	0.40978	-2783.5354019	-2783.1217183	-1167.45
N-Ag-TS22'	0.517796	-3242.6288328	-3242.1071332	-1229.76
N-Ag-TS29'	0.518053	-3242.6229531	-3242.1009965	-1221.57
L-Ag-TS35'	0.568412	-2998.4406497	-2997.8683341	-1153.61
L-Ag-TS50'	0.674057	-3457.5318934	-3456.8539328	-986.74
L-Ag-TS55'	0.674245	-3457.5297688	-3456.8516202	-925.38

VII. Cartesian coordinates of all the structures.

Pd₃(OAc)₆

Pd	-1.61859900	0.92687400	0.01603000
C	0.07011500	2.59622000	1.86704400
O	-1.02604200	2.43653800	1.25291000
O	1.16871400	1.99882100	1.65011000
C	2.26224700	-1.25584500	-1.89474100
O	1.57060500	-2.11863600	-1.27646400
O	2.31372100	-0.00669300	-1.67729500
C	3.15559100	-1.78167600	-2.99682000
H	3.40091700	-0.98430800	-3.69915900
H	4.08369200	-2.14379000	-2.54194700
H	2.67349000	-2.61808700	-3.50506600
C	0.08508500	3.64160400	2.96057000
H	-0.91396300	3.77101400	3.37785600
H	0.80022400	3.36154300	3.73565900
H	0.41152500	4.59123400	2.52344700
Pd	0.00120900	-1.86983900	0.00007800
C	2.25578900	-1.34550500	1.84188300
O	2.65808400	-0.32323400	1.20900200
O	1.19855600	-2.01434100	1.63392300
C	-0.07334800	2.59622200	-1.86705400
O	-1.17114700	1.99731900	-1.65024400
O	1.02300200	2.43787400	-1.25291200
C	-0.08961000	3.64178700	-2.96038200

H	0.90908000	3.77168800	-3.37838200
H	-0.80522300	3.36162000	-3.73498700
H	-0.41602100	4.59121400	-2.52279300
C	3.12966500	-1.80011300	2.99008800
H	2.94576800	-1.14028100	3.84423000
H	2.89584600	-2.82722800	3.27030900
H	4.18123900	-1.70190400	2.71339200
Pd	1.61741500	0.92886900	-0.01612700
C	-2.25395300	-1.34846700	-1.84185700
O	-2.65755000	-0.32665400	-1.20905900
O	-1.19597600	-2.01606300	-1.63372300
C	-3.12723200	-1.80422500	-2.99006100
H	-2.94433400	-1.14402500	-3.84413100
H	-2.89196300	-2.83097600	-3.27040700
H	-4.17893400	-1.70755800	-2.71329700
C	-2.26086800	-1.25851800	1.89468800
O	-2.31408200	-0.00946700	1.67709600
O	-1.56783700	-2.12037500	1.27668100
C	-3.15365100	-1.78548600	2.99668500
H	-4.08131300	-2.14862300	2.54173300
H	-2.67060600	-2.62137300	3.50489300
H	-3.39993800	-0.98845500	3.69907200

1

C	0.21010900	-1.21256000	-0.16883100
C	1.58247800	-1.20876000	0.08410700
C	2.27111400	-0.00033400	0.21340100
C	1.58297300	1.20841300	0.08440700
C	0.21060600	1.21284000	-0.16850300
C	-0.47094700	0.00029500	-0.29631300
H	-0.34327200	-2.13937100	-0.28269800
H	2.11486500	-2.15100300	0.17715600
H	3.33928500	-0.00057300	0.40828600
H	2.11575400	2.15040900	0.17770100
H	-0.34243000	2.13988700	-0.28211200
O	-1.82191400	0.00066100	-0.58571500
C	-2.65934100	-0.00035900	0.56878000
H	-2.48990400	0.89108400	1.18849700
H	-3.69079700	0.00011100	0.20981900
H	-2.49013300	-0.89303500	1.18678500

S,O-ligand

C	2.25540700	0.20402300	0.51773100
C	3.64961400	-0.32775800	0.17682500
O	4.19283000	-1.25981200	0.72297000
O	4.23278900	0.38903700	-0.81310000
C	-0.36247000	0.03784600	-0.58462600
C	-1.01957500	-1.19025300	-0.42440200
C	-1.10776300	1.19989100	-0.34254100
C	-2.35856300	-1.26259000	-0.04844300
C	-2.44685200	1.14853200	0.03635700
C	-3.07351600	-0.08811000	0.17748500
F	-0.54105300	2.40775700	-0.45182400
F	-3.13384300	2.27351300	0.26275700
F	-4.35576200	-0.14810400	0.53958100
F	-2.96076300	-2.44697900	0.10121000
F	-0.36410500	-2.34025400	-0.60824300
C	1.61777100	-0.69355500	1.57747300
H	2.26745600	-0.72411400	2.45599100
H	0.64599600	-0.29556900	1.87762700
H	1.49019000	-1.71387400	1.21266100
C	2.34363200	1.66615200	0.98479600
H	2.83906100	2.28838500	0.23837000
H	1.34088700	2.06334300	1.15542800
H	2.90534500	1.72299300	1.92458900
H	5.09729200	-0.02170600	-0.98259300
S	1.32640200	0.11051700	-1.13601800

N1

C	0.03223700	-0.38894800	0.21134800
C	-0.76605600	0.85405600	0.58360500
C	-2.23789400	-0.80286000	0.13652500
C	-0.84786100	-1.37248800	-0.05564400
C	-1.97215800	0.19423500	1.29261400
H	-2.80502200	0.88391300	1.46996300
H	-1.69990800	-0.30071800	2.22921000
C	-1.44309500	1.34404400	-0.74034500
H	-1.95879300	2.29493100	-0.57302800
H	-0.70881200	1.49872000	-1.53481800
C	-2.45634300	0.19926800	-1.05519200
H	-3.48806000	0.56500000	-1.04725200
H	-2.27956600	-0.27498200	-2.02392300

H	-0.21471600	1.62282800	1.12393600
H	-0.60274900	-2.35040600	-0.45380300
C	1.48387200	-0.48441600	-0.00481400
O	2.09232200	-1.49890200	-0.28900100
C	3.50695200	0.72224800	-0.04844200
H	3.75348200	0.38838200	-1.06015900
H	3.82946100	1.75220300	0.10490600
H	3.99759900	0.05510300	0.66566500
O	2.08552500	0.72409400	0.15329800
H	-3.04360600	-1.52733300	0.26698900

N2

C	-1.81146300	-0.08279900	-0.25200600
C	-1.51707700	1.41554700	-0.26280200
C	0.47173900	0.33643700	-0.02549400
C	-0.63167900	-0.70837100	-0.10224600
C	-0.14085300	1.41795800	-0.96027800
H	0.36959900	2.38525900	-0.89920300
H	-0.18629100	1.09306800	-2.00415400
C	-1.09752000	1.79370200	1.19655100
H	-0.96277700	2.87671300	1.28568300
H	-1.85111600	1.49032300	1.92864700
C	0.25564800	1.04030200	1.37105300
H	1.07363600	1.73855600	1.57325300
H	0.23234900	0.31436700	2.18680600
H	-2.28037600	2.06532800	-0.69975900
H	-0.50944100	-1.77502100	0.04517000
C	-3.12292400	-0.77913900	-0.21836600
O	-3.21295200	-2.00520600	-0.25447600
N	-4.21938600	0.04272600	-0.14291600
H	-4.07692900	1.03816600	-0.08101400
C	-5.57304100	-0.47143900	-0.06857700
H	-6.04078200	-0.23799200	0.89551700
H	-6.19673600	-0.05951300	-0.86993800
H	-5.51756200	-1.55478400	-0.18011100
C	1.88899100	-0.16654500	-0.33462100
C	2.90583800	0.96789800	-0.56981900
C	2.41753700	-1.13017500	0.74723000
H	1.81989000	-0.73494700	-1.27596600
C	4.29783400	0.41939000	-0.92066100
H	2.98214100	1.58482800	0.33649400

H	2.55680700	1.62915800	-1.37083800
C	3.80490800	-1.68536300	0.39313600
H	2.48259900	-0.59147300	1.70263300
H	1.70996400	-1.95301600	0.90193900
C	4.81055300	-0.55065100	0.15229100
H	5.00411600	1.24690300	-1.05755000
H	4.24232200	-0.10725600	-1.88399900
H	4.15985300	-2.34987900	1.18974200
H	3.72697900	-2.29846400	-0.51587400
H	5.78705000	-0.95776900	-0.13554800
H	4.96307800	-0.00048100	1.09193100

HOAc

O	0.77710500	-1.04697900	-0.00000900
C	0.09305000	0.12625500	-0.00004000
O	0.64398000	1.20378800	0.00000600
C	-1.39576300	-0.11034300	-0.00001300
H	-1.67859500	-0.69219300	0.88204400
H	-1.91522200	0.84676700	-0.00120600
H	-1.67842900	-0.69446400	-0.88060300
H	1.71983900	-0.81005700	0.00011000

ArI

C	-0.07922900	-1.13254500	0.00006400
C	1.31209500	-1.05016700	0.00009100
C	1.94598200	0.19888200	0.00007600
C	1.17534400	1.36790100	0.00001000
C	-0.21597600	1.29896900	-0.00002000
C	-0.82876000	0.04462600	0.00001200
H	1.68291300	2.32673500	-0.00001000
H	-0.80896100	2.20644200	-0.00007000
H	1.90817700	-1.95540600	0.00013100
H	-0.56768000	-2.10002400	0.00008100
I	-2.97761100	-0.08160000	-0.00001800
C	3.42936400	0.34282500	0.00011400
O	4.06200900	-0.85224300	-0.00001100
O	4.01633300	1.40725600	0.00001700
C	5.49731600	-0.78171900	-0.00013500
H	5.85645000	-0.25507700	0.88816800
H	5.84264200	-1.81560100	-0.00021500
H	5.85629400	-0.25499100	-0.88845100

Ag₂OAc₂

O	2.11646800	1.13830200	-0.00654400
C	2.68210300	-0.00041500	-0.00619400
O	2.11631800	-1.13905900	-0.00649100
C	4.19852900	-0.00029000	0.03575000
H	4.51306200	0.00562500	1.08500500
H	4.59352800	-0.90152200	-0.43481900
H	4.59322800	0.89616200	-0.44421400
Ag	0.00009100	1.39321100	-0.00597800
O	-2.11650400	-1.13912400	-0.00644000
C	-2.68210200	-0.00038800	-0.00604000
O	-2.11628200	1.13823900	-0.00645100
C	-4.19853000	0.00008400	0.03579400
H	-4.51312000	0.00835100	1.08501500
H	-4.59296500	0.89567900	-0.44600500
H	-4.59374100	-0.90198200	-0.43297700
Ag	-0.00009100	-1.39285200	-0.00594700

Ag₂I₂

Ag	0.00092900	1.46358700	0.00007500
Ag	-0.00036200	-1.46279700	0.00013500
I	2.43127000	-0.00069500	-0.00007500
I	-2.43177300	-0.00000600	-0.00011100

int0

Pd	0.90855300	-0.89059200	-0.34801400
C	0.49345500	1.05010200	-2.50495000
O	-0.09439100	1.63631200	-3.39953500
O	0.03671000	-0.03897200	-1.93962800
C	1.88045600	1.61568100	-2.07782700
Pd	-1.06577700	-0.22363400	1.74961600
C	1.56239500	-1.65122500	2.39806300
O	1.94544100	-1.75473000	1.18707400
O	0.50777900	-1.09433100	2.80802700
C	2.48767600	-2.22749700	3.44734100
H	3.08438600	-1.40981100	3.86516400
H	1.90355700	-2.66616400	4.25793200
H	3.15671900	-2.96698300	3.00601100
C	-1.40390700	-2.75394700	0.34277400
O	-0.39967500	-2.51424300	-0.38465300

O	-1.83585500	-2.06918900	1.33267600
C	-2.23643700	-3.95842100	-0.03773700
H	-1.59507600	-4.75926300	-0.40876100
H	-2.84134000	-4.29843100	0.80346400
H	-2.89786400	-3.64955100	-0.85545200
C	-2.16578200	2.54241800	0.62597400
C	-0.71057500	2.58760600	1.18851700
O	-0.04245300	3.56738700	0.89323400
O	-0.27722700	1.61733500	1.95341700
C	-4.12761200	0.36535600	0.19774600
C	-5.48940600	0.64192500	0.38631200
C	-3.77725400	-0.49427200	-0.84968600
C	-6.46810800	0.06318000	-0.41671100
C	-4.74527300	-1.10510500	-1.64110200
C	-6.09311400	-0.82240700	-1.42703700
F	-2.50318900	-0.76211500	-1.12022400
F	-4.38228900	-1.96588400	-2.59574900
F	-7.02324800	-1.39365100	-2.18814700
F	-7.75844300	0.34184100	-0.21888600
F	-5.88035700	1.47295600	1.35789000
C	-2.94091700	3.77302800	1.10679100
H	-2.43461700	4.66116100	0.71994300
H	-3.96947600	3.75247700	0.73333600
H	-2.96438800	3.83644600	2.19800500
C	-2.13745600	2.44602800	-0.89905500
H	-1.69151000	1.51595200	-1.24673400
H	-3.14618400	2.53070100	-1.31332400
H	-1.53992200	3.27856500	-1.27716800
S	-2.97820700	1.00899500	1.39638300
C	2.90645400	1.13418700	-3.10883300
H	3.90530700	1.51995400	-2.88657100
H	2.94288700	0.04447600	-3.16802900
H	2.59163000	1.52329100	-4.08091100
C	1.84441000	3.14153500	-1.96773000
H	1.50240100	3.53831000	-2.92699500
H	1.15972500	3.47240000	-1.18296800
H	2.84180900	3.53436200	-1.74576500
S	2.25699100	0.95857900	-0.33119400
C	3.95535600	0.40816500	-0.36361000
C	4.38722900	-0.81792800	-0.88601500
C	4.91330400	1.23583100	0.23765100

C	5.71705200	-1.21622200	-0.79510400
C	6.24964000	0.85437700	0.33093400
C	6.64922300	-0.37674100	-0.18550000
F	3.53690100	-1.64590600	-1.50327500
F	4.56053700	2.42244700	0.73749300
F	6.10713800	-2.38901900	-1.29847300
F	7.92434500	-0.75020000	-0.10251100
F	7.14485500	1.65895700	0.90743800

int1

C	-4.11312600	4.23041200	0.32135200
C	-4.97014200	3.14793000	0.13580700
C	-4.56451200	1.96563000	-0.50375900
C	-3.25697800	1.85968200	-0.94303500
C	-2.33043600	2.92280500	-0.74396300
C	-2.79680200	4.14138500	-0.15547600
H	-1.41459400	2.95559000	-1.33440800
Pd	-1.28388000	2.25998000	1.13421400
Pd	-0.79117500	-0.63565300	1.08562100
C	-3.28644900	0.49188900	2.33740400
O	-3.02483900	1.69623000	2.02257700
O	-2.52449700	-0.51485800	2.20235700
C	-4.66720000	0.21299700	2.87624500
H	-4.61300900	-0.52124700	3.68229200
H	-5.14791200	1.13099100	3.21429500
H	-5.23710000	-0.22968800	2.05185800
C	0.40270300	0.96420900	3.26168200
O	-0.29186200	1.97115300	2.96214500
O	0.42662100	-0.15739900	2.65182800
C	1.33778400	1.09031300	4.44411200
H	1.48318600	0.12234300	4.92572100
H	2.30540800	1.44356700	4.07136100
H	0.95247200	1.82467300	5.15242900
C	1.06913900	2.74866900	-0.69838100
O	0.47173400	2.64627900	-1.77191800
O	0.56428100	2.77720900	0.49313000
H	-2.91740300	0.95353200	-1.42984700
H	-5.99192100	3.22967300	0.49700000
H	-5.25046700	1.13907500	-0.62939100
C	0.10802400	-1.53604400	-1.83889800
C	-1.33641500	-1.94750700	-1.47667600

O	-1.95360300	-2.69875100	-2.20960500
O	-1.88651700	-1.34701700	-0.43862300
C	1.83884300	-2.32983900	0.43591500
C	1.23403500	-3.57588200	0.63056300
C	3.15276400	-2.17172700	0.88600500
C	1.92666700	-4.64288600	1.19236000
C	3.86959500	-3.22822000	1.43805700
C	3.25405700	-4.46929300	1.58804500
F	3.75580600	-0.97708900	0.82643000
F	5.12951800	-3.04745500	1.83601200
F	3.92584100	-5.48672800	2.12127700
F	1.33175000	-5.82504500	1.35533900
F	-0.04350100	-3.76493800	0.27474300
C	0.87623800	-2.64549800	-2.54704300
H	0.33446500	-2.87363200	-3.46797200
H	1.88853600	-2.32004700	-2.79462900
H	0.91597600	-3.56345200	-1.96078600
C	0.00376100	-0.27691400	-2.71922800
H	-0.47764100	0.55293400	-2.20005300
H	0.99207100	0.06136900	-3.03561600
H	-0.59493200	-0.53652400	-3.59750400
S	1.02073000	-0.91452000	-0.28461100
O	-1.91120400	5.15854600	-0.15499000
C	-2.21406300	6.33408100	0.59532600
H	-1.33251400	6.96983800	0.51629100
H	-3.08121900	6.86069900	0.17981800
H	-2.39809800	6.08780200	1.64786100
H	-4.47524700	5.12892200	0.80478600
C	2.61157900	2.93888200	-0.70125200
C	4.68318800	1.18865300	-1.73136700
C	5.85734600	1.89378800	-1.43225300
C	4.75691100	-0.20542500	-1.63980200
C	7.02337300	1.25449700	-1.02099700
C	5.90257900	-0.86768400	-1.21184100
C	7.04568100	-0.13565100	-0.90768600
F	3.68436600	-0.97129100	-1.91068800
F	5.88925900	-2.19915100	-1.05488900
F	8.15242400	-0.75604300	-0.49445200
F	8.12007100	1.96152400	-0.72727600
F	5.87299800	3.23313600	-1.49170600
C	2.88439900	4.43552500	-0.92579600

H	2.48328200	5.00457000	-0.07898000
H	3.95778600	4.61735400	-1.00237000
H	2.39909800	4.78364400	-1.84055300
C	3.26837300	2.43773000	0.58379700
H	3.12806600	1.36373500	0.71972300
H	4.33736800	2.66188500	0.58948500
H	2.80281300	2.95249100	1.42714100
S	3.16971500	1.96909200	-2.24424200
C	-4.99181000	-2.03909700	-1.15605600
H	-4.28065600	-2.83452500	-1.40824300
C	-6.26841700	-2.68778600	-0.62337600
C	-5.22402200	-1.25421400	-2.45285600
O	-4.51617600	-1.18377800	-0.15969600
H	-3.53390600	-1.25122600	-0.16545000
F	-5.57776800	-2.05533700	-3.47104700
F	-6.18166400	-0.31073700	-2.31228700
F	-4.08300100	-0.61671500	-2.80456100
F	-7.14612700	-1.76466100	-0.18557400
F	-5.96931300	-3.49497200	0.41172600
F	-6.88066300	-3.43115500	-1.56684900

TS1_{ortho}

C	-3.54492800	4.74995300	-0.66630800
C	-4.40733700	3.89244400	-1.35213600
C	-4.14676700	2.52279400	-1.46488300
C	-3.00732000	2.00364600	-0.86419900
C	-2.09470000	2.82827000	-0.16010300
C	-2.40191700	4.21786000	-0.06100400
H	-0.85835600	2.80402400	-0.69666900
Pd	-1.18300200	2.03252900	1.53889300
Pd	-0.89827700	-0.87639400	1.26520500
C	-3.39261200	0.28847400	2.41605700
O	-3.06092800	1.48199400	2.14127200
O	-2.66306800	-0.75365200	2.32472900
C	-4.81903300	0.05715400	2.85156400
H	-4.85733400	-0.72348900	3.61365100
H	-5.26755300	0.98245000	3.21367400
H	-5.36140000	-0.29780200	1.96862000
C	0.19231600	0.38415000	3.68615000
O	-0.38444400	1.46761400	3.42262700
O	0.24532300	-0.65320600	2.93526200

C	0.87812400	0.24380000	5.02792800
H	0.21256000	-0.30764900	5.70013100
H	1.79976300	-0.33229300	4.92307500
H	1.08171700	1.22599700	5.45501300
C	1.11361200	2.80458400	-0.14240300
O	0.33122600	2.94675400	-1.13399100
O	0.75204400	2.50274200	1.02823200
H	-2.81272800	0.93945400	-0.93404700
H	-5.30179100	4.30768900	-1.80916000
H	-4.82909900	1.87451000	-1.99873100
C	0.03376800	-1.42282000	-1.74596900
C	-1.41878200	-1.85760200	-1.44469600
O	-2.02693200	-2.51549300	-2.27035700
O	-1.97575100	-1.38296000	-0.35050300
C	1.84546400	-2.41300500	0.37510100
C	1.28082600	-3.68716200	0.49071400
C	3.19402500	-2.26514500	0.71023100
C	2.04038300	-4.78684900	0.87482500
C	3.97611100	-3.35289400	1.08406800
C	3.39603300	-4.61773000	1.16377700
F	3.77142700	-1.05455200	0.70226400
F	5.26693100	-3.18355500	1.37490500
F	4.13253000	-5.66567500	1.52512600
F	1.48637400	-5.99621800	0.96363100
F	-0.01738900	-3.87001600	0.21779500
C	0.78435300	-2.47694100	-2.55220000
H	0.24374000	-2.60261300	-3.49309800
H	1.80714300	-2.16278400	-2.76316800
H	0.78984700	-3.44631200	-2.05413800
C	-0.04230400	-0.08247700	-2.50037300
H	-0.53046900	0.69365700	-1.90828900
H	0.95549500	0.26793900	-2.77029400
H	-0.63502400	-0.24087300	-3.40608700
S	0.93143100	-0.96644400	-0.12142800
O	-1.48837000	4.96234900	0.61481100
C	-1.67526800	6.37017300	0.70891200
H	-0.82110900	6.74567500	1.27321900
H	-1.69312400	6.83942500	-0.28263300
H	-2.59971500	6.61511900	1.24570500
H	-3.77844800	5.80587100	-0.60150000
C	2.60911200	3.08686800	-0.36143500

C	4.52108600	1.41960300	-1.75490300
C	5.74940900	2.04421400	-1.49871000
C	4.52336000	0.02173200	-1.78949100
C	6.91037200	1.31723900	-1.25306300
C	5.66524400	-0.72805600	-1.52922100
C	6.86717400	-0.07760500	-1.26705500
F	3.38959400	-0.65704400	-2.03133300
F	5.59690100	-2.06549300	-1.49375300
F	7.97019700	-0.78161200	-1.01352500
F	8.06232200	1.94254900	-0.99247700
F	5.82275300	3.38055300	-1.42829200
C	2.78045000	4.61301800	-0.47415000
H	2.47112000	5.08664800	0.46485400
H	3.82939900	4.84878500	-0.66519600
H	2.17103300	5.01645000	-1.28572600
C	3.45164500	2.51398000	0.77719900
H	3.38675200	1.42531000	0.82576700
H	4.49501800	2.81238000	0.66543400
H	3.07622900	2.91633700	1.72052700
S	3.02225700	2.32244600	-2.05683200
C	-5.03451400	-1.80128700	-1.31769200
H	-4.31754400	-2.59907100	-1.54246400
C	-6.34542200	-2.45452400	-0.88414900
C	-5.17283600	-0.99047800	-2.61042400
O	-4.60622300	-0.96713900	-0.28143600
H	-3.64405200	-1.13151100	-0.17482800
F	-5.45106800	-1.77195100	-3.66798900
F	-6.13839100	-0.04819400	-2.52601100
F	-4.00939900	-0.34751400	-2.86550500
F	-7.25760200	-1.54390800	-0.50020300
F	-6.11670700	-3.27472100	0.15992100
F	-6.88291500	-3.18997300	-1.87976500

int2_{ortho}

C	-2.87179300	4.91306200	-1.02784500
C	-3.73293500	4.18314100	-1.85165900
C	-3.84989800	2.80247300	-1.71181100
C	-3.09863600	2.14138000	-0.73291500
C	-2.21873300	2.84306800	0.10032600
C	-2.12490200	4.24712800	-0.04731400
H	-0.55783300	3.05814400	-0.98388100

Pd	-1.24573500	1.98372100	1.61537700
Pd	-0.94003300	-0.96292600	1.31323900
C	-3.38982800	0.17046700	2.57412100
O	-3.07431000	1.37058100	2.31498100
O	-2.66512200	-0.87021100	2.43379600
C	-4.79978700	-0.07483200	3.05600100
H	-4.81307100	-0.88308000	3.78948900
H	-5.23144400	0.83781500	3.46730300
H	-5.37597500	-0.39406300	2.18074500
C	0.30963600	0.26173800	3.67517500
O	-0.23843300	1.35874500	3.42840000
O	0.27316700	-0.78777800	2.93480900
C	1.07706700	0.10038600	4.97068200
H	0.42942700	-0.40446900	5.69505700
H	1.95846700	-0.52578500	4.81756800
H	1.35840500	1.07621400	5.36758100
C	1.13718600	2.85140000	-0.15647000
O	0.40638000	3.15880700	-1.20517500
O	0.68950400	2.46106600	0.92459000
H	-3.22106400	1.07136300	-0.61118700
H	-4.31539800	4.70730800	-2.60400200
H	-4.52548700	2.23561300	-2.34031200
C	-0.13900600	-1.29211600	-1.74821900
C	-1.54498100	-1.84583200	-1.41551700
O	-2.15294400	-2.47848000	-2.26101300
O	-2.06841400	-1.48767800	-0.26431100
C	1.75592500	-2.44663900	0.22762100
C	1.21249200	-3.73465900	0.20850400
C	3.09019600	-2.31050100	0.61933400
C	1.98249700	-4.85309800	0.51087900
C	3.88206500	-3.41453500	0.91406000
C	3.32544500	-4.69089300	0.85611600
F	3.64513900	-1.09366200	0.74133500
F	5.16140100	-3.25088100	1.25590600
F	4.07154000	-5.75608700	1.13920100
F	1.44776200	-6.07358500	0.47181000
F	-0.07483000	-3.91319600	-0.11079200
C	0.62195300	-2.18671800	-2.71775100
H	0.00903300	-2.27568900	-3.61769700
H	1.58909200	-1.75509100	-2.97880300
H	0.76180800	-3.19379600	-2.32443900

C	-0.35032900	0.11970600	-2.32777200
H	-0.88689800	0.76448000	-1.62851800
H	0.60260600	0.58295700	-2.59288400
H	-0.97086500	0.02283600	-3.22340900
S	0.83537400	-0.96535200	-0.14132100
O	-1.23723300	4.87759900	0.79335500
C	-1.07856500	6.28350400	0.68236000
H	-0.34840200	6.56290100	1.44359100
H	-0.69975400	6.57247700	-0.30764800
H	-2.01964100	6.81381100	0.87531900
H	-2.79856400	5.98766500	-1.14810500
C	2.63631500	3.07028800	-0.34260200
C	4.54310400	1.33231900	-1.66359200
C	5.76600100	1.95874700	-1.38455600
C	4.54684600	-0.06581900	-1.70286400
C	6.92300400	1.23375200	-1.11782400
C	5.68756900	-0.81286100	-1.42761600
C	6.88287000	-0.16124000	-1.13924400
F	3.42234300	-0.74632800	-1.97061000
F	5.62502500	-2.14973800	-1.40963600
F	7.98212700	-0.86346400	-0.87084600
F	8.06760700	1.86096800	-0.83438500
F	5.83681900	3.29560800	-1.31516900
C	2.88606700	4.58446800	-0.47652900
H	2.57222800	5.09220100	0.44292500
H	3.95111200	4.76020700	-0.63513100
H	2.32798800	5.00348300	-1.31613600
C	3.40347500	2.47155100	0.83508800
H	3.28864300	1.38735300	0.88603500
H	4.46162700	2.72436800	0.76266000
H	3.00974400	2.89709100	1.76116500
S	3.05649100	2.23865500	-2.00873000
C	-5.13449900	-1.69164800	-1.26604700
H	-4.46770900	-2.50682800	-1.56938900
C	-6.49986800	-2.29555500	-0.94070600
C	-5.18186500	-0.72691200	-2.45640400
O	-4.68110000	-1.01911200	-0.12746900
H	-3.72716600	-1.23582200	-0.03597500
F	-5.52809000	-1.34971400	-3.59709300
F	-6.04191200	0.29270600	-2.25958100
F	-3.95416000	-0.18293800	-2.64381100

F	-7.36876100	-1.36659500	-0.50470200
F	-6.36459100	-3.22267100	0.02656500
F	-7.04096800	-2.89927900	-2.01966200

int3

C	-0.19844700	4.26118600	-0.85933500
C	-1.13217700	4.05106400	-1.88073200
C	-1.41515800	2.76261300	-2.32385300
C	-0.75979800	1.66967800	-1.73682000
C	0.16187200	1.85891700	-0.70912900
C	0.44838900	3.16571900	-0.27648200
Pd	0.95777600	0.31835400	0.33575900
H	-0.96030500	0.66133400	-2.08640300
H	-1.63301100	4.90654000	-2.32489700
H	-2.13641800	2.59873500	-3.11950200
O	1.37641500	3.26859100	0.73532000
C	1.67291500	4.55773100	1.24883200
H	2.40866300	4.40507100	2.04009000
H	2.10229800	5.21232400	0.47854900
H	0.78171700	5.04038300	1.67137500
H	0.00924000	5.27201200	-0.52694800
C	2.26630200	-0.84913200	-1.08661400
C	3.57296700	-1.33051800	-0.46802900
C	3.88574000	0.82888200	-1.08727000
C	2.46074100	0.47262600	-1.46201700
C	4.10849200	-0.03261300	0.17355400
H	5.16385100	-0.10790000	0.45402700
H	3.52516900	0.28927400	1.03875400
C	4.53790100	-1.45499300	-1.69582500
H	5.47858800	-1.91306400	-1.37670700
H	4.11877100	-2.08208900	-2.48731400
C	4.74710600	0.03096500	-2.13252700
H	5.79565900	0.33205900	-2.04725600
H	4.43164000	0.22358000	-3.16209800
H	3.48399100	-2.20680000	0.16694000
H	1.90424900	0.97660100	-2.24094600
C	1.23188300	-1.75114700	-1.67366300
O	0.26098800	-1.39020800	-2.31847600
C	0.53886900	-3.99113100	-1.87183100
H	0.46809300	-3.96039100	-2.96242400
H	0.90271700	-4.96070800	-1.53431500

H	-0.43973300	-3.77250400	-1.44230600
C	-0.36666200	-0.72339600	3.10371000
C	0.76749100	-1.67196300	2.58438400
O	1.54234800	-1.23540500	1.64310000
O	0.90481700	-2.72463100	3.19483100
C	-2.10781900	-0.16103900	0.75126400
C	-2.01794200	-1.42878300	0.16680900
C	-3.14547300	0.67538400	0.32577600
C	-2.91833800	-1.85082600	-0.80240900
C	-4.05281700	0.27121900	-0.65091500
C	-3.93973200	-0.99642600	-1.21554800
F	-3.25989500	1.91312000	0.81521900
F	-5.01991100	1.09880300	-1.05548700
F	-4.80468300	-1.39330200	-2.14900500
F	-2.80366200	-3.06806400	-1.34573900
F	-1.03066600	-2.26796600	0.50780500
C	-1.58199600	-1.49631100	3.60440900
H	-1.23082400	-2.18913900	4.37207500
H	-2.33678700	-0.82751500	4.02946300
H	-2.03444400	-2.09409100	2.81149600
C	0.25893400	0.13504800	4.22044700
H	1.08797400	0.74015500	3.83978200
H	-0.48074100	0.79164600	4.68854400
H	0.65859500	-0.54804200	4.97514700
S	-0.86639600	0.56546000	1.81814600
O	1.51027900	-3.03506500	-1.40422300
H	4.10682700	1.89475600	-1.02704000

TS2

C	-1.16093700	3.53818200	0.24204400
C	-1.93106500	3.36003700	-0.91095100
C	-1.61308800	2.35981000	-1.83105700
C	-0.51871300	1.52863900	-1.58580100
C	0.25243700	1.66774200	-0.42065300
C	-0.06174200	2.70380700	0.48451100
Pd	0.96969900	-0.13855300	0.35261000
H	-0.23843300	0.75739200	-2.29975500
H	-2.78368500	4.01028900	-1.08314600
H	-2.20672300	2.22955600	-2.73077200
O	0.72805700	2.78852800	1.59596200
C	0.42379500	3.77067700	2.57690800

H	1.17428200	3.65202600	3.35956300
H	0.48665500	4.78688500	2.16636700
H	-0.57453600	3.61409900	3.00432800
H	-1.43156900	4.31494200	0.94720600
C	2.72984400	0.08453000	-0.77968300
C	3.97081800	0.17126900	0.11122700
C	3.23858400	2.30230100	-0.17839400
C	2.28620400	1.43537300	-0.98108200
C	3.62002600	1.38552400	1.00206700
H	4.48346900	1.76087300	1.56106900
H	2.78923300	1.20973700	1.68890900
C	5.07869800	0.79168800	-0.79323000
H	6.03835600	0.79081700	-0.26682900
H	5.21020400	0.22906400	-1.72095900
C	4.56044600	2.24840900	-1.02368700
H	5.26309500	2.99286800	-0.63769900
H	4.38870200	2.47980400	-2.07940500
H	4.23462000	-0.76183300	0.60553700
H	1.97000500	1.75555500	-1.96444900
C	2.53628600	-0.92800900	-1.84909200
O	1.70118700	-0.84229200	-2.73796000
C	3.11400800	-3.09983900	-2.54949200
H	3.13436500	-2.80841900	-3.60263300
H	3.90389900	-3.81685100	-2.32843700
H	2.13651100	-3.52427800	-2.30704500
C	-0.57408800	-2.21968700	2.30136400
C	0.59340300	-2.85621200	1.46943000
O	1.46757600	-2.06735000	0.92401300
O	0.66110000	-4.07838900	1.49471700
C	-2.24418200	-0.50303500	0.52621200
C	-2.19661000	-1.31367100	-0.61300400
C	-3.26818100	0.44580100	0.60380700
C	-3.13787500	-1.20148200	-1.62975700
C	-4.20963400	0.58465400	-0.41225200
C	-4.14758900	-0.24508600	-1.52776500
F	-3.33852500	1.28790300	1.64195100
F	-5.15686300	1.52464500	-0.32955000
F	-5.04271200	-0.11356500	-2.50855100
F	-3.06733500	-1.98410200	-2.70944400
F	-1.21289000	-2.20938500	-0.75847900
C	-1.82740300	-3.08873100	2.28619400

H	-1.55008900	-4.06883000	2.67920400
H	-2.62058900	-2.65668700	2.90421500
H	-2.20021500	-3.24222000	1.27268600
C	-0.03958900	-2.03747900	3.73576400
H	0.81666300	-1.35609000	3.76248800
H	-0.81673100	-1.66255800	4.40864300
H	0.29863400	-3.01554700	4.08969000
S	-0.95773900	-0.44575300	1.75928100
O	3.37345100	-1.96690000	-1.70110000
H	2.88240600	3.30536700	0.05247600

int4

C	0.31144900	3.47431500	-0.52836600
C	-0.80728200	3.00173000	-1.23312800
C	-0.75026300	1.79965100	-1.91554100
C	0.43667000	1.04199100	-1.87852600
C	1.59663600	1.48336300	-1.17951900
C	1.50159000	2.74797000	-0.50252200
Pd	0.79968200	-0.08873000	0.24672400
H	0.52647600	0.14933500	-2.49132900
H	-1.72053800	3.58848100	-1.22548600
H	-1.60566000	1.42822100	-2.46980500
O	2.61585400	3.17932000	0.13683300
C	2.55313400	4.36262000	0.92356100
H	3.54097600	4.47021000	1.37270300
H	2.33583100	5.24495600	0.30896000
H	1.79878200	4.27493900	1.71540300
H	0.23987600	4.41983200	-0.00636000
C	2.55437100	-0.71653100	-0.63652100
C	3.69778300	-0.91785300	0.36202500
C	4.21141300	1.01688200	-0.71736100
C	2.86931200	0.61273600	-1.37621200
C	4.04080000	0.53805700	0.74183900
H	4.96677200	0.61610900	1.32209500
H	3.24224700	1.05301800	1.28066300
C	4.95513100	-1.30465100	-0.46596900
H	5.77096300	-1.58545400	0.20863400
H	4.77280400	-2.15677200	-1.12495800
C	5.28157400	0.01716100	-1.23460600
H	6.28310400	0.38270600	-0.98736800
H	5.24115600	-0.10471400	-2.32207500

H	3.44924800	-1.60499700	1.16965300
H	2.99264600	0.46387600	-2.45422100
C	2.09837000	-1.87258200	-1.45591000
O	1.56224300	-1.79443800	-2.55536800
C	1.73701100	-4.20138100	-1.45992500
H	2.12424100	-4.32546000	-2.47484400
H	2.01712900	-5.04616000	-0.83136000
H	0.64857300	-4.10406100	-1.50212000
C	-1.07232600	-0.55204600	2.83738700
C	-0.15928900	-1.77235000	2.47913400
O	0.80497800	-1.60664500	1.62158500
O	-0.34349300	-2.79362700	3.12634800
C	-2.54856900	0.20455300	0.40334900
C	-2.64570800	-1.06046300	-0.18728700
C	-3.52049900	1.15180600	0.06247100
C	-3.66420400	-1.37533300	-1.08157700
C	-4.54259700	0.85944700	-0.83729300
C	-4.61682800	-0.41011600	-1.40687700
F	-3.46934600	2.39173200	0.56745800
F	-5.44966200	1.78874400	-1.15526300
F	-5.59494000	-0.70064200	-2.26468200
F	-3.73101900	-2.58943300	-1.63223100
F	-1.73766500	-2.00382300	0.08624600
C	-2.46157000	-0.99988400	3.28158700
H	-2.34014500	-1.67121700	4.13358800
H	-3.08023200	-0.14502300	3.57147900
H	-2.97165600	-1.56286400	2.49736300
C	-0.34733900	0.22253000	3.95551800
H	0.62386900	0.59803500	3.61753600
H	-0.95080600	1.06006300	4.31829200
H	-0.16891400	-0.47265300	4.78089900
S	-1.18929200	0.71589200	1.43768500
O	2.31254500	-3.04635600	-0.83087400
H	4.48062700	2.06192400	-0.85993700

int5

C	3.79083500	1.94184000	-0.08002400
C	3.68421000	2.19909900	-1.44953800
C	3.21698500	1.22607200	-2.32404200
C	2.87572100	-0.03076200	-1.81768100
C	2.99493200	-0.35248400	-0.43396600

C	3.45796300	0.69017400	0.43897600
Pd	0.73335300	-0.17273800	-0.34985200
H	2.57677500	-0.82620900	-2.49353700
H	3.10933400	1.43066500	-3.38322200
C	1.30470300	-2.12910500	-0.14835000
C	0.95055200	-2.78012500	1.19183100
C	3.17995600	-2.37920700	1.33436200
C	2.82825100	-1.85899300	-0.08213000
C	1.91113200	-2.06129500	2.15690100
H	1.92907900	-2.52159600	3.15094000
H	1.70948300	-0.99592400	2.27037700
C	1.56574200	-4.20854700	1.17043900
H	1.21019800	-4.77515900	2.03748000
H	1.28173500	-4.77288600	0.27823300
C	3.10108000	-3.92778400	1.26230100
H	3.52966800	-4.36651000	2.16863300
H	3.65723300	-4.33331100	0.41083300
H	-0.10783300	-2.74776700	1.42834200
H	3.37629400	-2.42050900	-0.84523900
C	0.75236500	-2.72840500	-1.39820700
O	1.27145900	-2.67716500	-2.50387100
C	-3.39354300	-1.62329600	0.52662800
C	-2.26693900	-1.04476600	-0.34715200
O	-1.19365500	-0.78384900	0.27226200
O	-2.49849200	-0.85594100	-1.57678800
C	-2.67408900	0.85944900	1.88487000
C	-1.61336400	0.54413000	2.74380800
C	-2.55510300	2.03876700	1.13672200
C	-0.48097000	1.34588600	2.83233200
C	-1.45192100	2.87755400	1.25311100
C	-0.40411300	2.52090200	2.09245700
F	-3.48279700	2.37037200	0.22956500
F	-1.35982900	3.97945500	0.49766800
F	0.69764400	3.27728200	2.15485900
F	0.56902400	0.96760200	3.58446100
F	-1.62173600	-0.59039700	3.45540200
C	-4.59393300	-2.07021600	-0.31235200
H	-4.29795800	-2.91942600	-0.93665800
H	-5.41493600	-2.39461400	0.33505100
H	-4.94249100	-1.27067800	-0.96613300
C	-2.86908100	-2.76822200	1.40115800

H	-2.09791800	-2.41900200	2.08392900
H	-3.68710900	-3.19608200	1.98710700
H	-2.44221800	-3.55063200	0.76318100
S	-4.06571000	-0.21669300	1.63246500
Ag	-1.21991500	0.62759100	-2.45492800
O	0.60905400	2.02761900	-0.52990800
C	0.46637400	2.75754800	-1.55352900
O	-0.06041400	2.40148100	-2.65797900
C	0.94649800	4.19369400	-1.47056000
H	1.39337000	4.39494200	-0.49758100
H	1.67245800	4.37564800	-2.26760500
H	0.09897400	4.86352700	-1.63556800
H	4.12235400	-1.99860000	1.72597600
O	-0.44442800	-3.32496000	-1.18286600
C	-1.14165300	-3.76900900	-2.35996300
H	-2.01345200	-4.31216600	-1.99416000
H	-1.46012600	-2.90472200	-2.94800600
H	-0.50735700	-4.41851100	-2.96718200
H	3.96099300	3.18092600	-1.82178100
H	4.13523000	2.72639600	0.58144000
O	3.56751000	0.39190900	1.75450600
C	3.67408000	1.45407500	2.70255100
H	2.86108800	2.17520100	2.57285600
H	3.58685300	0.97982400	3.68035600
H	4.64439500	1.95998400	2.63113900

TS3

C	3.31239400	2.92960600	-2.26736000
C	2.62894800	2.07242000	-3.13973600
C	1.94543100	0.97291100	-2.64381800
C	1.92153800	0.72918900	-1.25318700
C	2.55790900	1.62171300	-0.36005000
C	3.29061200	2.70294900	-0.88656200
Pd	0.32925900	-0.22075800	-0.35641500
H	2.25365000	-0.57260500	-1.10263000
H	1.46228400	0.27240200	-3.31923100
C	1.33569500	0.26158000	1.38842700
C	0.30642900	0.93583400	2.31548300
C	1.83899800	2.56553300	1.94512500
C	2.41397100	1.36727300	1.11599300
C	0.31827100	2.38684700	1.78811900

H	-0.26288400	3.07132400	2.41556300
H	-0.01747600	2.48539100	0.75401400
C	0.98150900	1.12265700	3.70724700
H	0.22634700	1.44565500	4.43130900
H	1.41622700	0.19539600	4.09032200
C	2.03912100	2.23966500	3.44353500
H	1.83945900	3.12443200	4.05641200
H	3.06108400	1.91381600	3.66021700
H	-0.65045700	0.41685400	2.35828000
H	3.38403300	1.06299000	1.52412600
C	1.91874900	-1.04359700	1.86018700
O	3.10603000	-1.31504800	1.84617300
C	-3.72207900	-1.84659400	0.31509900
C	-2.20359300	-1.88046500	0.06714100
O	-1.55451700	-0.86819700	0.46990600
O	-1.73054700	-2.88981300	-0.53380700
C	-3.69093600	0.78405000	-0.82825900
C	-4.23742200	1.72732600	0.05184100
C	-2.50379500	1.13689400	-1.48192800
C	-3.61574400	2.94948900	0.30050400
C	-1.87686000	2.35718400	-1.26166800
C	-2.42740700	3.25939300	-0.35507500
F	-1.89122000	0.26781000	-2.30789800
F	-0.71343000	2.64813200	-1.85890000
F	-1.79778800	4.40812500	-0.09898400
F	-4.14370400	3.81775700	1.17029100
F	-5.36981200	1.46406700	0.71215500
C	-4.36775900	-3.22355000	0.13224300
H	-3.95774600	-3.90985000	0.87928500
H	-5.45009200	-3.16013200	0.27701200
H	-4.15320700	-3.63959000	-0.85325600
C	-4.04286100	-1.25154200	1.68781000
H	-3.58441200	-0.27086100	1.81380000
H	-5.12307700	-1.16679400	1.82477600
H	-3.63773200	-1.90888300	2.46611200
S	-4.45626400	-0.79875000	-1.08470100
Ag	0.37660100	-3.16455100	-0.64304100
O	3.16024400	-1.56713400	-1.33874900
C	3.33708800	-2.69044100	-0.77886200
O	2.43530200	-3.54111100	-0.48807700
C	4.75726700	-3.05805000	-0.40529100

H	4.94474600	-2.61394000	0.57762100
H	4.87953900	-4.14003100	-0.33875900
H	5.46099300	-2.62700500	-1.11928400
H	2.25192200	3.52478000	1.63981700
O	0.98039700	-1.89693900	2.33007800
C	1.48673700	-3.16854600	2.78524700
H	0.60614700	-3.74506300	3.06811500
H	2.03866400	-3.66386300	1.98296200
H	2.14693900	-3.02767900	3.64545600
H	2.66166600	2.26600700	-4.20799400
H	3.86738900	3.76515100	-2.67703300
O	3.95939800	3.47676100	0.02250900
C	4.70746700	4.58764400	-0.44841900
H	4.06828900	5.31857800	-0.96131900
H	5.14450000	5.05172700	0.43702200
H	5.51232800	4.27512100	-1.12642600

int6

C	-4.40884200	-1.90676400	1.14118600
C	-3.25726900	-2.70151100	1.20860000
C	-1.98677500	-2.14595800	1.05709400
C	-1.85047200	-0.76139600	0.85122400
C	-2.99969600	0.04160100	0.77016400
C	-4.27523300	-0.53297500	0.91503900
Pd	-0.10681100	0.14912300	0.59180300
H	-2.39664200	0.07235900	-2.19688000
H	-1.11877800	-2.79331500	1.09536800
H	-5.38413100	-2.36348900	1.26148800
C	-1.31034400	1.79920100	0.15820200
C	-0.94003400	2.92585800	1.14226700
C	-3.10165000	2.46307400	1.65487500
C	-2.81468600	1.49435300	0.46501700
C	-1.74664000	2.50383500	2.39138000
H	-1.71667000	3.25530400	3.18788500
H	-1.44092400	1.53643600	2.79955000
C	-1.70187000	4.21950900	0.72464300
H	-1.32076500	5.06709300	1.30385500
H	-1.56061500	4.46335200	-0.33069200
C	-3.18640700	3.89896200	1.09227500
H	-3.56297200	4.59001000	1.85355100
H	-3.85954000	3.96348400	0.23100700

H	0.13459400	3.06858300	1.26003200
H	-3.44993500	1.76671100	-0.38771000
C	-0.97747600	1.98228600	-1.27521600
O	-1.52776100	1.40107700	-2.22713000
C	3.98469300	1.41569100	-0.70861800
C	2.51740300	0.95296000	-0.79826200
O	1.81343900	1.12303200	0.23440900
O	2.16527400	0.37653000	-1.87347500
C	3.70470600	-0.95147300	0.86429700
C	3.37396300	-0.53043100	2.16003300
C	2.91252300	-1.95802100	0.29635900
C	2.28963300	-1.05928100	2.85120700
C	1.82043200	-2.50090200	0.97233300
C	1.51067300	-2.05257200	2.25760400
F	3.14015200	-2.39904000	-0.94606200
F	1.07061200	-3.45173700	0.39474400
F	0.48848800	-2.58490400	2.92821900
F	1.96323300	-0.60354000	4.06432700
F	4.05927400	0.45189100	2.75097600
C	4.57392700	1.74683900	-2.08224800
H	4.08907900	2.64942300	-2.47087300
H	5.64640600	1.95210900	-2.00430800
H	4.40913200	0.93316500	-2.78814300
C	4.16151900	2.56994300	0.27946900
H	3.78854800	2.30747300	1.26710900
H	5.21770800	2.84168800	0.35714900
H	3.60180200	3.44216900	-0.07845900
S	4.94969000	-0.12350600	-0.09986100
Ag	0.41062200	-0.86769000	-2.05207200
O	-3.04806500	-0.69616800	-2.28773500
C	-2.51318800	-1.87847400	-2.42696400
O	-1.29605900	-2.11786800	-2.51981200
C	-3.52074400	-2.99272400	-2.46241000
H	-3.93606200	-3.09254300	-1.45485500
H	-4.33880400	-2.73906000	-3.14086400
H	-3.04181200	-3.92432900	-2.76065200
H	-3.97178800	2.15482000	2.23627900
O	0.00632000	2.86119400	-1.49618900
C	0.45861000	3.00692700	-2.85713000
H	1.17419000	3.82879600	-2.83196200
H	0.94881700	2.08748300	-3.18316900

H	-0.37783800	3.24219600	-3.51854100
O	-5.32622800	0.34015500	0.80261200
C	-6.64272700	-0.17787700	0.89222100
H	-7.31326800	0.67297800	0.75888600
H	-6.84084600	-0.91997400	0.10698400
H	-6.83368100	-0.63635100	1.87192700
H	-3.36155400	-3.77041900	1.37912900

int7

C	-0.04185900	2.62305500	3.61524700
C	-0.46581700	1.29194400	3.52810300
C	-0.27024900	0.54711200	2.36682600
C	0.36702500	1.14867800	1.26598500
C	0.82481100	2.47576800	1.34359100
C	0.60364500	3.21294600	2.52388700
Pd	0.75549800	0.15212400	-0.41700300
H	-0.61911200	-0.47621200	2.30885300
O	1.06378500	4.50461000	2.50128200
C	0.88188600	5.30414000	3.65827400
H	1.31883300	6.27678800	3.42529700
H	-0.18165100	5.43542400	3.89888100
H	1.39456500	4.87799700	4.53124200
H	-0.21471100	3.17982100	4.52847000
C	1.60098000	1.99493800	-1.01032800
C	3.10468300	1.89246500	-1.34853200
C	3.07558000	3.29608000	0.42709700
C	1.55758400	3.03577300	0.16604600
C	3.71945200	1.94101600	0.06605600
H	4.81473000	1.97931200	0.05596100
H	3.39417000	1.11349800	0.70269100
C	3.60325500	3.24030300	-1.94378100
H	4.61211100	3.11735800	-2.35342500
H	2.96681100	3.59008800	-2.76006200
C	3.60465300	4.19797400	-0.70937400
H	4.61688000	4.54939400	-0.48229500
H	2.97675900	5.08274400	-0.85654100
H	3.36365000	1.03282000	-1.96604500
H	1.07894700	3.97127100	-0.14955500
C	0.65505900	2.28754900	-2.10620100
O	-0.48836700	2.76863800	-1.98211900
C	0.16926900	2.05872300	-4.41126200

H	0.71227100	1.74441300	-5.30269000
H	-0.69007700	1.40499800	-4.23377500
H	-0.18527900	3.08635700	-4.51834700
C	-2.32027700	-3.01813400	0.33177600
C	-1.62410100	-1.70044300	-0.08054700
O	-2.35609300	-0.82928600	-0.63242900
O	-0.38587800	-1.60703200	0.17830800
C	-4.54377500	-1.49202300	1.29286100
C	-4.30112200	-0.11498900	1.33418800
C	-5.73766900	-1.90778700	0.68957300
C	-5.15443400	0.80207500	0.73611400
C	-6.62517000	-0.99993800	0.11323200
C	-6.32260600	0.36050500	0.12068300
F	-6.04500200	-3.20693200	0.61279000
F	-7.75200700	-1.42689400	-0.46863600
F	-7.14664800	1.23451700	-0.46042900
F	-4.81874600	2.10476400	0.69556200
F	-3.18741600	0.36824800	1.90201600
C	-3.20967000	-3.53063800	-0.80307900
H	-2.57787100	-3.80056700	-1.65767800
H	-3.77028200	-4.41324000	-0.48738400
H	-3.90243300	-2.75765100	-1.13609600
C	-1.32016000	-4.08565400	0.78589500
H	-0.70465200	-3.73269000	1.61585600
H	-1.84135100	-5.00053400	1.08250800
H	-0.65109900	-4.32111100	-0.04739500
S	-3.33744900	-2.65080300	1.89251700
Ag	-1.75558200	1.36418900	-0.52432600
C	3.58697400	-2.83842300	1.17241900
C	4.92334700	-2.43925000	1.04428700
C	5.36069900	-1.83262900	-0.13986000
C	4.46922600	-1.62096300	-1.19173600
C	3.14521400	-2.02574200	-1.03414400
C	2.68188100	-2.63456200	0.13275100
H	3.26513400	-3.29736600	2.10110600
H	6.39436200	-1.52143900	-0.23559300
H	4.80103400	-1.13629500	-2.10244400
H	1.63681500	-2.89769700	0.24634300
I	1.72453300	-1.57887300	-2.59878500
C	5.83298300	-2.67627300	2.20238500
O	5.49684800	-3.21468400	3.23870200

O	7.08588000	-2.22272300	1.97458500
C	8.00895000	-2.41551700	3.05941000
H	7.66002900	-1.89707100	3.95642900
H	8.11552500	-3.47915100	3.28879900
H	8.95617200	-1.99849400	2.71765800
H	-0.96290000	0.83666900	4.38058500
H	3.26647300	3.68250900	1.42912400
O	1.11150600	1.95232800	-3.33063800

TS4

C	0.03630800	2.22407700	3.65237800
C	-0.15401100	0.84113000	3.52954500
C	0.09115800	0.18382100	2.32786400
C	0.55690400	0.92522300	1.22468200
C	0.79054100	2.31072100	1.33809500
C	0.50182000	2.95929000	2.55890900
Pd	0.97934700	0.03039500	-0.53135400
H	-0.09678900	-0.87827500	2.22809500
O	0.72161200	4.31005300	2.56761700
C	0.46524700	5.02779100	3.76592600
H	0.70727100	6.06957200	3.55025800
H	-0.58930700	4.95575000	4.06286300
H	1.09568000	4.67333300	4.59200000
H	-0.17815800	2.70863700	4.59728100
C	1.57833500	2.04474500	-1.05351800
C	3.05680800	2.23509100	-1.42332500
C	2.82594600	3.56216100	0.39744200
C	1.37935800	3.02402800	0.16335700
C	3.69225800	2.35780600	-0.01902700
H	4.76271400	2.58980000	-0.05102600
H	3.53530700	1.47814600	0.60834200
C	3.28573000	3.67211700	-1.98006000
H	4.29191300	3.73760800	-2.40733700
H	2.58410300	3.92653400	-2.77685300
C	3.14405900	4.57936900	-0.71775100
H	4.07869600	5.10735100	-0.50173200
H	2.35905800	5.33564500	-0.82225700
H	3.43292200	1.46482700	-2.09597700
H	0.72521600	3.85774300	-0.12062000
C	0.57306400	2.24701300	-2.12933200
O	-0.61993400	2.54842700	-1.94371000

C	0.07440000	2.02803800	-4.42849400
H	0.65188500	1.89963300	-5.34322900
H	-0.59682100	1.17826000	-4.27619300
H	-0.50750600	2.95155600	-4.46111800
C	-2.34832500	-3.09436200	-0.20058700
C	-1.61240900	-1.73909400	-0.32062200
O	-2.31428200	-0.75891900	-0.70861400
O	-0.38559300	-1.71876900	-0.01815700
C	-4.42969100	-1.67509400	1.15458800
C	-4.04642000	-0.38500000	1.53643400
C	-5.65776100	-1.80243900	0.49360300
C	-4.80480600	0.73315100	1.21816600
C	-6.44885500	-0.69444600	0.19158100
C	-6.01088900	0.58176500	0.53971100
F	-6.09432400	-3.00057600	0.09351900
F	-7.61120900	-0.84493600	-0.45327900
F	-6.73953600	1.65313800	0.22039500
F	-4.33412700	1.96573300	1.49333400
F	-2.87842200	-0.17365300	2.16047400
C	-3.26262900	-3.31349800	-1.40829000
H	-2.64748100	-3.38479200	-2.31301800
H	-3.83355100	-4.23797900	-1.29542200
H	-3.94824700	-2.47667300	-1.54048000
C	-1.37640800	-4.26313000	-0.01448600
H	-0.75087400	-4.12951500	0.87034400
H	-1.92126600	-5.20815100	0.06803600
H	-0.71651600	-4.31510800	-0.88552600
S	-3.34609500	-3.05854100	1.41447300
Ag	-1.62326400	1.30299700	-0.21438400
C	3.37575600	-2.88031200	1.24714200
C	4.67095600	-2.34549100	1.24999500
C	4.99929200	-1.33453100	0.33661100
C	4.04266100	-0.84466100	-0.54976000
C	2.74045700	-1.33977600	-0.47283300
C	2.40618000	-2.40791200	0.36584400
H	3.13931700	-3.68148400	1.93994500
H	6.00815100	-0.93869300	0.30759900
H	4.31229700	-0.09012700	-1.27303100
H	1.40921400	-2.82518400	0.35969200
I	1.65595600	-1.40039700	-2.79786100
C	5.65578200	-2.90560100	2.21252400

O	5.41542600	-3.79364700	3.00838000
O	6.87059200	-2.31472200	2.11183900
C	7.86619600	-2.81664000	3.01651500
H	7.55096200	-2.67527500	4.05399400
H	8.03868900	-3.88304100	2.84699000
H	8.76992100	-2.24360700	2.80824000
H	-0.51654200	0.27889300	4.38559600
H	2.96981000	3.94470500	1.40836200
O	1.04614500	2.07247300	-3.36702600

int8

C	0.33407100	1.79708000	-4.01491000
C	0.60653700	0.46533400	-3.68331400
C	0.18101000	-0.08017100	-2.47537200
C	-0.53416200	0.72781100	-1.58318900
C	-0.83715100	2.05391700	-1.89388700
C	-0.38113200	2.59203800	-3.11705800
Pd	-0.98233900	0.14743500	0.30806000
H	0.43877000	-1.10139400	-2.22808500
O	-0.69744400	3.90717500	-3.32349800
C	-0.26660100	4.52407300	-4.52799900
H	-0.61470800	5.55694500	-4.47828700
H	0.82747500	4.51471100	-4.61764300
H	-0.70343500	4.03728500	-5.40975300
H	0.68257400	2.19638800	-4.95955900
C	-1.86195100	2.12978300	0.43292100
C	-3.38594000	2.24154800	0.61587100
C	-3.05625000	3.24164800	-1.39124400
C	-1.61072200	2.88435700	-0.92459500
C	-3.87577900	2.06081000	-0.84027400
H	-4.95681000	2.20529000	-0.93874300
H	-3.60651100	1.10259700	-1.28276400
C	-3.80137300	3.72843000	0.85818100
H	-4.86097500	3.74545000	1.13304100
H	-3.25317200	4.20210700	1.67143500
C	-3.56635300	4.41023200	-0.52558200
H	-4.49760400	4.81692200	-0.93281400
H	-2.84554000	5.23342500	-0.47714900
H	-3.78803700	1.56980600	1.37082100
H	-1.04981100	3.80892000	-0.74095000
C	-0.97779300	2.64892500	1.51877100

O	0.25693300	2.83525000	1.37887100
C	-0.73205800	3.30619300	3.77661200
H	-1.42313400	3.53762300	4.58514600
H	-0.10675800	2.45029700	4.03854600
H	-0.11447200	4.17053000	3.52515400
C	2.12218500	-3.09827600	-0.08755400
C	1.43680700	-1.77237400	0.29596400
O	2.19432900	-0.89604800	0.82251500
O	0.21064400	-1.66138300	0.02649500
C	4.33480100	-1.60373600	-1.12993300
C	4.11672400	-0.22077000	-1.13298000
C	5.55278300	-2.05334900	-0.60283500
C	5.02611200	0.66875400	-0.57672500
C	6.49339000	-1.17325800	-0.06911200
C	6.22129400	0.19322500	-0.04276800
F	5.83444800	-3.35926400	-0.56166100
F	7.64275900	-1.63241900	0.43770300
F	7.09921800	1.04199200	0.49444400
F	4.72955200	1.97833700	-0.50757200
F	2.98195100	0.29628200	-1.62317300
C	3.04510900	-3.57950200	1.03297600
H	2.43847700	-3.82405600	1.91210900
H	3.59268900	-4.47113000	0.72021700
H	3.75157100	-2.80215300	1.32475800
C	1.10989800	-4.17429600	-0.49013200
H	0.47515200	-3.84657200	-1.31579000
H	1.62699700	-5.09591300	-0.77124500
H	0.45534600	-4.38153400	0.36096100
S	3.08688400	-2.74128500	-1.68574400
Ag	1.55127600	1.11925400	1.02917100
C	-3.65980100	-2.49920700	-1.74635100
C	-4.74635800	-2.61134400	-0.87271200
C	-4.74846800	-1.87455300	0.31813400
C	-3.68538400	-1.02496800	0.62762900
C	-2.62029100	-0.91828600	-0.26640400
C	-2.58810900	-1.65635400	-1.44860200
H	-3.66458300	-3.07586400	-2.66571600
H	-5.57466300	-1.97193800	1.01334600
H	-3.69039000	-0.48931800	1.56615700
H	-1.76025600	-1.58689900	-2.13800000
I	-1.00289800	-0.48818800	3.06732100

C	-5.85730700	-3.52530000	-1.25459600
O	-5.88915300	-4.18268700	-2.27754000
O	-6.84750100	-3.54956600	-0.33192600
C	-7.94730600	-4.41825400	-0.64404900
H	-8.42260200	-4.11675700	-1.58158900
H	-7.60575400	-5.45225900	-0.74320300
H	-8.64446700	-4.32238200	0.18850000
H	1.17741800	-0.14996700	-4.37306800
H	-3.10715700	3.41905700	-2.46606200
O	-1.57386100	2.94764300	2.65576000

int9

C	-5.51616200	0.50293800	-1.63217300
C	-4.65963000	0.31909000	-2.72370300
C	-3.27402700	0.35877700	-2.56650900
C	-2.75200000	0.58503400	-1.28847400
C	-3.58128100	0.78414100	-0.18393400
C	-4.97747900	0.75150800	-0.36552200
Pd	-0.77490500	0.63280000	-1.02017200
H	-5.08538100	0.14118600	-3.70741800
H	-2.62169200	0.20373800	-3.42198500
O	-5.71397600	0.98875400	0.76125800
C	-7.12947100	1.02211900	0.64920000
H	-7.50508700	1.25155600	1.64756200
H	-7.46014500	1.80075100	-0.05018400
H	-7.53274500	0.05344400	0.32581300
H	-6.58806700	0.46720900	-1.78415300
C	-1.40459600	1.28982000	0.92743300
C	-0.82914600	0.43577200	2.05467300
C	-3.07297800	0.24779300	2.34863100
C	-2.94276400	1.18225200	1.10813600
C	-1.87056000	-0.69823300	2.18867800
H	-1.68960000	-1.31729700	3.07348400
H	-1.93817800	-1.34394700	1.31673900
C	-1.10263500	1.22003700	3.38381300
H	-0.53495800	0.72975600	4.18024200
H	-0.76207100	2.25655200	3.34293100
C	-2.64496100	1.07123900	3.58631900
H	-2.86941800	0.52610800	4.50843200
H	-3.15798400	2.03632500	3.64116600
H	0.21683600	0.16559500	1.93615200

H	-3.33116700	2.17570100	1.35881900
C	-0.92489300	2.72805700	0.79612800
O	-1.65091400	3.64986200	0.48590200
C	0.89578900	4.19941100	0.96729900
H	1.97022300	4.10071900	1.09883000
H	0.64984900	4.58155800	-0.02419000
H	0.46075300	4.85155000	1.72950300
C	2.79959900	2.49597400	-2.04646500
C	1.42919300	1.95685900	-1.62371300
O	1.38607400	0.76063600	-1.16702900
O	0.37902900	2.63149600	-1.78388900
C	3.78114700	0.97994800	0.29631500
C	3.16781700	0.97168200	1.55615400
C	4.20238900	-0.25623000	-0.20973500
C	2.92475700	-0.21146300	2.24909700
C	3.96757500	-1.44927300	0.46695500
C	3.32340800	-1.42659600	1.70148400
F	4.82332600	-0.33292500	-1.39255400
F	4.32650100	-2.62182000	-0.06785200
F	3.05607800	-2.57238200	2.33473900
F	2.27032800	-0.18681700	3.42022300
F	2.77879200	2.10798600	2.14241800
C	3.32864800	1.62027000	-3.19332300
H	2.66449400	1.72817200	-4.05958300
H	4.33283300	1.94013700	-3.48287300
H	3.35994800	0.57069300	-2.90900400
C	2.72687700	3.96705500	-2.47104700
H	2.04837300	4.05532500	-3.32324500
H	2.34181100	4.60077700	-1.67087400
H	3.71428100	4.33078600	-2.77206600
S	4.00650500	2.51481800	-0.57711000
C	-1.43425000	-3.64439900	-1.04967900
C	-0.24510300	-4.09722900	-0.46687800
C	0.69991800	-3.16625400	-0.01452700
C	0.45498400	-1.80328400	-0.14520700
C	-0.73850700	-1.35467000	-0.72523300
C	-1.69207500	-2.27618300	-1.17284000
H	-2.16663400	-4.36266600	-1.40109900
H	1.62168300	-3.52205600	0.43354100
H	1.19882000	-1.09327400	0.18619300
H	-2.62596200	-1.94960700	-1.60997400

C	0.06701900	-5.54396200	-0.30310300
O	1.08171300	-5.97619600	0.20842500
O	-0.91107500	-6.34302300	-0.79162500
C	-0.66273600	-7.75177800	-0.66589800
H	-1.52954800	-8.24471600	-1.10646500
H	0.25097300	-8.03092900	-1.19770500
H	-0.55328500	-8.03187200	0.38543000
O	0.37204600	2.86177300	1.10782300
H	-4.05902000	-0.21128600	2.42387700

TS5

C	3.87111600	-3.75447300	-1.17782300
C	3.95581900	-2.77063200	-2.16906000
C	3.13797100	-1.64731300	-2.13019300
C	2.20645700	-1.51139400	-1.08880200
C	2.06759900	-2.51241500	-0.10707700
C	2.91838000	-3.63239400	-0.16041500
Pd	0.58832400	-0.22402700	-1.05840400
H	4.68658900	-2.87947900	-2.96509500
H	3.24769100	-0.86402400	-2.87209000
O	2.71398600	-4.56166200	0.81919100
C	3.43636400	-5.78416200	0.75774500
H	3.07112700	-6.39060400	1.58780500
H	3.25321900	-6.31224900	-0.18664700
H	4.51532700	-5.62228400	0.87831100
H	4.53500200	-4.60940900	-1.21729400
C	-0.25358300	-1.63131100	0.24030200
C	-0.87155700	-0.96266300	1.45975200
C	0.91830100	-2.07761600	2.30292800
C	0.86818800	-2.51672500	0.79988300
C	0.37120100	-0.62780500	2.30256700
H	0.10996000	-0.28543900	3.30968400
H	1.00759600	0.12281600	1.84221900
C	-1.50981200	-2.10177700	2.32578500
H	-2.16059600	-1.65455700	3.08000000
H	-2.12818500	-2.78062400	1.73308200
C	-0.27155500	-2.80123400	2.97953200
H	-0.25631000	-2.63709700	4.06151100
H	-0.25325100	-3.88171300	2.80924400
H	-1.54393800	-0.15171700	1.20486500
H	0.51258900	-3.55365400	0.76862200

C	-1.16191000	-2.31714200	-0.76140200
O	-0.82281000	-3.26452400	-1.44235500
C	-3.26257500	-2.26628000	-1.82126600
H	-4.19359100	-1.72022300	-1.69275700
H	-2.81316500	-2.05431400	-2.79313200
H	-3.41547900	-3.34183300	-1.70486900
C	-2.73073600	1.82469200	-2.62285100
C	-1.63775000	0.85008800	-2.15362900
O	-1.10505800	1.08519400	-1.00514400
O	-1.24542900	-0.06512100	-2.90509800
C	-3.82737100	1.43313200	0.14466200
C	-4.34471400	0.30233400	0.79236000
C	-3.05942100	2.30935600	0.92257000
C	-4.10883600	0.05226100	2.14081600
C	-2.77940800	2.05539400	2.26159200
C	-3.31064300	0.92310500	2.87367400
F	-2.55945500	3.43134100	0.39676400
F	-1.99730600	2.88650400	2.96196400
F	-3.00934600	0.63944500	4.14661600
F	-4.58538400	-1.05873800	2.72004900
F	-5.10137300	-0.58407700	0.13148800
C	-2.15202500	3.24801400	-2.64885900
H	-1.34198300	3.28926800	-3.38766500
H	-2.92164000	3.96662500	-2.94366300
H	-1.75169000	3.52908000	-1.67837500
C	-3.25911500	1.42930200	-4.00871000
H	-2.44209300	1.49718200	-4.73152900
H	-3.62900200	0.40314900	-4.01626300
H	-4.05996900	2.10550400	-4.32591400
S	-4.28757600	1.73363200	-1.54422100
C	4.03604800	1.44677600	1.06775600
C	4.22662300	2.49354300	0.15422800
C	3.54280200	2.47336800	-1.06797200
C	2.67636600	1.42630600	-1.36877400
C	2.44197100	0.41341800	-0.42033700
C	3.15794700	0.40482500	0.78184500
H	4.58692400	1.44504400	2.00151100
H	3.71235700	3.27704300	-1.77666600
H	2.18839200	1.41074200	-2.34382300
H	3.05276100	-0.41824700	1.47557500
C	5.15295700	3.62806100	0.41345500

O	5.35844000	4.54010900	-0.36466200
O	5.75190700	3.53932900	1.62361500
C	6.65728700	4.61067400	1.93394100
H	7.04589900	4.38940500	2.92803700
H	7.46944000	4.65265100	1.20302600
H	6.13348400	5.57035700	1.92966800
O	-2.38892000	-1.76964400	-0.78358400
H	1.88537900	-2.24989200	2.77977800

int10

C	0.90109200	3.99614400	-2.38658500
C	0.05378500	3.32677800	-3.26447200
C	-0.93273600	2.47517000	-2.77870000
C	-1.08767800	2.23341700	-1.39563700
C	-0.16475400	2.82587900	-0.46114700
C	0.78220500	3.77393400	-1.00995600
Pd	1.00570500	0.93917700	-0.71710300
H	0.14583500	3.49264600	-4.33366800
H	-1.63110200	2.00334800	-3.46089700
O	1.50588000	4.45114900	-0.10817300
C	2.76335600	5.01857600	-0.47910700
H	3.26216900	5.24954700	0.46018200
H	3.36268200	4.29017800	-1.03416000
H	2.62603400	5.93082300	-1.07182500
H	1.63859800	4.69468900	-2.76065900
C	0.95339500	1.43705700	1.26858000
C	0.26761100	0.45397000	2.21467600
C	-1.25451200	2.10811600	1.93784800
C	-0.05527600	2.60391900	1.08389000
C	-1.20904000	0.56804500	1.81179500
H	-1.87752200	0.06583100	2.51628100
H	-1.41203700	0.18408600	0.81592500
C	0.24341500	1.15215800	3.61044600
H	-0.07063100	0.42081700	4.36130700
H	1.22320300	1.52924600	3.91469700
C	-0.82028600	2.27920000	3.41881700
H	-1.68020300	2.12679400	4.07809300
H	-0.42264000	3.27804400	3.62384100
H	0.73140400	-0.52524800	2.23514000
H	0.34868900	3.52810000	1.49783900
C	2.40317700	1.71001100	1.58561700

O	2.96696700	2.78591900	1.52619200
C	4.41758600	0.66623500	2.23693500
H	4.63653600	1.45762500	2.95854300
H	4.70306400	-0.30814900	2.63334400
H	4.92942000	0.85834800	1.29297100
C	3.76956900	-2.33633700	-1.18499000
C	3.22715700	-0.92536700	-0.84633800
O	1.92915000	-0.86794000	-0.79762100
O	4.00467300	0.02179500	-0.74593800
C	1.30800000	-3.36063300	0.12370800
C	0.84974600	-2.99636000	1.39489200
C	0.34716200	-3.43834500	-0.89152400
C	-0.49236400	-2.72595100	1.64756100
C	-0.98840000	-3.11870900	-0.66962100
C	-1.41418800	-2.76764600	0.60892600
F	0.69405500	-3.78498400	-2.13801300
F	-1.86760100	-3.13573800	-1.68718700
F	-2.69336000	-2.45502500	0.83949200
F	-0.89001900	-2.35257900	2.87420400
F	1.70266500	-2.83553200	2.41423700
C	3.49978700	-2.59268200	-2.67736500
H	4.02564100	-1.83419400	-3.26970800
H	3.86816700	-3.57996900	-2.96980700
H	2.43586000	-2.53604700	-2.89993700
C	5.27098900	-2.42317500	-0.88250300
H	5.79410500	-1.68197800	-1.49074700
H	5.47754500	-2.20267300	0.16683400
H	5.66194900	-3.41715700	-1.12412400
S	3.03303800	-3.71613900	-0.11440600
C	-4.61005800	1.44860900	-0.23091300
C	-4.73165000	0.09874200	-0.58431000
C	-3.65721600	-0.55706000	-1.19815400
C	-2.46959100	0.12372300	-1.43821200
C	-2.32689200	1.46709400	-1.05463000
C	-3.41825200	2.12705500	-0.47374900
H	-5.44815700	1.96047500	0.22759400
H	-3.75836100	-1.60321400	-1.45694800
H	-1.63128100	-0.39728000	-1.89038800
H	-3.33159400	3.17890100	-0.21957900
C	-5.97211300	-0.68729500	-0.33223300
O	-6.12105400	-1.85382100	-0.63890000

O	-6.93040900	0.04334900	0.28414800
C	-8.15135400	-0.66363900	0.55526000
H	-8.80603000	0.05588900	1.04710800
H	-8.60223000	-1.02328800	-0.37366300
H	-7.96250300	-1.52145000	1.20634600
O	3.00135000	0.57730700	1.99961400
H	-2.20177100	2.59020600	1.70530100

TS6

C	0.05017800	5.25255900	-1.49800500
C	-1.26868900	5.28775300	-1.95467900
C	-2.11381500	4.19796900	-1.76710200
C	-1.66040100	3.04319600	-1.10898300
C	-0.33572500	2.99807000	-0.60869200
C	0.51205200	4.12053400	-0.82111500
Pd	0.61227600	1.14017500	-0.52996300
H	-1.62951800	6.16947600	-2.47587000
H	-3.12456700	4.21040800	-2.16319500
O	1.75354300	4.00127100	-0.29492600
C	2.66423100	5.09153200	-0.34077300
H	3.53796700	4.75224300	0.21470300
H	2.94797700	5.32981100	-1.37319900
H	2.24345500	5.98532500	0.13770200
H	0.70590300	6.09937800	-1.66249600
C	0.77940200	1.24076900	1.55119900
C	-0.08826800	0.32063900	2.40779400
C	-1.32709500	2.18256600	2.06449500
C	-0.00611100	2.44636500	1.35404300
C	-1.50703700	0.65386200	1.92048500
H	-2.28452000	0.26029400	2.58119100
H	-1.70501700	0.31926300	0.90353600
C	-0.09622100	0.99814000	3.81659700
H	-0.57864500	0.32621700	4.53226100
H	0.91039500	1.20605300	4.18908100
C	-0.94109100	2.28749700	3.57744200
H	-1.85232700	2.29110400	4.18273200
H	-0.39217100	3.20627900	3.80458300
H	0.22591200	-0.71251900	2.42840600
H	0.50868300	3.38871700	1.49775500
C	2.25876900	1.29064700	1.81849500
O	2.92863700	2.30140500	1.88047100

C	4.14078100	-0.09197600	2.18134600
H	4.50245500	0.54461400	2.99282700
H	4.29835900	-1.14522600	2.40482000
H	4.62080400	0.17827100	1.23978800
C	3.20604300	-1.82925300	-2.27653600
C	2.75474500	-0.66856000	-1.35389700
O	1.45895800	-0.60459300	-1.20252700
O	3.57689600	0.10832500	-0.87369400
C	1.63770600	-3.31937300	-0.31944300
C	1.80560700	-3.14320200	1.05886500
C	0.32421700	-3.33671700	-0.80596700
C	0.71827700	-2.99546200	1.91355900
C	-0.77264100	-3.15671500	0.02921200
C	-0.57159600	-2.97649800	1.39428700
F	0.08037000	-3.49245400	-2.11252200
F	-2.01654900	-3.13560600	-0.46844300
F	-1.61248200	-2.74172900	2.20340700
F	0.90686600	-2.78532300	3.22617300
F	3.02716700	-3.09212300	1.60299400
C	2.36738800	-1.84819500	-3.56148700
H	2.51146100	-0.90336400	-4.10076700
H	2.68533600	-2.66730100	-4.21302500
H	1.30920300	-1.96308400	-3.33828900
C	4.70067400	-1.71301300	-2.59389700
H	4.86935800	-0.80658900	-3.18316400
H	5.29054400	-1.63422900	-1.68053100
H	5.04391200	-2.57215100	-3.18022100
S	3.05920500	-3.49054700	-1.36823600
C	-4.59763500	0.80684900	-0.22509200
C	-4.21194700	-0.40502600	-0.81483100
C	-3.02509600	-0.46822600	-1.55603000
C	-2.21588000	0.65751100	-1.66767200
C	-2.56877700	1.86625500	-1.03884600
C	-3.78912200	1.93375700	-0.35146700
H	-5.52354200	0.85628100	0.33611200
H	-2.74361300	-1.40706200	-2.01739200
H	-1.31099700	0.60503500	-2.26738300
H	-4.08254500	2.86815800	0.11780900
C	-5.02675900	-1.64764700	-0.69500700
O	-4.78647500	-2.68720500	-1.27533200
O	-6.07792300	-1.49434100	0.14452600

C	-6.89961900	-2.66208300	0.30412500
H	-7.68712500	-2.37584800	1.00139900
H	-7.32589100	-2.96731900	-0.65538200
H	-6.31232400	-3.49260300	0.70501200
O	2.71330500	0.04579700	2.03247100
H	-2.15401800	2.82379700	1.76434800

int11

C	-5.47677700	-0.48379300	-1.25119200
C	-5.42655700	-1.85113900	-1.54200800
C	-4.23527800	-2.55902900	-1.43289900
C	-3.05940000	-1.90320000	-1.02435700
C	-3.10037400	-0.53026500	-0.72584400
C	-4.31852300	0.17586700	-0.82635800
Pd	-1.36975400	0.44184000	-0.44223400
H	-6.33044100	-2.35780100	-1.86698800
H	-4.19087600	-3.61427800	-1.68542600
O	-4.26445800	1.49396900	-0.48371500
C	-5.45123300	2.27505100	-0.52458100
H	-5.15739500	3.26766800	-0.18328100
H	-5.85284200	2.34005400	-1.54368500
H	-6.22288800	1.87024000	0.14344500
H	-6.41229700	0.05421400	-1.35093600
C	-1.15983600	0.99541400	1.75359600
C	-0.24532900	0.12540300	2.59913200
C	-2.16334400	-1.04400500	2.31776100
C	-2.35657500	0.27628200	1.58903300
C	-0.64447300	-1.29383800	2.15838400
H	-0.27107700	-2.06801400	2.83496100
H	-0.33955800	-1.53470300	1.13855700
C	-0.90979800	0.17993600	4.02067100
H	-0.24128800	-0.29940200	4.74147600
H	-1.07861600	1.20554100	4.35971200
C	-2.22860800	-0.63219000	3.82737000
H	-2.24445700	-1.52854800	4.45453800
H	-3.12536900	-0.05044300	4.05925000
H	0.79990900	0.40030900	2.60076500
H	-3.31268800	0.77726400	1.50594900
C	-1.07215800	2.49143400	1.75974800
O	-2.01799700	3.23777500	1.61796300
C	0.44937400	4.28796600	1.97110300

H	-0.24031000	4.81716500	2.63299600
H	1.47984300	4.39370800	2.30365800
H	0.33380100	4.63573800	0.94366700
C	1.54602500	2.56971400	-2.76049700
C	0.58362000	2.39832000	-1.55624500
O	0.39915800	1.14759400	-1.22149600
O	0.06797900	3.36766800	-1.01013200
C	3.23264200	1.52368400	-0.66896700
C	3.16596800	2.11591000	0.59795500
C	3.18041600	0.12485000	-0.72932800
C	3.06736500	1.35403800	1.75749000
C	3.07554000	-0.65189400	0.41856500
C	3.02791200	-0.03215800	1.66372700
F	3.19238900	-0.50976400	-1.90872800
F	2.99419700	-1.98678700	0.34467700
F	2.88205600	-0.77187900	2.77156500
F	2.94555300	1.94250800	2.95509600
F	3.16694500	3.44618600	0.73443300
C	1.35609700	1.45378300	-3.79515700
H	0.32649300	1.47705600	-4.17392700
H	2.03547400	1.59942400	-4.64000700
H	1.54322100	0.47545200	-3.35652200
C	1.37144800	3.95537200	-3.38918100
H	0.38433700	4.01363300	-3.85996000
H	1.43220900	4.73521700	-2.63027900
H	2.12674600	4.13302700	-4.16207200
S	3.33417900	2.54264100	-2.11845300
C	-0.43380300	-4.45151400	-0.02886900
C	0.70306600	-3.95024200	-0.67938900
C	0.59839200	-2.80199300	-1.47369700
C	-0.63084400	-2.16328100	-1.60938400
C	-1.77475200	-2.64312500	-0.94000800
C	-1.66018900	-3.80618200	-0.16465200
H	-0.34725600	-5.34130300	0.58415600
H	1.48539300	-2.41831000	-1.96478000
H	-0.71423100	-1.30893200	-2.27779200
H	-2.53490400	-4.18298200	0.35720200
C	2.03390000	-4.61397500	-0.58378400
O	2.99137700	-4.33929400	-1.27811600
O	2.06331200	-5.57146400	0.37331100
C	3.32421300	-6.24563900	0.51257800

H	3.18495800	-6.96991400	1.31529900
H	3.59732900	-6.74930100	-0.41875000
H	4.11276500	-5.53266100	0.76794200
O	0.19024600	2.86936000	2.01028900
H	-2.84014600	-1.84665300	2.02630000

int12

C	2.26986800	-0.06651800	-2.71459600
C	1.60400500	-1.24349700	-3.08072500
C	0.27133000	-1.44815600	-2.74160700
C	-0.41975700	-0.48199800	-1.97942200
C	0.22537300	0.70848900	-1.54323000
C	1.57271900	0.88657500	-1.96775900
H	2.13525000	-1.99856600	-3.64820500
H	-0.23586500	-2.34956700	-3.06119400
O	2.13702100	2.06294800	-1.54625400
C	3.50129700	2.33804100	-1.85349500
H	3.70040700	3.32646400	-1.43705100
H	4.17776900	1.61220000	-1.38544300
H	3.67831900	2.35011700	-2.93564100
H	3.30581400	0.07296800	-2.99257900
C	0.19956200	-0.33770100	3.12053000
C	0.25007700	1.20731600	3.36332100
O	0.53735000	1.56077100	4.50091900
O	-0.11399800	2.00006400	2.40740600
C	1.81117200	-1.19351100	0.76599900
C	2.92407200	-0.35127900	0.86577300
C	1.97265200	-2.41178000	0.09846300
C	4.14807200	-0.70022200	0.30874400
C	3.19324800	-2.77645400	-0.46479100
C	4.28208800	-1.91607200	-0.36059900
F	0.94008700	-3.24921400	-0.05174400
F	3.31223700	-3.92786400	-1.13101900
F	5.44750600	-2.24281400	-0.91831500
F	5.18494000	0.14476900	0.36746100
F	2.82339000	0.83005800	1.48230900
C	1.34940700	-1.05480700	3.81783400
H	1.26800500	-0.82937300	4.88336200
H	1.29791100	-2.13785700	3.66923500
H	2.31990500	-0.68629100	3.48122100
C	-1.16817000	-0.83442200	3.62399200

H	-1.99267200	-0.36962500	3.07446300
H	-1.25351200	-1.92185200	3.54076900
H	-1.25666800	-0.54494100	4.67477600
S	0.15995400	-0.72467900	1.26133800
C	-4.09581200	-0.00592300	-1.13970600
C	-4.44933300	-1.28950500	-0.69984700
C	-3.48724100	-2.30752800	-0.70117500
C	-2.19286800	-2.04590200	-1.13449000
C	-1.82115500	-0.76022500	-1.56632000
C	-2.79807600	0.25101700	-1.56700200
H	-4.84013900	0.78189700	-1.14365100
H	-3.77233000	-3.29277400	-0.34789100
H	-1.44108100	-2.82694700	-1.08869400
H	-2.54864100	1.24785600	-1.90958500
C	-5.81732000	-1.62481900	-0.21551300
O	-6.15658200	-2.72295300	0.18305500
O	-6.65700800	-0.56559300	-0.26415800
C	-7.99194300	-0.82566400	0.19794300
H	-7.98144500	-1.14931900	1.24232500
H	-8.52899300	0.11707100	0.09335500
H	-8.46269700	-1.60700700	-0.40494300
Pd	-0.10411700	1.42168500	0.44472700
C	-1.12532900	5.22182700	-1.41205900
H	-1.15014600	5.73957000	-0.45448000
H	-2.07591300	5.32388000	-1.94122900
H	-0.33951400	5.65019800	-2.04880600
C	-0.81258400	3.77735400	-1.15567200
O	-0.47653300	3.40546400	-0.03486700
O	-0.89667700	2.95019600	-2.18976000
H	-0.60858900	2.27181600	-2.03227300

TS7

C	2.27622200	-0.06317900	-2.70792900
C	1.60624400	-1.22902400	-3.08199900
C	0.27352200	-1.44679300	-2.73291500
C	-0.42447200	-0.48813200	-1.98638100
C	0.22485500	0.71333100	-1.58093200
C	1.58329800	0.89910200	-1.96519800
H	2.13860900	-1.98262100	-3.65599400
H	-0.22699100	-2.35374600	-3.05439500
O	2.13478200	2.06410300	-1.54693800

C	3.49816800	2.34774700	-1.84965500
H	3.68973000	3.33613100	-1.43227800
H	4.17106500	1.62285100	-1.37740700
H	3.67406100	2.36709900	-2.93195800
H	3.31219000	0.07783800	-2.99065700
C	0.19994700	-0.34669000	3.11966700
C	0.24397800	1.19219900	3.36753100
O	0.52472900	1.54819700	4.50216800
O	-0.11738700	1.99273100	2.40702900
C	1.81270900	-1.19430000	0.76270800
C	2.92459700	-0.35086800	0.86291400
C	1.97561900	-2.41184600	0.09406900
C	4.14906300	-0.69798300	0.30567200
C	3.19661700	-2.77467200	-0.46946800
C	4.28454400	-1.91316300	-0.36453600
F	0.94425600	-3.25075100	-0.05619900
F	3.31703600	-3.92553900	-1.13640500
F	5.45033800	-2.23829400	-0.92236900
F	5.18496300	0.14811900	0.36546200
F	2.82281600	0.82973900	1.48068300
C	1.35336300	-1.06063600	3.81436400
H	1.27082500	-0.83914900	4.88064600
H	1.30704600	-2.14341900	3.66215100
H	2.32204800	-0.68637000	3.47887700
C	-1.16515800	-0.85148600	3.62216300
H	-1.99212900	-0.39071800	3.07293700
H	-1.24436400	-1.93927200	3.53756900
H	-1.25544500	-0.56367300	4.67323300
S	0.16122900	-0.72789800	1.25928200
C	-4.09554500	-0.00511500	-1.14214500
C	-4.44809500	-1.28951000	-0.70393700
C	-3.48518500	-2.30678300	-0.70622900
C	-2.19088400	-2.04355400	-1.13877100
C	-1.82573100	-0.75699500	-1.57434300
C	-2.79786500	0.25902600	-1.56858300
H	-4.84055600	0.78207200	-1.14540000
H	-3.76956700	-3.29268900	-0.35422300
H	-1.43845000	-2.82400500	-1.09371700
H	-2.53786300	1.25651100	-1.90422100
C	-5.81588400	-1.62634200	-0.22029300
O	-6.15443200	-2.72521700	0.17687900

O	-6.65625700	-0.56759700	-0.26812300
C	-7.99117400	-0.82876600	0.19348500
H	-7.98068300	-1.15447800	1.23721900
H	-8.52835900	0.11409200	0.09070700
H	-8.46181900	-1.60899100	-0.41093300
Pd	-0.10558700	1.42000000	0.45377800
C	-1.12392300	5.23053700	-1.38615500
H	-1.14162400	5.75797700	-0.43283200
H	-2.08279000	5.33355400	-1.90002800
H	-0.35323100	5.66003000	-2.03329500
C	-0.82079300	3.76305300	-1.18035100
O	-0.47475200	3.39879300	-0.01551400
O	-0.92062500	2.98909000	-2.18319700
H	-0.42570800	1.81211900	-1.79379600

mono-p^m

C	2.28056800	-0.07721800	-2.70389600
C	1.60400500	-1.23279700	-3.08072500
C	0.27133000	-1.45885600	-2.72020700
C	-0.43045700	-0.50339800	-1.99012200
C	0.22537300	0.70848900	-1.61813000
C	1.59411900	0.89727500	-1.96775900
H	2.13525000	-1.98786600	-3.65890500
H	-0.22516500	-2.37096700	-3.03979400
O	2.13702100	2.05224800	-1.55695400
C	3.50129700	2.33804100	-1.85349500
H	3.68970700	3.32646400	-1.43705100
H	4.16706900	1.61220000	-1.37474300
H	3.67831900	2.36081700	-2.93564100
H	3.31651400	0.06226800	-2.99257900
C	-4.09581200	-0.00592300	-1.13970600
C	-4.44933300	-1.28950500	-0.69984700
C	-3.48724100	-2.30752800	-0.70117500
C	-2.19286800	-2.04590200	-1.13449000
C	-1.83185500	-0.76022500	-1.57702000
C	-2.79807600	0.26171700	-1.56700200
H	-4.84013900	0.78189700	-1.14365100
H	-3.77233000	-3.29277400	-0.34789100
H	-1.44108100	-2.82694700	-1.08869400
H	-2.52724100	1.25855600	-1.89888500
C	-5.81732000	-1.62481900	-0.21551300

O	-6.15658200	-2.72295300	0.18305500
O	-6.65700800	-0.56559300	-0.26415800
C	-7.99194300	-0.82566400	0.19794300
H	-7.98144500	-1.14931900	1.24232500
H	-8.52899300	0.11707100	0.09335500
H	-8.46269700	-1.60700700	-0.40494300
H	-0.25548900	1.38371600	-1.58287300

TS1_{para}

C	3.77142900	-4.52495400	0.01101700
C	4.46311800	-3.65056300	-0.85419300
C	3.88910300	-2.42380300	-1.22559200
C	2.65836000	-2.07063200	-0.69509700
C	1.93819000	-2.90742200	0.19025400
C	2.54764900	-4.14869000	0.53252900
H	0.65133300	-3.16072700	-0.30583300
Pd	1.00961200	-1.93357500	1.77590400
Pd	0.75620100	0.92960000	1.11879200
C	3.24743300	-0.09430100	2.38808300
O	2.89378100	-1.30837900	2.29384100
O	2.53422400	0.93691500	2.15449200
C	4.67979400	0.17740300	2.77912300
H	5.20835800	0.46376600	1.86462200
H	4.72429300	1.01747800	3.47527200
H	5.13777700	-0.71283800	3.21029700
C	-0.33906100	0.01796900	3.69332700
O	0.19969100	-1.10765300	3.56938200
O	-0.35941700	0.95579600	2.81787000
C	-1.01855100	0.35081900	5.00443500
H	-1.91362800	0.95042700	4.82682500
H	-1.26504600	-0.56284800	5.54582100
H	-0.32859600	0.94856300	5.60909500
C	-1.28918300	-3.02150600	0.25224200
O	-0.49664100	-3.40695100	-0.67060900
O	-0.92684700	-2.46820200	1.32418800
H	2.25193100	-1.10294400	-0.95827500
H	4.40750000	-1.72449400	-1.86521600
C	-0.25045300	1.00677700	-1.92744600
C	1.24304500	1.37387400	-1.75323300
O	1.87797600	1.72903700	-2.73254000
O	1.79884400	1.17844000	-0.57951800

C	-2.00764600	2.32267500	0.06300200
C	-1.43413900	3.59760500	0.02573300
C	-3.36095300	2.22551800	0.39847100
C	-2.18863400	4.74034900	0.26790300
C	-4.13807900	3.35559200	0.63008800
C	-3.54798900	4.61656500	0.56299600
F	-3.94676200	1.02646200	0.53065300
F	-5.43295600	3.23138300	0.92542200
F	-4.27867200	5.70576100	0.78793800
F	-1.62656800	5.94803200	0.21482900
F	-0.13345500	3.73852700	-0.25915100
C	-0.96447500	2.01103300	-2.82827700
H	-0.47743000	1.96524300	-3.80509500
H	-2.02065600	1.76145100	-2.94015000
H	-0.86161200	3.03291900	-2.46306800
C	-0.30695700	-0.41400600	-2.52121100
H	0.11437500	-1.16418700	-1.84816900
H	-1.33604700	-0.69821800	-2.74140100
H	0.28059500	-0.41466600	-3.44356900
S	-1.10093000	0.81718100	-0.22614800
H	4.23620800	-5.47215400	0.26508200
C	-2.78773800	-3.31388800	0.07667700
C	-4.68134000	-1.81827600	-1.52718600
C	-5.91511400	-2.39053200	-1.18666800
C	-4.67361800	-0.43936700	-1.75928400
C	-7.07075600	-1.62779600	-1.04825700
C	-5.81013600	0.34805900	-1.60999000
C	-7.01707300	-0.24926000	-1.25968100
F	-3.53639200	0.19186400	-2.09711600
F	-5.73107100	1.67617100	-1.76493900
F	-8.11425700	0.49206500	-1.10970200
F	-8.22708800	-2.20156600	-0.70374600
F	-5.99871500	-3.70284100	-0.92891900
C	-2.98484400	-4.83813000	0.16785100
H	-2.68732400	-5.18895400	1.16313900
H	-4.03722100	-5.08055500	0.00682000
H	-2.38087200	-5.35662600	-0.57953800
C	-3.61804400	-2.57892900	1.12788200
H	-3.53203200	-1.49471600	1.03406700
H	-4.66671900	-2.86960300	1.05316300
H	-3.25183300	-2.86051800	2.11766200

S	-3.19598200	-2.77576500	-1.70576200
O	5.67409900	-4.07526200	-1.27261400
C	6.46792000	-3.19033100	-2.06778900
H	6.66712900	-2.24967000	-1.54435600
H	7.40431900	-3.71911500	-2.24853300
H	5.98205000	-2.96949400	-3.02541200
H	2.03549400	-4.82499800	1.21282700
C	4.98280100	1.56036200	-1.32835800
H	4.29728300	1.97066000	-2.08179200
C	5.44191600	2.72702500	-0.44544300
C	6.13569000	0.88970700	-2.07379300
O	4.38386300	0.58272600	-0.53477300
H	3.42968000	0.81544700	-0.46893300
F	6.85386400	1.77230900	-2.78963900
F	6.97431000	0.24787700	-1.23612600
F	5.64753400	-0.03473800	-2.93705100
F	6.34674100	2.33395800	0.47475300
F	4.37652400	3.22558500	0.21321700
F	5.98777200	3.72427200	-1.16811300

int2_{para}

C	3.42559000	-4.62374000	0.07747600
C	4.02081100	-3.91138100	-0.97565900
C	3.63776400	-2.58735600	-1.21856500
C	2.69861400	-1.97975300	-0.38614100
C	2.11539700	-2.66019100	0.68931100
C	2.49431400	-4.00092600	0.90795300
H	0.52360000	-3.39177800	-0.15785700
Pd	1.06512400	-1.65185100	2.05171300
Pd	0.74476700	1.18234600	1.16629300
C	3.20642200	0.35378500	2.60670000
O	2.87684000	-0.86876100	2.63496200
O	2.48579400	1.34226400	2.24296400
C	4.62465600	0.69135900	3.00021100
H	5.19413900	0.78621100	2.06980200
H	4.65582200	1.64999400	3.52101700
H	5.05440800	-0.10320600	3.61056900
C	-0.50790900	0.43739300	3.73021800
O	0.00642200	-0.70185900	3.69847400
O	-0.43909400	1.33298200	2.80939900
C	-1.27691400	0.86024500	4.96514300

H	-2.14037800	1.46907900	4.68907100
H	-1.58667000	-0.01588400	5.53559500
H	-0.61917100	1.47542300	5.58796400
C	-1.21845800	-3.04355600	0.51295000
O	-0.42941200	-3.60520400	-0.37320600
O	-0.82638600	-2.36244100	1.46766300
H	2.46313600	-0.94057600	-0.56040400
H	4.08607600	-2.00154000	-2.00793500
C	-0.13565200	0.91021800	-1.90643300
C	1.33541000	1.35773500	-1.71637700
O	1.99443800	1.62396000	-2.70803300
O	1.84741700	1.32852200	-0.50832000
C	-2.02389200	2.35610800	-0.13197500
C	-1.50048400	3.64351500	-0.28812900
C	-3.38085500	2.23779500	0.17964300
C	-2.30687900	4.77213000	-0.18665700
C	-4.20860600	3.35125600	0.27363000
C	-3.66794400	4.62236900	0.08769600
F	-3.92223000	1.03402000	0.42368500
F	-5.50539400	3.20303300	0.54990500
F	-4.44785700	5.69668500	0.17935600
F	-1.79190800	5.99031900	-0.35331000
F	-0.19867500	3.80967100	-0.55175100
C	-0.84784700	1.77991600	-2.93910000
H	-0.31501900	1.65328800	-3.88431800
H	-1.88710400	1.47350000	-3.06669600
H	-0.80288000	2.83808500	-2.68182900
C	-0.11288700	-0.56777700	-2.34195300
H	0.34469200	-1.21073700	-1.58634400
H	-1.12225900	-0.92822200	-2.54497600
H	0.49281200	-0.63907100	-3.24961100
S	-1.05018800	0.86793400	-0.22990700
H	3.73162600	-5.65116400	0.24784000
C	-2.70566500	-3.34043300	0.33524700
C	-4.56960700	-1.98006800	-1.41515400
C	-5.80633800	-2.53465600	-1.05570500
C	-4.56296900	-0.62384900	-1.75556600
C	-6.96966800	-1.77327200	-1.00539900
C	-5.70960200	0.16137500	-1.70019200
C	-6.91999200	-0.41625900	-1.32901700
F	-3.42154500	-0.01443500	-2.11266400

F	-5.63831600	1.47163800	-1.96501900
F	-8.02478500	0.32457300	-1.26584300
F	-8.12883000	-2.32654800	-0.64005900
F	-5.88528300	-3.82252900	-0.69434000
C	-2.93297700	-4.84807200	0.55456000
H	-2.65673300	-5.11891300	1.58036400
H	-3.98855200	-5.07816700	0.39984100
H	-2.33496500	-5.44380300	-0.13774500
C	-3.52819100	-2.49862200	1.31008200
H	-3.42657600	-1.42940600	1.11510700
H	-4.57973000	-2.78156700	1.25508500
H	-3.17267200	-2.69073200	2.32519700
S	-3.07960800	-2.94175500	-1.49366900
O	4.96489200	-4.57825400	-1.69599900
C	5.69147100	-3.84011100	-2.67397200
H	6.17682800	-2.95765200	-2.23892500
H	6.44951300	-4.52243900	-3.06159600
H	5.04316500	-3.51465400	-3.49832000
H	2.07680000	-4.56079000	1.74165500
C	5.08017700	1.41522000	-1.32629500
H	4.39363200	1.92906400	-2.01100800
C	5.87336300	2.48601600	-0.57039200
C	5.96552500	0.50686300	-2.18297400
O	4.41292500	0.61102500	-0.40242200
H	3.48939200	0.94080000	-0.34475500
F	6.78962000	1.21522900	-2.97826300
F	6.71423100	-0.32614000	-1.43908000
F	5.18903400	-0.25912300	-2.98830700
F	6.80425300	1.93859200	0.23789700
F	5.02608200	3.19616100	0.20251800
F	6.49393900	3.34504300	-1.40169200

int13

C	-2.53340400	2.51293100	0.41856500
C	-2.66760600	3.33641500	-0.70820900
C	-1.69121100	3.29688700	-1.71043000
C	-0.59595400	2.43128600	-1.58135900
C	-0.45866800	1.59933500	-0.46828400
C	-1.43891900	1.65895700	0.53477200
Pd	0.99257400	0.17684700	-0.39628200
H	0.15136300	2.41159400	-2.37073100

H	-1.76805400	3.92317100	-2.59167400
H	-3.29738800	2.56032100	1.18866800
C	2.83362000	1.03952000	0.60565600
C	3.04233800	0.49870200	2.01453900
C	1.51244400	2.16881100	2.15511600
C	1.89784100	2.05718500	0.69301900
C	1.64040500	0.70329900	2.62884400
H	1.63841800	0.60759100	3.71913800
H	0.88558800	0.03482900	2.20497800
C	3.83504900	1.63552900	2.74203600
H	4.13731300	1.29647200	3.73726500
H	4.74106200	1.91202300	2.19716100
C	2.78755500	2.79263600	2.82805700
H	2.56101100	3.05472500	3.86586500
H	3.11500900	3.70560500	2.32257900
H	3.48049400	-0.49527800	2.06143300
H	1.80544200	2.86713700	-0.01954400
C	3.82309300	0.92937900	-0.50358800
O	3.67986400	1.40888800	-1.61379400
C	5.89078600	0.00606000	-1.13268400
H	6.25496600	0.94901400	-1.54897600
H	6.69649100	-0.53914300	-0.64241500
H	5.45207200	-0.59476600	-1.93312500
C	0.57843600	-2.77826100	-1.64455900
C	1.81791500	-2.69287300	-0.69083800
O	2.24965500	-1.51896600	-0.35484900
O	2.35866100	-3.75748600	-0.42015700
C	-1.74869400	-1.52440900	-0.28887600
C	-3.07173200	-1.18484400	-0.58932400
C	-1.46034800	-1.92741500	1.01910900
C	-4.07288900	-1.23920300	0.37834100
C	-2.44680700	-1.99472500	1.99604000
C	-3.75915900	-1.64887300	1.67165500
F	-0.20294500	-2.22877200	1.36962600
F	-2.14523800	-2.37607800	3.24022700
F	-4.71051700	-1.70639900	2.60312600
F	-5.32647400	-0.89653100	0.07280600
F	-3.40140500	-0.75692300	-1.81045300
C	1.12446300	-2.72228000	-3.08462100
H	1.83767800	-3.54382600	-3.19735200
H	0.32588800	-2.83892000	-3.82335300

H	1.65702000	-1.78529000	-3.27574600
C	-0.24173600	-4.04074000	-1.40562400
H	-0.61909800	-4.08974200	-0.38282400
H	-1.07922500	-4.11624100	-2.10617400
H	0.42878700	-4.89160200	-1.54270600
S	-0.50934900	-1.22990900	-1.53923400
O	-3.77774500	4.13458200	-0.72755300
C	-3.97616300	4.97657200	-1.85132100
H	-4.91040300	5.51039300	-1.66869800
H	-3.16187800	5.70547900	-1.96368100
H	-4.06725800	4.39917200	-2.78137100
H	-1.35928200	1.02918200	1.41783200
O	4.90980600	0.24822000	-0.10876500
H	0.57849900	2.69281400	2.35692200

TS8

C	-2.23672600	2.42254300	0.31818100
C	-2.41569400	3.02245100	-0.93839200
C	-1.37749800	2.97860000	-1.88135900
C	-0.18645000	2.31963600	-1.56841000
C	-0.01675200	1.66959900	-0.33738900
C	-1.04973000	1.76259500	0.61334200
Pd	1.15272800	-0.06055200	-0.34879000
H	0.61644000	2.29654400	-2.30095400
H	-1.48380100	3.44832800	-2.85203600
H	-3.04395600	2.48583400	1.04105100
C	2.81837900	0.95344400	0.46128600
C	3.13255300	0.56730800	1.90689400
C	1.71592000	2.34091600	1.99618500
C	1.92445300	2.06774700	0.51726900
C	1.80326100	0.92425100	2.60930100
H	1.89224400	0.94411300	3.69986300
H	0.97915800	0.26261500	2.32910700
C	4.05163000	1.70811500	2.43778000
H	4.41085100	1.46503400	3.44255400
H	4.92685800	1.85588100	1.80048600
C	3.08987300	2.93909300	2.46086500
H	2.98003400	3.34784500	3.46970200
H	3.42326800	3.75564200	1.81319400
H	3.51182700	-0.44501100	2.03069200
H	2.01778000	2.87864100	-0.19392100

C	3.79724400	0.84733900	-0.65361500
O	3.67662100	1.39626700	-1.73760200
C	5.77887000	-0.19568400	-1.37696200
H	6.20615800	0.73822100	-1.75183400
H	6.55002300	-0.82453200	-0.93324400
H	5.28546500	-0.71892400	-2.20001000
C	0.26654400	-3.03780600	-1.30256300
C	1.54251400	-3.00264300	-0.39221500
O	2.15473900	-1.87094300	-0.22460700
O	1.94064100	-4.08887800	0.00813400
C	-1.88598900	-1.32279600	-0.18353800
C	-3.15626300	-0.88750000	-0.57543700
C	-1.67423800	-1.55866500	1.17902100
C	-4.17680900	-0.68987900	0.35205400
C	-2.68161500	-1.37503000	2.11902600
C	-3.93877400	-0.93790000	1.70153500
F	-0.46632000	-1.94139200	1.61712600
F	-2.44939000	-1.59699300	3.41625500
F	-4.90905300	-0.75107600	2.59693800
F	-5.37672700	-0.25847800	-0.04546700
F	-3.41279500	-0.60619800	-1.85654300
C	0.76197400	-3.26988000	-2.74320900
H	1.35646900	-4.18798200	-2.74518200
H	-0.07336500	-3.38187700	-3.44083900
H	1.40432800	-2.45121400	-3.08291100
C	-0.70955100	-4.12596500	-0.86827400
H	-1.04650600	-3.97892700	0.15924400
H	-1.57853500	-4.17286000	-1.53192300
H	-0.17321500	-5.07633900	-0.89889500
S	-0.58856100	-1.34883600	-1.40498100
O	-3.61965400	3.62716700	-1.13472500
C	-3.87558300	4.22671500	-2.39725400
H	-4.88905100	4.62647100	-2.34048900
H	-3.17544300	5.04639000	-2.60563900
H	-3.82116800	3.49207300	-3.21121700
H	-0.93617300	1.29803100	1.58783800
O	4.83777100	0.06323400	-0.32145800
H	0.85015100	2.95559500	2.24197700

int14

C	-1.46332100	-2.46973000	0.39045700

C	-1.63216500	-2.04836400	1.73184200
C	-0.52864600	-1.64341400	2.47199900
C	0.75084000	-1.62688500	1.86741200
C	0.93448300	-2.04023600	0.52285800
C	-0.21966800	-2.46198100	-0.19857300
Pd	1.09939300	0.26115000	0.38370500
H	1.62758200	-1.42859200	2.47835700
H	-0.62374400	-1.32857300	3.50341000
H	-2.34468400	-2.78717200	-0.15703500
C	2.86357700	-0.67501500	-0.14079500
C	3.24261600	-0.47727100	-1.61151500
C	2.52628700	-2.63137800	-1.48767700
C	2.36542800	-2.13790300	-0.03153100
C	2.20049100	-1.36944600	-2.32324000
H	2.41833300	-1.50329800	-3.38798000
H	1.17662500	-1.00128900	-2.22099600
C	4.54054500	-1.29596700	-1.85977800
H	4.93094100	-1.07704300	-2.85901800
H	5.32827800	-1.05058600	-1.14348000
C	4.04804500	-2.77660900	-1.75330200
H	4.21692400	-3.31995900	-2.68808400
H	4.55109700	-3.33486900	-0.95699200
H	3.28752800	0.56814500	-1.91147200
H	2.96846900	-2.72989400	0.66501300
C	3.77182200	-0.20156400	0.93582700
O	3.81952600	-0.66449500	2.06949400
C	5.36284100	1.42405600	1.55403400
H	6.04501800	0.68444700	1.98212800
H	5.91808200	2.21919500	1.05691700
H	4.74146000	1.83516100	2.35480800
C	-0.43060900	3.11568500	0.16990500
C	0.75481900	2.92785800	-0.83243200
O	1.62525900	1.99073100	-0.58722700
O	0.86061400	3.75837800	-1.72370900
C	-2.21572200	0.78817700	-0.11051900
C	-3.45455200	0.44959600	0.44340100
C	-1.99122700	0.44411900	-1.44857300
C	-4.41961100	-0.23991500	-0.28543600
C	-2.94705700	-0.23015000	-2.19922700
C	-4.16531300	-0.57624600	-1.61265000
F	-0.82279900	0.73487700	-2.03426400

F	-2.70136300	-0.56396700	-3.46921400
F	-5.08248000	-1.23297000	-2.32347800
F	-5.58200300	-0.57431400	0.28047500
F	-3.73402800	0.75090600	1.71823900
C	0.12593000	3.91693300	1.36259300
H	0.53795800	4.85339900	0.97477900
H	-0.65789500	4.14788800	2.09016400
H	0.93518300	3.37595900	1.86275500
C	-1.61656500	3.82137700	-0.47765800
H	-2.00738900	3.25491100	-1.32559000
H	-2.42109600	3.98896800	0.24497700
H	-1.26488500	4.77940100	-0.86489800
S	-0.96669900	1.47896600	0.95569300
O	4.54166500	0.83275700	0.53625800
H	1.95872500	-3.53792000	-1.71564800
H	-0.11620300	-2.78673200	-1.22722600
O	-2.91571700	-2.07146500	2.17712900
C	-3.17881700	-1.61675700	3.50194300
H	-2.85666500	-0.57810500	3.63324000
H	-4.26024800	-1.67627900	3.62639200
H	-2.68770400	-2.25536400	4.24638400

int15

C	-4.19690900	0.03942000	1.34471700
C	-4.44530400	-0.44459600	0.04037200
C	-3.81676300	0.14317400	-1.05659000
C	-2.93168200	1.20684000	-0.84959600
C	-2.66513200	1.71316100	0.45202900
C	-3.32868600	1.09038600	1.54710900
Pd	-0.67762300	0.62124000	0.16803700
H	-2.50455700	1.72232500	-1.70443500
H	-3.98028800	-0.21714300	-2.06315000
H	-4.69493900	-0.44936300	2.17510600
C	-0.41389300	2.65414000	0.18053700
C	0.43519300	3.10346800	1.37654600
C	-1.69080000	3.64407500	1.96374800
C	-1.86952800	3.02925800	0.55679000
C	-0.52188400	2.82530300	2.55908400
H	-0.15392900	3.23763200	3.50445200
H	-0.73945500	1.76282700	2.70403100
C	0.45228800	4.65809500	1.37700400

H	1.16901000	5.01900600	2.12199400
H	0.75518600	5.06844300	0.41081600
C	-1.01485100	5.02653300	1.77256700
H	-1.04306000	5.59315900	2.70821200
H	-1.52079800	5.62852000	1.01103800
H	1.41778800	2.63932500	1.41776200
H	-2.30674600	3.75126500	-0.14015800
C	0.00874700	2.99640300	-1.20655600
O	-0.74561400	3.08585800	-2.16422600
C	3.68661300	0.56471100	-0.68800300
C	2.17973500	0.36157400	-0.93084600
O	1.44686900	0.44536300	0.10184500
O	1.79589900	0.08474000	-2.10557500
C	3.01385300	-1.80893800	0.81594900
C	2.65639800	-1.38361200	2.10093400
C	2.19326400	-2.77123400	0.21265800
C	1.52894000	-1.87424300	2.74969600
C	1.08986900	-3.30605600	0.86644200
C	0.74868300	-2.84749100	2.13364100
F	2.41943200	-3.17716200	-1.04551900
F	0.31532100	-4.21227500	0.25192900
F	-0.33762500	-3.31920400	2.74965100
F	1.16950300	-1.39220600	3.94718100
F	3.36627000	-0.43750600	2.72851000
C	4.45163100	0.83467800	-1.98798100
H	4.17487000	1.81911300	-2.37481100
H	5.53031100	0.84109000	-1.80064900
H	4.21928500	0.08717800	-2.74624100
C	3.94081900	1.66161900	0.35027800
H	3.47109200	1.41884800	1.30105700
H	5.01541400	1.78529600	0.50957800
H	3.52129400	2.60568000	-0.01368000
S	4.37631400	-1.10405500	-0.07581700
Ag	-0.02825600	-1.06509100	-2.16327400
O	-1.34128000	-1.46403200	0.50138500
C	-1.80959400	-2.32716200	-0.29937600
O	-1.65212300	-2.33003000	-1.56559900
C	-2.62745200	-3.45129800	0.30676600
H	-3.56912900	-3.04643200	0.68537300
H	-2.82867400	-4.22680400	-0.43281700
H	-2.07907400	-3.86869000	1.15117300

H	-3.14894500	1.44693100	2.55490500
O	-5.29797400	-1.49557300	-0.03610000
C	-5.48551800	-2.11830400	-1.30888200
H	-6.13191100	-2.97702300	-1.12572300
H	-5.97698100	-1.43753500	-2.01440000
H	-4.52911100	-2.45538900	-1.72494800
H	-2.61287400	3.68673800	2.54923800
O	1.34344300	3.19585800	-1.31410400
C	1.82578200	3.43235300	-2.65056600
H	2.85442300	3.77383700	-2.53302000
H	1.79355500	2.49997200	-3.21962200
H	1.22310100	4.19249300	-3.15144200

TS9

C	4.01795400	2.79127900	0.27681900
C	3.23281800	2.85935000	-0.88762300
C	2.29904200	1.85544100	-1.13955200
C	2.13243100	0.79165800	-0.22494900
C	2.90229000	0.75025300	0.96167800
C	3.84921500	1.75605900	1.18840800
Pd	0.27840100	-0.05857800	0.11130700
H	2.10892700	-0.33834400	-0.99757600
H	1.70449800	1.86434000	-2.04538000
H	4.75027700	3.57456900	0.44529900
C	1.28360700	-1.08112100	1.61123600
C	0.45216000	-0.95028900	2.89940600
C	2.39792700	0.09336600	3.40925600
C	2.63609900	-0.36703000	1.93634000
C	0.89486900	0.43583000	3.41803300
H	0.51121200	0.65143000	4.42086300
H	0.62778000	1.26271300	2.75459200
C	1.10005000	-1.88532000	3.96538100
H	0.43817200	-1.94733900	4.83526200
H	1.24354200	-2.90540400	3.59896000
C	2.43794900	-1.16059900	4.31337000
H	2.46780900	-0.87159400	5.36863700
H	3.31757000	-1.78130100	4.11652600
H	-0.61342800	-1.12070400	2.75646100
H	3.45970200	-1.08915000	1.89202700
C	1.44941200	-2.46373100	1.04277100
O	2.50735700	-2.93247500	0.66174600

C	-4.06235700	-0.89033400	0.43897400
C	-2.62558400	-1.03853800	-0.08807600
O	-1.70995300	-0.63182400	0.68662700
O	-2.47324400	-1.49535600	-1.25871700
C	-3.11118100	1.78657800	-0.04727300
C	-2.55077600	2.27252300	1.14172900
C	-2.40001700	2.02072800	-1.23304200
C	-1.35083300	2.97601300	1.15434900
C	-1.20062900	2.73227000	-1.23802200
C	-0.68346200	3.22634700	-0.04237800
F	-2.83564100	1.54512100	-2.40158300
F	-0.53971800	2.93407900	-2.39054500
F	0.45610000	3.91801400	-0.03541100
F	-0.80847200	3.38205200	2.30887900
F	-3.13621800	2.03309900	2.31911800
C	-5.03428500	-1.84690100	-0.25830700
H	-4.79208900	-2.87557600	0.02946600
H	-6.06378900	-1.64473400	0.05420300
H	-4.96015600	-1.76455800	-1.34243500
C	-4.12190500	-1.03362700	1.96230700
H	-3.47113600	-0.31321400	2.45312100
H	-5.14680600	-0.88374000	2.31198600
H	-3.80088800	-2.04278300	2.24641000
S	-4.62494300	0.85651100	-0.07850300
Ag	-0.51977900	-2.00085500	-1.94030400
O	2.69615900	-1.10335700	-1.91064700
C	2.47699200	-2.31049100	-2.23718800
O	1.34084400	-2.84832100	-2.42596800
C	3.68761100	-3.20134700	-2.40969400
H	4.53225000	-2.62492700	-2.79070000
H	3.94406300	-3.57150000	-1.41171900
H	3.46420600	-4.04773800	-3.06049200
H	4.45942100	1.74046200	2.08715800
O	3.46290100	3.93557100	-1.69027000
C	2.62221000	4.10966700	-2.82490800
H	2.93250700	5.04785000	-3.28736600
H	2.74684600	3.29332700	-3.54891300
H	1.56814700	4.17259900	-2.53295600
H	3.07495500	0.88931700	3.72614600
O	0.28997600	-3.16066200	1.01327700
C	0.39475600	-4.49516900	0.47616600

H	-0.62143700	-4.88903800	0.48079500
H	0.79791400	-4.46453300	-0.53899700
H	1.04724500	-5.10692300	1.10507500

int16

C	4.71620000	0.98733100	0.98571200
C	3.71433600	1.95832800	0.84427900
C	2.36925900	1.57906600	0.77659800
C	2.02213700	0.22136000	0.83143100
C	3.02833700	-0.75610500	0.92575700
C	4.36811900	-0.35879700	1.02006100
Pd	0.15044600	-0.38358400	0.64405400
H	2.50349700	-0.93200200	-2.03890500
H	1.60415000	2.33128200	0.65062600
H	5.75084500	1.31037600	1.03694100
C	1.06419000	-2.25435600	0.46102500
C	0.46243100	-3.17944900	1.53372800
C	2.64675900	-3.02988100	2.12674000
C	2.58728200	-2.18468100	0.81678400
C	1.27554400	-2.75353500	2.77763300
H	1.08282500	-3.38948700	3.64834200
H	1.12583600	-1.70699500	3.05704600
C	1.00557000	-4.62160900	1.30141400
H	0.45104100	-5.32651300	1.92945000
H	0.88160900	-4.94808800	0.26611400
C	2.50171000	-4.51964400	1.74146200
H	2.70413200	-5.16190300	2.60469800
H	3.19685200	-4.81093000	0.94696600
H	-0.62464700	-3.12581100	1.60052000
H	3.17820000	-2.68341100	0.03591300
C	0.75062800	-2.51211300	-0.96418900
O	1.42583800	-2.13037400	-1.93570200
C	-4.10877600	-0.88872000	-0.63537700
C	-2.57687200	-0.75340900	-0.72613400
O	-1.93172200	-0.96202800	0.33729100
O	-2.10611000	-0.36925800	-1.84162000
C	-3.33079700	1.56380800	0.61677000
C	-3.06410200	1.25907900	1.95896300
C	-2.37895800	2.33346400	-0.06652000
C	-1.90072800	1.68324800	2.59327600
C	-1.20889300	2.76948500	0.55257700

C	-0.97242100	2.44977800	1.88948300
F	-2.53609600	2.64071100	-1.35841200
F	-0.30327600	3.48721300	-0.13284700
F	0.13172900	2.88645100	2.49958700
F	-1.64782000	1.33925000	3.85954100
F	-3.90089900	0.49156400	2.66159800
C	-4.73895900	-1.25367800	-1.98212100
H	-4.45018500	-2.27739900	-2.24586200
H	-5.83139000	-1.22150000	-1.91999300
H	-4.39912200	-0.58224400	-2.77027100
C	-4.53620700	-1.85166900	0.47341000
H	-4.12878500	-1.55154200	1.43644200
H	-5.62694800	-1.88746900	0.54175500
H	-4.16814400	-2.85808500	0.24169200
S	-4.73189500	0.87966300	-0.24010500
Ag	-0.12406600	0.44049200	-2.10377700
O	3.27006200	-0.29876100	-2.21061300
C	2.93290500	0.92686600	-2.50304200
O	1.76756600	1.33955700	-2.64925800
C	4.09124700	1.87255000	-2.66069500
H	4.21715300	2.41955200	-1.72089500
H	5.01295500	1.33023900	-2.87226800
H	3.86847600	2.59168000	-3.45059400
H	5.15143700	-1.11045000	1.08939700
O	4.14880000	3.25579200	0.72961200
C	3.16245500	4.27544400	0.63630900
H	3.70694200	5.22093200	0.61072500
H	2.56217800	4.17829200	-0.27858000
H	2.48648100	4.26599500	1.50105500
H	3.52755900	-2.80316900	2.73266000
O	-0.37264300	-3.21793300	-1.14786200
C	-0.82114400	-3.39654600	-2.50573900
H	-1.64343100	-4.10930500	-2.44299000
H	-1.17694600	-2.44350500	-2.90371700
H	-0.01623100	-3.78775700	-3.13112200

int17

C	0.18513700	-1.25838400	4.34273700
C	0.59263600	-0.05103800	3.76043300
C	0.32573000	0.20155900	2.40606300
C	-0.33702200	-0.75636200	1.63345300

C	-0.76888300	-1.97079300	2.21592700
C	-0.49497200	-2.20134900	3.56483600
Pd	-0.81207000	-0.43284400	-0.27389000
H	0.65672900	1.14161200	1.98223000
C	-1.63287200	-2.37483000	-0.12873900
C	-3.14805300	-2.40972900	-0.42511000
C	-3.02959100	-3.09209700	1.72895800
C	-1.52809900	-2.92251000	1.34032200
C	-3.71515300	-1.95781700	0.93746500
H	-4.80892200	-2.00580400	0.98445900
H	-3.38551400	-0.95642100	1.22748900
C	-3.63970700	-3.88385800	-0.48644700
H	-4.66508100	-3.92102600	-0.87082200
H	-3.02510900	-4.49519900	-1.15145900
C	-3.57707800	-4.34265300	1.00573100
H	-4.57277200	-4.59933400	1.38268900
H	-2.93591000	-5.21819200	1.15348700
H	-3.44495000	-1.82417000	-1.29468200
H	-1.03437000	-3.90341600	1.35188200
C	-0.71266400	-3.03144400	-1.07854400
O	0.44091000	-3.42948600	-0.82547100
C	-0.28845500	-3.61881300	-3.33120900
H	0.56118800	-2.93447300	-3.41680200
H	0.08460000	-4.61547300	-3.08474700
H	-0.85836300	-3.64055700	-4.26019700
C	2.17652700	2.81898600	-0.93980100
C	1.50222800	1.43855600	-0.76984800
O	2.22313600	0.42810300	-1.01092000
O	0.28883100	1.43785600	-0.39840400
C	4.48344500	1.78548500	0.40121700
C	4.27858300	0.53577500	0.99571300
C	5.62951500	1.92954300	-0.39155000
C	5.11907000	-0.54218700	0.75262000
C	6.50445300	0.86838200	-0.62048500
C	6.23732500	-0.37933500	-0.06013000
F	5.89996500	3.09337800	-0.99214700
F	7.58407000	1.03212100	-1.39401100
F	7.04664400	-1.41223300	-0.30308200
F	4.81164100	-1.75702500	1.24553600
F	3.21129500	0.31166100	1.77406700
C	2.98312400	2.86175100	-2.23949800

H	2.29581000	2.77019700	-3.08914300
H	3.52748500	3.80459200	-2.32690100
H	3.68501600	2.02945000	-2.29214500
C	1.16997100	3.97144200	-0.86624800
H	0.61173600	3.95824200	0.07197400
H	1.67903200	4.93383800	-0.97291400
H	0.45019900	3.86745900	-1.68385400
S	3.28796800	3.08867700	0.57432400
Ag	1.72746700	-1.56683700	-0.01682400
C	-3.78290000	2.80437900	0.22546400
C	-5.11658400	2.37642800	0.22253000
C	-5.53802800	1.40964900	-0.69901500
C	-4.63322300	0.86858500	-1.61243000
C	-3.31269500	1.31245000	-1.58509800
C	-2.86468600	2.27567100	-0.67993300
H	-3.47348300	3.54677200	0.95336900
H	-6.56974400	1.07796200	-0.69808100
H	-4.95241800	0.10847000	-2.31596100
H	-1.82282500	2.57376200	-0.65234800
I	-1.87648700	0.38672500	-2.90422400
C	-6.04245500	2.97872600	1.22502700
O	-5.72130800	3.83048300	2.02998000
O	-7.29235900	2.47061100	1.14125700
C	-8.23322600	3.00999000	2.08462700
H	-7.89965400	2.82346600	3.10887600
H	-8.34350100	4.08849300	1.94314600
H	-9.17472100	2.49765500	1.88701800
H	-0.81831500	-3.13214300	4.02597700
H	0.38444600	-1.47291900	5.38585200
O	1.26109300	0.94375200	4.41976400
C	1.56677000	0.75115000	5.78989000
H	2.09374700	1.65097300	6.11205500
H	0.65928200	0.62934100	6.39735800
H	2.21731100	-0.12094300	5.94398600
O	-1.20699800	-3.15303800	-2.32804300
H	-3.18837200	-3.09451200	2.81045400
TS10			
C	0.41178100	0.92747500	4.00132300
C	0.44648100	1.81265500	2.91461600
C	-0.02115500	1.39976600	1.65936200

C	-0.51672600	0.10980200	1.49769500
C	-0.59901400	-0.77937600	2.58588300
C	-0.11678300	-0.35428300	3.82635400
Pd	-1.08936500	-0.53649200	-0.30808100
H	0.05012300	2.09489600	0.83261800
C	-1.69780300	-2.28091600	0.85454400
C	-3.20809000	-2.56165500	0.94639000
C	-2.62601500	-2.23484000	3.10629100
C	-1.26280800	-2.10187100	2.35787800
C	-3.61178500	-1.61245900	2.09473400
H	-4.65985700	-1.72222800	2.39401300
H	-3.40574400	-0.56136500	1.88174000
C	-3.45322500	-3.95000900	1.60940700
H	-4.51327000	-4.20950500	1.51745200
H	-2.88733300	-4.75119500	1.13071900
C	-3.05415000	-3.71645100	3.09921000
H	-3.90537200	-3.87648100	3.76890100
H	-2.24865400	-4.38006500	3.43135300
H	-3.72323500	-2.46685900	-0.00820500
H	-0.59187100	-2.91796500	2.65632700
C	-0.89355000	-3.26960400	0.10721100
O	0.33485500	-3.47793100	0.26107700
C	-0.81308200	-4.78826700	-1.70511000
H	-0.14481200	-4.15179600	-2.29181000
H	-0.22734600	-5.53483100	-1.16508900
H	-1.55097900	-5.26240100	-2.35067100
C	2.26697300	2.24944200	-1.87268000
C	1.54423200	0.95335700	-1.44582800
O	2.29724300	-0.06092500	-1.28799300
O	0.29932200	1.00976900	-1.27173700
C	4.31282700	1.68328000	0.05617300
C	4.01422400	0.61014700	0.90399000
C	5.58598000	1.69378000	-0.52831100
C	4.90160100	-0.43858900	1.10685600
C	6.50266000	0.66529700	-0.31452200
C	6.15230300	-0.41355100	0.49501200
F	5.95097400	2.68732200	-1.34517000
F	7.70710200	0.69597500	-0.89656200
F	7.01031300	-1.41863300	0.68150500
F	4.53240300	-1.49787900	1.84718000
F	2.82272100	0.52368700	1.50935000

C	3.28197900	1.96902000	-2.98224800
H	2.74742100	1.63642100	-3.87983800
H	3.84800000	2.87148200	-3.22329800
H	3.97070600	1.17439300	-2.69437600
C	1.28198300	3.35152400	-2.27361600
H	0.58920600	3.58735000	-1.46283900
H	1.81964900	4.25896100	-2.56229700
H	0.69128200	3.00904900	-3.12843500
S	3.10249700	2.93125800	-0.31070600
Ag	1.56403000	-1.70442100	-0.13930300
C	-3.35085900	2.89585200	-0.89592800
C	-4.61063600	2.59163600	-0.36310300
C	-5.00606800	1.25133200	-0.25395000
C	-4.14726200	0.22717800	-0.64576700
C	-2.86814700	0.55861900	-1.09413600
C	-2.47915800	1.88706200	-1.29771700
H	-3.06514100	3.93752800	-1.00074000
H	-5.99195000	1.00768600	0.12555400
H	-4.46861600	-0.80151600	-0.58976400
H	-1.50893700	2.12408300	-1.71012200
I	-2.03060500	-1.08234700	-2.86119300
C	-5.49044900	3.72151900	0.03584200
O	-5.19530400	4.89686400	-0.06972500
O	-6.67550000	3.30104300	0.53948400
C	-7.56852000	4.34985700	0.94471900
H	-7.10993300	4.96741400	1.72182900
H	-7.82244200	4.99008300	0.09533700
H	-8.45800900	3.84880800	1.32707700
H	-0.16213200	-1.02849000	4.67885700
H	0.77979900	1.22341300	4.97629800
O	0.93115000	3.08842600	2.96620100
C	1.47847100	3.55044500	4.18935100
H	1.81963600	4.56984700	4.00159800
H	0.72925100	3.56437900	4.99282400
H	2.33260100	2.93800600	4.50949300
O	-1.57624000	-3.97831800	-0.79049200
H	-2.60162500	-1.77716300	4.09816400
int18			
C	0.54105700	-0.02556800	4.37702300
C	0.74627000	1.05045700	3.50192700

C	0.21901300	1.00719000	2.20373400
C	-0.49853900	-0.10717200	1.78479900
C	-0.72791900	-1.18793100	2.64954500
C	-0.18977500	-1.13043100	3.93908900
Pd	-1.05006400	-0.38621500	-0.14489600
H	0.43465200	1.83988400	1.54692600
C	-1.89610000	-2.23643100	0.63414700
C	-3.42640700	-2.40324100	0.62885100
C	-2.93023000	-2.48488500	2.83683900
C	-1.53049700	-2.35289300	2.16292000
C	-3.81484600	-1.62992800	1.91024700
H	-4.88218600	-1.70840200	2.14092900
H	-3.53162300	-0.57772400	1.89253200
C	-3.82074000	-3.85350600	1.05276100
H	-4.89654300	-3.97681900	0.89146300
H	-3.32011600	-4.62414000	0.46807100
C	-3.47033600	-3.90439500	2.57221700
H	-4.35870700	-4.10123200	3.18068500
H	-2.73321600	-4.67864300	2.81197900
H	-3.90046100	-2.10091900	-0.30170800
H	-0.95319600	-3.27117100	2.33015400
C	-1.07927100	-3.16951500	-0.19653700
O	0.16332400	-3.30631200	-0.06715600
C	-0.97388800	-4.70008600	-1.99782900
H	-0.37751200	-4.03997100	-2.63083900
H	-0.33135300	-5.39386000	-1.45233700
H	-1.71490600	-5.23278500	-2.59110700
C	2.01920500	2.69104800	-1.30012500
C	1.32754500	1.33812000	-1.04799600
O	2.07056900	0.31294000	-1.17186100
O	0.11245400	1.36599100	-0.71326900
C	4.27668400	1.73896100	0.18635000
C	4.06254500	0.50431800	0.81117900
C	5.45949500	1.87795000	-0.55225200
C	4.93605000	-0.56301200	0.65122200
C	6.36588100	0.82829200	-0.69730900
C	6.09441800	-0.40335500	-0.10495200
F	5.73836200	3.02470000	-1.18017100
F	7.48053900	0.98774400	-1.41916600
F	6.93646200	-1.42591400	-0.26471800
F	4.63340100	-1.76328300	1.17766400

F	2.95979100	0.27966300	1.53813400
C	2.87778600	2.63480400	-2.56453800
H	2.22385900	2.48900200	-3.43180900
H	3.43246600	3.56702300	-2.69042900
H	3.57621900	1.79839800	-2.53344000
C	1.01799200	3.84862800	-1.34713000
H	0.42828300	3.91231100	-0.43055600
H	1.54016000	4.79528400	-1.51121600
H	0.32133100	3.68102800	-2.17323500
S	3.06118600	3.03496600	0.25063600
Ag	1.45357500	-1.60329600	-0.49153200
C	-3.70472000	2.87356700	0.69922900
C	-4.83132400	2.59113600	-0.08006500
C	-4.86664700	1.41149700	-0.83372700
C	-3.79541700	0.51759300	-0.80075100
C	-2.68918000	0.81426300	-0.00522800
C	-2.62479100	1.99045600	0.73995400
H	-3.68385200	3.79163700	1.27756300
H	-5.72397600	1.19519900	-1.46111200
H	-3.82372800	-0.36752700	-1.41968700
H	-1.76525400	2.23195400	1.34678700
I	-1.20333800	-0.96558200	-2.91513400
C	-5.94633200	3.57727300	-0.07957600
O	-5.95145800	4.61285100	0.55834400
O	-6.97293100	3.19706200	-0.87585500
C	-8.07635300	4.11450400	-0.92381900
H	-8.50573900	4.25378200	0.07215100
H	-7.75213800	5.08760100	-1.30286600
H	-8.80554500	3.66396200	-1.59736100
H	-0.35053900	-1.96372900	4.61941800
H	0.94046100	-0.01424600	5.38379000
O	1.45116000	2.17731500	3.80581000
C	2.06893400	2.26313300	5.08013500
H	2.59109000	3.22097100	5.09748500
H	1.33073800	2.24152000	5.89319100
H	2.79473800	1.45321600	5.23411000
O	-1.74381100	-3.89611300	-1.07332200
H	-2.90933500	-2.19556600	3.89035000
int19			
C	3.55046200	-2.08613100	-3.35815000

C	2.27915500	-1.57254000	-3.66494600
C	1.45093800	-1.09569100	-2.63793400
C	1.94191800	-1.15391800	-1.33778400
C	3.19126100	-1.65914300	-0.98696300
C	3.99077700	-2.13096100	-2.04135000
Pd	0.78276600	-0.65376700	0.18225900
H	0.45608500	-0.71333800	-2.82434900
C	2.50071200	-0.96506800	1.32777500
C	3.25323700	0.23731600	1.95224500
C	4.86323900	-0.84375100	0.78153200
C	3.59124700	-1.67992800	0.46439200
C	4.28109800	0.58158800	0.85524700
H	5.00774600	1.33110000	1.18580300
H	3.82730300	0.91433000	-0.07909000
C	4.19204400	-0.32054400	3.06030200
H	4.63468100	0.52076100	3.60332300
H	3.67519300	-0.94396700	3.79419500
C	5.27137100	-1.10734100	2.24990100
H	6.27607700	-0.72164100	2.44850800
H	5.27187800	-2.17487700	2.48960600
H	2.60242800	1.04007900	2.29517700
H	3.70537300	-2.71539800	0.80349500
C	1.81751600	-1.84054000	2.34978600
O	2.15658200	-2.94496800	2.70643200
C	-0.16732600	-1.99641700	3.65241100
H	-0.95629700	-1.32015700	3.97459200
H	-0.58181300	-2.80959200	3.05302200
H	0.38263200	-2.39979200	4.50477000
C	-2.44888200	-3.06349800	-0.54993100
C	-1.19128300	-2.21346900	-0.37984400
O	-1.18682700	-1.02624700	-0.84462100
O	-0.19760700	-2.66972500	0.26751600
C	-3.85251800	-0.87139800	0.65432000
C	-3.02676300	0.10901900	1.21880000
C	-4.94770700	-0.42578200	-0.09726700
C	-3.27939300	1.46658600	1.06453600
C	-5.21214000	0.93054500	-0.27657900
C	-4.37634500	1.87830300	0.30990600
F	-5.77064300	-1.30139300	-0.68377900
F	-6.26228400	1.32815600	-1.00317100
F	-4.62635200	3.17820700	0.15164900

F	-2.48311200	2.37944800	1.63411700
F	-1.93684900	-0.23930300	1.92588700
C	-3.14544900	-2.77570000	-1.88008300
H	-2.48826700	-3.08086200	-2.70284500
H	-4.08108000	-3.33485500	-1.94947600
H	-3.35069600	-1.71131000	-1.99657000
C	-2.15381400	-4.55479600	-0.36285300
H	-1.48593900	-4.88775800	-1.16326800
H	-1.65186100	-4.74595800	0.58698600
H	-3.07712200	-5.13876800	-0.41702800
S	-3.55589200	-2.60413800	0.91711900
C	1.56563600	3.38499900	-1.14355400
C	0.94141000	4.10380300	-0.11514300
C	0.37784300	3.41432800	0.96596100
C	0.44765500	2.02375200	1.02430600
C	1.06664600	1.31107200	-0.01076200
C	1.62840200	1.99170100	-1.09500100
H	2.00006900	3.91865300	-1.98165900
H	-0.11394900	3.98006600	1.74990900
H	-0.00016400	1.50557300	1.86799900
H	2.10945600	1.44838600	-1.89964800
C	0.84288700	5.58844800	-0.12050300
O	0.31240100	6.24908300	0.75227800
O	1.41478500	6.14188000	-1.21679700
C	1.34876600	7.57478400	-1.27729300
H	1.84780200	7.85443100	-2.20536700
H	0.30898500	7.91328500	-1.28215400
H	1.85611200	8.02114400	-0.41757700
O	0.71103300	-1.19897300	2.82781300
H	5.66569100	-1.00134900	0.05651200
H	4.97493100	-2.53662300	-1.82062200
O	1.93242900	-1.58477400	-4.98286600
C	0.65610800	-1.07588700	-5.34355100
H	0.54922900	-0.01844900	-5.06731700
H	0.58781700	-1.17363600	-6.42800700
H	-0.15533300	-1.64983000	-4.87636700
H	4.16858800	-2.44887100	-4.17233400
TS11			
C	4.77624800	-3.00273200	0.66565800
C	4.71679700	-2.42849800	-0.61614900

C	3.62543700	-1.63050800	-0.96571100
C	2.59089200	-1.42130700	-0.03896200
C	2.61173800	-2.04274400	1.22842000
C	3.72380000	-2.83095300	1.55380800
Pd	0.70082500	-0.73002700	-0.50299200
H	3.59039700	-1.12842100	-1.92380200
C	0.11460300	-1.77943300	1.20884300
C	-0.78233000	-0.92364500	2.09496400
C	1.11638300	-1.16284100	3.31582300
C	1.35649200	-2.07489100	2.06462500
C	0.23541700	-0.00345600	2.78905100
H	-0.21619200	0.57317800	3.60300900
H	0.72028700	0.68957500	2.10750000
C	-1.22268200	-1.82965900	3.29141100
H	-2.05165800	-1.33889400	3.80645600
H	-1.58082400	-2.80849900	2.96338300
C	0.06514600	-1.90840800	4.17891900
H	-0.08192900	-1.39110700	5.13216200
H	0.36151600	-2.93715700	4.40593300
H	-1.60208800	-0.46024000	1.56187100
H	1.27335700	-3.11961600	2.38919100
C	-0.47869900	-2.99161200	0.51599800
O	0.14847600	-3.99494300	0.23960600
C	-2.42994200	-3.84390700	-0.49998400
H	-3.46046800	-3.50748900	-0.60605200
H	-1.94139900	-3.91188900	-1.47420100
H	-2.37696600	-4.80767500	0.01300000
C	-2.77701300	-0.47236100	-2.84025100
C	-1.54906200	-0.80734700	-1.97307100
O	-1.28661000	-0.02090400	-0.99047300
O	-0.80549000	-1.76355700	-2.28497300
C	-4.21245400	0.56310500	-0.52029100
C	-3.96988300	0.12691900	0.78834800
C	-4.36548900	1.94245400	-0.71126500
C	-3.81405500	1.02155200	1.84267200
C	-4.20990100	2.85322000	0.33086100
C	-3.92457200	2.38987600	1.61288600
F	-4.65777800	2.43797000	-1.91997600
F	-4.34324400	4.16677000	0.11171400
F	-3.76771400	3.25354300	2.61915100
F	-3.53011400	0.57499900	3.07716400

F	-3.85463600	-1.17461700	1.06730300
C	-2.58312600	0.93016200	-3.43187500
H	-1.69269600	0.92197300	-4.07258700
H	-3.44604000	1.21910300	-4.03576700
H	-2.42820300	1.67161800	-2.64895700
C	-2.96897600	-1.51479700	-3.94932600
H	-2.07360600	-1.53435900	-4.57480500
H	-3.10186000	-2.51804600	-3.53876600
H	-3.83180400	-1.26033000	-4.57211100
S	-4.37406500	-0.61143900	-1.84358500
C	3.36401800	2.45508300	0.94638300
C	3.36992700	3.14394100	-0.27502900
C	2.83653600	2.52745400	-1.41418300
C	2.30294000	1.24503500	-1.33057700
C	2.24456500	0.58166400	-0.08947200
C	2.81504200	1.17914300	1.04098700
H	3.80369800	2.91817600	1.82250300
H	2.86053900	3.06086600	-2.35860300
H	1.93167900	0.77107400	-2.24029000
H	2.86077300	0.64156700	1.97838500
C	3.94723900	4.50601600	-0.42774700
O	3.98891700	5.12190600	-1.47599100
O	4.42902600	4.99648000	0.73766900
C	5.00051800	6.31195200	0.65352000
H	5.33926800	6.55108000	1.66158600
H	5.83904200	6.32325800	-0.04808500
H	4.25308900	7.03518800	0.31634600
O	-1.78617600	-2.82080900	0.28048500
H	2.03146900	-0.89113000	3.84814700
H	3.74759200	-3.34491600	2.51157700
O	5.77738100	-2.68929200	-1.42881400
C	5.75966800	-2.16064700	-2.74760100
H	5.75918500	-1.06229000	-2.74289300
H	6.67311100	-2.51594100	-3.22659200
H	4.89008300	-2.51916000	-3.31388500
H	5.64358600	-3.60124300	0.92294400

int20

C	1.12274200	-4.23124000	0.80074200
C	2.14035100	-4.27976100	-0.14907700
C	2.90179500	-3.12015100	-0.40094700

C	2.64662900	-1.91136900	0.24782100
C	1.55576900	-1.81326200	1.17294200
C	0.83324500	-3.02048700	1.44401200
Pd	-0.39891400	-1.62637100	-0.01593800
H	3.73203100	-3.15179900	-1.09555200
H	0.56427400	-5.13068100	1.03374500
C	-0.35604600	-0.32306000	1.55059300
C	-0.38859900	1.12403300	1.08127000
C	1.73206100	0.81252600	1.81510000
C	1.10114700	-0.58944000	2.02130700
C	1.03613000	1.32735800	0.53538700
H	1.25894500	2.37758200	0.32152900
H	1.24472500	0.73691000	-0.35788400
C	-0.33707700	2.00490700	2.36384500
H	-0.48462700	3.05232900	2.08813600
H	-1.11846000	1.74869400	3.08244900
C	1.11031300	1.74853800	2.88845800
H	1.68143300	2.67981100	2.94510100
H	1.12433300	1.29691800	3.88557400
H	-1.21712800	1.32383600	0.41395300
H	1.13117100	-0.88659100	3.07453100
C	-1.48673600	-0.81225300	2.41359100
O	-1.37625900	-1.67212000	3.27226800
C	-3.82060100	-0.70752500	2.75037800
H	-4.62142500	-0.04350500	2.43428600
H	-3.99172200	-1.72117900	2.38512300
H	-3.70913900	-0.70525300	3.83722500
C	-4.28489000	-1.17007100	-1.77495500
C	-3.13114200	-1.49589100	-0.79586200
O	-2.01128000	-0.89140800	-1.08130600
O	-3.30025200	-2.30398700	0.11794800
C	-3.77053800	1.67211400	-0.96152200
C	-3.82129900	2.30194600	0.29134200
C	-2.77552400	2.11061600	-1.84615800
C	-2.93851700	3.31943300	0.64310200
C	-1.86216100	3.10159200	-1.49916600
C	-1.95049000	3.71413600	-0.25207200
F	-2.67431600	1.59238200	-3.07461600
F	-0.89285200	3.46146700	-2.35089900
F	-1.04297700	4.62768000	0.11516100
F	-2.98474400	3.86881100	1.86437700

F	-4.74084200	1.95207500	1.20009800
C	-3.80291500	-1.25308500	-3.22821900
H	-3.48464500	-2.28186600	-3.43799200
H	-4.61480200	-0.99795200	-3.91518500
H	-2.96084400	-0.59025900	-3.40389700
C	-5.46469100	-2.12449000	-1.54065900
H	-5.14954400	-3.14153900	-1.79136200
H	-5.77623600	-2.11881700	-0.49614600
H	-6.31318500	-1.86077600	-2.18111100
S	-5.05281700	0.51991700	-1.39095700
C	5.58059500	0.46962000	0.56723900
C	5.51451500	1.16414400	-0.64867200
C	4.50879500	0.85171600	-1.57145400
C	3.57222800	-0.13546000	-1.27880300
C	3.61385000	-0.81356600	-0.05260000
C	4.63892900	-0.51353100	0.85729700
H	6.36696800	0.70331500	1.27549800
H	4.47727700	1.39528300	-2.50964500
H	2.78973900	-0.37470600	-1.99292200
H	4.68743900	-1.05094000	1.79991800
C	6.48565200	2.23534600	-1.01261700
O	6.47194400	2.84650000	-2.06329900
O	7.39418400	2.46048600	-0.03676100
C	8.35549300	3.48928900	-0.32546000
H	9.00123800	3.54332900	0.55094900
H	8.93510000	3.23501600	-1.21694900
H	7.85442200	4.44603700	-0.49523000
O	-2.63230300	-0.17996200	2.12230000
H	2.81810300	0.82612900	1.81813600
H	0.11021800	-3.01979400	2.25471900
O	2.34757700	-5.47423300	-0.75446200
C	3.37750300	-5.58271400	-1.73216000
H	4.36629000	-5.38398100	-1.29996800
H	3.34158800	-6.61277600	-2.08804000
H	3.20518300	-4.90206200	-2.57525000

TS12

C	3.63554600	-3.96997900	0.22804600
C	4.79338900	-3.22459200	-0.05771300
C	4.70682000	-1.83658000	-0.22057100
C	3.47047100	-1.17885600	-0.11631100

C	2.30562200	-1.93068000	0.16426700
C	2.41817800	-3.32481800	0.36773900
Pd	0.48112100	-1.31454700	-0.52894700
H	5.58211200	-1.24680600	-0.46571800
H	3.72674300	-5.04333300	0.35723500
C	-0.25790000	-1.19116300	1.40527200
C	-0.76439900	0.20982100	1.70969300
C	1.39964100	0.16887700	2.37124700
C	1.11108300	-1.22239400	1.83730200
C	0.49723800	1.07196600	1.50496500
H	0.38451200	2.07752600	1.92163700
H	0.81667000	1.15225800	0.46623200
C	-0.89617400	0.26588800	3.26113700
H	-1.36557100	1.20983900	3.55239800
H	-1.51438900	-0.54506800	3.65337600
C	0.59452400	0.19150200	3.72555800
H	0.88611300	1.07847900	4.29519500
H	0.80425100	-0.68242500	4.34949400
H	-1.64736300	0.46810400	1.14698900
H	1.49796200	-2.09141100	2.35201300
C	-1.12527900	-2.40551200	1.54491400
O	-0.69834400	-3.53337600	1.71217300
C	-3.36293000	-3.15788600	1.42713400
H	-4.34049900	-2.68644000	1.50346500
H	-3.24553000	-3.66108800	0.46593300
H	-3.19157200	-3.85644000	2.24926800
C	-3.21975200	-1.22103800	-2.75503400
C	-2.08254400	-1.63976400	-1.79140900
O	-1.23925600	-0.68953900	-1.51949300
O	-2.00808100	-2.80278300	-1.38606200
C	-3.86888100	0.76920100	-0.59307100
C	-4.28229100	0.61063200	0.73944600
C	-3.01819300	1.85076500	-0.86312700
C	-3.88369200	1.48499600	1.74788600
C	-2.58230200	2.71456300	0.13803000
C	-3.02570700	2.53709200	1.44583100
F	-2.59495200	2.09753300	-2.10614100
F	-1.71701300	3.69814300	-0.14138300
F	-2.55649200	3.31994200	2.42693300
F	-4.25321000	1.27407800	3.01856400
F	-5.09052100	-0.39830900	1.08974800

C	-2.67111200	-0.39341300	-3.92267700
H	-1.97264600	-1.01246600	-4.49929300
H	-3.48301100	-0.08316500	-4.58677000
H	-2.13982100	0.48465500	-3.56819700
C	-3.96463200	-2.46019000	-3.27162600
H	-3.27705800	-3.05358100	-3.88161800
H	-4.30776200	-3.08694800	-2.44865900
H	-4.81652800	-2.17341600	-3.89753700
S	-4.58670900	-0.28544600	-1.83014100
C	4.08385400	2.54568300	0.24880600
C	3.26943400	3.06712300	-0.76613700
C	2.55726100	2.19465500	-1.59857300
C	2.63916300	0.82001300	-1.40113800
C	3.42340200	0.28648300	-0.36241500
C	4.16541500	1.16862300	0.43822800
H	4.64109100	3.22164600	0.88701700
H	1.94481700	2.61120600	-2.39095500
H	2.10645200	0.15109400	-2.07270400
H	4.78455500	0.76478400	1.23421800
C	3.13234700	4.53111600	-1.01177300
O	2.45863400	5.01825900	-1.89802400
O	3.84552500	5.27075800	-0.13170600
C	3.74898200	6.69292900	-0.31620800
H	4.36874800	7.13411400	0.46440400
H	4.11465900	6.97773300	-1.30642300
H	2.71141500	7.02328000	-0.21853800
O	-2.41915300	-2.06653100	1.48760800
H	2.45049500	0.43576800	2.46728200
H	1.53304100	-3.88563100	0.65867300
O	5.94347100	-3.94039000	-0.15333900
C	7.15515700	-3.25006300	-0.43163500
H	7.39100200	-2.51677300	0.35042700
H	7.93502400	-4.01215300	-0.45722600
H	7.11476700	-2.74071900	-1.40304000

int21

C	2.33286000	-4.24201700	-0.60629300
C	3.66088500	-3.90331300	-0.90265500
C	4.04497100	-2.56107100	-0.92113000
C	3.10441400	-1.54571000	-0.65679400
C	1.78119300	-1.90001000	-0.35566700

C	1.40403400	-3.24523100	-0.32761500
Pd	0.37654400	-0.51158000	-0.09406300
H	5.06115800	-2.26993300	-1.15974300
H	2.05435300	-5.29062700	-0.59041500
C	0.16695900	-0.48330200	2.08769000
C	-0.59078600	0.74314900	2.59934700
C	1.53853400	1.41208900	2.18497000
C	1.46903200	-0.06060000	1.82414900
C	0.11221900	1.90015100	1.85341600
H	-0.11003300	2.87433500	2.30051200
H	-0.11235400	1.94336900	0.78725500
C	-0.00000400	0.94791600	4.03733000
H	-0.56176700	1.73171800	4.55380700
H	-0.06589100	0.04110300	4.64509500
C	1.47232400	1.39157200	3.75360800
H	1.67165500	2.39504300	4.14161700
H	2.21241800	0.71482400	4.19045100
H	-1.67534100	0.67455400	2.55026900
H	2.33065700	-0.71525000	1.85697500
C	-0.20646100	-1.87822100	2.46327300
O	0.55538400	-2.81910800	2.55730600
C	-2.05349300	-3.25471200	2.98386600
H	-3.12948100	-3.11498700	3.07875500
H	-1.82381400	-3.94947200	2.17158300
H	-1.62581600	-3.64161200	3.91288600
C	-2.23409100	0.47659000	-3.06310900
C	-1.23532300	0.23082300	-1.93479800
O	-1.38618100	0.80850200	-0.81874500
O	-0.27585400	-0.59870500	-2.11919800
C	-4.31289200	-0.10609500	-1.19316200
C	-3.85260100	-0.58864000	0.04073600
C	-5.30708200	0.88092800	-1.17006400
C	-4.35298700	-0.09961300	1.24327500
C	-5.81920100	1.38069400	0.02484700
C	-5.33533400	0.88851800	1.23378500
F	-5.78430700	1.39335600	-2.30953200
F	-6.76315800	2.32888400	0.01950600
F	-5.81266600	1.36137500	2.38746800
F	-3.89425600	-0.55141900	2.41984700
F	-2.90569600	-1.53284400	0.09328500
C	-2.70848100	1.93018400	-3.07101200

H	-1.86728500	2.58175600	-3.33427500
H	-3.50629400	2.06821100	-3.80378500
H	-3.06414100	2.23341100	-2.08591400
C	-1.67823400	0.04406900	-4.42358200
H	-0.80803500	0.66167300	-4.66666300
H	-1.35238000	-0.99745400	-4.41000700
H	-2.43064900	0.18389100	-5.20494800
S	-3.66719200	-0.71752400	-2.73169600
C	4.99108500	1.62261000	0.22107100
C	4.28931400	2.58586600	-0.51799500
C	3.23478900	2.18299600	-1.34972600
C	2.87174700	0.84265300	-1.42613400
C	3.54676900	-0.12662400	-0.66052900
C	4.62196200	0.28197600	0.14492900
H	5.81142800	1.93078400	0.85920200
H	2.71389800	2.93750500	-1.92969700
H	2.06897700	0.53308700	-2.08815500
H	5.14818700	-0.46053100	0.73804900
C	4.61782400	4.03613500	-0.46114600
O	4.02578100	4.90295000	-1.07569500
O	5.66051700	4.29972800	0.36246500
C	6.02326100	5.68588100	0.45734000
H	6.86517900	5.72408500	1.14883200
H	6.31137300	6.07685200	-0.52231100
H	5.18619500	6.27881600	0.83618600
O	-1.53099000	-1.95151900	2.68891700
H	2.37850800	1.96259400	1.76199600
H	0.38924500	-3.52565600	-0.06697000
O	4.49694800	-4.95392100	-1.15773200
C	5.85494400	-4.67160300	-1.45180100
H	6.35283200	-4.15491800	-0.61971800
H	6.33725000	-5.63730000	-1.61259900
H	5.95702900	-4.06264500	-2.36044300

int22

C	2.46822500	-1.35743900	-2.17268700
C	1.80554700	-2.56162000	-1.89040400
C	0.45725300	-2.53924700	-1.52408600
C	-0.22264900	-1.31803300	-1.35598400
C	0.45895600	-0.09193500	-1.55367400
C	1.79881900	-0.15289200	-1.99757300

H	-0.08143400	-3.46429800	-1.35780800
C	-0.09731500	2.04955500	2.56531000
C	0.01127100	3.40217900	1.77985000
O	0.24243700	4.38953900	2.46510000
O	-0.25789400	3.39895700	0.51223700
C	1.68995900	-0.08373500	1.41302200
C	2.82677800	0.68922500	1.15690500
C	1.85034800	-1.47135900	1.48231700
C	4.07855500	0.10982700	0.98388600
C	3.09016400	-2.07070900	1.28093900
C	4.20844900	-1.27828000	1.04033600
F	0.80041000	-2.27408100	1.70122700
F	3.20117800	-3.40448200	1.29801700
F	5.39872400	-1.84409500	0.84606800
F	5.14759600	0.86767900	0.72809000
F	2.71674200	2.01629200	1.02281900
C	0.92475100	1.95065000	3.69060300
H	0.75314900	2.80303100	4.35145600
H	0.81262900	1.02065900	4.25698300
H	1.94607400	2.03120400	3.31722900
C	-1.53857300	1.95392100	3.09968600
H	-2.27044500	1.95179700	2.28595200
H	-1.68264300	1.05858900	3.71200700
H	-1.71877300	2.84170900	3.71232600
S	0.02080500	0.55938600	1.38833500
C	-3.90820300	-0.47365800	-0.99980300
C	-4.30096000	-1.34365700	0.02618700
C	-3.35946200	-2.22100600	0.58083900
C	-2.04694900	-2.21983100	0.11880600
C	-1.63829300	-1.34352000	-0.90134800
C	-2.59568200	-0.47505500	-1.45631800
H	-4.64919200	0.19307500	-1.42779900
H	-3.65765200	-2.89055700	1.37945400
H	-1.31451800	-2.87062900	0.58325900
H	-2.31090900	0.19242300	-2.26161600
C	-5.71738900	-1.29171800	0.48088900
O	-6.56421000	-0.55337900	0.01514600
O	-5.97198800	-2.16499500	1.48391100
C	-7.32467800	-2.15638500	1.96651000
H	-8.02187000	-2.41364600	1.16440900
H	-7.35964100	-2.90298500	2.76008100

H	-7.58897100	-1.16884100	2.35443700
Pd	-0.05870900	1.66433800	-0.63168800
C	-0.82339800	3.47252500	-4.64528500
H	-0.13950200	3.32159400	-5.48503700
H	-0.74255000	4.48811600	-4.26142100
H	-1.83810800	3.28684400	-5.01041800
C	-0.50806700	2.49011100	-3.55654700
O	-0.24931900	2.85879100	-2.40391300
O	-0.53918400	1.22793700	-3.93728300
H	-0.26094700	0.65494500	-3.16885600
O	2.55846800	-3.69099700	-1.99561600
C	2.03645500	-4.89411500	-1.44255400
H	2.84015700	-5.62862800	-1.51087300
H	1.75904400	-4.75283600	-0.39081800
H	1.16864800	-5.25998300	-2.00600400
H	3.50672000	-1.39465300	-2.48607500
H	2.34665800	0.77192100	-2.16817600

TS13

C	2.29656000	0.84945700	2.43212600
C	1.73686300	2.10305500	2.12431100
C	0.39323900	2.19910600	1.73866700
C	-0.38610200	1.04458300	1.58308100
C	0.17356100	-0.24026900	1.84079000
C	1.51837400	-0.28550700	2.29440800
H	-0.05288300	3.16700500	1.54940500
C	0.17918400	-1.47289800	-2.80643000
C	0.24408100	-2.95025900	-2.30840700
O	0.54425000	-3.78991200	-3.14399200
O	-0.12706000	-3.21045600	-1.08917800
C	1.86565300	0.32043700	-1.13896400
C	2.95323100	-0.51924200	-0.87737000
C	2.09040400	1.70062100	-1.11709700
C	4.21658600	-0.01044800	-0.59564000
C	3.34626600	2.22764900	-0.83158800
C	4.41117300	1.37077800	-0.56893300
F	1.08930100	2.56497700	-1.34164100
F	3.52544900	3.55317600	-0.78884500
F	5.61312600	1.86893900	-0.28667100
F	5.23590200	-0.83127200	-0.33582300
F	2.78928700	-1.84586800	-0.87563700

C	1.29220100	-1.15959600	-3.79825700
H	1.18356400	-1.85631400	-4.63217200
H	1.22434300	-0.13209800	-4.16913900
H	2.27961700	-1.32553100	-3.36423600
C	-1.21387800	-1.26315600	-3.42913300
H	-2.01046600	-1.41877300	-2.69484000
H	-1.31377500	-0.26080200	-3.85617600
H	-1.33615400	-2.00593200	-4.22241900
S	0.19088800	-0.26404400	-1.34231200
C	-4.10571300	0.48297100	1.07679000
C	-4.39506000	1.41069200	0.06696700
C	-3.37023700	2.22383000	-0.43507700
C	-2.07944700	2.10801300	0.07051400
C	-1.77895600	1.17887600	1.08274600
C	-2.81420600	0.36435700	1.57675400
H	-4.91058300	-0.13613700	1.45839800
H	-3.58772900	2.93337800	-1.22507700
H	-1.28119200	2.70614900	-0.35617600
H	-2.60872300	-0.35468700	2.36102900
C	-5.79603000	1.48560200	-0.43281800
O	-6.71295300	0.80328000	-0.01809400
O	-5.94685600	2.40769100	-1.41258200
C	-7.27945200	2.52422800	-1.93613600
H	-7.98028900	2.80822700	-1.14638100
H	-7.22896700	3.29849400	-2.70183600
H	-7.60763200	1.57516400	-2.36874900
Pd	-0.13610400	-1.78527000	0.37336400
C	-1.47359800	-4.24203400	3.70836500
H	-1.14539200	-4.12413900	4.74308700
H	-1.10586700	-5.17592400	3.28420600
H	-2.56853000	-4.25125300	3.70336900
C	-1.00561100	-3.06712900	2.88383500
O	-0.55394700	-3.30144000	1.72483500
O	-1.10913500	-1.90306000	3.39732700
H	-0.57569000	-1.09530900	2.57984300
O	2.58189100	3.15763300	2.21649400
C	2.11493800	4.44768100	1.82236900
H	2.97406900	5.11245600	1.91355500
H	1.77112700	4.44120600	0.78255200
H	1.31013200	4.79909300	2.47877000
H	3.33008600	0.80786500	2.75966300

H	1.95623600	-1.25288300	2.52941900
TS1_{meta}			
C	-2.78062800	5.50316200	-0.75423700
C	-3.65891200	4.78616800	-1.58014900
C	-3.46841200	3.41326300	-1.78201300
C	-2.42193100	2.74244500	-1.16353000
C	-1.52077100	3.44998300	-0.32887200
C	-1.72095300	4.83197800	-0.13424700
H	-0.23463700	3.26061400	-0.68905600
Pd	-0.86596200	2.44079000	1.40049900
Pd	-1.09270300	-0.42702800	0.89720800
C	-3.41639200	1.08407500	1.96294700
O	-2.85690400	2.21467000	1.80683300
O	-2.88635800	-0.06211900	1.83150000
C	-4.88312200	1.08820000	2.32601000
H	-5.44004600	0.69206900	1.47199300
H	-5.05171200	0.41172600	3.16710700
H	-5.22313100	2.09526400	2.56610500
C	-0.06683200	0.41505000	3.51455900
O	-0.36880000	1.61432400	3.28355900
O	-0.14682800	-0.56643400	2.69653900
C	0.41472000	0.06184500	4.90511900
H	-0.43699700	-0.32232200	5.47618600
H	1.16944000	-0.72547600	4.85704900
H	0.80721600	0.94642900	5.40729400
C	1.66742500	2.89121500	-0.01639000
O	1.00104800	3.21702400	-1.04754000
O	1.15916800	2.61057200	1.10651000
H	-2.30736700	1.67353900	-1.30128200
H	-4.15917700	2.87019400	-2.42080300
C	0.08215800	-1.00138600	-2.02643800
C	-1.45564000	-1.06664500	-1.89494600
O	-2.09935500	-1.54867300	-2.82981900
O	-2.02062500	-0.49439800	-0.87875500
C	1.44020500	-2.37145800	0.22689600
C	0.64916400	-3.52474800	0.25433300
C	2.75879900	-2.47608200	0.67876600
C	1.16224700	-4.74868400	0.67016900
C	3.29707300	-3.69251100	1.08495700
C	2.49460800	-4.83198700	1.07879800

F	3.54375500	-1.39107200	0.75762100
F	4.56676200	-3.76407500	1.48849600
F	2.99638900	-6.00061500	1.47049600
F	0.39510100	-5.83904700	0.67469400
F	-0.62889500	-3.46921800	-0.13673700
C	0.65618000	-2.20551100	-2.76398400
H	0.23668300	-2.19335100	-3.77261100
H	1.74422100	-2.14896900	-2.82657300
H	0.35868700	-3.14708100	-2.30335800
C	0.41495000	0.31511800	-2.75213800
H	0.06376600	1.19017800	-2.20099000
H	1.49109700	0.41294900	-2.89925600
H	-0.08807100	0.29754900	-3.72357700
S	0.84513000	-0.77217000	-0.28634200
C	3.20253900	2.91155400	-0.10565800
C	4.91946100	1.00073500	-1.44241800
C	6.20389300	1.40477300	-1.05268300
C	4.70606900	-0.37547800	-1.56752300
C	7.21109800	0.48922700	-0.76351000
C	5.68918900	-1.31151300	-1.26541600
C	6.95077800	-0.87788900	-0.86926500
F	3.50690100	-0.85195700	-1.94224600
F	5.40881300	-2.61992700	-1.32002900
F	7.90220900	-1.76351100	-0.57473000
F	8.41978300	0.90702000	-0.37596900
F	6.47818100	2.70708000	-0.89378500
C	3.64610300	4.38616300	-0.12208200
H	3.35462800	4.86835400	0.81830800
H	4.73153200	4.43835800	-0.22723800
H	3.18266400	4.92641700	-0.95045900
C	3.83122700	2.15155600	1.06151800
H	3.57524200	1.09057100	1.04335400
H	4.91597800	2.26526200	1.04892100
H	3.45127700	2.57455500	1.99393000
S	3.61760500	2.15322500	-1.80380900
H	-1.04481100	5.41304900	0.48650100
H	-4.48716500	5.28368900	-2.07105300
O	-2.87148400	6.83945100	-0.49640900
C	-3.94948200	7.56524800	-1.06934100
H	-4.92141500	7.17653300	-0.73744600
H	-3.83773300	8.59362800	-0.72273900

H	-3.91216700	7.54945900	-2.16688000
C	-5.05999100	-2.61776800	-1.47355200
H	-4.57150900	-3.44850800	-2.00183900
C	-4.66582500	-2.75980800	0.01008100
C	-6.56865400	-2.80039600	-1.68186100
O	-4.71865200	-1.36474500	-1.96452200
H	-3.79469500	-1.39291700	-2.29922000
F	-6.96404700	-4.04348100	-1.33336500
F	-7.28482600	-1.92049300	-0.95834300
F	-6.87683300	-2.62487000	-2.97844200
F	-5.12758700	-1.74421200	0.75465500
F	-3.31733600	-2.78486700	0.12135900
F	-5.12600100	-3.91213300	0.54398800

int2_{meta}

C	-1.27175000	5.64380300	-1.24456400
C	-2.08547400	5.08642400	-2.23576200
C	-2.53980900	3.77170700	-2.07947700
C	-2.18754600	2.99902400	-0.97367900
C	-1.34854500	3.54737000	0.01062200
C	-0.89804500	4.86855400	-0.12541000
H	0.70498800	3.87296400	-0.75063200
Pd	-0.78583500	2.49725700	1.58989800
Pd	-1.18545600	-0.36577400	1.08540700
C	-3.37356500	1.24666500	2.27298700
O	-2.77356000	2.34942700	2.08130800
O	-2.90451200	0.07572500	2.12021700
C	-4.81961000	1.32037100	2.70654900
H	-5.43728900	1.03605400	1.84969200
H	-5.00359800	0.59274000	3.49981200
H	-5.07614100	2.32750900	3.03433400
C	0.05785800	0.30033500	3.63945100
O	-0.14818800	1.51801900	3.43118200
O	-0.17534200	-0.66532400	2.82320600
C	0.60828700	-0.12424100	4.98537900
H	-0.23501900	-0.38098300	5.63519900
H	1.23717700	-1.01068400	4.88380900
H	1.16271500	0.69655900	5.44209400
C	2.02469400	2.86939800	0.19653800
O	1.65646800	3.59414900	-0.83778300
O	1.28145400	2.52353200	1.11827300

H	-2.56637400	1.98897600	-0.87360000
H	-3.18678800	3.34384600	-2.84100800
C	-0.14757300	-0.65262100	-1.92448300
C	-1.68505600	-0.61727500	-1.76334200
O	-2.37523900	-0.84674000	-2.76124100
O	-2.19409900	-0.23900400	-0.63808000
C	1.02681400	-2.53561100	0.03040400
C	0.08649900	-3.55809800	-0.13237500
C	2.31183900	-2.89366600	0.44582100
C	0.42258200	-4.89275400	0.06802300
C	2.67349500	-4.22212300	0.64129400
C	1.72415300	-5.22436500	0.44955900
F	3.23666000	-1.95202500	0.69158100
F	3.91575700	-4.53173200	1.01716100
F	2.05597700	-6.49980100	0.63552800
F	-0.48437700	-5.85364400	-0.10813200
F	-1.16379500	-3.26293200	-0.50428000
C	0.30436600	-1.74585900	-2.88696400
H	-0.13637100	-1.51726500	-3.85998500
H	1.39112900	-1.76982800	-2.97991400
H	-0.06319000	-2.72799700	-2.59089000
C	0.29894400	0.73973700	-2.40892500
H	-0.00493400	1.52762200	-1.71576800
H	1.38187300	0.77361000	-2.54382400
H	-0.19410900	0.93721100	-3.36520300
S	0.66458300	-0.80595400	-0.20479100
C	3.51314200	2.52803000	0.23224900
C	5.00277700	0.55499800	-1.25068200
C	6.32590100	0.69703400	-0.80883000
C	4.55524700	-0.74651300	-1.49744700
C	7.15455100	-0.40154900	-0.60133000
C	5.35951400	-1.86098100	-1.28357600
C	6.66699100	-1.68777200	-0.83926400
F	3.29937700	-0.96805900	-1.91392600
F	4.86636000	-3.09130300	-1.46904200
F	7.44760200	-2.74556400	-0.62659400
F	8.40661100	-0.23603300	-0.16696200
F	6.81619600	1.91173800	-0.53042900
C	4.29131000	3.82637100	0.52521400
H	4.00761000	4.21334900	1.51089100
H	5.36153400	3.61329000	0.52283700

H	4.08166500	4.58999700	-0.22646400
C	3.78384900	1.45965100	1.29086800
H	3.28869300	0.51596500	1.05676000
H	4.85705900	1.28826100	1.38790300
H	3.40188900	1.81253800	2.25174700
S	3.93743200	1.94676200	-1.53292500
H	-0.30260200	5.35512400	0.64380200
H	-2.38133500	5.65750800	-3.10714500
O	-0.77850700	6.91404800	-1.26057800
C	-1.12439300	7.75582500	-2.35202500
H	-2.20964600	7.90662200	-2.41710400
H	-0.63901100	8.71367800	-2.15907400
H	-0.76019300	7.35154900	-3.30581000
C	-5.37570200	-1.89343300	-1.45925500
H	-4.90585500	-2.68129700	-2.06385800
C	-5.05064900	-2.22645700	0.01155600
C	-6.88205200	-1.97276100	-1.74130000
O	-4.95256100	-0.61190400	-1.78582300
H	-4.04387500	-0.65839100	-2.15747000
F	-7.34422100	-3.23221700	-1.58728900
F	-7.58779000	-1.16980400	-0.92396900
F	-7.13058600	-1.60290600	-3.00954300
F	-5.43186800	-1.24585600	0.84429400
F	-3.71890100	-2.40770700	0.15677400
F	-5.64838300	-3.36997600	0.41326100

int23

C	2.40255000	2.81945100	-0.35761700
C	2.84667300	2.67629300	0.96228100
C	2.02955600	2.01501900	1.88459000
C	0.80296500	1.46682800	1.50711700
C	0.37855700	1.59061500	0.17316300
C	1.15255300	2.30310800	-0.74144100
Pd	-1.06526500	0.31636400	-0.45841900
H	0.19430200	0.93043700	2.22835000
H	3.80909700	3.06379800	1.27348300
H	2.36748400	1.91324800	2.91310300
C	-2.95093700	0.75756400	0.67985900
C	-4.18439200	0.76586400	-0.21657600
C	-3.19615800	2.79737600	-0.42450400
C	-2.34578900	2.00057600	0.54642700

C	-3.72900200	1.69357800	-1.36374500
H	-4.56220300	2.03307800	-1.98716100
H	-2.95798400	1.24922900	-1.99907300
C	-5.17898100	1.71474100	0.53164700
H	-6.15133000	1.69904200	0.03064200
H	-5.33743600	1.40601100	1.56821000
C	-4.49465200	3.11423400	0.40259900
H	-5.11910700	3.81879400	-0.15495800
H	-4.26671200	3.57099300	1.37005100
H	-4.56253000	-0.21831500	-0.47855200
H	-1.71071000	2.45679400	1.29418400
C	-2.77988700	-0.14279700	1.85539000
O	-1.87993900	-0.06663300	2.67440300
C	-3.62682400	-2.05476800	2.93126500
H	-3.59487900	-1.58744400	3.91884300
H	-4.50228500	-2.69484700	2.83044400
H	-2.71115300	-2.63016200	2.77425200
C	-0.28600800	-2.32862900	-2.21640300
C	-1.62610900	-2.46580200	-1.41571100
O	-2.20923000	-1.37325900	-1.02943900
O	-2.08484900	-3.59624100	-1.31938900
C	1.84290800	-1.10614900	-0.50515900
C	1.54347700	-1.77085200	0.68757100
C	3.10163800	-0.50814200	-0.62107400
C	2.46451600	-1.85953300	1.72369200
C	4.02440700	-0.56056400	0.41906800
C	3.70990900	-1.24559200	1.58860100
F	3.43436100	0.18594700	-1.71501500
F	5.20112200	0.06686500	0.30218900
F	4.59023900	-1.29875400	2.58880700
F	2.15274600	-2.49241200	2.85742000
F	0.32578600	-2.29867600	0.87056700
C	0.61151900	-3.55089900	-2.06282400
H	0.04253700	-4.41570600	-2.41047200
H	1.52711000	-3.45394700	-2.65434300
H	0.86883300	-3.73326400	-1.01930800
C	-0.67564200	-2.09934900	-3.68972200
H	-1.26431000	-1.18483600	-3.81137100
H	0.20567100	-2.04680200	-4.33592800
H	-1.29810900	-2.94267800	-4.00284600
S	0.62682100	-0.73337600	-1.75716700

H	0.86776100	2.39901100	-1.78430100
O	3.13069300	3.40502300	-1.35311500
C	4.53404500	3.52065300	-1.15362300
H	4.95245900	3.82806200	-2.11369300
H	4.78172700	4.27974000	-0.39979400
H	4.96779800	2.55764800	-0.85403900
O	-3.75929200	-1.05728900	1.90196000
H	-2.71566100	3.66691900	-0.87408600

TS14

C	1.84523700	2.92041500	-0.40692300
C	2.46770700	2.69524700	0.82860100
C	1.80402000	1.94522100	1.80637600
C	0.54589600	1.40221900	1.56498500
C	-0.06921000	1.62149000	0.31582500
C	0.55332200	2.42066100	-0.64366000
Pd	-1.15737600	-0.03061200	-0.36372100
H	0.03321600	0.81513100	2.32212900
H	3.45908600	3.08123300	1.03109900
H	2.28776400	1.78029000	2.76550300
C	-2.92019300	0.71823600	0.50968700
C	-3.98659400	1.02871400	-0.54290000
C	-2.74720000	2.91857400	-0.30778400
C	-2.15087700	1.91793300	0.66475000
C	-3.22811600	2.01525400	-1.46321900
H	-3.89025300	2.53854100	-2.16002600
H	-2.40944700	1.55031700	-2.02151000
C	-4.97929800	2.00320300	0.16062700
H	-5.84180800	2.19262700	-0.48593300
H	-5.35500700	1.59223500	1.10102600
C	-4.11983300	3.29441500	0.35234200
H	-4.55212400	4.14911300	-0.17613600
H	-4.00778100	3.58244100	1.40193100
H	-4.43686400	0.15096500	-1.00281600
H	-1.84494400	2.23710900	1.65213100
C	-3.11669000	-0.19931400	1.66181600
O	-2.38937300	-0.23603600	2.64259100
C	-4.31312100	-2.07744800	2.42375600
H	-4.35627600	-1.68932600	3.44439900
H	-5.24146700	-2.58269400	2.15954800
H	-3.46655900	-2.76185600	2.32752500

C	0.00486700	-2.58706400	-2.01082900
C	-1.27882400	-2.87979700	-1.15919000
O	-2.00979200	-1.87310200	-0.78400300
O	-1.57045300	-4.05903900	-1.01211400
C	1.98736800	-1.00072500	-0.43624500
C	1.82744500	-1.66033800	0.78706600
C	3.15829700	-0.26025400	-0.62368400
C	2.80662000	-1.61827000	1.77312400
C	4.13393900	-0.17970000	0.36407700
C	3.96407800	-0.86901400	1.56065700
F	3.34577100	0.45294300	-1.74236400
F	5.20939200	0.59793000	0.17937600
F	4.89152600	-0.78962700	2.51648200
F	2.63038400	-2.25503200	2.93359400
F	0.69425900	-2.32549900	1.04411800
C	1.06669500	-3.66801500	-1.84274600
H	0.61366600	-4.61881700	-2.13040000
H	1.93919400	-3.47229000	-2.47372000
H	1.38275300	-3.76433500	-0.80362100
C	-0.46105200	-2.48353200	-3.47658700
H	-1.17355700	-1.66400800	-3.61296900
H	0.38401000	-2.34132300	-4.15674900
H	-0.97127400	-3.41732900	-3.73018800
S	0.70282100	-0.86074100	-1.66131200
H	0.10361800	2.59982000	-1.61505600
O	2.42143600	3.58743800	-1.44537500
C	3.82644500	3.81088700	-1.38912500
H	4.10867100	4.19770000	-2.36949800
H	4.09111000	4.55221500	-0.62375800
H	4.36646900	2.87628600	-1.19306100
O	-4.17492400	-1.00349600	1.47507400
H	-2.11076400	3.76941300	-0.55273600

int24

C	0.73997400	3.43345200	-0.94683000
C	-0.29985900	2.91319000	-1.75123200
C	-0.16705500	1.64848400	-2.29836200
C	0.97829600	0.86093000	-2.04902000
C	2.04281800	1.39732200	-1.26762100
C	1.89713000	2.69066300	-0.72315500
Pd	0.92751300	-0.10785400	0.11135400

H	1.13053500	-0.07117000	-2.58517900
H	-1.19581900	3.49077400	-1.94135100
H	-0.95669900	1.24855900	-2.92758800
C	2.86025000	-0.70866400	-0.31582200
C	3.75795800	-0.73536000	0.92607400
C	4.44706300	1.09474500	-0.23386600
C	3.30932800	0.54078500	-1.12009300
C	3.96065100	0.77235300	1.19926400
H	4.72665200	0.96594000	1.95766000
H	3.04180100	1.28986700	1.48740100
C	5.18405200	-1.13375100	0.45216000
H	5.82994600	-1.30058500	1.32050700
H	5.18254300	-2.05665300	-0.13247000
C	5.64463600	0.11737300	-0.36593000
H	6.54588000	0.56438300	0.06490000
H	5.86673900	-0.11885500	-1.41163100
H	3.35640300	-1.34223800	1.73624200
H	3.66701000	0.27987600	-2.12199000
C	2.63236600	-1.95907900	-1.08720400
O	2.34677700	-2.00893300	-2.27746900
C	2.37234500	-4.29649900	-0.93733800
H	2.98869000	-4.48862000	-1.81984100
H	2.53005000	-5.06376500	-0.17985100
H	1.32105400	-4.26804400	-1.23717700
C	-1.06130300	-0.03544100	2.60679600
C	-0.24830700	-1.36743100	2.51036300
O	0.75785200	-1.41607400	1.68425000
O	-0.54691400	-2.26013400	3.29151600
C	-2.58197100	-0.00946000	0.13221200
C	-2.47593100	-1.17569900	-0.63679600
C	-3.85487000	0.56484500	0.25688100
C	-3.58486400	-1.73912900	-1.26497500
C	-4.97452700	0.01412200	-0.35906100
C	-4.83626700	-1.14291300	-1.12404600
F	-4.02691600	1.67108500	0.99113700
F	-6.17557400	0.58339200	-0.22101300
F	-5.90104000	-1.67786400	-1.72007500
F	-3.45449900	-2.84625300	-1.99950400
F	-1.30156800	-1.79302400	-0.80467200
C	-2.44362800	-0.26294600	3.20988900
H	-2.31336200	-0.67823700	4.21096500

H	-3.00939900	0.67122600	3.26754900
H	-3.01370900	-0.99417100	2.63254200
C	-0.23525600	0.95898200	3.44333300
H	0.73319600	1.16794800	2.97898100
H	-0.77440000	1.90018900	3.58816700
H	-0.04899600	0.50512200	4.42142700
S	-1.20036300	0.80689700	0.91343900
O	2.74451700	-3.05789200	-0.31414300
H	4.70904900	2.13514100	-0.44444500
H	2.67707900	3.13098700	-0.11422100
O	0.69951700	4.65342800	-0.34735600
C	-0.46996600	5.45005800	-0.49502500
H	-1.35703800	4.93962000	-0.09866300
H	-0.28808300	6.35641700	0.08379000
H	-0.64492200	5.72245900	-1.54384200

int25

C	-2.02090300	3.52945100	-0.88372500
C	-1.07002800	3.48077800	-1.93005100
C	0.22686300	3.09743500	-1.64899000
C	0.61128700	2.73712200	-0.33306800
C	-0.36398900	2.76867300	0.71228700
C	-1.67153000	3.15513300	0.41980600
Pd	0.43973000	0.51143200	-0.15791700
H	1.67060300	2.70402400	-0.09730500
H	0.98682000	3.04910800	-2.42058500
C	0.76041100	0.91060400	1.84549600
C	-0.01305100	-0.03734100	2.76480700
C	-0.97338100	1.98606400	3.13561500
C	0.11136200	2.30711400	2.08051800
C	-1.43262500	0.56916800	2.72449100
H	-2.11033200	0.11018000	3.45147200
H	-1.89288200	0.52423500	1.73492100
C	0.41571600	0.30949200	4.22309200
H	0.01871100	-0.45296800	4.90094400
H	1.50113700	0.31796500	4.34989900
C	-0.24892800	1.70027100	4.47281800
H	-0.97046800	1.65283300	5.29393400
H	0.47907100	2.47906300	4.72032000
H	0.09059900	-1.08724000	2.50838700
H	0.84963200	3.02286000	2.45745700

C	2.26682000	0.88980000	1.87452600
O	2.96467700	1.88377400	1.76261200
C	-0.29320000	-3.87591000	0.09603300
C	0.50938000	-2.61106400	-0.26935500
O	0.02771300	-1.52579500	0.18635800
O	1.54654500	-2.74974000	-0.96606200
C	-2.55918700	-2.35548500	-0.80098600
C	-3.44140200	-2.10693500	0.25739300
C	-2.28786200	-1.29018300	-1.66907700
C	-4.01701400	-0.85411900	0.45515000
C	-2.88137500	-0.04361700	-1.50741400
C	-3.74170800	0.17916100	-0.43657100
F	-1.39910500	-1.42379700	-2.66026100
F	-2.59216500	0.95774700	-2.35588400
F	-4.28502100	1.38438100	-0.25039800
F	-4.81912000	-0.62970000	1.50305800
F	-3.73139500	-3.06638300	1.14329700
C	0.48445400	-5.15564700	-0.22807700
H	1.38472800	-5.19127300	0.39239900
H	-0.12226900	-6.03902100	-0.00688100
H	0.79824300	-5.17866300	-1.27248300
C	-0.71959100	-3.83714400	1.56684700
H	-1.31368000	-2.95131400	1.78707800
H	-1.30259700	-4.72674200	1.81627100
H	0.17441000	-3.81270800	2.20175000
S	-1.79831100	-3.94180000	-1.04729000
Ag	2.92697600	-1.14049500	-1.18906600
O	2.81788000	1.62338200	-1.97499400
C	3.94791600	1.46910000	-1.47186100
O	4.43605900	0.33277500	-1.09659600
C	4.83431000	2.67113700	-1.18856300
H	4.71405500	2.92039200	-0.12811100
H	5.88582800	2.43226000	-1.36208500
H	4.52987900	3.52720500	-1.79285900
H	-1.75042500	2.74934200	3.21564000
O	2.75866600	-0.34927800	2.05634500
C	4.20395000	-0.44027600	2.09781000
H	4.41798100	-1.50309500	2.20655600
H	4.62999300	-0.04640900	1.17268600
H	4.58602400	0.11975100	2.95547900
H	-1.35112400	3.73487500	-2.94410800

H	-2.45011200	3.15600400	1.17215900
O	-3.30456100	3.91213600	-1.04958800
C	-3.81909700	4.06402200	-2.37143600
H	-3.69471300	3.13922400	-2.94452800
H	-4.88109900	4.27961800	-2.25034300
H	-3.34062700	4.89758800	-2.89916700

TS15

C	-2.02090300	3.52945100	-0.88372500
C	-1.07002800	3.48077800	-1.93005100
C	0.22686300	3.09743500	-1.64899000
C	0.61128700	2.73712200	-0.33306800
C	-0.36398900	2.76867300	0.71228700
C	-1.67153000	3.15513300	0.41980600
Pd	0.43973000	0.51143200	-0.15791700
H	1.67060300	2.70402400	-0.09730500
H	0.98682000	3.04910800	-2.42058500
C	0.76041100	0.91060400	1.84549600
C	-0.01305100	-0.03734100	2.76480700
C	-0.97338100	1.98606400	3.13561500
C	0.11136200	2.30711400	2.08051800
C	-1.43262500	0.56916800	2.72449100
H	-2.11033200	0.11018000	3.45147200
H	-1.89288200	0.52423500	1.73492100
C	0.41571600	0.30949200	4.22309200
H	0.01871100	-0.45296800	4.90094400
H	1.50113700	0.31796500	4.34989900
C	-0.24892800	1.70027100	4.47281800
H	-0.97046800	1.65283300	5.29393400
H	0.47907100	2.47906300	4.72032000
H	0.09059900	-1.08724000	2.50838700
H	0.84963200	3.02286000	2.45745700
C	2.26682000	0.88980000	1.87452600
O	2.96467700	1.88377400	1.76261200
C	-0.29320000	-3.87591000	0.09603300
C	0.50938000	-2.61106400	-0.26935500
O	0.02771300	-1.52579500	0.18635800
O	1.54654500	-2.74974000	-0.96606200
C	-2.55918700	-2.35548500	-0.80098600
C	-3.44140200	-2.10693500	0.25739300
C	-2.28786200	-1.29018300	-1.66907700

C	-4.01701400	-0.85411900	0.45515000
C	-2.88137500	-0.04361700	-1.50741400
C	-3.74170800	0.17916100	-0.43657100
F	-1.39910500	-1.42379700	-2.66026100
F	-2.59216500	0.95774700	-2.35588400
F	-4.28502100	1.38438100	-0.25039800
F	-4.81912000	-0.62970000	1.50305800
F	-3.73139500	-3.06638300	1.14329700
C	0.48445400	-5.15564700	-0.22807700
H	1.38472800	-5.19127300	0.39239900
H	-0.12226900	-6.03902100	-0.00688100
H	0.79824300	-5.17866300	-1.27248300
C	-0.71959100	-3.83714400	1.56684700
H	-1.31368000	-2.95131400	1.78707800
H	-1.30259700	-4.72674200	1.81627100
H	0.17441000	-3.81270800	2.20175000
S	-1.79831100	-3.94180000	-1.04729000
Ag	2.92697600	-1.14049500	-1.18906600
O	2.81788000	1.62338200	-1.97499400
C	3.94791600	1.46910000	-1.47186100
O	4.43605900	0.33277500	-1.09659600
C	4.83431000	2.67113700	-1.18856300
H	4.71405500	2.92039200	-0.12811100
H	5.88582800	2.43226000	-1.36208500
H	4.52987900	3.52720500	-1.79285900
H	-1.75042500	2.74934200	3.21564000
O	2.75866600	-0.34927800	2.05634500
C	4.20395000	-0.44027600	2.09781000
H	4.41798100	-1.50309500	2.20655600
H	4.62999300	-0.04640900	1.17268600
H	4.58602400	0.11975100	2.95547900
H	-1.35112400	3.73487500	-2.94410800
H	-2.45011200	3.15600400	1.17215900
O	-3.30456100	3.91213600	-1.04958800
C	-3.81909700	4.06402200	-2.37143600
H	-3.69471300	3.13922400	-2.94452800
H	-4.88109900	4.27961800	-2.25034300
H	-3.34062700	4.89758800	-2.89916700
int26			
C	-4.70329900	-1.14968900	0.73020500

C	-3.72333300	-2.14240000	0.60146100
C	-2.36961900	-1.77741300	0.55682000
C	-1.97267600	-0.43981000	0.65095000
C	-2.97668600	0.54927900	0.75504400
C	-4.32314800	0.19688800	0.79768500
Pd	-0.08541700	0.16570600	0.60274700
H	-2.20700300	1.23573900	-2.14501600
H	-1.63517800	-2.56645400	0.44243800
C	-0.96315000	2.06109600	0.59209300
C	-0.46007600	2.82352800	1.83494100
C	-2.69870100	2.68431900	2.16592700
C	-2.51414400	1.97643100	0.78871400
C	-1.41509400	2.28284700	2.92262200
H	-1.30475100	2.80358100	3.87982800
H	-1.32320500	1.20564300	3.08605800
C	-0.93615100	4.30376600	1.73656000
H	-0.45333500	4.89294400	2.52323600
H	-0.67137200	4.76460200	0.78247100
C	-2.47793400	4.20083500	1.96825500
H	-2.78182500	4.75336700	2.86317100
H	-3.05935700	4.59527600	1.12807900
H	0.61129000	2.71882700	2.00948500
H	-3.03219400	2.54507900	0.00508700
C	-0.51152000	2.52356500	-0.74251900
O	-1.09383500	2.31151200	-1.82108200
C	4.23208400	0.85756000	-0.39362700
C	2.70872300	0.71425200	-0.57684900
O	2.00835700	0.79215600	0.46869300
O	2.29857300	0.45704900	-1.75082500
C	3.44631400	-1.69594700	0.60248000
C	3.15013500	-1.52041200	1.96154100
C	2.49880500	-2.37185700	-0.17785900
C	1.95721400	-1.96731300	2.51836700
C	1.29600500	-2.82648700	0.36131200
C	1.02684300	-2.62800200	1.71649000
F	2.68870100	-2.56089900	-1.48800800
F	0.40145700	-3.45805000	-0.41461200
F	-0.10413000	-3.08865400	2.25292700
F	1.67556400	-1.74300800	3.80530900
F	3.98774900	-0.85229900	2.75895500
C	4.92338500	1.36646200	-1.66145900

H	4.62928900	2.40765500	-1.83554400
H	6.01160100	1.34308300	-1.54499000
H	4.63723500	0.77469700	-2.53064700
C	4.58421500	1.71088700	0.82626300
H	4.13185800	1.31451200	1.73275100
H	5.66898100	1.75238200	0.95710700
H	4.21167900	2.73088200	0.67458600
S	4.86698900	-0.93298200	-0.14880100
Ag	0.32822200	-0.29707700	-2.20163400
O	-3.00005600	0.66717400	-2.41352100
C	-2.72211300	-0.55200800	-2.78625900
O	-1.58009100	-1.02587100	-2.92226700
C	-3.93642000	-1.40060600	-3.03496000
H	-4.72350700	-0.81523700	-3.51383100
H	-3.67066800	-2.27129700	-3.63362000
H	-4.30322300	-1.72912300	-2.05693200
H	-3.64628000	2.42452000	2.64394100
O	0.62971200	3.22086800	-0.71606400
C	1.19706700	3.59572300	-1.98707800
H	2.04240500	4.23884200	-1.74211600
H	1.53897800	2.70364200	-2.51602200
H	0.46516800	4.13348700	-2.59334200
H	-3.99045200	-3.19087500	0.53496100
H	-5.10211900	0.95074800	0.86931200
O	-6.05173000	-1.38817000	0.77606500
C	-6.49281800	-2.73405500	0.73127200
H	-6.09653600	-3.32207800	1.57022800
H	-7.58160000	-2.69958800	0.80069300
H	-6.20987500	-3.22722100	-0.20960300

int27

C	-1.04505800	2.80780400	3.66964500
C	-1.12024600	1.41208700	3.56197200
C	-0.64686000	0.78262800	2.40641400
C	-0.10470300	1.52849600	1.34747900
C	-0.01682500	2.93760300	1.47488000
C	-0.49040000	3.56307300	2.62610500
Pd	0.73980400	0.68456400	-0.25360900
H	-0.70561200	-0.29707000	2.33013300
C	1.08057900	2.69701500	-0.79685900
C	2.57691300	3.03121600	-0.98914400

C	1.96119100	4.39067800	0.71416000
C	0.62398000	3.68251200	0.34038500
C	3.00575900	3.28036800	0.47307400
H	4.03702400	3.63980100	0.56274100
H	2.86994600	2.40591000	1.11571500
C	2.72086300	4.45637200	-1.59438400
H	3.75920800	4.63139100	-1.89653500
H	2.10083600	4.59014300	-2.48393500
C	2.31019300	5.39014700	-0.41098600
H	3.14265300	6.03354500	-0.10721600
H	1.46662000	6.04333600	-0.65850100
H	3.13403900	2.27249200	-1.53859200
H	-0.08730000	4.42122900	-0.05143100
C	0.19261100	2.71766800	-1.98035100
O	-1.03914900	2.88551900	-1.96614100
C	-0.01106300	2.35464200	-4.31049200
H	-0.70339400	1.51704100	-4.18263700
H	-0.58885600	3.26559300	-4.48274500
H	0.66890300	2.16823900	-5.14196600
C	-1.39875200	-3.23938200	0.07365700
C	-1.06680500	-1.74924100	-0.17854800
O	-1.94155000	-1.07590900	-0.79174700
O	0.05201600	-1.33172400	0.25528500
C	-4.04994600	-2.43495900	0.79848900
C	-4.18579000	-1.05412000	0.97392100
C	-5.00595700	-3.06926600	-0.00492200
C	-5.16870800	-0.32148500	0.32323900
C	-6.02142700	-2.35622300	-0.64097300
C	-6.09119100	-0.97234900	-0.49140400
F	-4.94782600	-4.38766300	-0.21947000
F	-6.91325900	-2.98685000	-1.41369900
F	-7.03504400	-0.27498500	-1.12634200
F	-5.18343300	1.02111500	0.42446400
F	-3.31511600	-0.37061100	1.73067000
C	-1.95655700	-3.88027300	-1.19920700
H	-1.17602600	-3.88170200	-1.96951800
H	-2.26688700	-4.91028100	-1.00995000
H	-2.80071400	-3.30983800	-1.58645000
C	-0.19909000	-4.02291900	0.61491200
H	0.18957400	-3.58005000	1.53415400
H	-0.47210000	-5.06570100	0.80167500

H	0.60317500	-4.00437700	-0.12879100
S	-2.66483600	-3.30822900	1.48782400
Ag	-1.99896900	1.20426100	-0.46794400
C	4.13255200	-2.50036100	1.09719700
C	5.50174100	-2.39790600	0.82186200
C	5.93014600	-1.80746300	-0.37399000
C	4.99752000	-1.32042000	-1.28976500
C	3.64135300	-1.43763300	-0.98871500
C	3.18534200	-2.02076700	0.19334700
H	3.82028000	-2.95624900	2.03084600
H	6.99012300	-1.72562700	-0.58473800
H	5.32764000	-0.85385500	-2.21114600
H	2.12537600	-2.08226300	0.41233900
I	2.20218100	-0.63258700	-2.38030600
C	6.45740900	-2.92842900	1.83667500
O	6.12631500	-3.45721500	2.87960800
O	7.74689200	-2.75581300	1.46934900
C	8.71837900	-3.24174900	2.41072300
H	8.60911800	-2.73255800	3.37195600
H	8.59655000	-4.31677200	2.56799300
H	9.69077900	-3.02501100	1.96865700
H	-0.43556900	4.64161600	2.74314200
O	0.82929200	2.49410900	-3.15160800
H	1.94291000	4.83076000	1.71436000
H	-1.54145400	0.80815600	4.35678300
O	-1.48053900	3.52564700	4.74651500
C	-2.05858900	2.82094600	5.83413700
H	-2.33650000	3.57714000	6.57036000
H	-2.95710300	2.26801700	5.52857600
H	-1.34640000	2.11971100	6.28925400

TS16

C	-0.15773700	-1.95555000	3.81604400
C	0.16308900	-0.61624100	3.54149600
C	-0.01960500	-0.11388900	2.25287100
C	-0.51834900	-0.93104500	1.22213500
C	-0.85687100	-2.27809700	1.51477000
C	-0.66490000	-2.77921100	2.80046000
Pd	-1.00312900	-0.17658100	-0.58536900
H	0.23875900	0.91721000	2.03999300
C	-1.61018400	-2.22881600	-0.91102500

C	-3.08788400	-2.44885000	-1.27396900
C	-2.87275900	-3.61776100	0.65244500
C	-1.42906200	-3.09245700	0.39350600
C	-3.73619400	-2.45339200	0.12953200
H	-4.80616500	-2.68765300	0.10794000
H	-3.58351300	-1.52503600	0.68334300
C	-3.31473700	-3.92757600	-1.70984500
H	-4.31923900	-4.02853900	-2.13415300
H	-2.60995100	-4.24843000	-2.47893000
C	-3.17988000	-4.72640100	-0.37584200
H	-4.11432000	-5.23737300	-0.12225100
H	-2.39199300	-5.48606500	-0.41293400
H	-3.46083100	-1.73850000	-2.01059300
H	-0.75984600	-3.93921900	0.19212700
C	-0.59767700	-2.53399000	-1.95947600
O	0.59134400	-2.82322400	-1.74283700
C	-0.08967300	-2.51987800	-4.26605600
H	0.61571100	-1.69088500	-4.16232700
H	0.45532800	-3.46605900	-4.23926500
H	-0.65878600	-2.42523500	-5.19012200
C	2.29766500	2.99827600	-0.60651200
C	1.58025000	1.62745900	-0.58421500
O	2.28834800	0.62235600	-0.88274200
O	0.35767700	1.62265300	-0.25854500
C	4.41186300	1.74366500	0.85676300
C	4.05488000	0.49835100	1.38387400
C	5.62201000	1.81190800	0.15521700
C	4.81693600	-0.64095500	1.16547600
C	6.41825600	0.68534800	-0.04814200
C	6.00363900	-0.55112000	0.44305300
F	6.03446000	2.96483500	-0.38037800
F	7.56289600	0.77771800	-0.73408700
F	6.73697800	-1.64325300	0.21991200
F	4.36911500	-1.84059800	1.58409100
F	2.90790300	0.34603700	2.06308200
C	3.19545100	3.11225000	-1.84052900
H	2.56967200	3.09053200	-2.74033800
H	3.75585500	4.04972400	-1.82256600
H	3.88988200	2.27452800	-1.90086400
C	1.31225300	4.16739500	-0.52061600
H	0.69892200	4.11159200	0.38093900

H	1.84516900	5.12268300	-0.53623000
H	0.64140900	4.12777700	-1.38383700
S	3.31328300	3.13314000	0.99287600
Ag	1.58463400	-1.37037900	-0.12059400
C	-3.38301200	2.87427800	0.95922000
C	-4.67741100	2.34137700	1.02560600
C	-5.01702400	1.25763600	0.20445800
C	-4.07147500	0.69391900	-0.64956500
C	-2.76806900	1.19260300	-0.63251700
C	-2.42536400	2.32878400	0.10806400
H	-3.13813200	3.73129300	1.57837100
H	-6.02605000	0.86141900	0.22179800
H	-4.35063700	-0.11840600	-1.30345600
H	-1.42930100	2.74419900	0.05097200
I	-1.71245400	1.04498800	-2.96093600
C	-5.64836900	2.97986900	1.95260400
O	-5.39554600	3.92838300	2.67121700
O	-6.86548000	2.38648600	1.91605200
C	-7.84767700	2.96228700	2.79094800
H	-7.52127200	2.89800300	3.83264800
H	-8.01609500	4.01380800	2.54280600
H	-8.75692700	2.38087500	2.63712700
H	-0.91000600	-3.80824400	3.04566600
O	-1.06649300	-2.46318600	-3.20988800
H	-3.03641700	-3.91034300	1.69237700
H	0.55826300	0.03555000	4.31098500
O	-0.01226900	-2.54925500	5.03221400
C	0.50426500	-1.77576100	6.10691800
H	0.53708300	-2.44403100	6.96866700
H	1.51774800	-1.41210300	5.89262700
H	-0.14327800	-0.91996700	6.33768000

int28

C	0.50742900	-0.91655600	4.23511800
C	0.71396200	0.33055800	3.62700800
C	0.21426300	0.56525600	2.34502700
C	-0.48739300	-0.42919700	1.66238100
C	-0.71422600	-1.67077800	2.27712600
C	-0.20465900	-1.91079000	3.55350000
Pd	-1.03348800	-0.27280600	-0.27797400
H	0.41212000	1.52413100	1.88190000

C	-1.86907400	-2.25651600	0.07133700
C	-3.39967400	-2.42706200	0.03050400
C	-2.89832700	-2.99933300	2.16356600
C	-1.50106000	-2.70692500	1.53592300
C	-3.79056700	-1.96432100	1.45275900
H	-4.85672000	-2.10132900	1.66062900
H	-3.51527500	-0.93293600	1.67118300
C	-3.78518900	-3.93772900	0.11839000
H	-4.86110600	-4.02737800	-0.06300400
H	-3.28408500	-4.55505200	-0.62583600
C	-3.42755900	-4.32668100	1.58600300
H	-4.31132400	-4.66305900	2.13721100
H	-2.68381500	-5.12886700	1.64273200
H	-3.87470400	-1.92435500	-0.80799100
H	-0.90946800	-3.63022400	1.49845300
C	-1.05710400	-2.98328900	-0.94947500
O	0.18456100	-3.15157000	-0.86025900
C	-0.96060600	-4.06560500	-3.04936000
H	-0.34260100	-3.28580600	-3.49858200
H	-0.33944800	-4.88445100	-2.68116400
H	-1.70352600	-4.42309800	-3.76003800
C	2.04198500	2.97925100	-0.71210000
C	1.34852000	1.60370700	-0.75502600
O	2.09156300	0.62630700	-1.08610800
O	0.13114600	1.56428800	-0.42952500
C	4.30119300	1.75787300	0.55697800
C	4.09214900	0.41224400	0.88212400
C	5.49217700	2.07260000	-0.11076100
C	4.98089900	-0.58371500	0.50009000
C	6.41351300	1.09088700	-0.47351600
C	6.14799900	-0.24548000	-0.18048800
F	5.76366000	3.33453200	-0.45747900
F	7.53697300	1.41897700	-1.12053100
F	7.00606800	-1.19674700	-0.55213900
F	4.68782900	-1.87400100	0.73878800
F	2.98402200	0.02404100	1.52726100
C	2.92012200	3.18376300	-1.94761100
H	2.27876200	3.22568100	-2.83503700
H	3.47928000	4.11850500	-1.86883900
H	3.61470100	2.35427400	-2.08170300
C	1.04011500	4.12331700	-0.53383700

H	0.43482000	3.99693600	0.36606500
H	1.56248900	5.08298600	-0.49071000
H	0.35685500	4.13000900	-1.38751000
S	3.06761000	2.99414100	0.88883800
Ag	1.47427300	-1.39285600	-0.84024800
C	-3.76590400	2.64238700	1.28903100
C	-4.88404300	2.52253400	0.45738100
C	-4.88420900	1.55864000	-0.55847200
C	-3.78773400	0.71333500	-0.73250900
C	-2.69198800	0.83748600	0.12173400
C	-2.66129600	1.80499900	1.12567000
H	-3.77279500	3.39518800	2.07072000
H	-5.73497300	1.47557100	-1.22532100
H	-3.78862900	-0.00003700	-1.54438400
H	-1.81075300	1.91577900	1.78092000
I	-1.15272200	-0.21821900	-3.10919800
C	-6.02996800	3.44376200	0.68973000
O	-6.06510700	4.29682200	1.55606900
O	-7.04820400	3.23003400	-0.17611300
C	-8.18264400	4.09358500	-0.00537300
H	-8.61214300	3.97315900	0.99301900
H	-7.89366600	5.13995800	-0.13669900
H	-8.89903400	3.79422400	-0.77055400
H	-0.35518500	-2.86835600	4.04352700
O	-1.72737800	-3.49211900	-1.96438200
H	-2.87749800	-2.95499700	3.25490300
H	1.27570200	1.11420800	4.12066100
O	0.95688700	-1.25747900	5.47551400
C	1.70045600	-0.29585300	6.21044200
H	1.96058300	-0.77495700	7.15555100
H	2.62132800	-0.00853500	5.68584000
H	1.10819600	0.60590800	6.41415600

int29

C	4.20957400	-1.50998100	-2.77973800
C	2.93524300	-1.23581300	-3.29590200
C	1.89460100	-0.88827900	-2.42364000
C	2.15670000	-0.81862300	-1.06491800
C	3.41744200	-1.09188000	-0.51920400
C	4.44189900	-1.44032000	-1.39817700
Pd	0.72014400	-0.47608500	0.24821300

H	2.73347800	-1.29425900	-4.35856400
H	0.89976300	-0.68652900	-2.80629500
C	2.27882500	-0.47255100	1.63770000
C	2.72083200	0.85231600	2.30935400
C	4.64460800	0.03576800	1.43376000
C	3.58870900	-1.00926900	0.97485200
C	3.83194800	1.34355900	1.35917400
H	4.36772000	2.21058800	1.75940000
H	3.47679700	1.57832600	0.35513200
C	3.56080800	0.48353600	3.56571500
H	3.77305200	1.39794400	4.12904600
H	3.04775600	-0.20291800	4.24397300
C	4.86413600	-0.12602300	2.95637900
H	5.75072900	0.42754400	3.28060600
H	5.00358800	-1.17314600	3.24098900
H	1.90280500	1.54062300	2.51640300
H	3.81887600	-2.00426400	1.37068200
C	1.60923700	-1.43527300	2.58946800
O	2.07171800	-2.46492900	3.02368700
C	-0.49682900	-1.90520100	3.59624400
H	-1.38222400	-1.33461700	3.86866600
H	-0.76324300	-2.72101900	2.92063500
H	0.01306200	-2.29326300	4.47955400
C	-1.97864100	-3.39827600	-0.72785800
C	-0.89601800	-2.35201200	-0.46640000
O	-1.01729900	-1.19781300	-0.99278000
O	0.06739000	-2.61955100	0.31864500
C	-3.84850500	-1.45109200	0.24358800
C	-3.26358400	-0.32112200	0.82891400
C	-4.93319100	-1.23162800	-0.61608500
C	-3.73429800	0.96400400	0.58874300
C	-5.41324100	0.04918100	-0.88192700
C	-4.81265500	1.14948600	-0.27418900
F	-5.53681900	-2.25829200	-1.22321400
F	-6.44704000	0.22873400	-1.71112100
F	-5.27007200	2.37819900	-0.51481000
F	-3.16633100	2.02148900	1.18155400
F	-2.20403800	-0.44517200	1.64808200
C	-2.57838300	-3.25342900	-2.12608100
H	-1.80392100	-3.46326800	-2.87271200
H	-3.40190200	-3.95773800	-2.26375500

H	-2.93719100	-2.23851000	-2.29856800
C	-1.46830600	-4.81791800	-0.46132600
H	-0.68262200	-5.05381700	-1.18579600
H	-1.03488800	-4.90624700	0.53626300
H	-2.27655000	-5.54545300	-0.57895900
S	-3.28349700	-3.09608400	0.61204100
C	1.05625100	3.59983000	-1.15707200
C	0.16921000	4.23257200	-0.27571800
C	-0.44489600	3.48765800	0.73908600
C	-0.16589200	2.12948600	0.87879300
C	0.71660200	1.50176400	-0.00985700
C	1.33000000	2.23751900	-1.02803800
H	1.52927300	4.17578800	-1.94473200
H	-1.14063400	3.98425400	1.40682200
H	-0.65721400	1.56635000	1.66738600
H	2.01369200	1.76035300	-1.71982800
C	-0.16080000	5.68003800	-0.37320700
O	-0.92191300	6.26746900	0.37197700
O	0.48427900	6.29094100	-1.39609500
C	0.20180500	7.69089000	-1.54157800
H	0.78984700	8.02341100	-2.39728600
H	-0.86464400	7.85287000	-1.72110500
H	0.49002200	8.23872600	-0.64012600
O	0.36052000	-0.97758100	2.89382700
H	5.56171200	0.00077200	0.84093600
O	5.29191800	-1.85622100	-3.53579100
C	5.12633800	-1.95777100	-4.94168600
H	4.82545000	-0.99938100	-5.38591500
H	6.10031900	-2.24645900	-5.33995100
H	4.38636400	-2.72392000	-5.20927900
H	5.43866900	-1.66549500	-1.03125200

TS17

C	5.17102200	-2.23885600	-0.03634000
C	4.91480000	-1.61940300	-1.26943500
C	3.67491000	-1.02231000	-1.48705500
C	2.68046200	-1.03929900	-0.50192700
C	2.92074800	-1.71992300	0.72099200
C	4.16150000	-2.30580800	0.93696700
Pd	0.69996400	-0.56591200	-0.75305400
H	5.66762900	-1.58171300	-2.04706400

H	3.49883300	-0.50095100	-2.42285800
C	0.41460300	-1.79784300	0.91072500
C	-0.49526800	-1.12902200	1.93360400
C	1.51616800	-1.22174600	2.98008400
C	1.75556200	-1.99580000	1.63956900
C	0.46148600	-0.14538900	2.62575300
H	0.01637200	0.30391900	3.51981500
H	0.79740700	0.65593600	1.97415000
C	-0.72266000	-2.16948600	3.07905800
H	-1.55265000	-1.82186000	3.69843700
H	-0.99567500	-3.15657800	2.69853800
C	0.63968200	-2.15936200	3.85155100
H	0.51928600	-1.74229400	4.85626200
H	1.07366200	-3.15811000	3.96008800
H	-1.40432200	-0.73179900	1.50247100
H	1.83874500	-3.06373800	1.87432000
C	-0.09457000	-3.02700100	0.18118100
O	0.61732400	-3.92692000	-0.21877500
C	-2.01721700	-4.04084500	-0.73747500
H	-3.08501600	-3.82544200	-0.73447700
H	-1.61302700	-3.98371300	-1.75028300
H	-1.80859700	-5.02328500	-0.30603400
C	-3.01608200	-0.57984300	-2.70943200
C	-1.66937000	-0.80674200	-1.99784200
O	-1.39689400	-0.05508800	-0.99183500
O	-0.85454100	-1.64039100	-2.45313900
C	-4.30957300	0.11299900	-0.18712400
C	-3.87596100	-0.36291600	1.05662300
C	-4.65297900	1.46925700	-0.26228900
C	-3.71765700	0.48170400	2.15098900
C	-4.49984600	2.33029200	0.82166400
C	-4.02171400	1.83468600	2.03227700
F	-5.13290300	1.99201800	-1.39748800
F	-4.81880300	3.62540100	0.71131700
F	-3.86537100	2.65115000	3.07735300
F	-3.24697800	0.00515500	3.31517000
F	-3.57154700	-1.65265600	1.22972200
C	-3.06385100	0.87211200	-3.20225900
H	-2.25792700	1.02338300	-3.93085600
H	-4.01924100	1.08711100	-3.68553000
H	-2.91110300	1.57166600	-2.38121600

C	-3.19993600	-1.56320500	-3.87240500
H	-2.38253200	-1.42614700	-4.58410000
H	-3.16461000	-2.60030300	-3.53169200
H	-4.15003500	-1.38195900	-4.38385800
S	-4.46448700	-0.99281000	-1.56927600
C	3.00638200	2.87165400	0.71608600
C	2.79603600	3.63559800	-0.44139900
C	2.25338800	3.02412100	-1.57863900
C	1.91619800	1.67370300	-1.55449400
C	2.06528900	0.93048100	-0.36834000
C	2.65629500	1.52485400	0.75292600
H	3.45672200	3.33450000	1.58697600
H	2.11375800	3.61696800	-2.47645100
H	1.53264200	1.21186600	-2.46527300
H	2.86653100	0.93879900	1.63764500
C	3.14803300	5.07739700	-0.52826900
O	3.00211200	5.76364300	-1.52213800
O	3.65397900	5.55641500	0.63230300
C	4.00709100	6.94863300	0.61241900
H	4.39264800	7.16920200	1.60789400
H	4.76873000	7.14237400	-0.14780000
H	3.13080400	7.56485200	0.39354900
O	-1.42933400	-3.00187700	0.06537100
H	2.43537700	-0.88073800	3.46306000
O	6.34898000	-2.82494000	0.30325500
C	7.40204200	-2.83636100	-0.65230300
H	7.71644100	-1.81890200	-0.91856300
H	8.23388800	-3.35643900	-0.17543400
H	7.11316600	-3.37504300	-1.56382700
H	4.36285800	-2.86898200	1.84339500

int30

C	1.67686700	2.42856000	-1.30625100
C	0.40215600	2.66827700	-1.83617800
C	-0.38488800	1.58320200	-2.19510000
C	0.08496800	0.25957400	-1.95306300
C	1.37996300	0.02371800	-1.38856500
C	2.19956500	1.15423500	-1.08827500
H	0.06687800	3.68736400	-1.97736000
C	-2.74068200	0.86217500	3.27360200
C	-1.75914800	0.54456300	2.14807900

O	-1.53662000	1.39854700	1.23969600
O	-1.22333800	-0.61651600	2.09355900
C	-4.36773800	0.28611200	0.98121900
C	-4.71019200	1.49119600	0.35444800
C	-3.97189300	-0.77647600	0.15508600
C	-4.66825900	1.63472400	-1.02835900
C	-3.91448600	-0.64322600	-1.23012800
C	-4.27959700	0.56014900	-1.82267000
F	-3.61490900	-1.95382600	0.67597800
F	-3.49823000	-1.65785000	-1.99892400
F	-4.25124200	0.68785300	-3.15159300
F	-4.98753800	2.80390900	-1.60570500
F	-5.07769400	2.55617900	1.07607000
C	-2.35872000	0.13993900	4.57098000
H	-1.42865400	0.56759900	4.96078100
H	-3.13458700	0.27569300	5.33129900
H	-2.20458300	-0.92502800	4.39483700
C	-2.89125900	2.37119600	3.47590300
H	-3.19440800	2.86511400	2.55432500
H	-3.63717200	2.57264400	4.24931700
H	-1.93209500	2.79579200	3.79365800
S	-4.40344700	0.09836600	2.74839500
C	5.97536900	0.76485600	-1.02653500
C	6.26929800	1.10383600	0.30200300
C	5.23006600	1.45289700	1.17353800
C	3.91234300	1.45431200	0.72590400
C	3.60637300	1.09474500	-0.59464500
C	4.65542000	0.76634800	-1.46772400
H	6.78127100	0.50667600	-1.70370900
H	5.47678800	1.71837200	2.19601400
H	3.10537900	1.72332800	1.40113300
H	4.42608700	0.50361600	-2.49636300
C	7.65997500	1.11779600	0.83603700
O	7.95585300	1.40816300	1.97923300
O	8.57576600	0.76839700	-0.09703600
C	9.93769800	0.76468400	0.35985800
H	10.06575900	0.05614300	1.18269900
H	10.53669100	0.46682300	-0.50079400
H	10.22988300	1.75935900	0.70739500
Pd	-0.40249300	-0.25373700	0.16534000
C	0.54919700	-1.99854600	-0.30593500

C	1.22925000	-2.60008000	0.93372900
C	2.94667400	-1.91237800	-0.38226800
C	1.71166200	-1.47354100	-1.20717700
C	2.47784200	-1.70525600	1.07440200
H	3.19470100	-2.08656900	1.80890400
H	2.24473500	-0.66748400	1.32174700
C	1.88243300	-3.93840800	0.49275700
H	2.28618100	-4.45524800	1.36981800
H	1.17112100	-4.61755900	0.01769800
C	3.02215500	-3.46163200	-0.46202700
H	4.00167200	-3.80608400	-0.11688700
H	2.89261400	-3.82497400	-1.48674400
H	0.56860700	-2.68024300	1.79682600
H	1.70495200	-1.94559500	-2.19539300
C	-0.49674700	-2.82172200	-0.98997600
O	-0.71477500	-2.82616800	-2.19153300
C	-2.23813700	-4.38662500	-0.66761400
H	-1.84030400	-5.05195500	-1.43847800
H	-2.63509500	-4.95993300	0.16980700
H	-3.01283200	-3.75389000	-1.09971600
H	3.87904300	-1.43203100	-0.66377900
O	-1.18801500	-3.57626100	-0.11103700
O	-1.60270300	1.66090300	-2.77311500
C	-2.16117100	2.95663100	-2.99791900
H	-1.53304600	3.54324700	-3.67873900
H	-3.13559600	2.78163000	-3.44742500
H	-2.29041200	3.49667400	-2.05296500
H	-0.44801300	-0.55607400	-2.43638900
H	2.30329000	3.28272700	-1.06484700

TS18

C	1.32285000	-2.35378600	-2.63230400
C	0.13882200	-3.02762900	-2.93321200
C	-0.91129800	-3.01558100	-2.00667100
C	-0.74882600	-2.33490800	-0.79451500
C	0.42130200	-1.61402300	-0.52577200
C	1.49892200	-1.62777900	-1.44619500
H	0.04948300	-3.55734600	-3.87398700
C	-1.29719300	3.78024000	-0.68944700
C	-0.70859000	2.44447300	-0.25423300
O	-0.35189900	1.60080300	-1.13490900

O	-0.63755300	2.14855300	0.98490900
C	-3.42283100	1.80344500	-0.66035100
C	-3.22068900	1.02950700	-1.81192700
C	-3.85457700	1.13260000	0.49242900
C	-3.42901900	-0.34641500	-1.81681900
C	-4.11209600	-0.23510300	0.49250400
C	-3.88816400	-0.97877600	-0.66300700
F	-4.03654900	1.79229200	1.64363600
F	-4.57263700	-0.83596300	1.59523700
F	-4.10350500	-2.29397400	-0.65510200
F	-3.19394500	-1.06092900	-2.92678400
F	-2.80022200	1.59812900	-2.94558300
C	-0.97210700	4.88767900	0.31947800
H	0.10260700	5.09984500	0.29102600
H	-1.50350100	5.80966900	0.06339200
H	-1.24240000	4.58449400	1.33118100
C	-0.86522600	4.14656600	-2.11199500
H	-1.12337500	3.35376000	-2.81229900
H	-1.35180900	5.07493900	-2.42378900
H	0.21993300	4.29779400	-2.14029200
S	-3.19305100	3.56434400	-0.64289600
C	5.19917100	-0.94459700	-0.98905500
C	5.22573000	0.45401400	-0.89781000
C	4.03026200	1.17506900	-1.01606900
C	2.82033900	0.51187300	-1.19785500
C	2.77977000	-0.89220000	-1.25498100
C	3.98762000	-1.60479500	-1.17420100
H	6.12398300	-1.50442800	-0.90995300
H	4.07042100	2.25818000	-0.96660900
H	1.90209200	1.07744400	-1.31178900
H	3.96518900	-2.68918000	-1.23800000
C	6.48542100	1.21923700	-0.68875300
O	6.55146900	2.43063800	-0.60378600
O	7.57178700	0.41498100	-0.59871300
C	8.81779000	1.09972400	-0.39716300
H	8.79627600	1.67406200	0.53314100
H	9.57876500	0.32050700	-0.35001700
H	9.01930400	1.78537500	-1.22473500
Pd	-0.02644600	0.13746000	0.50906300
C	0.21600100	-0.86173200	2.30316500
C	1.32965800	-0.29581100	3.18797000

C	2.29047200	-1.90224000	1.90327400
C	0.82314800	-1.90162500	1.50843300
C	2.55879000	-0.42602800	2.26270900
H	3.50421200	-0.29498500	2.79810400
H	2.54304400	0.24511300	1.40358400
C	1.62955500	-1.42363400	4.22271600
H	2.33823000	-1.06126600	4.97364600
H	0.72879200	-1.74943200	4.74957500
C	2.26399400	-2.54334700	3.33620100
H	3.28880500	-2.76951200	3.64459100
H	1.70049400	-3.48097300	3.36324400
H	1.11880700	0.68296100	3.61594000
H	0.31117600	-2.84844700	1.40176300
C	-1.18746200	-1.03012400	2.77489800
O	-1.98774700	-1.81807800	2.29618400
C	-2.83720400	-0.18817900	4.24464600
H	-3.17076200	-1.20824400	4.44777600
H	-2.83498800	0.41097700	5.15472000
H	-3.48472000	0.26004900	3.49041200
H	2.97140600	-2.38519400	1.20557000
O	-1.47048600	-0.18568200	3.78168600
O	-2.10054800	-3.65227800	-2.17158300
C	-2.45622500	-4.08495000	-3.47659900
H	-1.82563200	-4.91636900	-3.81864000
H	-3.48960600	-4.42734300	-3.40604400
H	-2.39546200	-3.25954300	-4.19622600
H	-1.54617400	-2.38720500	-0.05996200
H	2.13362100	-2.36285800	-3.35578200

int31

C	1.14669500	-3.62642000	-1.21345500
C	-0.03065600	-4.35350300	-1.03463800
C	-1.09285000	-3.76948100	-0.33456600
C	-0.96213100	-2.46253700	0.16561600
C	0.18753200	-1.73021000	-0.09316900
C	1.29123900	-2.30808700	-0.75745600
H	-0.10008700	-5.36073200	-1.42662600
C	-1.10258500	3.08782900	-2.24755200
C	-0.54831400	2.06891100	-1.26358700
O	-0.38569900	0.86176700	-1.65925600
O	-0.30219700	2.37967900	-0.05899100

C	-3.33790300	1.42775100	-1.36915100
C	-3.20871900	0.23590100	-2.09770600
C	-3.78883700	1.32151600	-0.04584600
C	-3.49534000	-1.00285600	-1.53385700
C	-4.13179900	0.09486400	0.51607100
C	-3.97883600	-1.06977600	-0.22916400
F	-3.90421600	2.40832400	0.73103400
F	-4.59902900	0.02825000	1.76890200
F	-4.26169700	-2.25058700	0.31975700
F	-3.30387200	-2.12919400	-2.22920900
F	-2.77492900	0.25712100	-3.36110200
C	-0.69850700	4.51437800	-1.85949100
H	0.38082400	4.63596800	-2.00212700
H	-1.20664800	5.24375800	-2.49798100
H	-0.93739100	4.71971100	-0.81590300
C	-0.70475300	2.74969100	-3.68821900
H	-1.02097800	1.74337800	-3.95569500
H	-1.16097800	3.46411800	-4.37890200
H	0.38456100	2.81507300	-3.79365300
S	-3.00211500	3.02349300	-2.07386000
C	4.98799100	-1.54150200	-0.46594300
C	5.06823500	-0.26503000	-1.04069200
C	3.91347700	0.32032600	-1.57802800
C	2.69302100	-0.34423100	-1.52090200
C	2.59301300	-1.60763900	-0.90972200
C	3.76346800	-2.20148000	-0.40569300
H	5.88098800	-2.00219500	-0.05903100
H	3.99583100	1.29751100	-2.04246900
H	1.81079400	0.10398500	-1.96380900
H	3.69723800	-3.17856400	0.06431700
C	6.33944000	0.50349600	-1.11221100
O	6.44934000	1.61621600	-1.59176000
O	7.38507700	-0.17147500	-0.57545300
C	8.64050800	0.52338700	-0.61634900
H	8.57812300	1.46675400	-0.06670400
H	9.36390900	-0.14571500	-0.14984100
H	8.92792300	0.74113000	-1.64869400
Pd	0.13066000	0.22330400	0.32357300
C	0.25099700	0.48668500	2.48939300
C	1.19059300	1.62586800	2.88167600
C	2.49289900	-0.18301400	2.45871300

C	1.05724400	-0.62017300	2.22163900
C	2.45035300	1.30412600	2.04810700
H	3.32950000	1.86010100	2.38811100
H	2.32673200	1.45735900	0.97355000
C	1.68704800	1.21164700	4.30803300
H	2.27439900	2.02594700	4.74231700
H	0.85504500	1.00709400	4.98675800
C	2.57533400	-0.04256800	4.02012800
H	3.61495100	0.12374400	4.31760300
H	2.22438800	-0.94101500	4.53617400
H	0.76700000	2.62458000	2.80312300
H	0.72782400	-1.64594500	2.32985000
C	-1.17692000	0.40095300	2.91504200
O	-1.90189800	-0.56295200	2.74864900
C	-2.93304900	1.61499000	3.93976100
H	-3.21965200	0.70404800	4.46938500
H	-2.98765400	2.48367000	4.59523500
H	-3.57683600	1.74624200	3.07017800
H	3.25938200	-0.80969900	2.00483800
O	-1.55498700	1.54166700	3.51603100
O	-2.28010500	-4.37933200	-0.06945600
C	-2.51588400	-5.66330400	-0.62498800
H	-1.81415600	-6.41209400	-0.23323500
H	-3.53074300	-5.93597800	-0.33149800
H	-2.44803900	-5.64644600	-1.72074000
H	-1.76741600	-2.05819100	0.76651500
H	1.98004900	-4.08828500	-1.73695100

int32

C	-2.52206400	-1.97379900	1.42246500
C	-1.85576400	-3.12192100	0.97498400
C	-0.49208500	-3.04975800	0.69368300
C	0.23192700	-1.85351400	0.81318700
C	-0.44410600	-0.68757800	1.26239100
C	-1.80290000	-0.78143800	1.59299700
H	-2.38045700	-4.05929100	0.83785200
H	0.02147000	-3.94500300	0.35389600
C	0.40052800	2.50639400	-2.02696500
C	0.38169400	3.57693900	-0.88216800
O	0.25994800	4.73791900	-1.24970600
O	0.60724600	3.18081200	0.33113000

C	-1.63408500	0.34147800	-1.51215500
C	-2.67570400	1.13272500	-1.01619600
C	-1.93989500	-0.96513400	-1.90678200
C	-3.97450900	0.64941800	-0.91063300
C	-3.23144500	-1.47190500	-1.78757000
C	-4.24831500	-0.66335200	-1.29130600
F	-0.98142300	-1.78896200	-2.34714400
F	-3.49234700	-2.74666200	-2.10348400
F	-5.47918800	-1.15884800	-1.14858400
F	-4.94559100	1.41544700	-0.41013700
F	-2.42142100	2.36545200	-0.56172200
C	-0.57677500	2.83755100	-3.14781800
H	-0.30480000	3.82544700	-3.52582900
H	-0.51988700	2.10673000	-3.96075900
H	-1.60286200	2.90084500	-2.78401100
C	1.84938100	2.42634400	-2.54456800
H	2.54154000	2.10904500	-1.75830700
H	1.93690700	1.74235400	-3.39410300
H	2.13794400	3.43212300	-2.86252100
S	0.09825000	0.75852800	-1.34506000
C	3.94517500	-1.05560900	0.71549900
C	4.31816100	-1.62554300	-0.51003100
C	3.35563900	-2.29148500	-1.28077500
C	2.04040200	-2.37793300	-0.83898800
C	1.65157600	-1.80306200	0.38377200
C	2.62834900	-1.14772300	1.15440500
H	4.68902700	-0.54791500	1.31857200
H	3.65818600	-2.72054000	-2.23018500
H	1.28863900	-2.85169500	-1.46195000
H	2.35344700	-0.71985400	2.11245500
C	5.70726000	-1.55269900	-1.03872900
O	6.06985900	-2.03488300	-2.09519000
O	6.54212900	-0.88255200	-0.20990600
C	7.89848400	-0.77647900	-0.66922300
H	7.94104300	-0.25022600	-1.62673600
H	8.42780900	-0.21539200	0.10105900
H	8.34104100	-1.76828400	-0.79656500
Pd	0.22586500	1.21264500	0.91322500
C	0.89888300	1.74963800	5.31039100
H	1.83357000	1.32868000	5.69226900
H	0.10858200	1.49281300	6.02172400

H	0.98266200	2.83032700	5.20868700
C	0.58711600	1.13625400	3.97767000
O	0.43955300	1.82564700	2.96221900
O	0.49062800	-0.18050500	3.99822900
H	0.21678000	-0.49740700	3.09911800
O	-3.86135300	-1.89724000	1.66728500
C	-4.67465600	-3.01103500	1.31074200
H	-5.70291700	-2.70339600	1.50329300
H	-4.56513100	-3.25891300	0.24826200
H	-4.44032700	-3.89415600	1.91830800
H	-2.36205300	0.09352600	1.91555200

TS19

C	-2.39130100	-1.65084300	1.82500900
C	-1.78946000	-2.82508400	1.35160600
C	-0.43182100	-2.82732700	1.02544100
C	0.35943000	-1.67972300	1.14887700
C	-0.23938200	-0.48906000	1.65936400
C	-1.60276400	-0.50790400	2.00250500
H	-2.36528600	-3.73359700	1.22220300
H	0.01419000	-3.74812700	0.66208500
C	0.19821600	1.86915000	-2.50343300
C	0.20898300	3.18500000	-1.66951000
O	0.07001500	4.22806200	-2.28871300
O	0.47194600	3.11258500	-0.39465100
C	-1.81256800	-0.00714700	-1.36670400
C	-2.79520400	0.90069600	-0.95435300
C	-2.19647500	-1.33407500	-1.57980700
C	-4.10969900	0.50522300	-0.73768100
C	-3.50664000	-1.74878800	-1.35599700
C	-4.46063300	-0.83006600	-0.93245300
F	-1.29957800	-2.25598500	-1.94782800
F	-3.84044900	-3.03955800	-1.48639000
F	-5.70461000	-1.23807600	-0.67830600
F	-5.02414900	1.38128900	-0.32124600
F	-2.47197000	2.17665100	-0.72263100
C	-0.83254600	1.91671600	-3.62463300
H	-0.58613000	2.77584600	-4.25235800
H	-0.81077200	1.00428500	-4.22853100
H	-1.84181800	2.07351100	-3.23976700
C	1.62476300	1.66216300	-3.04774100

H	2.35409000	1.55618100	-2.23857300
H	1.68143300	0.78175700	-3.69445300
H	1.88940800	2.55114300	-3.62692400
S	-0.06551600	0.36364300	-1.38720200
C	4.08596600	-0.98566100	0.90384200
C	4.41051700	-1.64243400	-0.29175000
C	3.41006800	-2.32799300	-0.99301200
C	2.10744500	-2.35164400	-0.50965900
C	1.76860400	-1.69109200	0.68589500
C	2.78081700	-1.00879200	1.38543800
H	4.85937600	-0.46033700	1.45220900
H	3.67327500	-2.82378200	-1.92136400
H	1.32924700	-2.84348900	-1.08463900
H	2.54541800	-0.50065100	2.31361300
C	5.78503900	-1.64034500	-0.86344500
O	6.10024300	-2.19183700	-1.90111900
O	6.66253900	-0.95032500	-0.09902000
C	8.00690300	-0.90924500	-0.60281100
H	8.03494800	-0.43311500	-1.58674900
H	8.57569300	-0.32668300	0.12194000
H	8.41584300	-1.91938100	-0.69216800
Pd	0.26409200	1.39353600	0.66525000
C	1.37782600	2.87285000	4.59189000
H	2.44880300	2.73434800	4.77011700
H	0.85041000	2.57733100	5.50187500
H	1.17922100	3.91628000	4.34983100
C	0.96160400	1.97233600	3.45249500
O	0.63265700	2.52394800	2.35751900
O	0.97395100	0.71589500	3.64763100
H	0.45723100	0.17534800	2.56043700
O	-3.71678700	-1.51833500	2.11212300
C	-4.55753800	-2.66145600	1.98006100
H	-5.55854000	-2.32719100	2.25366000
H	-4.57430400	-3.03502300	0.94970200
H	-4.24399700	-3.46803300	2.65446700
H	-2.07833500	0.38087700	2.40797900
mono-p^p			
C	4.29093500	-0.27375800	-0.05873000
C	3.66381500	0.89403000	0.39213100
C	2.27094600	0.97456300	0.38658900

C	1.47123000	-0.08726600	-0.05753200
C	2.12465100	-1.25203900	-0.50478200
C	3.50779800	-1.34737200	-0.50850600
H	4.24152800	1.73487900	0.75615000
H	1.79886100	1.87656700	0.76417800
C	-2.19274100	-1.01282100	0.27265600
C	-2.82250200	0.19845100	-0.04491400
C	-2.03826300	1.31382600	-0.36828200
C	-0.65267500	1.21944700	-0.37565200
C	-0.00613600	0.01110100	-0.05531500
C	-0.80524500	-1.10061200	0.26858500
H	-2.79461000	-1.87602000	0.53215400
H	-2.53782500	2.24264800	-0.62205600
H	-0.05887200	2.08290600	-0.65882700
H	-0.32938100	-2.03584600	0.54664700
C	-4.30058700	0.35695100	-0.05516900
O	-4.88434400	1.38941100	-0.32584000
O	-4.94727200	-0.78774100	0.27471700
C	-6.37987400	-0.69373000	0.28347600
H	-6.75449000	-0.41446900	-0.70499000
H	-6.73880800	-1.68393600	0.56423800
H	-6.71304600	0.05573700	1.00647300
H	1.53699900	-2.08364100	-0.88140200
O	5.63974300	-0.46790300	-0.10165200
C	6.48562900	0.58635800	0.33435600
H	7.50702000	0.22423600	0.20914800
H	6.34767300	1.49298600	-0.26928200
H	6.31686600	0.83076900	1.39135200
H	4.01118500	-2.23973200	-0.86505000

int33

C	-0.30701400	2.05756900	-1.31949300
C	0.44376500	2.22420000	-0.15666700
C	-0.22045000	2.54483400	1.05701300
C	-1.60444200	2.63472300	1.10818100
C	-2.38486400	2.41580400	-0.06795800
C	-1.71252700	2.16860700	-1.28533300
H	-3.44238100	2.65176700	-0.02941300
Pd	-2.69318800	0.15170500	-0.50549000
C	-2.81279400	-2.73846900	-0.01451800
O	-2.98080300	-3.92553400	-0.23998700

O	-3.24371500	-1.77787500	-0.79031400
C	-5.34893300	0.78465200	-0.94571100
O	-5.38286400	0.71167500	0.28251500
O	-4.24868800	0.71566300	-1.66556300
H	0.36835300	2.73083700	1.94492100
H	0.16902000	1.78694800	-2.25349400
C	-2.12991200	-2.32642600	1.31715000
C	0.36926000	-1.22111300	0.25401000
C	1.47103900	-1.46008600	1.08532100
C	0.58910500	-1.24763900	-1.12896000
C	2.74200500	-1.69153200	0.57485100
C	1.86391200	-1.44472800	-1.65610500
C	2.94290400	-1.66099700	-0.80215400
F	-0.40400400	-1.04044500	-1.99697700
F	2.05674900	-1.40848900	-2.97566500
F	4.17058100	-1.80813300	-1.29617800
F	3.78223600	-1.85537600	1.39691500
F	1.33142700	-1.40733300	2.41776900
C	-3.22700400	-1.93308000	2.32460500
H	-3.86019600	-2.81163000	2.48162400
H	-2.79278300	-1.64098600	3.28585200
H	-3.86263200	-1.12501800	1.94870700
C	-1.21690400	-3.41949900	1.85542400
H	-0.44542700	-3.68977900	1.13094400
H	-0.74328900	-3.11562900	2.79289200
H	-1.82712700	-4.30970000	2.02244000
S	-1.15655900	-0.72033100	1.03901100
C	3.93033100	1.20513500	0.94817900
C	4.64670600	1.30231700	-0.25011200
C	4.00658800	1.79685600	-1.39435900
C	2.66336300	2.14660300	-1.35099300
C	1.91146100	1.99644700	-0.16893400
C	2.58094800	1.54410200	0.98285400
H	4.41616300	0.81025100	1.83203900
H	4.57857900	1.88420700	-2.31175300
H	2.19091600	2.53861100	-2.24526200
H	2.02794500	1.38078600	1.90190000
C	6.05985600	0.84722600	-0.37963900
O	6.71092700	0.92028100	-1.40316100
O	6.53645900	0.32311400	0.77002500
C	7.88560700	-0.16893700	0.70219100

H	8.57601100	0.63703300	0.43977000
H	8.10704000	-0.55808700	1.69577400
H	7.96666800	-0.95906700	-0.04896400
O	-2.32368200	2.92469600	2.21249700
C	-1.63876000	3.09364000	3.45066800
H	-1.07808700	2.18966600	3.71900500
H	-0.95559300	3.95146600	3.41534000
H	-2.41301500	3.27687500	4.19549500
C	-6.59949900	0.94939200	-1.79144200
H	-6.84338800	-0.01824300	-2.24170900
H	-7.42993500	1.27397500	-1.16308700
H	-6.43122100	1.65976800	-2.60459900
H	-2.28044900	2.14702900	-2.20934800

TS20

C	0.83155000	1.90937400	-0.92790500
C	1.56687700	1.49411800	0.19988600
C	0.88722800	1.23809400	1.40321700
C	-0.50391700	1.35929000	1.46954700
C	-1.26727100	1.75588400	0.33755600
C	-0.54747500	2.04636000	-0.84355100
H	-2.18385800	2.65606500	0.60585600
Pd	-3.09520000	0.68912400	-0.08907300
C	-4.78512700	-1.71260400	-0.54462100
O	-5.75504500	-2.38707800	-0.85702000
O	-4.73745700	-0.41483000	-0.59332300
C	-3.90142900	3.48652400	-0.17475400
O	-2.98201100	3.71099800	0.66862700
O	-4.09161700	2.36928000	-0.75712200
H	1.45863000	0.96158300	2.27998200
H	1.33869500	2.08349200	-1.87080300
C	-3.52170200	-2.52325500	-0.10014900
C	-0.68424400	-1.62856800	0.00891100
C	0.30540400	-2.16692100	0.84030800
C	-0.30357800	-1.25121200	-1.28424100
C	1.61567200	-2.32751700	0.40529600
C	1.00583300	-1.39715600	-1.73203000
C	1.96874700	-1.94117100	-0.88552400
F	-1.18593700	-0.70499900	-2.12789200
F	1.34798600	-0.98641700	-2.95448200
F	3.22885600	-2.06107600	-1.29419800

F	2.55241100	-2.79010700	1.24241900
F	0.02142400	-2.50066900	2.10756100
C	-3.89945900	-3.53939300	0.98255000
H	-4.69571200	-4.17058700	0.58058600
H	-3.04137400	-4.16186700	1.25583600
H	-4.27867400	-3.04808000	1.88298100
C	-2.93648300	-3.21573800	-1.33278700
H	-2.66393900	-2.50177200	-2.11064000
H	-2.06501000	-3.82524200	-1.07549800
H	-3.71878900	-3.86900700	-1.72772200
S	-2.29431400	-1.31537900	0.71484000
C	5.05219200	0.08593700	0.72780600
C	5.81644200	0.90216600	-0.11574100
C	5.18791800	1.92664500	-0.83548900
C	3.81735800	2.12428300	-0.72365500
C	3.03505600	1.30758900	0.11429100
C	3.68232000	0.29341400	0.84464600
H	5.53163200	-0.71363900	1.28025300
H	5.79460700	2.55906900	-1.47466900
H	3.34908000	2.93558300	-1.27112900
H	3.10805400	-0.36705900	1.48402600
C	7.28671200	0.72956500	-0.28583000
O	7.98052500	1.42344400	-1.00373700
O	7.77482200	-0.29358200	0.45124900
C	9.18999200	-0.51149900	0.32722900
H	9.74476200	0.37478800	0.64674500
H	9.41509300	-1.36002000	0.97323800
H	9.45487000	-0.73478000	-0.70972200
O	-1.22339100	1.09751600	2.58820800
C	-0.56075200	0.56588700	3.73305300
H	-0.07520600	-0.38862000	3.49700700
H	0.17763200	1.27024100	4.13480500
H	-1.34205900	0.40107800	4.47506900
C	-4.86669400	4.59875000	-0.51530800
H	-5.78675000	4.43916900	0.05631200
H	-4.44415200	5.56788700	-0.24973300
H	-5.12211100	4.55801000	-1.57563300
H	-1.10350700	2.37040800	-1.71922100
int34			
C	1.11259600	1.77118300	-0.98692300

C	1.85013200	1.26456400	0.09213200
C	1.16207400	0.85341300	1.24688700
C	-0.23311400	0.89481500	1.29493100
C	-0.99431000	1.33876800	0.18837300
C	-0.28343500	1.80772300	-0.92613100
H	-1.80211500	3.00095200	1.05285700
Pd	-2.97437100	0.91223600	-0.02515400
C	-5.28186500	-0.96579800	-0.45168400
O	-6.41164800	-1.39740100	-0.63037900
O	-4.94906500	0.28275500	-0.34361100
C	-3.17127600	3.91887400	0.14700100
O	-2.21938000	3.89982100	1.05922800
O	-3.53263200	2.92149800	-0.49207000
H	1.73277900	0.50524100	2.09910700
H	1.62258800	2.07839800	-1.89450000
C	-4.13587100	-2.04985000	-0.44471500
C	-1.14154400	-1.86016700	-0.05896100
C	-0.30285300	-2.51754400	0.85006600
C	-0.57961500	-1.46533500	-1.28096100
C	1.04153900	-2.74251000	0.57203100
C	0.75792900	-1.70023600	-1.58213600
C	1.56997700	-2.34531300	-0.65293600
F	-1.29384600	-0.78203100	-2.17973700
F	1.27099100	-1.28258600	-2.74029700
F	2.85871900	-2.55071900	-0.91853900
F	1.84112100	-3.29490500	1.49253800
F	-0.75506900	-2.87640300	2.05887300
C	-4.56918100	-3.31646500	0.29295600
H	-5.48338100	-3.68019500	-0.18197500
H	-3.79578300	-4.09001800	0.23736900
H	-4.79439500	-3.11463500	1.34319700
C	-3.76990400	-2.34445000	-1.90076200
H	-3.49906400	-1.43795800	-2.44063100
H	-2.94915000	-3.06552700	-1.97125900
H	-4.65608700	-2.77940600	-2.37152500
S	-2.72094000	-1.28621400	0.55802000
C	5.33972700	-0.16600700	0.47400200
C	6.11894800	0.81162300	-0.15922700
C	5.49489600	1.94120600	-0.70569300
C	4.11625900	2.09148200	-0.61937400
C	3.32297200	1.11930000	0.01591800

C	3.96040900	-0.01104900	0.55999600
H	5.81767400	-1.04718800	0.88604400
H	6.11204700	2.69251200	-1.18682800
H	3.64476600	2.98083200	-1.02590300
H	3.36857600	-0.79237000	1.02593900
C	7.59848600	0.70365300	-0.28086200
O	8.30799500	1.52961300	-0.82294800
O	8.08277000	-0.42730500	0.28404700
C	9.50725400	-0.58816400	0.19683500
H	10.01964500	0.23674200	0.69946900
H	9.72799800	-1.53498300	0.68995300
H	9.82894600	-0.61359900	-0.84788000
O	-0.95387300	0.47026000	2.38057700
C	-0.26192200	-0.06926200	3.50034900
H	0.32017100	-0.95708200	3.22573800
H	0.40029300	0.67404700	3.96145900
H	-1.03455600	-0.35820700	4.21341700
C	-3.80127300	5.26288300	-0.06233300
H	-4.24596500	5.59854600	0.87926200
H	-3.03197600	5.98873500	-0.34024300
H	-4.56507700	5.19718100	-0.83527900
H	-0.83461500	2.15640900	-1.79600400

int35

C	1.84122000	1.29908900	-1.16990600
C	2.46101300	1.04943800	0.06826100
C	1.65475300	0.83940400	1.19413400
C	0.26124300	0.83657300	1.07531600
C	-0.35591300	1.02179500	-0.16306500
C	0.44709400	1.29937600	-1.28342600
Pd	-2.28749300	0.44805200	-0.36356400
H	-0.35359400	0.66660800	1.95501600
H	2.11324600	0.68507500	2.16628400
O	-0.21587000	1.50295200	-2.46860000
C	0.53274100	1.42492700	-3.67436100
H	-0.19543200	1.48514400	-4.48475100
H	1.24332600	2.25637000	-3.77059400
H	1.07552300	0.47349700	-3.73777200
H	2.46267900	1.44218300	-2.04578500
C	-3.53515400	1.81984300	0.89928300
C	-4.81578800	2.25485900	0.19535900

C	-3.14924600	3.59275000	-0.56737600
C	-2.51693800	2.63852900	0.42638000
C	-4.27566900	2.72747500	-1.17177600
H	-5.00829300	3.31773300	-1.73123900
H	-3.90997400	1.91263600	-1.80177900
C	-5.14937800	3.63512800	0.85395700
H	-6.12247400	3.98702300	0.49894200
H	-5.20130200	3.56796000	1.94379300
C	-3.99181800	4.55580800	0.34658200
H	-4.37151400	5.38821800	-0.25348100
H	-3.39550000	4.98099000	1.15909300
H	-5.61057800	1.51432800	0.19931500
H	-1.60985000	2.86210500	0.97169500
C	-3.50123200	1.10952300	2.20905200
O	-2.49742300	0.89662600	2.86741900
C	-4.80742300	-0.05065500	3.78431200
H	-4.25641300	-0.98504600	3.65213400
H	-4.38657100	0.49934500	4.62998800
H	-5.86716700	-0.25015600	3.93735100
C	-3.05446700	-2.46839300	-1.63307900
C	-4.13394400	-1.88051200	-0.66234400
O	-4.11762200	-0.59972500	-0.45018800
O	-4.99149000	-2.66007700	-0.27031600
C	-0.27880700	-2.09638000	-0.57694600
C	-0.51386100	-2.38567500	0.77011100
C	1.04203300	-2.13508000	-1.03397100
C	0.52296900	-2.70293900	1.63841000
C	2.09609400	-2.43724400	-0.17639500
C	1.83256600	-2.72156200	1.15976400
F	1.33369200	-1.82176500	-2.30317700
F	3.35406100	-2.42532400	-0.62203100
F	2.84421900	-2.96733000	1.99665400
F	0.28010800	-2.94417300	2.92859400
F	-1.75519100	-2.29099200	1.26534900
C	-2.72015700	-3.92191400	-1.31913000
H	-3.65137900	-4.48818800	-1.38775100
H	-1.99211800	-4.32899700	-2.02753300
H	-2.34497300	-4.03959700	-0.30248100
C	-3.61833100	-2.31794700	-3.05945900
H	-3.79771400	-1.26801400	-3.31069900
H	-2.94679100	-2.75521900	-3.80439400

H	-4.57853800	-2.84089600	-3.09323400
S	-1.50124100	-1.38321700	-1.66097900
C	6.14263100	1.80773000	-0.45987600
C	6.74799900	0.83387600	0.34648900
C	5.94289700	-0.06324600	1.06150900
C	4.55856500	0.01018500	0.97287800
C	3.93819600	0.98416600	0.16797300
C	4.75608300	1.87879900	-0.54465800
H	6.76202200	2.50890200	-1.00737200
H	6.42490200	-0.81852100	1.67311900
H	3.95192400	-0.71429400	1.50539500
H	4.29502600	2.65315600	-1.15035100
C	8.22378200	0.70551800	0.47891900
O	8.78699100	-0.12392200	1.16805400
O	8.89284200	1.62351000	-0.26003300
C	10.32347100	1.54812500	-0.16929600
H	10.68134400	0.57363300	-0.51304000
H	10.70254700	2.34421000	-0.81052700
H	10.65322500	1.69531200	0.86289500
H	-2.46191800	4.09127500	-1.25099000
O	-4.73423800	0.73593100	2.58092600

TS21

C	-1.58574100	-1.49657600	-0.97581600
C	-2.22885900	-1.11468500	0.21739500
C	-1.44115300	-0.81318000	1.34014800
C	-0.05245500	-0.88682000	1.26413000
C	0.59818200	-1.24386300	0.07273800
C	-0.19233300	-1.57924900	-1.04729400
Pd	2.40609900	-0.25728600	-0.25088000
H	0.55455900	-0.67720500	2.14205500
H	-1.91476000	-0.54956200	2.28022300
O	0.48878700	-1.90859000	-2.18475300
C	-0.23679100	-2.01483500	-3.40362000
H	0.50797900	-2.20186600	-4.17822100
H	-0.95073700	-2.84827500	-3.38160900
H	-0.77106000	-1.08266900	-3.62599900
H	-2.18730000	-1.68309200	-1.85656600
C	3.42171500	-1.80299600	0.75495000
C	4.43928400	-2.47762500	-0.16841500
C	2.48826800	-3.61306100	-0.42808900

C	2.19815500	-2.53888300	0.60385000
C	3.53472600	-2.93655300	-1.33661000
H	4.03585300	-3.64872800	-2.00026700
H	3.11663300	-2.11903300	-1.92882000
C	4.75154900	-3.84873200	0.50481100
H	5.55711800	-4.35758400	-0.03380600
H	5.07161100	-3.72963900	1.54297000
C	3.39938100	-4.61975400	0.36060200
H	3.51631800	-5.53394000	-0.22868200
H	2.96565500	-4.90609600	1.32357300
H	5.30491400	-1.86300500	-0.40827600
H	1.60463600	-2.77809500	1.47570500
C	3.75623800	-1.18703100	2.06450300
O	2.93479500	-0.90913100	2.92599200
C	5.46771900	-0.17330600	3.32202200
H	5.01904100	0.82162700	3.26669700
H	5.15382200	-0.66277100	4.24752100
H	6.55353700	-0.10414900	3.26724200
C	2.85612200	2.65108000	-1.63783300
C	3.98196200	2.21627500	-0.63589200
O	4.08315700	0.95998200	-0.32482000
O	4.77143300	3.09311100	-0.31007600
C	0.12164700	2.06960500	-0.59037500
C	0.32183500	2.42924000	0.74622900
C	-1.19177400	2.05281400	-1.07101300
C	-0.73948500	2.77204300	1.57572900
C	-2.26828100	2.39002000	-0.25568200
C	-2.03745400	2.75106500	1.06837600
F	-1.45159400	1.66436600	-2.32629200
F	-3.51626200	2.34029900	-0.72804300
F	-3.06969600	3.02921100	1.87092600
F	-0.52830100	3.08934300	2.85525000
F	1.55510500	2.41496500	1.26687900
C	2.38301000	4.07818400	-1.38255400
H	3.25516900	4.72960300	-1.46567100
H	1.62618200	4.38469900	-2.11125100
H	1.98609900	4.19828400	-0.37391200
C	3.45018100	2.50574800	-3.05239500
H	3.72917500	1.46931300	-3.26679600
H	2.75034500	2.85352200	-3.81819900
H	4.35870600	3.11336300	-3.09426800

S	1.40539200	1.42762600	-1.64357200
C	-5.90208400	-1.82889900	-0.41767300
C	-6.52146500	-0.83808100	0.35623000
C	-5.72907300	0.05130800	1.09347700
C	-4.34405000	-0.04316500	1.05469100
C	-3.70721700	-1.02725600	0.27520700
C	-4.51488000	-1.91960500	-0.45378200
H	-6.51142000	-2.52754400	-0.97936700
H	-6.21947600	0.81875700	1.68262100
H	-3.75386600	0.67513900	1.61115000
H	-4.04884100	-2.71025600	-1.03349900
C	-7.99982300	-0.68380500	0.43176700
O	-8.57206300	0.15951900	1.09547500
O	-8.65487100	-1.59305100	-0.32829100
C	-10.08712100	-1.49138300	-0.29564600
H	-10.41214300	-0.51192600	-0.65713100
H	-10.45419800	-2.28318000	-0.94885600
H	-10.46019000	-1.62816800	0.72303500
H	1.61529900	-4.05790900	-0.90398500
O	5.07271400	-0.94913800	2.17604100

int36

C	-0.23028500	2.73785900	0.24275700
C	-0.98308500	2.01139100	-0.70850600
C	-0.30187800	1.29101200	-1.68613000
C	1.10204200	1.26353500	-1.69450400
C	1.88632900	1.97665200	-0.74427300
C	1.16155300	2.74472700	0.22975600
Pd	2.02721700	-0.12715600	0.05659100
H	1.62127500	0.78095900	-2.51767300
H	-0.84162600	0.76041200	-2.46223500
O	1.90350700	3.44225300	1.12413200
C	1.25078600	4.13750000	2.18006400
H	2.04780100	4.58882100	2.77167200
H	0.59156700	4.92601700	1.79644700
H	0.67094100	3.45184500	2.81035900
H	-0.75920800	3.26613900	1.02404600
C	3.83241200	0.48078800	-0.73520100
C	4.93678200	0.54485900	0.32516200
C	4.38127800	2.71777400	-0.05363000
C	3.41774600	1.95588100	-0.99627500

C	4.50268200	1.76950100	1.15974900
H	5.27264400	2.08930000	1.87040300
H	3.56261600	1.62794600	1.69834100
C	6.20325300	1.11112700	-0.37583000
H	7.05768700	1.05968700	0.30741900
H	6.47149200	0.54598400	-1.27147900
C	5.80046000	2.59249000	-0.67225700
H	6.48397600	3.29497100	-0.18545600
H	5.80468600	2.82496300	-1.74223700
H	5.08520800	-0.39744700	0.85115900
H	3.57703300	2.24906000	-2.03940700
C	4.01688100	-0.40622900	-1.91557600
O	3.50596200	-0.23615000	-3.01596200
C	4.90508900	-2.45818200	-2.65976300
H	5.30782600	-2.02768200	-3.58066700
H	5.57458200	-3.22065600	-2.26274800
H	3.92085000	-2.88680200	-2.86731600
C	0.98077800	-1.86408500	2.53156900
C	2.12441500	-2.56117700	1.72438600
O	2.80308700	-1.84012700	0.87744600
O	2.38092500	-3.72272900	2.00880400
C	-1.16902600	-1.55804400	0.59827200
C	-0.92188500	-2.23352400	-0.60341900
C	-2.48348400	-1.55686900	1.08248200
C	-1.94692100	-2.85366600	-1.31465700
C	-3.51974400	-2.17149900	0.38647600
C	-3.25008200	-2.81523000	-0.81858200
F	-2.78278400	-0.92857300	2.22300200
F	-4.77591800	-2.10463000	0.83711400
F	-4.24217900	-3.38375400	-1.50390400
F	-1.69040600	-3.48342400	-2.46356300
F	0.31020100	-2.29355400	-1.11821400
C	0.00301400	-2.87758300	3.11736000
H	0.55864600	-3.54344500	3.78032600
H	-0.79427400	-2.37969900	3.67757100
H	-0.44077000	-3.49920000	2.33659800
C	1.63885200	-1.01257300	3.63303300
H	2.29605900	-0.24581000	3.21185600
H	0.88632800	-0.53428800	4.26746400
H	2.25118000	-1.67514600	4.25242800
S	0.05800900	-0.59950300	1.46343000

C	-4.56345400	0.78628100	-0.91219100
C	-5.27497900	1.89083600	-0.42639000
C	-4.57863200	3.05042800	-0.06132300
C	-3.19334900	3.10072700	-0.16317300
C	-2.46419200	1.99511700	-0.63716500
C	-3.17893800	0.84649500	-1.02167100
H	-5.09499900	-0.11960100	-1.18015500
H	-5.14521000	3.90222300	0.29941600
H	-2.67251500	4.01428900	0.10620400
H	-2.63815400	-0.02301100	-1.37609800
C	-6.75703800	1.88712600	-0.27637400
O	-7.40789300	2.82649600	0.13934400
O	-7.30896200	0.71295000	-0.65570100
C	-8.73868500	0.64239200	-0.53093500
H	-9.21658300	1.40559500	-1.15106700
H	-9.01464900	-0.35640500	-0.86877000
H	-9.04164900	0.79578400	0.50829500
O	4.80519200	-1.46091800	-1.63160600
H	4.08017300	3.74263700	0.15623500

int37

C	1.94159700	-2.03142500	1.25223900
C	2.56729800	-1.91018900	-0.00757800
C	1.85138000	-2.25596200	-1.14890500
C	0.52138300	-2.69233000	-1.04099600
C	-0.13040900	-2.82247300	0.21842400
C	0.63350600	-2.47987500	1.38229000
Pd	-1.01621800	-0.77737200	-0.50637700
H	-0.00043400	-3.05190500	-1.92265900
H	2.31298900	-2.19277600	-2.12763200
C	-2.43267900	-2.25136200	-0.35550000
C	-3.58600300	-2.11281100	0.63994500
C	-2.30347600	-3.78065200	1.49560900
C	-1.55735400	-3.40843500	0.18957000
C	-2.88329400	-2.42950000	1.97173500
H	-3.58713500	-2.54517600	2.80344700
H	-2.13139500	-1.69137100	2.24036200
C	-4.47608900	-3.37816800	0.45797900
H	-5.40766900	-3.25056100	1.01900000
H	-4.75323200	-3.55309900	-0.58569600
C	-3.59507700	-4.52003900	1.06060500

H	-4.07944500	-4.97297500	1.93121900
H	-3.39539200	-5.32302100	0.34396300
H	-4.13158300	-1.17511400	0.56404900
H	-1.54276000	-4.25740400	-0.50095400
C	-2.77010000	-2.29053500	-1.81700100
O	-2.23201700	-2.99863600	-2.65235600
C	-4.06573800	-1.30149100	-3.52865000
H	-4.86581900	-0.56425900	-3.59026200
H	-3.18733100	-0.96677000	-4.08808400
H	-4.39432900	-2.26583000	-3.92373500
C	-3.62142300	1.92283100	2.02877500
C	-3.09142000	1.33327100	0.71002800
O	-2.14412900	0.50255000	0.83223800
O	-3.59651100	1.74470500	-0.37418400
C	-0.91123500	2.91942100	1.77448500
C	-0.04394800	2.03209300	2.42330600
C	-0.49339400	3.41496900	0.53026400
C	1.18260300	1.67235400	1.87637700
C	0.73641100	3.07488300	-0.02155900
C	1.57889000	2.19719500	0.65111000
F	-1.29415800	4.20681500	-0.19569500
F	1.08395400	3.53265600	-1.23241500
F	2.74326300	1.83799100	0.11261100
F	1.98029800	0.79810200	2.51583700
F	-0.38577800	1.46573800	3.59110600
C	-5.01994600	2.52560100	1.86655600
H	-5.73578900	1.72138900	1.66590400
H	-5.33010600	3.03118800	2.78673300
H	-5.05195100	3.22987100	1.03553200
C	-3.57671700	0.89534100	3.16304000
H	-2.56684300	0.51928600	3.31189800
H	-3.92917600	1.34938900	4.09311500
H	-4.22930600	0.04891500	2.91982200
S	-2.48581700	3.39486000	2.44677300
Ag	-2.26328800	1.42569500	-2.02223600
O	0.61590600	0.50004600	-1.41882300
C	0.54144900	0.99046000	-2.58281100
O	-0.53206000	1.24082900	-3.22745900
C	1.84519700	1.30402700	-3.29257400
H	2.55424600	1.71901200	-2.57496400
H	2.26209900	0.37468000	-3.69605600

H	1.68183800	2.00036500	-4.11526200
O	0.01833600	-2.61941300	2.58434000
C	0.62336500	-2.05579900	3.74610500
H	0.80433500	-0.98422300	3.61656800
H	-0.09394700	-2.21306200	4.55256600
H	1.56338200	-2.56279500	3.99724300
C	6.22574900	-1.30903400	0.79250900
C	6.59378300	-0.43137800	-0.23665300
C	5.64023100	-0.04769600	-1.18923800
C	4.34073900	-0.53228000	-1.11376000
C	3.95948400	-1.41123200	-0.08616300
C	4.92288200	-1.79108200	0.86424500
H	6.96425900	-1.61363500	1.52501400
H	5.93728000	0.64118100	-1.97287900
H	3.59543800	-0.20384000	-1.82605100
H	4.65363600	-2.48953700	1.65085200
C	7.96989800	0.12160700	-0.36430200
O	8.32838700	0.88445800	-1.24112200
O	8.79787300	-0.31924500	0.61240300
C	10.14227800	0.18006800	0.53964900
H	10.15316500	1.27094100	0.61458200
H	10.66953300	-0.26786400	1.38215100
H	10.61013200	-0.10894900	-0.40545500
H	2.49090500	-1.72469200	2.13121000
H	-1.69486100	-4.32677800	2.21464700
O	-3.75056200	-1.40790100	-2.12729300

TS22

C	3.10917800	-1.58966400	1.84449500
C	3.16715700	-0.97327600	0.57976900
C	1.99428600	-0.87267700	-0.16744800
C	0.76763900	-1.31964500	0.35755000
C	0.69843300	-1.85980400	1.66102600
C	1.89868200	-2.04370900	2.37478900
Pd	-0.99055700	-0.37715500	-0.16003600
H	0.17480000	-2.04456600	-0.62124700
H	2.03056600	-0.47890500	-1.17896600
C	-1.79290600	-1.60357300	1.30998200
C	-2.62037900	-0.69737200	2.23855700
C	-0.98912000	-1.50110400	3.59369500
C	-0.65797200	-2.18523400	2.22341700

C	-1.52649800	-0.12389100	3.16450600
H	-1.93745500	0.45635600	3.99764800
H	-0.78386900	0.48405600	2.64272200
C	-3.39175500	-1.62138800	3.22879300
H	-4.11552100	-1.02004600	3.78851100
H	-3.95532300	-2.40709400	2.71810300
C	-2.26358400	-2.17184500	4.15605800
H	-2.42593100	-1.87061100	5.19584400
H	-2.19563700	-3.26385500	4.13740700
H	-3.25909800	0.00743300	1.70813200
H	-0.76114600	-3.27220100	2.31469700
C	-2.54164400	-2.65369100	0.53506100
O	-2.19293700	-3.81618700	0.43324500
C	-4.42759300	-3.14388700	-0.79115300
H	-5.26061200	-2.58760900	-1.22054000
H	-3.80202800	-3.58062400	-1.57316000
H	-4.79366400	-3.93815000	-0.13481600
C	-3.79086900	2.71267200	-1.57234400
C	-3.06044900	1.35976300	-1.58271900
O	-2.65288700	0.94969600	-0.45347900
O	-2.89872900	0.78392700	-2.69824100
C	-1.51586500	3.65611300	-0.07365400
C	-1.92081600	4.11891200	1.18558500
C	-0.34362500	2.89031800	-0.11998100
C	-1.21374600	3.81172500	2.34628400
C	0.39889400	2.60743600	1.02067200
C	-0.04967000	3.05284100	2.26066600
F	0.07488900	2.34201700	-1.27579500
F	1.50717000	1.85726900	0.94744700
F	0.62030500	2.72293600	3.36679600
F	-1.64671500	4.23394300	3.53917400
F	-3.03100700	4.85302400	1.31600700
C	-4.54692900	2.97260900	-2.87900600
H	-5.33695800	2.22314400	-2.98631600
H	-5.01151800	3.96287300	-2.86240600
H	-3.88996000	2.89049800	-3.74602400
C	-4.71008100	2.83498900	-0.35523300
H	-4.16601700	2.66581700	0.57306800
H	-5.17208000	3.82420700	-0.32600500
H	-5.49908100	2.07690500	-0.42428100
S	-2.43068500	4.03263500	-1.55087100

Ag	-2.13431200	-1.20412500	-2.76939500
O	0.25714900	-3.08412800	-1.49732400
C	-0.64413600	-3.73522300	-2.10714200
O	-1.62097700	-3.24474800	-2.75901900
C	-0.55985900	-5.24553500	-2.04963600
H	0.48322900	-5.56568600	-2.02686200
H	-1.03530000	-5.54830900	-1.11110800
H	-1.09160000	-5.70226200	-2.88537800
O	1.78802800	-2.66310600	3.58889600
C	2.96153600	-2.85778500	4.36486500
H	3.43081500	-1.90297100	4.63630500
H	2.63875700	-3.37040000	5.27217300
H	3.69479700	-3.48247500	3.83843400
C	6.84990900	-0.61111800	-0.26542300
C	6.86053500	0.62699100	-0.92288000
C	5.65984000	1.33172900	-1.08515100
C	4.46816000	0.80896100	-0.59804800
C	4.44573200	-0.43383700	0.06087600
C	5.65466900	-1.13239500	0.21958000
H	7.77634800	-1.16111600	-0.14650800
H	5.68674400	2.29324100	-1.58683700
H	3.54634200	1.37440500	-0.69388700
H	5.64986900	-2.10433600	0.70428800
C	8.10593500	1.23878900	-1.46062900
O	8.15734700	2.31115000	-2.03249200
O	9.19808700	0.46755600	-1.24370700
C	10.43122400	1.00917100	-1.74137300
H	10.64741400	1.97202000	-1.27023600
H	11.19852000	0.27707300	-1.48882000
H	10.37960500	1.15509400	-2.82383300
H	4.02353500	-1.67908900	2.41827300
H	-0.14493900	-1.50343900	4.28020800
O	-3.67283300	-2.17658900	-0.03169500

int38

C	3.32958600	-1.54385700	1.69750900
C	3.27050900	-0.42461400	0.84738000
C	2.02986300	-0.03087000	0.31855200
C	0.86188500	-0.74248500	0.63781300
C	0.92718700	-1.86187600	1.48589300
C	2.16895200	-2.25651200	2.01293800

Pd	-0.91123900	-0.22485400	-0.05067600
H	1.48325700	-2.01037300	-1.06752300
H	1.98381400	0.82377500	-0.35218900
C	-1.50501000	-1.97185300	0.89868100
C	-2.56925400	-1.57638900	1.94380600
C	-0.89963300	-2.46405600	3.19760800
C	-0.34807200	-2.60008300	1.74386600
C	-1.68406600	-1.13767700	3.13279700
H	-2.26320100	-0.93574000	4.04018200
H	-1.05325400	-0.27255900	2.91794200
C	-3.19561500	-2.88486200	2.51089000
H	-4.06604700	-2.63398200	3.12620900
H	-3.54390200	-3.55415700	1.72030600
C	-2.04211500	-3.48980500	3.37396800
H	-2.33381500	-3.56313400	4.42665300
H	-1.74825700	-4.49184900	3.04499700
H	-3.30748700	-0.86417600	1.57245100
H	-0.21423100	-3.65809900	1.48982100
C	-1.93969000	-2.78735100	-0.27593900
O	-1.25356000	-3.61016500	-0.86935100
C	-3.66430700	-3.15597400	-1.84640200
H	-4.70509300	-2.85589800	-1.96753700
H	-3.07384400	-2.82587900	-2.70795200
H	-3.58174900	-4.24262500	-1.76044500
C	-4.00192500	2.15516000	-2.11492800
C	-2.91958400	1.07295100	-1.95434000
O	-2.80824900	0.56838300	-0.80270100
O	-2.21388700	0.78915300	-2.97348400
C	-2.88262000	3.25935700	0.30565800
C	-3.84472700	3.25193200	1.32382700
C	-1.58835500	2.85588300	0.65681500
C	-3.54627500	2.82590800	2.61645600
C	-1.26114800	2.45520500	1.94742900
C	-2.24998500	2.42262300	2.92683600
F	-0.61989300	2.77293500	-0.27670300
F	-0.02080600	2.04167000	2.24261500
F	-1.95613800	1.99290400	4.15579100
F	-4.49487900	2.79913300	3.55930800
F	-5.10394800	3.62711800	1.07321400
C	-4.25389200	2.52042400	-3.58049700
H	-4.64580200	1.64227500	-4.10246400

H	-4.99252900	3.32416300	-3.65482900
H	-3.33329100	2.82203200	-4.08245200
C	-5.29259400	1.73859000	-1.40575700
H	-5.10817200	1.48845500	-0.36190000
H	-6.03449900	2.53846900	-1.46040900
H	-5.69928500	0.84616800	-1.89656600
S	-3.27820400	3.73977400	-1.36007100
Ag	-0.77108500	-0.80350700	-2.85785400
O	1.71836900	-2.92341200	-1.34494200
C	1.10864100	-3.29464600	-2.44903700
O	0.49455100	-2.53250700	-3.20759700
C	1.21005000	-4.76366800	-2.72109700
H	2.15898500	-5.16724000	-2.36457400
H	0.39631500	-5.22809800	-2.15335600
H	1.06789200	-4.96087200	-3.78326300
O	2.14032900	-3.35961200	2.82187500
C	3.35953800	-3.81816300	3.38515700
H	3.81420100	-3.06146300	4.03818200
H	3.10562300	-4.69815000	3.97840600
H	4.08299200	-4.10201400	2.60932400
C	6.87920500	0.36199700	-0.02860900
C	6.84893500	1.76058000	-0.11996400
C	5.64255600	2.43766600	0.10553400
C	4.48840900	1.73055000	0.41950000
C	4.50478600	0.32657500	0.51457300
C	5.72066600	-0.34175200	0.28297200
H	7.80819900	-0.16558200	-0.21231300
H	5.63578700	3.52051300	0.03976300
H	3.56577900	2.26650800	0.62011300
H	5.74717100	-1.42653500	0.32314000
C	8.05302800	2.56947300	-0.44795000
O	8.06839700	3.78268900	-0.53706800
O	9.15513700	1.80471100	-0.64137000
C	10.34970300	2.53363900	-0.96092800
H	10.60529800	3.22811300	-0.15580400
H	11.13064400	1.78259700	-1.08230300
H	10.21818700	3.10493500	-1.88405800
H	4.28418900	-1.82861900	2.12182200
H	-0.11137000	-2.53482900	3.94850800
O	-3.21234700	-2.51053700	-0.64918900

int39

C	0.77046500	2.16126700	3.17342200
C	1.22177300	2.13485100	1.83908500
C	0.58118600	1.29424700	0.91670200
C	-0.51028300	0.50901200	1.31871800
C	-0.99410300	0.57190800	2.63570600
C	-0.32650700	1.39323500	3.56535000
Pd	-1.51620500	-0.64240100	0.04102700
H	0.90956500	1.27143300	-0.11467300
O	-0.83322100	1.36539500	4.83788800
C	-0.21896800	2.17514100	5.82785000
H	-0.78247200	2.00683500	6.74712200
H	0.82951200	1.89231400	5.99085200
H	-0.26450500	3.24082300	5.56606600
H	1.29824700	2.77209600	3.89477800
C	-2.69825500	-1.05892400	1.74101200
C	-4.17422200	-0.64222500	1.56095000
C	-3.47529700	0.67151600	3.26755100
C	-2.22023800	-0.21236800	2.97571800
C	-4.08399400	0.86840300	1.86327500
H	-5.06373600	1.35891600	1.88917900
H	-3.43159500	1.40674000	1.17020500
C	-5.01359400	-1.14390100	2.77010300
H	-6.08147700	-1.01002900	2.56459100
H	-4.85646400	-2.20665300	2.96835300
C	-4.54083800	-0.22194900	3.93989000
H	-5.36690900	0.38680900	4.32249100
H	-4.13015800	-0.78382400	4.78521600
H	-4.59837500	-0.92261300	0.59692700
H	-2.01675900	-0.85299000	3.84283200
C	-2.38301400	-2.49770900	1.84909700
O	-1.35452000	-2.98601500	2.35922500
C	-2.97048800	-4.70586400	1.23247200
H	-3.82750700	-5.18966800	0.76397000
H	-2.06962500	-4.84907400	0.62801800
H	-2.79503900	-5.11373300	2.23038500
C	1.79848600	-0.95578700	-2.94996500
C	0.87951000	-1.18026700	-1.72739900
O	1.17031400	-2.16017300	-0.98298000
O	-0.08128800	-0.36628100	-1.57722500
C	4.06131200	-1.54571900	-1.28820900

C	3.74814600	-1.62097900	0.07290500
C	4.83113600	-2.58878900	-1.81876800
C	4.11074200	-2.70784600	0.85571500
C	5.23475300	-3.67411400	-1.04182600
C	4.85778000	-3.74221700	0.29813100
F	5.17279000	-2.59219400	-3.11117200
F	5.95975400	-4.66166500	-1.57877800
F	5.20794200	-4.79296700	1.04138800
F	3.68369900	-2.79030900	2.12903800
F	3.01439200	-0.66448300	0.66478800
C	2.03292200	-2.27625200	-3.68707600
H	1.07902400	-2.62973100	-4.09656600
H	2.73991500	-2.14086200	-4.50862400
H	2.40556800	-3.04330100	-3.00795900
C	1.26109400	0.12614200	-3.89135100
H	1.11654100	1.07579900	-3.37222800
H	1.93929100	0.27302200	-4.73690600
H	0.28871300	-0.19345300	-4.27804900
S	3.43239900	-0.23262900	-2.30681800
Ag	0.52843600	-2.13866000	1.20149200
C	-3.08267700	2.48967700	-2.67462400
C	-4.37503600	2.91402900	-2.34108000
C	-5.34339600	1.97458400	-1.96554000
C	-5.02452200	0.61722600	-1.91847600
C	-3.72991400	0.22516100	-2.25311200
C	-2.74551300	1.13813200	-2.63346700
H	-2.34402800	3.23349200	-2.95379600
H	-6.34213600	2.30518000	-1.70535800
H	-5.76776800	-0.10996600	-1.61304900
H	-1.73404700	0.81268400	-2.84667400
I	-3.19015100	-1.85777200	-2.05590200
C	-4.66117500	4.37720800	-2.39662000
O	-3.85467400	5.21965200	-2.73758000
O	-5.92673600	4.66909100	-2.02275900
C	-6.26103000	6.06714100	-2.04815900
H	-5.61160200	6.62875800	-1.37144200
H	-6.14767300	6.47078100	-3.05780800
H	-7.29970300	6.12733200	-1.72350800
H	-3.22945800	1.57342700	3.82986400
O	-3.30928700	-3.30987800	1.30268300
C	4.31188100	3.38386800	0.02168000

C	4.50187400	4.64246200	0.60970400
C	3.60766800	5.07748000	1.59737500
C	2.54862500	4.26886800	1.99088300
C	2.35303000	2.99806500	1.41698600
C	3.25437800	2.57498400	0.42247700
H	4.99878700	3.03971200	-0.74332300
H	3.75587900	6.05897700	2.03533100
H	1.84559800	4.63557300	2.73242900
H	3.13692800	1.59774700	-0.02819200
C	5.61651800	5.54862700	0.22947900
O	5.81586800	6.64577600	0.71741300
O	6.40901200	5.02089600	-0.73573100
C	7.50320600	5.85414500	-1.14383600
H	8.16478300	6.06562800	-0.29900200
H	8.03215500	5.29151200	-1.91357600
H	7.13768000	6.80382400	-1.54451900

TS23

C	0.86643800	1.47388200	3.23905300
C	1.20451200	1.73963000	1.89604600
C	0.43824400	1.16926800	0.87242400
C	-0.67064600	0.36932400	1.18663500
C	-1.04943600	0.15331500	2.52338600
C	-0.24516200	0.69223300	3.55059600
Pd	-1.80041200	-0.45240500	-0.26212700
H	0.69284700	1.34996400	-0.16424900
O	-0.64718400	0.39080100	4.82307100
C	0.11013400	0.90211200	5.91079200
H	-0.38774400	0.55009200	6.81549500
H	1.14176700	0.52699500	5.89647700
H	0.12758200	1.99988600	5.91043600
H	1.49433800	1.87304500	4.02544800
C	-2.98069500	-1.07908400	1.44830100
C	-4.40773800	-0.51538800	1.53098100
C	-3.44390800	0.29548100	3.41252800
C	-2.31711800	-0.58888200	2.78996300
C	-4.13496400	0.86962600	2.16013300
H	-5.05128700	1.42405800	2.39142200
H	-3.47839500	1.49887200	1.55581100
C	-5.19188000	-1.21537600	2.68159300
H	-6.24976700	-0.94017400	2.61576600

H	-5.14141600	-2.30395700	2.61934200
C	-4.53403800	-0.63944400	3.97422200
H	-5.25745900	-0.07273500	4.56940100
H	-4.11640900	-1.41705400	4.62228900
H	-4.93954200	-0.55787500	0.58107600
H	-2.11530100	-1.43912000	3.45308900
C	-2.84188800	-2.54173800	1.23503500
O	-1.84305300	-3.21867400	1.54906800
C	-3.73096100	-4.48807200	0.23285800
H	-4.68041400	-4.76290400	-0.22476200
H	-2.91960600	-4.55180700	-0.49721700
H	-3.50668300	-5.13450500	1.08406500
C	1.83259200	-1.06118300	-3.02313600
C	0.83159100	-1.23034300	-1.85619200
O	0.99020300	-2.26052700	-1.13612500
O	-0.04614700	-0.33431500	-1.71511500
C	3.92470900	-1.76835400	-1.19388600
C	3.48614000	-1.79923800	0.13394500
C	4.67187600	-2.86608000	-1.63934900
C	3.71048600	-2.89073800	0.96071100
C	4.93767700	-3.95849500	-0.81422600
C	4.43892100	-3.97866900	0.48700500
F	5.12515600	-2.91435000	-2.89543400
F	5.64459100	-4.99781400	-1.27092400
F	4.65331500	-5.03544300	1.27212000
F	3.15947700	-2.92593800	2.18869200
F	2.75332800	-0.79455800	0.63964400
C	2.03244600	-2.39018800	-3.75470400
H	1.08476200	-2.68859100	-4.21791800
H	2.79050500	-2.29048800	-4.53495300
H	2.32453300	-3.17997500	-3.06231000
C	1.41198200	0.05502900	-3.98314900
H	1.32228000	1.01464300	-3.46957300
H	2.12961800	0.15042500	-4.80306000
H	0.43176100	-0.19112300	-4.40221300
S	3.46762100	-0.44049400	-2.28229900
Ag	0.15317900	-2.25522700	0.91072800
C	-2.15817700	3.14721400	-2.34917800
C	-3.29688700	3.76717000	-1.81804100
C	-4.26604700	2.98811800	-1.17181900
C	-4.09109400	1.61265000	-1.03367000

C	-2.90898100	1.03822000	-1.50019600
C	-1.96604100	1.77318700	-2.22532700
H	-1.42696500	3.75539700	-2.87188400
H	-5.16628300	3.45427300	-0.78759900
H	-4.85695600	1.01555200	-0.56285800
H	-1.09095100	1.29437900	-2.64085400
I	-3.32009500	-1.34462000	-2.38775100
C	-3.43890300	5.23678600	-1.99610900
O	-2.63614400	5.94190400	-2.57710100
O	-4.57302200	5.71792100	-1.43376600
C	-4.76551600	7.13429100	-1.57308900
H	-3.94338000	7.68248400	-1.10493500
H	-4.81508500	7.41452600	-2.62884900
H	-5.70854500	7.35452200	-1.07250000
H	-3.05584300	1.01637100	4.13299000
O	-3.89622900	-3.12202100	0.65931100
C	4.25584400	3.17219500	0.15501800
C	4.56346900	4.26790600	0.97374400
C	3.76187400	4.53488900	2.09172800
C	2.67658100	3.71919800	2.38719400
C	2.36284400	2.61121300	1.57814700
C	3.17087800	2.35557500	0.45527700
H	4.87349500	2.95840500	-0.70994900
H	4.00223900	5.39375900	2.70942700
H	2.04563400	3.95714400	3.23815300
H	2.96441500	1.49829500	-0.17382500
C	5.71287100	5.17356400	0.70848400
O	6.01171000	6.13200000	1.39624500
O	6.40971200	4.81695300	-0.39704100
C	7.53219700	5.65722300	-0.70373100
H	8.25280200	5.65457100	0.11886900
H	7.97768400	5.23732400	-1.60583200
H	7.20749300	6.68678100	-0.87825100

int40

C	1.04764400	1.86359700	3.25467300
C	1.45003200	1.95952800	1.90845500
C	0.65256300	1.37963200	0.91187600
C	-0.54775200	0.75237800	1.25823500
C	-0.97658900	0.68880700	2.58394900
C	-0.14527700	1.22799100	3.58936900

Pd	-1.68359600	-0.27247300	-0.07467700
H	0.96434900	1.43314100	-0.12345300
O	-0.60905400	1.07540000	4.86641700
C	0.16410600	1.60314800	5.93553700
H	-0.38841100	1.37314500	6.84768600
H	1.15609400	1.13606700	5.98540500
H	0.28292400	2.69098000	5.84830100
H	1.68912000	2.27148300	4.02520000
C	-2.96472500	-0.59761400	1.65632900
C	-4.36877100	0.03268200	1.65621200
C	-3.37232400	1.05130300	3.41879300
C	-2.28322700	0.05185000	2.91715900
C	-4.04870700	1.47778000	2.10359300
H	-4.95182600	2.07680400	2.25996600
H	-3.38257800	2.01382500	1.42837100
C	-5.18721100	-0.45922100	2.89328400
H	-6.21954400	-0.11371500	2.77731900
H	-5.22289600	-1.54390500	2.98406100
C	-4.49095000	0.24021400	4.10180600
H	-5.18244300	0.90335500	4.63126100
H	-4.09565200	-0.47078700	4.83513800
H	-4.90962100	-0.09832200	0.72176800
H	-2.10857300	-0.71126500	3.68552500
C	-2.86095300	-2.08722200	1.68760400
O	-1.79795500	-2.70193500	1.95490600
C	-3.88117000	-4.19006700	1.32970500
H	-4.90532100	-4.52674600	1.17970000
H	-3.26654300	-4.42823800	0.45913900
H	-3.45106200	-4.62408500	2.23426100
C	1.72219600	-0.73854900	-2.99823200
C	0.75006500	-0.96582700	-1.82443600
O	0.91251900	-2.05876900	-1.19295000
O	-0.10676600	-0.07220500	-1.58933600
C	3.78789600	-1.77039100	-1.28167400
C	3.35471100	-1.86808600	0.04667600
C	4.43635800	-2.88767000	-1.82231800
C	3.49596600	-3.03638300	0.78190400
C	4.61949000	-4.05892100	-1.08742300
C	4.13088200	-4.13869700	0.21485800
F	4.86909000	-2.87689500	-3.08626100
F	5.23393600	-5.11400500	-1.63247300

F	4.26227300	-5.26752500	0.91349200
F	2.94977800	-3.12929100	2.00860600
F	2.69903900	-0.85604400	0.63453000
C	1.78474900	-1.99145700	-3.87595500
H	0.79037500	-2.18391300	-4.29483500
H	2.49380900	-1.84550700	-4.69405100
H	2.07622200	-2.86752300	-3.29613600
C	1.35628700	0.50628700	-3.81100800
H	1.32469500	1.40185600	-3.18756000
H	2.07134500	0.65425500	-4.62529300
H	0.35968300	0.36702600	-4.23854100
S	3.42803700	-0.33453000	-2.26561400
Ag	-0.11518100	-2.49555500	0.60074700
C	-2.37776500	3.66889400	-1.63192100
C	-3.69214300	3.60833300	-2.10553600
C	-4.42618500	2.42706800	-1.94302300
C	-3.86060900	1.32393800	-1.30215800
C	-2.55454000	1.41447000	-0.82110100
C	-1.79825400	2.57314000	-0.99001500
H	-1.81372100	4.58649500	-1.76469500
H	-5.43759200	2.36083300	-2.32782200
H	-4.43193200	0.41098200	-1.21662400
H	-0.78253400	2.64827100	-0.63285900
I	-2.87912900	-2.15653900	-1.81245900
C	-4.25085900	4.81626900	-2.77279400
O	-3.64275000	5.85658400	-2.93705200
O	-5.52815300	4.63594800	-3.18272800
C	-6.12106100	5.76815900	-3.83757200
H	-6.14604400	6.63152700	-3.16694200
H	-5.55228100	6.03763600	-4.73167600
H	-7.13188100	5.45893900	-4.10389800
H	-2.94813600	1.84464500	4.03506000
O	-3.97526400	-2.75181400	1.45854000
C	4.67091700	2.94443800	0.16008800
C	5.05295400	4.08063300	0.88674100
C	4.24734500	4.51976700	1.94597400
C	3.08444800	3.83363900	2.27381500
C	2.69565200	2.68606400	1.55733500
C	3.50887200	2.25723500	0.49409500
H	5.28933300	2.59745200	-0.66004600
H	4.54674900	5.40842100	2.49149200

H	2.45365900	4.20637200	3.07507400
H	3.24114600	1.36868100	-0.06268800
C	6.28620800	4.85466700	0.58199200
O	6.65138700	5.84137400	1.19331900
O	6.97574600	4.34063800	-0.46409000
C	8.17654600	5.04901400	-0.80620200
H	8.87610900	5.05147900	0.03435100
H	8.60109300	4.51647000	-1.65745000
H	7.95044200	6.08489300	-1.07369600

int41

C	3.96966500	-2.34545900	0.99176500
C	3.95401100	-1.12599400	0.28770900
C	2.72801900	-0.60207800	-0.15046100
C	1.54896100	-1.29368800	0.12785900
C	1.54724900	-2.50372600	0.82083000
C	2.78180700	-3.03291300	1.24698700
Pd	-0.18727200	-0.70556900	-0.64157300
H	2.69774800	0.34825600	-0.67515800
O	2.70699500	-4.23614900	1.89015500
C	3.91019400	-4.83364000	2.35373100
H	3.61577900	-5.76715200	2.83542500
H	4.59665400	-5.05382500	1.52609400
H	4.42173000	-4.19424600	3.08481400
H	4.92161400	-2.76030300	1.29814900
C	-0.92163800	-2.41989300	0.33602500
C	-1.94615200	-2.21972100	1.45416600
C	-0.25437200	-3.30409600	2.50208700
C	0.24466600	-3.21352000	1.02639900
C	-1.02146800	-1.97799000	2.66779700
H	-1.57865000	-1.91996700	3.60814100
H	-0.39341400	-1.09142200	2.57173700
C	-2.56948500	-3.60005800	1.82999500
H	-3.40878800	-3.41636500	2.50795100
H	-2.95853400	-4.13109600	0.96344300
C	-1.39990500	-4.33924700	2.55319300
H	-1.65830300	-4.57591200	3.59011500
H	-1.12669500	-5.27943400	2.06268400
H	-2.69974700	-1.46611000	1.23641500
H	0.32254400	-4.22511800	0.60617500
C	-1.40647000	-2.98000500	-0.97818000

O	-2.43691600	-3.53972800	-1.24720300
C	-0.89777300	-2.78045200	-3.31780800
H	-0.05021600	-2.45429100	-3.91853500
H	-1.15078600	-3.82078900	-3.52678600
H	-1.76742400	-2.13915000	-3.47333900
C	0.21075200	2.43228800	2.30125100
C	-1.12350400	2.81050400	2.49135000
C	-2.13634000	2.12645900	1.80741800
C	-1.81677600	1.07915300	0.94673200
C	-0.47990500	0.70450800	0.76429600
C	0.53720800	1.38018100	1.44183100
H	0.99811800	2.95936900	2.82853500
H	-3.16825700	2.42943400	1.95309800
H	-2.60653800	0.57308900	0.40999200
H	1.57486000	1.10146000	1.31817200
C	-1.52247800	3.92311300	3.39618300
O	-2.66936900	4.28083600	3.58363100
O	-0.45990100	4.50651300	3.99954000
C	-0.78481200	5.58918600	4.88523000
H	0.16736500	5.94171800	5.28207500
H	-1.29680700	6.38958900	4.34405100
H	-1.43525700	5.24381200	5.69349500
C	-2.11763500	1.97693100	-3.08613600
C	-1.31957100	0.88976000	-2.35493800
O	-1.92550500	-0.07645400	-1.78729800
O	-0.06753500	1.02595200	-2.23613400
C	-4.52873800	0.93222200	-1.86513500
C	-4.60854000	-0.43682200	-1.56418800
C	-4.90936400	1.83069100	-0.86229900
C	-4.97871000	-0.88540500	-0.30068600
C	-5.29046500	1.39799600	0.40727000
C	-5.30838400	0.03627800	0.69195600
F	-4.87226400	3.15193500	-1.07448200
F	-5.58333900	2.28624400	1.36764900
F	-5.61880600	-0.39159800	1.91858200
F	-4.96637900	-2.19214700	-0.00761900
F	-4.27512800	-1.35784600	-2.46756100
C	-2.04475800	3.24474100	-2.21362500
H	-0.99834000	3.54932900	-2.11957800
H	-2.62202200	4.05049500	-2.67219100
H	-2.43404300	3.06592800	-1.20993900

C	-1.50943700	2.23932800	-4.47395600
H	-1.56133500	1.35136900	-5.11071000
H	-2.03003000	3.06146600	-4.97392800
H	-0.45915500	2.51257100	-4.34683500
S	-3.89748300	1.47215200	-3.44191200
C	7.42942100	0.32208000	0.74080600
C	7.62372200	0.98447600	-0.47858100
C	6.61085100	0.95319800	-1.44717000
C	5.42682600	0.26724700	-1.19760400
C	5.22047000	-0.40121700	0.02247000
C	6.24378200	-0.35931000	0.98723500
H	8.21783500	0.36354200	1.48485400
H	6.76107300	1.45896800	-2.39399400
H	4.65907100	0.22704900	-1.96412500
H	6.09219900	-0.84296300	1.94737200
C	8.91228400	1.69924100	-0.68627600
O	9.81344900	1.74812900	0.12958200
O	8.98168400	2.30090300	-1.89715300
C	10.20428200	3.00892000	-2.15410900
H	10.35132600	3.80384800	-1.41780300
H	11.05996300	2.32961000	-2.10902400
H	10.09820300	3.42735500	-3.15512100
H	0.56319500	-3.49340400	3.19862400
O	-0.46070200	-2.65548700	-1.93999700

TS24

C	3.47949400	-1.65749100	1.95953400
C	3.64798200	-1.05371800	0.69985500
C	2.55377600	-0.42379500	0.09769300
C	1.30232500	-0.41319100	0.73003800
C	1.10913500	-1.08018000	1.96259000
C	2.22457600	-1.68153900	2.57460200
Pd	-0.51480700	-0.02907400	-0.20763100
H	2.69263600	0.12640300	-0.82589300
O	1.96698900	-2.30690200	3.75966100
C	3.00798800	-3.04822800	4.38284100
H	2.56580800	-3.49195800	5.27579700
H	3.38219200	-3.84539400	3.72790600
H	3.84374700	-2.40087900	4.67803400
H	4.32718100	-2.14608400	2.42297100
C	-1.24509100	-1.30638700	1.23968500

C	-2.55774400	-0.77232900	1.84113500
C	-1.07629900	-0.64116900	3.55897800
C	-0.28522100	-1.39849400	2.43766300
C	-2.02175400	0.31465600	2.79182400
H	-2.80648000	0.72080700	3.43924200
H	-1.54837900	1.14107200	2.26809600
C	-3.09151000	-1.82499500	2.86392800
H	-4.12013400	-1.56651500	3.12902400
H	-3.10320500	-2.83751500	2.45799400
C	-2.11781500	-1.66584300	4.08117700
H	-2.64245600	-1.26337700	4.95348600
H	-1.65741200	-2.61206100	4.37934600
H	-3.28042600	-0.45426100	1.09244800
H	-0.23440200	-2.44800800	2.74694400
C	-1.31575200	-2.61163700	0.46105400
O	-1.31316600	-3.71417800	0.96239600
C	-1.30805000	-3.57150100	-1.71270500
H	-1.23912900	-3.19062300	-2.72896300
H	-0.44094800	-4.18361800	-1.45595000
H	-2.22489900	-4.14449200	-1.57612600
C	1.01422200	3.35824700	2.15477700
C	1.32952000	4.18481400	1.06884600
C	1.34611300	3.63828500	-0.22095700
C	1.03966700	2.29781400	-0.42930600
C	0.66785000	1.48454700	0.65882500
C	0.69934200	2.01696500	1.95574300
H	1.03133300	3.76275000	3.16051600
H	1.60698800	4.27876000	-1.05702400
H	1.05965500	1.90291700	-1.43878700
H	0.51709400	1.38506500	2.81260500
C	1.67213700	5.62278000	1.22441100
O	1.95452700	6.36809200	0.30534600
O	1.63641600	6.02652900	2.51684800
C	1.95951700	7.40961400	2.72895800
H	1.88682800	7.56807400	3.80507300
H	2.97067600	7.62789200	2.37465200
H	1.25654400	8.05576300	2.19606600
C	-3.07052200	1.80495600	-2.92189900
C	-2.04052100	1.01964600	-2.09682300
O	-2.44272500	0.51058900	-0.98772800
O	-0.84028000	0.94974300	-2.45632200

C	-4.95843700	-0.21442600	-2.10207500
C	-4.43471000	-1.47789400	-1.80284700
C	-5.86819300	0.33355000	-1.19162500
C	-4.76445300	-2.14991500	-0.63248000
C	-6.21480600	-0.32599000	-0.01380600
C	-5.65772000	-1.57109900	0.26502700
F	-6.41016600	1.53785400	-1.40805000
F	-7.07042000	0.22982000	0.85296700
F	-5.95596700	-2.19874500	1.40744000
F	-4.19333500	-3.32779800	-0.32941900
F	-3.55391900	-2.05335000	-2.62745700
C	-3.66683600	2.91206900	-2.04127000
H	-2.86462800	3.58808100	-1.72087000
H	-4.40840500	3.48710100	-2.60128100
H	-4.13733500	2.49923600	-1.14945500
C	-2.43991100	2.38131900	-4.19376100
H	-1.98482600	1.59827100	-4.80301400
H	-3.18731400	2.91746500	-4.78683900
H	-1.65163200	3.08367300	-3.91035100
S	-4.42508300	0.64706200	-3.56174700
C	7.39778100	-0.90758000	0.15040100
C	7.48697100	-1.08200700	-1.23697400
C	6.31416900	-1.24288300	-1.98756100
C	5.07496100	-1.23279300	-1.35594400
C	4.97364600	-1.05999500	0.03576600
C	6.15756300	-0.89574400	0.77718800
H	8.31374900	-0.77357700	0.71594400
H	6.38070100	-1.38462600	-3.06005700
H	4.17316500	-1.38506400	-1.94112300
H	6.09948000	-0.72977600	1.84863300
C	8.84210100	-1.08720800	-1.85339400
O	9.88098100	-0.95415900	-1.23476400
O	8.79945300	-1.25880100	-3.19511600
C	10.07899400	-1.27201300	-3.84736000
H	10.60336800	-0.32621500	-3.68589300
H	10.69976000	-2.08533000	-3.46161100
H	9.86845000	-1.41854700	-4.90682500
H	-0.44402600	-0.20599600	4.33598100
O	-1.34638500	-2.39720300	-0.87051600

int42

C	2.39272200	-0.46212300	2.42677500
C	3.16335600	-0.13911600	1.30950500
C	2.83350500	1.00542700	0.57074100
C	1.72530500	1.80201300	0.87346300
C	0.85666200	1.44506900	1.96086300
C	1.27638200	0.31640800	2.75688600
Pd	-0.45232500	0.09195100	0.67760400
H	3.45266300	1.28761100	-0.27324700
O	0.53909700	0.09837800	3.87138300
C	0.65803600	-1.13728400	4.57033300
H	-0.10705500	-1.09883700	5.34553500
H	0.46766800	-1.98241500	3.89837600
H	1.64469900	-1.24405300	5.03554700
H	2.63610400	-1.34128400	3.00876300
C	-1.56527400	1.14734600	2.01068500
C	-2.61914600	2.03298400	1.31012300
C	-0.96536400	3.47776700	1.88191500
C	-0.44676700	2.13868000	2.46293000
C	-1.71957400	3.06595700	0.59910600
H	-2.29274400	3.89276000	0.16663300
H	-1.09218900	2.63359700	-0.17914700
C	-3.30606700	2.93480800	2.37315000
H	-4.13319800	3.47505400	1.90058000
H	-3.70852100	2.37397600	3.21690600
C	-2.15514500	3.90584000	2.78873300
H	-2.42049900	4.94769700	2.58469600
H	-1.91232300	3.82771000	3.85238800
H	-3.30723200	1.46393900	0.68089400
H	-0.38454200	2.20340800	3.55182300
C	-2.11105100	0.24708700	3.09609200
O	-2.38762800	0.61392600	4.22126200
C	-2.85144800	-1.93904500	3.62314400
H	-2.96548600	-2.87434300	3.08085900
H	-2.17912300	-2.05657300	4.47669500
H	-3.81899200	-1.58009700	3.97968000
C	1.75348600	5.35955300	-0.46508500
C	1.36049000	5.15099000	-1.79380800
C	1.08301200	3.85166500	-2.23927500
C	1.18429800	2.77582000	-1.36432300
C	1.54666200	2.98297600	-0.02335700
C	1.85082500	4.27997700	0.40975900

H	1.98465100	6.36266900	-0.12617100
H	0.78906100	3.70879400	-3.27369300
H	0.96593500	1.76520900	-1.69824600
H	2.16862200	4.44031400	1.43573000
C	1.23150700	6.26528200	-2.77482600
O	0.90622900	6.12338000	-3.93778800
O	1.51726000	7.47016900	-2.22978700
C	1.41007600	8.58489500	-3.12991500
H	1.66787500	9.46519900	-2.54105300
H	2.09899800	8.46801000	-3.97085900
H	0.39241700	8.66685200	-3.52116600
C	-1.01558900	-1.95884100	-2.85158700
C	-0.74124300	-1.18418200	-1.55930100
O	-1.73563100	-0.65499300	-0.95038500
O	0.43820300	-1.07317500	-1.11571800
C	-3.37456500	-3.07219500	-1.66972600
C	-3.52523800	-2.84965700	-0.29389600
C	-4.49382200	-2.85605000	-2.48416900
C	-4.72822400	-2.39880400	0.23902700
C	-5.70673600	-2.40935000	-1.96562000
C	-5.81974300	-2.17809000	-0.59756900
F	-4.42212500	-3.05191900	-3.80600600
F	-6.75803800	-2.20203400	-2.76815500
F	-6.97458400	-1.74673300	-0.08420100
F	-4.85738700	-2.17054100	1.55469800
F	-2.50734600	-3.05459100	0.54795300
C	-1.91710700	-1.14087700	-3.78079000
H	-1.38340800	-0.23368400	-4.08851300
H	-2.17768500	-1.71549300	-4.67219100
H	-2.82918500	-0.83039700	-3.27020800
C	0.28746400	-2.37045200	-3.54384800
H	0.92390800	-2.95885500	-2.87998300
H	0.07494800	-2.94280600	-4.45146400
H	0.84285800	-1.46944000	-3.81979000
S	-1.82528000	-3.59848800	-2.36141300
C	6.23739400	-2.34997400	1.43210900
C	6.40054000	-2.66993000	0.07758900
C	5.50203200	-2.15732100	-0.86840200
C	4.45822000	-1.33137800	-0.46340600
C	4.28958500	-1.00503300	0.89327000
C	5.19129800	-1.52864400	1.83528800

H	6.94605300	-2.75098900	2.14880400
H	5.62053200	-2.41683400	-1.91396500
H	3.74019000	-0.96500700	-1.19057800
H	5.08196600	-1.26716600	2.88375700
C	7.53800300	-3.55711600	-0.29486200
O	8.33671100	-4.02075300	0.49661700
O	7.59186900	-3.79784600	-1.62478300
C	8.66772600	-4.65177200	-2.04547300
H	9.63369000	-4.21011500	-1.78586800
H	8.59151900	-5.63143800	-1.56596100
H	8.56523700	-4.74396100	-3.12674000
H	-0.20959200	4.25193900	1.77211700
O	-2.29360800	-1.01938700	2.66792400

TS25

C	3.63929700	-1.82315800	0.03841800
C	4.19744200	-0.53642200	-0.04279900
C	3.34887100	0.57349200	0.05490700
C	1.96803300	0.43118000	0.24667600
C	1.40158500	-0.86168600	0.36834200
C	2.27051000	-1.98253200	0.24696800
Pd	-0.58049400	-1.15101100	-0.20512100
H	3.75847400	1.57538600	-0.02389900
O	1.65989200	-3.18127800	0.37511400
C	2.42233000	-4.37702200	0.47458800
H	1.69589800	-5.15344900	0.71187900
H	2.92472500	-4.60918100	-0.47243300
H	3.16897200	-4.30893800	1.27628100
H	4.27474700	-2.69110300	-0.08777000
C	-1.11485100	-1.69585300	1.73323600
C	-2.02652800	-0.72699700	2.48362700
C	0.09226200	-0.05309300	2.92402200
C	0.24250900	-1.27510900	2.02868700
C	-1.22516400	0.58668300	2.43030700
H	-1.61010000	1.34134200	3.12115500
H	-1.16292800	1.02171400	1.43275500
C	-1.84520200	-1.10980200	3.98784000
H	-2.56497400	-0.54656900	4.58887100
H	-2.02076600	-2.17242800	4.17486800
C	-0.37884100	-0.66725300	4.28538800
H	-0.33881700	0.10389900	5.06016500

H	0.25892800	-1.49408100	4.61242700
H	-3.05614300	-0.72639000	2.15010900
H	0.94917400	-2.05490700	2.28581100
C	-1.48333900	-3.15440700	1.68498200
O	-0.70564800	-4.07998000	1.80422000
C	-3.29860900	-4.62109000	1.35626200
H	-4.38476200	-4.53327000	1.34696100
H	-2.93488700	-4.99336700	0.39714900
H	-2.96700900	-5.27167600	2.16963700
C	-3.94953900	-2.29537700	-2.65716900
C	-2.78243800	-2.39267800	-1.64497500
O	-2.34856300	-1.23187300	-1.24047400
O	-2.30606600	-3.48729900	-1.34892200
C	-4.86084400	0.05435100	-1.16270800
C	-4.75988100	0.15938700	0.22971100
C	-4.51080400	1.18642200	-1.90773700
C	-4.32022000	1.32452300	0.84985900
C	-4.03878200	2.35158900	-1.30755000
C	-3.94225600	2.41921900	0.07966600
F	-4.60059200	1.18109200	-3.24420400
F	-3.67100300	3.39836300	-2.05767200
F	-3.49933500	3.52844700	0.68158500
F	-4.22797100	1.39560400	2.18875700
F	-5.06156000	-0.88019500	1.01830400
C	-3.45767400	-1.55289100	-3.90710000
H	-2.63751700	-2.12364700	-4.36004500
H	-4.26208800	-1.45579400	-4.64091400
H	-3.08847200	-0.56038100	-3.65569500
C	-4.47210000	-3.69097300	-3.01677700
H	-3.66068300	-4.26225900	-3.47409400
H	-4.79718800	-4.23450500	-2.12754800
H	-5.30195900	-3.62620300	-3.72793700
S	-5.46085500	-1.44797200	-1.89857900
C	0.56699700	3.84125800	1.15695900
C	-0.40500700	4.01832800	0.16353900
C	-0.58937600	3.02789600	-0.80912000
C	0.17241400	1.86438300	-0.77102600
C	1.14153300	1.66906200	0.23031500
C	1.34373400	2.68550400	1.17529600
H	0.71240100	4.61185300	1.90520200
H	-1.33170000	3.18835700	-1.58251100

H	0.04083800	1.11446100	-1.54685900
H	2.10248500	2.55384200	1.94108500
C	-1.24524900	5.24670500	0.07573700
O	-1.94580200	5.53322800	-0.87328400
O	-1.14471900	6.01693500	1.18360600
C	-1.95312500	7.20464300	1.16618800
H	-1.76802600	7.70199500	2.11834500
H	-1.67122600	7.85165600	0.33110300
H	-3.01013300	6.94399200	1.06512800
O	-2.81205400	-3.28037500	1.55147600
H	0.97220000	0.58340800	2.99915400
C	7.94230100	-1.04944100	0.22441400
C	8.43072100	-0.01868100	-0.58939600
C	7.52680000	0.84063100	-1.22875900
C	6.15759700	0.66918300	-1.05321900
C	5.65569700	-0.36048800	-0.23720500
C	6.57400500	-1.21748900	0.39704900
H	8.65458100	-1.70107400	0.71920900
H	7.90164400	1.63271100	-1.86662300
H	5.46577900	1.32297700	-1.57501100
H	6.20865400	-2.00255900	1.05198100
C	9.90676100	0.11457400	-0.73526100
O	10.71976500	-0.61212400	-0.19654000
O	10.25576700	1.14405800	-1.54067100
C	11.66980500	1.32340700	-1.72033000
H	12.15810300	1.51696100	-0.76136400
H	12.11743800	0.43106100	-2.16621500
H	11.77607900	2.18020000	-2.38573600

int43

C	3.77328200	-1.73910300	-0.17109600
C	4.32724400	-0.44571500	-0.23355100
C	3.47235600	0.66229500	-0.22043400
C	2.07943500	0.50127500	-0.14425900
C	1.52931700	-0.78914900	-0.09453100
C	2.39148000	-1.90770200	-0.08365000
Pd	-0.44702000	-1.08205800	-0.21245600
H	3.88244500	1.66692800	-0.25310000
O	1.76313800	-3.10641900	0.02078700
C	2.51405400	-4.28147100	0.29454200
H	1.77137900	-5.04898500	0.50978000

H	3.12430800	-4.57773500	-0.56809100
H	3.16495800	-4.14337300	1.16795000
H	4.42656000	-2.60237200	-0.21662000
C	-1.16570200	-1.76821200	1.79820900
C	-2.13425500	-0.79847500	2.45593500
C	-0.05261000	0.03417000	2.79730700
C	0.12203200	-1.24877800	2.00839100
C	-1.41233000	0.55480100	2.28210200
H	-1.83767200	1.33959100	2.91230100
H	-1.37883000	0.90734300	1.24797100
C	-1.90404000	-1.03721900	3.98853900
H	-2.65281400	-0.47200000	4.55063300
H	-2.00866700	-2.08976400	4.26475700
C	-0.46555900	-0.47689400	4.22237600
H	-0.46913900	0.36348200	4.92272200
H	0.22810000	-1.22791100	4.61168500
H	-3.16560800	-0.89023400	2.14185400
H	0.98752200	-1.89123300	2.10054900
C	-1.44289000	-3.23604300	1.66964200
O	-0.59016800	-4.09979800	1.64399900
C	-3.16833800	-4.81444300	1.40488200
H	-4.25131200	-4.82269900	1.52591500
H	-2.88933900	-5.07773600	0.38289000
H	-2.69154900	-5.49461800	2.11513700
C	-3.86058800	-2.26772100	-2.56630400
C	-2.73150200	-2.34276200	-1.50978800
O	-2.34042700	-1.18031800	-1.06217300
O	-2.22737600	-3.42664700	-1.21842300
C	-4.95111600	-0.00751000	-1.07992900
C	-4.87603200	0.08234400	0.31459500
C	-4.64938400	1.15045900	-1.80458000
C	-4.48624000	1.25279300	0.95671300
C	-4.23574000	2.32624900	-1.18282100
C	-4.14541900	2.37356100	0.20588700
F	-4.72902200	1.16205100	-3.14124100
F	-3.91668400	3.39772000	-1.91728800
F	-3.74322600	3.48828300	0.82877600
F	-4.40034600	1.30094300	2.29673300
F	-5.15075100	-0.97987300	1.08312600
C	-3.35478900	-1.45940900	-3.76940100
H	-2.49047100	-1.97526700	-4.20599600

H	-4.13222600	-1.37464800	-4.53293300
H	-3.04245800	-0.45983800	-3.47215300
C	-4.29184500	-3.67541500	-2.99483400
H	-3.43173100	-4.18948200	-3.43026700
H	-4.63007900	-4.26513300	-2.14063600
H	-5.08965500	-3.62708800	-3.74286300
S	-5.44555200	-1.53010100	-1.84847100
C	0.48260400	3.76339200	0.93890700
C	-0.55564600	3.89311600	0.00598300
C	-0.71214800	2.92844000	-0.99672400
C	0.14578800	1.83226500	-1.04719900
C	1.19017700	1.69030600	-0.11287100
C	1.35749000	2.68366300	0.86425700
H	0.59958600	4.51294400	1.71335200
H	-1.50695800	3.05482200	-1.72337300
H	0.04180700	1.10516400	-1.84970700
H	2.16428100	2.58532100	1.58467300
C	-1.49157600	5.05303400	0.01979100
O	-2.17335700	5.39728100	-0.92315900
O	-1.50500100	5.68253000	1.21713700
C	-2.43744700	6.77192100	1.31050700
H	-2.33146200	7.16576000	2.32138800
H	-2.20977600	7.54242700	0.56907700
H	-3.45534900	6.41041600	1.14089200
O	-2.76585700	-3.45510400	1.65768200
H	0.79192100	0.72090800	2.78095100
C	8.04040600	-0.92273300	0.36607600
C	8.59035700	0.09847200	-0.42040900
C	7.73855300	0.93764200	-1.15152600
C	6.36073300	0.75543000	-1.09331100
C	5.79670600	-0.26340400	-0.30466200
C	6.66361900	-1.09997000	0.42256100
H	8.71179300	-1.55923400	0.93263400
H	8.16132400	1.72177700	-1.76897000
H	5.71128900	1.39226800	-1.68579800
H	6.24862400	-1.87662300	1.05770700
C	10.07165200	0.24331100	-0.43945000
O	10.84138700	-0.46390000	0.18269100
O	10.48207600	1.26037400	-1.23272700
C	11.90466200	1.44905300	-1.29162600
H	12.30597300	1.66711900	-0.29811800

H	12.39669600	0.55191500	-1.67715100
H	12.06273700	2.29279000	-1.96349800
int44			
C	1.83657600	-1.46032100	1.41145000
C	2.29037300	-0.14947500	1.19025800
C	1.35327100	0.88249500	1.09111700
C	-0.02673400	0.61832900	1.12861500
C	-0.49844000	-0.70785500	1.27213400
C	0.46674400	-1.72396500	1.47005700
H	1.69519200	1.90181000	0.94275000
O	-0.03773000	-2.97536900	1.69456500
C	0.83477800	-4.09180900	1.56213700
H	0.19865100	-4.97586800	1.62107600
H	1.34836100	-4.07221900	0.59374100
H	1.57679100	-4.12726900	2.37015800
H	2.56233800	-2.25411200	1.53640100
C	-3.26207600	-1.48874200	-2.43372300
C	-4.42061700	-1.91204100	-1.45492600
O	-5.46454200	-2.25210000	-1.99305000
O	-4.17440800	-1.94190600	-0.18241700
C	-0.42927800	-0.60343300	-2.02006900
C	0.36406300	-1.71812100	-1.72238400
C	0.19800100	0.48182800	-2.64637900
C	1.72837400	-1.73165000	-1.98368400
C	1.56398400	0.48130000	-2.92009000
C	2.33462000	-0.62821700	-2.57863800
F	-0.49799600	1.57796100	-2.96330800
F	2.13694600	1.54346700	-3.49127600
F	3.64427800	-0.63542200	-2.81599700
F	2.46989700	-2.79062400	-1.62569000
F	-0.15734200	-2.79841400	-1.13267000
C	-2.58262000	-2.76856000	-2.92685200
H	-3.33520500	-3.33731400	-3.48019200
H	-1.74924200	-2.54670800	-3.60132700
H	-2.22338000	-3.38055900	-2.09931300
C	-3.78943800	-0.64467300	-3.59326200
H	-4.24377600	0.28432100	-3.23990100
H	-2.98959100	-0.40067500	-4.30057400
H	-4.56257200	-1.22507800	-4.10230100
S	-2.10137000	-0.37632500	-1.42650400

C	-3.05539400	2.88288000	1.49159700
C	-2.81929700	3.83039600	0.48552500
C	-1.65309000	3.74069000	-0.28422200
C	-0.74179700	2.71522500	-0.05867200
C	-0.97582500	1.74665600	0.93254500
C	-2.14260700	1.85684700	1.70976400
H	-3.95170600	2.95556100	2.09641200
H	-1.48576700	4.47699800	-1.06295900
H	0.14056400	2.63938700	-0.68483200
H	-2.33031400	1.13714100	2.49898900
C	-3.76480700	4.94343100	0.19375300
O	-3.59148200	5.78686400	-0.66523600
O	-4.85376800	4.91906100	0.99592200
C	-5.80968600	5.96397700	0.75628600
H	-6.18842800	5.91120000	-0.26799200
H	-6.61441600	5.79713900	1.47233500
H	-5.35361600	6.94584600	0.91004600
Pd	-2.36143300	-1.31754700	0.65024700
C	-3.21096800	-2.56631100	4.86045200
H	-4.09119100	-3.13578000	4.56666800
H	-3.47603400	-1.79444200	5.58793300
H	-2.47607400	-3.22573800	5.33239200
C	-2.59030500	-1.92913900	3.65238100
O	-3.00118200	-2.16611100	2.51137100
O	-1.59062600	-1.11246000	3.92493700
H	-1.18006200	-0.81462200	3.06849300
C	5.68324700	1.53331700	1.41273100
C	6.47587800	0.66164300	0.65307900
C	5.89383500	-0.47691600	0.08037100
C	4.54274900	-0.74340200	0.26668800
C	3.73777900	0.12476600	1.02686000
C	4.33021300	1.26593700	1.59445700
H	6.13352600	2.41110200	1.86163200
H	6.51721500	-1.13429800	-0.51624900
H	4.09591700	-1.61009100	-0.20865500
H	3.72628800	1.93419500	2.20074100
C	7.92787200	0.89449300	0.41954500
O	8.64698600	0.16096800	-0.23173700
O	8.37321000	2.02499100	1.01561100
C	9.76914700	2.30371700	0.82331300
H	9.99584400	2.41786100	-0.24021000

H	9.96084700	3.23343100	1.35915400
H	10.38281800	1.49314800	1.22574600

TS26

C	-1.65826200	-1.07018700	-1.83499800
C	-2.06002400	0.18008500	-1.33904100
C	-1.08387500	1.13465000	-1.00916600
C	0.27799600	0.85717100	-1.15185900
C	0.70993600	-0.42162100	-1.61227900
C	-0.29866200	-1.36200800	-1.96327100
H	-1.39256700	2.10175400	-0.62813500
O	0.16220800	-2.54555600	-2.43046500
C	-0.75691100	-3.61735100	-2.62389100
H	-0.14865300	-4.48374000	-2.88389400
H	-1.31428300	-3.82232100	-1.70250900
H	-1.45691000	-3.40542000	-3.44140700
H	-2.41118100	-1.78901700	-2.13018600
C	2.63254100	-1.81609400	2.60829700
C	3.91947000	-2.22769400	1.81575400
O	4.83822900	-2.67435700	2.48510700
O	3.91707500	-2.14351200	0.51772300
C	-0.06798700	-0.97731800	1.74500200
C	-0.73009200	-2.07072600	1.17577200
C	-0.84264200	-0.06050300	2.46828000
C	-2.10316200	-2.23651100	1.30954500
C	-2.21794100	-0.21738200	2.61930900
C	-2.84973100	-1.31546600	2.03942000
F	-0.27350000	1.01745600	3.02055400
F	-2.93049400	0.67786800	3.30532400
F	-4.16597800	-1.47236000	2.16005800
F	-2.72109600	-3.25068500	0.68605300
F	-0.06812600	-2.98521800	0.45638000
C	1.85212800	-3.09750400	2.91389600
H	2.50909400	-3.73661600	3.51003300
H	0.94904000	-2.88816400	3.49545500
H	1.58139600	-3.63318000	2.00337500
C	2.99035100	-1.05480200	3.88536400
H	3.52479400	-0.12741000	3.66403500
H	2.09246800	-0.81427800	4.46411100
H	3.64957200	-1.69113000	4.48063700
S	1.66380600	-0.61300200	1.50364300

C	3.37565500	3.05022000	-1.15944400
C	3.17217400	3.82543800	-0.00928800
C	2.01586000	3.63166000	0.75649500
C	1.07665300	2.68009900	0.37675000
C	1.27274200	1.89464700	-0.77340200
C	2.43812600	2.09370300	-1.53506000
H	4.26868300	3.20020300	-1.75488200
H	1.87880600	4.22905200	1.65145500
H	0.21044300	2.50710200	1.00661000
H	2.60700500	1.50248900	-2.42762600
C	4.14600300	4.85681600	0.44647200
O	4.00350400	5.54706700	1.43779700
O	5.22036400	4.94822200	-0.36945200
C	6.20152600	5.92165500	0.02181200
H	6.59711500	5.69104900	1.01464000
H	6.98969600	5.86363600	-0.72885700
H	5.76276500	6.92299200	0.04414000
Pd	2.39428600	-1.31357300	-0.56596800
C	4.01598000	-1.98867300	-4.54871700
H	4.36754900	-1.15762400	-5.16395600
H	3.37244700	-2.61721900	-5.17264300
H	4.85374600	-2.58001900	-4.18008200
C	3.19265200	-1.45653500	-3.39785800
O	3.38239600	-1.97567300	-2.25708500
O	2.34889000	-0.53755100	-3.64520400
H	1.60863900	-0.42333700	-2.55718700
C	-5.34106000	2.07192400	-1.13183000
C	-6.22185100	1.06335500	-0.71796900
C	-5.73857400	-0.23718900	-0.52810700
C	-4.39781700	-0.52629000	-0.74926600
C	-3.49892900	0.48030100	-1.14881700
C	-3.99723000	1.78169200	-1.34145300
H	-5.71512400	3.07658100	-1.29099400
H	-6.42880100	-1.00580000	-0.19788200
H	-4.03860900	-1.53396700	-0.57244600
H	-3.32997700	2.56631000	-1.68321900
C	-7.66914500	1.31371000	-0.46533800
O	-8.45949300	0.46354100	-0.10350200
O	-8.01521100	2.60213300	-0.68356800
C	-9.40133400	2.90740800	-0.45717400
H	-9.67582100	2.70012300	0.58064200

H	-9.50909700	3.96907400	-0.67891900
H	-10.03862500	2.30912100	-1.11383800
di-p^m			
C	1.17912500	2.58157500	-0.04272500
C	1.19784800	1.17652000	0.01372900
C	-0.01020900	0.47354800	0.04952400
C	-1.24087700	1.15133400	0.02842900
C	-1.24549800	2.54716800	-0.02997000
C	-0.04126900	3.26111600	-0.06505900
H	0.00244500	-0.60976300	0.09495000
O	-0.16913200	4.61804500	-0.12119100
C	1.01237100	5.40661300	-0.13582600
H	0.67997000	6.44522800	-0.16178900
H	1.61911600	5.24365100	0.76456200
H	1.62583200	5.20216700	-1.02303200
H	2.11647500	3.11985200	-0.09986100
C	-4.82230400	0.09938900	-0.65088000
C	-4.94131500	-1.03926600	0.15734300
C	-3.84458300	-1.45623700	0.92283100
C	-2.65015900	-0.74783800	0.88126100
C	-2.51758700	0.39586500	0.07401300
C	-3.62430000	0.80452800	-0.69004000
H	-5.66589600	0.42017400	-1.25084800
H	-3.95402300	-2.33398100	1.55057400
H	-1.81626400	-1.06504600	1.49940900
H	-3.53323300	1.67030900	-1.33838000
C	-6.19478200	-1.83683300	0.24180500
O	-6.33636600	-2.82995000	0.92941100
O	-7.18110000	-1.33565900	-0.53959600
C	-8.41741500	-2.06561100	-0.49947600
H	-8.82217800	-2.08275300	0.51595200
H	-9.09282800	-1.53862000	-1.17331600
H	-8.26755400	-3.09612500	-0.83244200
C	3.86815600	-1.42900400	-0.67709500
C	4.95146700	-0.92648100	0.05629700
C	4.80006900	0.26622000	0.77537100
C	3.58742600	0.94399300	0.76176900
C	2.49289600	0.45164900	0.02868100
C	2.65701300	-0.74568200	-0.68940800
H	3.98435700	-2.34693800	-1.24141000

H	5.64403000	0.63816700	1.34626600
H	3.47336400	1.85183300	1.34593200
H	1.83250300	-1.12772400	-1.28294800
C	6.27244700	-1.60980700	0.10789800
O	7.23739800	-1.20115300	0.72522600
O	6.29147300	-2.75459600	-0.61526100
C	7.54256900	-3.46022100	-0.60253300
H	7.81371300	-3.74507400	0.41752500
H	7.38828200	-4.34476800	-1.22032500
H	8.34078400	-2.83698600	-1.01446900
H	-2.17362700	3.10767100	-0.02068900

int45

C	-0.35743500	-1.93857300	2.06737700
C	-1.64126400	-2.51290800	2.19989500
C	-2.76719700	-1.70002900	2.35706800
C	-2.61040600	-0.31431500	2.41495900
C	-1.32605600	0.27626400	2.29379000
C	-0.17570400	-0.55766300	2.12641900
H	-1.19882300	1.31427500	2.57821300
Pd	-2.08225300	0.82650100	0.18810400
C	-2.34204700	0.98282800	-2.73392400
O	-2.37289700	1.49000300	-3.84307300
O	-2.46208600	1.65324000	-1.61966800
C	-3.84894800	2.74356100	1.29764500
O	-4.67990800	1.83611700	1.28549000
O	-2.57056200	2.60072500	1.02557800
H	-3.47567600	0.31585200	2.59006400
H	-3.74440200	-2.16144500	2.43914200
H	0.49127600	-2.57986600	1.87439700
C	-2.27902800	-0.56852400	-2.64915400
C	0.25731300	-1.08206700	-1.26020600
C	0.96558600	-2.27190400	-1.05501300
C	1.00160600	0.07015100	-1.53807200
C	2.35573800	-2.30989700	-1.06474300
C	2.39266800	0.04590500	-1.57634700
C	3.07178700	-1.14139500	-1.31786400
F	0.39205000	1.23978600	-1.73424300
F	3.08183800	1.16622500	-1.80066800
F	4.40154000	-1.15081900	-1.28797500
F	3.00144200	-3.45283900	-0.81344200

F	0.31147100	-3.41767900	-0.80365500
C	-3.72682600	-1.08732200	-2.56695600
H	-4.25439400	-0.74115000	-3.46049000
H	-3.75614500	-2.18069900	-2.53940900
H	-4.25002700	-0.68789800	-1.69282400
C	-1.51976500	-1.17630100	-3.82127800
H	-0.48879300	-0.81809600	-3.86511500
H	-1.51989600	-2.26958700	-3.77105000
H	-2.01578700	-0.85242900	-4.73865200
S	-1.51264500	-1.10397600	-1.00321600
C	2.55821100	1.86775100	1.12144600
C	3.70808800	1.08867600	1.30407100
C	3.58984800	-0.19155500	1.85893300
C	2.33872600	-0.70321600	2.17989200
C	1.16759300	0.03966000	1.93642100
C	1.30589600	1.34778500	1.42990700
H	2.64366300	2.85833700	0.69140200
H	4.49073100	-0.77603000	2.01171600
H	2.27248100	-1.69083400	2.62428700
H	0.42584800	1.94392500	1.21357500
C	5.06111000	1.53634700	0.86763700
O	6.06804100	0.86254500	0.96914400
O	5.04281400	2.77208400	0.32767500
C	6.31172600	3.24924000	-0.15084300
H	6.69899600	2.58739700	-0.93004600
H	6.11939300	4.24427400	-0.55128400
H	7.03767200	3.29388200	0.66529500
O	-1.87380400	-3.84302300	2.16252600
C	-0.77020600	-4.74422300	2.07301300
H	-1.20432100	-5.74387600	2.10162600
H	-0.22225700	-4.61041900	1.13551300
H	-0.08667100	-4.62148400	2.92237400
C	-4.21729600	4.18148300	1.62733700
H	-3.47184500	4.63320900	2.28663700
H	-4.22889000	4.75863400	0.69721700
H	-5.20629400	4.21447000	2.08611600
TS27			
C	-0.23090300	-2.55466800	0.85051300
C	-1.47875800	-2.66632100	1.47896100
C	-1.95188100	-1.62074200	2.29225400

C	-1.21688800	-0.45314900	2.38388800
C	-0.00111300	-0.25250400	1.67446700
C	0.50466200	-1.36567100	0.93858600
H	0.98911500	0.26186200	2.39305800
Pd	0.13617100	1.73260700	0.81268500
C	-0.80349900	4.03874800	-0.82492200
O	-0.82428800	5.14400000	-1.34328000
O	0.15310100	3.58647600	-0.06748200
C	2.67654700	1.42994300	2.25886000
O	2.11164400	0.55213800	2.98106300
O	2.10955800	2.06044200	1.31253200
H	-1.59226400	0.35229500	3.00963400
H	-2.89449000	-1.75162300	2.81334400
H	0.16727600	-3.37302900	0.26336900
C	-1.99155000	3.08395400	-1.19057500
C	-2.68251500	0.28172900	-0.50493400
C	-3.97308100	-0.14281600	-0.15898600
C	-1.89087900	-0.59699700	-1.25163700
C	-4.44790200	-1.40332000	-0.51121100
C	-2.34980700	-1.85987700	-1.60927000
C	-3.62526700	-2.26714300	-1.23023900
F	-0.64511000	-0.27099200	-1.60960000
F	-1.54874300	-2.71071600	-2.26262200
F	-4.04466600	-3.49544500	-1.53546100
F	-5.67119000	-1.79319900	-0.14814000
F	-4.77496400	0.65000800	0.55716700
C	-3.32123900	3.83623600	-1.22271600
H	-3.22641400	4.65103800	-1.94443900
H	-4.14049300	3.17481800	-1.52345700
H	-3.55915900	4.27352500	-0.24993000
C	-1.66905500	2.44598200	-2.54505500
H	-0.72337400	1.90397300	-2.52303300
H	-2.46562900	1.76880500	-2.86837900
H	-1.58892400	3.25920800	-3.27165300
S	-2.09226700	1.80847500	0.20766700
C	3.59934700	-0.36650700	-1.05481700
C	4.50796800	-1.34899300	-0.64021400
C	4.08886700	-2.34267000	0.25483000
C	2.78472600	-2.34439100	0.73471900
C	1.86952700	-1.35019000	0.34173800
C	2.29391800	-0.37277800	-0.57114700

H	3.91640600	0.40095000	-1.75111200
H	4.80424600	-3.09535800	0.56837200
H	2.47265500	-3.09868500	1.45060600
H	1.60107700	0.39190800	-0.89973700
C	5.92071300	-1.38672200	-1.11275200
O	6.73454000	-2.22774900	-0.78140600
O	6.20932900	-0.37158600	-1.95791000
C	7.56044700	-0.34928900	-2.44558200
H	7.78486900	-1.26497000	-2.99941900
H	7.62334600	0.52082300	-3.09896800
H	8.26730600	-0.26081200	-1.61612100
O	-2.30523600	-3.73253300	1.35693500
C	-1.91132600	-4.82127800	0.52026500
H	-2.73763800	-5.53139300	0.55359300
H	-1.75526000	-4.49446700	-0.51317600
H	-1.00038800	-5.30218100	0.89538100
C	4.14234800	1.71310700	2.48381500
H	4.70775500	1.04409200	1.82543900
H	4.37651500	2.74344100	2.21433200
H	4.41831100	1.50180200	3.51740600

int46

C	-0.28435200	-2.76298900	0.61618300
C	-1.52685400	-2.97098600	1.22281200
C	-2.08098600	-1.95940700	2.01761500
C	-1.45380800	-0.72058200	2.07893100
C	-0.26090400	-0.43650500	1.37774800
C	0.36113300	-1.51434800	0.69803300
H	1.12778500	-0.28357400	2.78772500
Pd	0.18920400	1.51771100	0.98246100
C	-0.33560100	4.12748900	-0.43552000
O	-0.20553200	5.26603500	-0.86187700
O	0.46498300	3.51667700	0.37927100
C	2.71193900	0.70327300	2.51034600
O	2.04782500	-0.23133100	3.15841200
O	2.19687800	1.47810300	1.69338200
H	-1.93415700	0.06906500	2.65184200
H	-3.02095400	-2.14750300	2.52650400
H	0.18884700	-3.55216800	0.04389400
C	-1.56096600	3.32566900	-1.02082100
C	-2.71389200	0.58376500	-0.54615500

C	-4.03249000	0.27500500	-0.18493500
C	-2.02189200	-0.35855300	-1.31712400
C	-4.62403300	-0.93684100	-0.53547000
C	-2.59206800	-1.57740900	-1.66280600
C	-3.89235600	-1.87306000	-1.26212400
F	-0.76292100	-0.13921500	-1.70656500
F	-1.88607400	-2.48538900	-2.34777100
F	-4.42697300	-3.05324800	-1.57134700
F	-5.87377600	-1.21372700	-0.15610800
F	-4.74584200	1.12353000	0.56112600
C	-2.80153500	4.20803500	-1.14659800
H	-2.54046600	5.05945800	-1.77952900
H	-3.63436600	3.65884500	-1.59867200
H	-3.11825700	4.59643500	-0.17557300
C	-1.13579000	2.74658400	-2.37184200
H	-0.24381000	2.12612000	-2.28220000
H	-1.93800500	2.15875300	-2.82891000
H	-0.90796800	3.59296700	-3.02585900
S	-1.94522500	1.98469300	0.26031300
C	3.43992900	-0.31590700	-1.22492300
C	4.39786400	-1.24354400	-0.79435000
C	4.01756100	-2.26545900	0.08646000
C	2.70341200	-2.34905300	0.53339600
C	1.73484300	-1.41423800	0.12143400
C	2.12666700	-0.40442500	-0.77262400
H	3.72781800	0.47643400	-1.90594900
H	4.76902000	-2.97580500	0.41479700
H	2.42111900	-3.12502400	1.23839400
H	1.40161600	0.32732600	-1.10469500
C	5.82228500	-1.18828300	-1.22604300
O	6.68764400	-1.95178800	-0.84043300
O	6.05847300	-0.18455400	-2.10013800
C	7.41839800	-0.07395800	-2.54998600
H	7.72948200	-0.98826200	-3.06263800
H	7.43429300	0.77487900	-3.23344500
H	8.09051800	0.09853700	-1.70500400
O	-2.27178100	-4.10470800	1.09357200
C	-1.90464000	-5.03350500	0.07809800
H	-2.69649000	-5.78357900	0.05839700
H	-1.84042600	-4.54133700	-0.89974400
H	-0.95016000	-5.52703800	0.30133300

C	4.18235700	0.73655100	2.79363500
H	4.65345700	-0.01231800	2.14661500
H	4.58394200	1.71963200	2.55069500
H	4.38438700	0.46944300	3.83209600

int47

C	-1.93892300	2.98009500	1.41627900
C	-1.02332400	3.99348600	1.10232900
C	0.22015500	3.65139700	0.56832800
C	0.55838500	2.30394600	0.32442500
C	-0.36536500	1.28601800	0.62334700
C	-1.60172700	1.65060300	1.18211200
Pd	-0.08120300	-0.68997600	0.21241200
H	0.94409400	4.41568600	0.31103200
H	-2.89918100	3.25627000	1.84059300
C	1.28403700	-1.55817700	1.80740900
C	0.75173700	-2.87407900	2.36456900
C	-0.36286300	-1.20129500	3.41930600
C	0.60126500	-0.54110800	2.45306000
C	-0.71471100	-2.51344100	2.68569700
H	-1.19058100	-3.24771400	3.34338600
H	-1.32805600	-2.38073500	1.79326900
C	1.34833300	-2.91381900	3.81424400
H	1.12840200	-3.88219300	4.27274500
H	2.43431900	-2.78374900	3.82342500
C	0.59168800	-1.75379400	4.54010500
H	-0.00675000	-2.12546500	5.37737800
H	1.26300900	-0.98297900	4.92930200
H	0.93058200	-3.74593200	1.74205100
H	0.99364500	0.45870800	2.58443300
C	2.66825300	-1.39349400	1.26331800
O	3.38171800	-0.43804800	1.49829500
C	4.36978900	-2.40563700	-0.01858900
H	4.44161100	-1.63954700	-0.79304400
H	5.09795100	-2.18625000	0.76656700
H	4.54387100	-3.39324200	-0.44409300
C	-1.11997300	-2.06126400	-2.54054200
C	-0.74943100	-3.11557100	-1.44505100
O	-0.07222100	-2.70355900	-0.42263400
O	-1.03939200	-4.27921700	-1.69238800
C	-2.95013900	-0.11922800	-1.23075900

C	-3.58926100	1.09258200	-1.51412800
C	-3.60714100	-1.02236800	-0.38863100
C	-4.83718800	1.39831400	-0.97532700
C	-4.85506400	-0.73674200	0.15388500
C	-5.47171700	0.47948400	-0.14284200
F	-3.02658300	-2.18280200	-0.05981300
F	-5.45982600	-1.61209700	0.96063500
F	-6.66596200	0.76257200	0.37584300
F	-5.42125800	2.56743400	-1.24688900
F	-2.99316000	2.00960500	-2.27987900
C	0.10639000	-1.93537700	-3.46531300
H	0.31562800	-2.92934400	-3.87105600
H	-0.07848800	-1.24465100	-4.29361500
H	0.99167300	-1.60884300	-2.91052400
C	-2.37604700	-2.44170000	-3.31410500
H	-3.24493300	-2.52008600	-2.65807700
H	-2.58822000	-1.72533500	-4.11372300
H	-2.20553100	-3.43180100	-3.74187700
S	-1.27629200	-0.32501500	-1.80983400
C	4.33379800	2.19790800	0.03580100
C	4.51634200	1.31123400	-1.03188300
C	3.39832700	0.81704800	-1.71635400
C	2.11794900	1.17139600	-1.31178000
C	1.91947900	2.00390700	-0.19605700
C	3.04840100	2.53395900	0.44753400
H	5.19763900	2.58310500	0.56499000
H	3.55351600	0.15186900	-2.55963500
H	1.26288000	0.81497100	-1.87159400
H	2.91019400	3.17502400	1.31293600
C	5.85459000	0.81460300	-1.43777500
O	6.03847900	-0.13284100	-2.18308600
O	6.86727900	1.51210100	-0.87542400
C	8.18459500	1.03982900	-1.19731800
H	8.35969400	1.09079100	-2.27535100
H	8.87203900	1.69731700	-0.66494900
H	8.31278800	0.00367400	-0.87192900
O	-1.43919100	5.26993500	1.35574100
C	-0.55116500	6.33491500	1.05551900
H	-0.30431400	6.36941700	-0.01418200
H	-1.07413400	7.25189200	1.33211500
H	0.38022600	6.26307100	1.63352400

H	-2.32395500	0.88081600	1.44455000
H	-1.18091100	-0.57697300	3.78097200
O	3.03727000	-2.45497200	0.52984800

TS28

C	-1.99426400	2.91931600	0.89984500
C	-1.18589900	3.89718800	0.29828300
C	0.10414800	3.55994700	-0.12666800
C	0.58496700	2.24945500	0.01777800
C	-0.22899700	1.25229400	0.60876900
C	-1.50895700	1.63047000	1.06354300
Pd	0.01014200	-0.75644300	0.02256200
H	0.74747200	4.29429400	-0.59672600
H	-2.99114300	3.19773000	1.22633100
C	1.21403700	-1.10231700	1.70301200
C	0.53330700	-2.10473700	2.64700000
C	-0.11850800	-0.03393300	3.32193100
C	0.79997300	0.20221500	2.13748700
C	-0.79305700	-1.37606400	2.96552000
H	-1.32305700	-1.81822900	3.81494700
H	-1.47022200	-1.32424900	2.10928900
C	1.27349200	-1.94367900	4.00854800
H	0.91558900	-2.69325200	4.72110600
H	2.35589200	-2.06853700	3.91512100
C	0.86905300	-0.50021300	4.44959700
H	0.34254500	-0.50213300	5.40860100
H	1.72806600	0.17006400	4.54727300
H	0.46647200	-3.11621200	2.25046200
H	1.52689000	1.00496300	2.15725000
C	2.64803700	-1.28843100	1.30372900
O	3.51662700	-0.45222100	1.47815000
C	4.23200500	-2.74663500	0.35736600
H	4.55335100	-2.01689700	-0.39018600
H	4.90772300	-2.69198500	1.21574700
H	4.22441800	-3.75158700	-0.06279000
C	-1.33660500	-2.31524600	-2.49159300
C	-0.74647100	-3.26978900	-1.39595900
O	0.03132700	-2.76643700	-0.49175500
O	-0.98421200	-4.46188000	-1.54768500
C	-3.02688400	-0.31482200	-1.07912600
C	-3.72242400	0.87875100	-1.30150000

C	-3.52509900	-1.17736800	-0.09594700
C	-4.86186500	1.20722900	-0.57074200
C	-4.66932700	-0.87331100	0.63387500
C	-5.34030200	0.32621900	0.39532100
F	-2.88359800	-2.31615800	0.19496700
F	-5.11677800	-1.71325400	1.57135100
F	-6.43039500	0.63240600	1.09989100
F	-5.48262200	2.37210700	-0.77784300
F	-3.26917500	1.77221900	-2.18630400
C	-0.28469700	-2.23659000	-3.61571400
H	-0.09012600	-3.25789400	-3.95502200
H	-0.64016000	-1.64022700	-4.46141900
H	0.66106700	-1.82029600	-3.25358900
C	-2.67964600	-2.80840100	-3.01923600
H	-3.42629300	-2.86538800	-2.22541000
H	-3.05308900	-2.16668500	-3.82319500
H	-2.53140000	-3.82235700	-3.39545800
S	-1.45823200	-0.52296700	-1.90210600
C	4.36585400	2.23735800	-0.09819800
C	4.61710500	1.16209700	-0.95853400
C	3.54958500	0.52444700	-1.60054100
C	2.24352800	0.91521300	-1.33709900
C	1.97419900	1.93786300	-0.41013600
C	3.05446900	2.62081600	0.16917700
H	5.19437200	2.73585200	0.39128000
H	3.76042000	-0.29234400	-2.28253800
H	1.42254400	0.42443000	-1.84656700
H	2.85663400	3.42036600	0.87754300
C	5.97992800	0.60881400	-1.16971200
O	6.21058300	-0.45128000	-1.72453200
O	6.95088000	1.39849600	-0.66029900
C	8.28528400	0.88216700	-0.78729800
H	8.54617300	0.74346000	-1.83995100
H	8.93448900	1.62590100	-0.32511800
H	8.37535700	-0.07972200	-0.27518400
O	-1.74344500	5.13160500	0.17942200
C	-0.97918800	6.16398600	-0.42949200
H	-0.71515100	5.91310400	-1.46496400
H	-1.61458700	7.05062800	-0.42454900
H	-0.06110500	6.37369500	0.13484900
H	-2.14409100	0.89164900	1.54310700

H	-0.75639300	0.80480600	3.60147800
O	2.87386200	-2.49713800	0.76992800
int48			
C	-1.84292300	1.21865300	2.24264100
C	-1.41536600	2.33951700	1.49947500
C	-0.13453800	2.35714500	0.96181800
C	0.74069800	1.25278500	1.12757800
C	0.30615000	0.09548000	1.84834200
C	-1.00867700	0.13502100	2.39990400
Pd	0.00032400	-0.74119000	-0.27547000
H	0.23110700	3.21426800	0.41124900
H	-2.84288900	1.22794800	2.66273800
C	1.41531900	-1.81188500	0.74149800
C	0.97845700	-3.27037700	0.99816900
C	0.72435200	-2.24081200	3.00687200
C	1.25751500	-1.09735700	2.10908100
C	-0.14581400	-3.07966900	2.04001200
H	-0.46892800	-4.02765600	2.48308100
H	-1.02210400	-2.56821500	1.63590500
C	2.06766300	-3.94550000	1.87740100
H	1.85038500	-5.01457400	1.96970600
H	3.07432400	-3.84802900	1.46477500
C	1.91205900	-3.21053000	3.24845800
H	1.66634300	-3.91291800	4.05090500
H	2.82258300	-2.67897300	3.54007400
H	0.71701500	-3.80231000	0.08384700
H	2.21407400	-0.72797600	2.48285000
C	2.77341800	-1.67201500	0.10577200
O	3.79294200	-1.42092200	0.72359200
C	4.04688000	-1.85700100	-1.86461700
H	4.48280300	-0.85955600	-1.76397000
H	4.73074800	-2.58790000	-1.42494200
H	3.85643600	-2.09124000	-2.91162500
C	-1.75103300	-0.79156800	-2.99159000
C	-1.31145500	-2.20481000	-2.48279500
O	-0.35399000	-2.27043500	-1.60546800
O	-1.82012000	-3.17166300	-3.03403800
C	-3.17721200	0.48382300	-0.75207300
C	-3.92321600	1.66322300	-0.65865800
C	-3.63607700	-0.62665800	-0.03324000

C	-5.05561500	1.75475600	0.14514800
C	-4.77503700	-0.56186800	0.76162900
C	-5.48614900	0.63546800	0.85255800
F	-2.96342000	-1.78243000	-0.06789000
F	-5.18254000	-1.63123100	1.45122900
F	-6.57312700	0.70738500	1.62147600
F	-5.72602900	2.90652300	0.23764600
F	-3.53839900	2.76492700	-1.31726200
C	-0.69437200	-0.34015800	-4.01754700
H	-0.64981700	-1.09559600	-4.80787400
H	-0.95545200	0.62424100	-4.46384000
H	0.29899600	-0.27432500	-3.56300300
C	-3.15110800	-0.81259900	-3.59397400
H	-3.89817900	-1.12978400	-2.86278800
H	-3.42777600	0.17072500	-3.98664600
H	-3.15896600	-1.54698600	-4.40148300
S	-1.63070700	0.52401600	-1.63398400
C	4.50684600	1.73644100	1.19120900
C	4.80471400	1.80697300	-0.17441500
C	3.76851300	1.74194500	-1.11475600
C	2.45459900	1.57533000	-0.69455900
C	2.15412100	1.45304300	0.67151600
C	3.19018500	1.56381600	1.60749000
H	5.30804000	1.79554500	1.91814200
H	4.01652300	1.80621000	-2.16883200
H	1.65429600	1.49867500	-1.42412900
H	2.96368000	1.49483900	2.66703000
C	6.19825400	1.91604500	-0.68711000
O	6.50155600	1.85632400	-1.86410300
O	7.10391500	2.08213200	0.30200500
C	8.47125600	2.16319400	-0.13127000
H	8.61225200	3.01420800	-0.80312300
H	9.06109000	2.28818400	0.77677000
H	8.76251400	1.25013700	-0.65745700
O	-2.33353200	3.33038500	1.36773500
C	-1.98432500	4.48477700	0.60650600
H	-1.71953900	4.21495500	-0.42123900
H	-2.87670800	5.11067300	0.59447300
H	-1.15622500	5.03152100	1.07351600
H	-1.36485200	-0.71961300	2.96132600
H	0.25138400	-1.89889000	3.93186800

O	2.76253000	-1.91350300	-1.21941500
int49			
C	-2.25135900	-3.15542000	0.39534800
C	-1.28163100	-4.15600300	0.56435600
C	-0.13963600	-4.14726100	-0.23986200
C	-0.01356800	-3.17950100	-1.22515800
C	-0.99320800	-2.15927900	-1.45218300
C	-2.12787700	-2.16075800	-0.57433900
Pd	0.44957600	-0.66003300	-0.52818400
H	0.83379800	-3.22567200	-1.90179800
H	0.62380600	-4.90155100	-0.08889800
C	0.39477700	-0.40987200	-2.55471300
C	-0.11632600	0.96751200	-2.99885800
C	-1.86699000	-0.42986200	-3.35376200
C	-0.78490000	-1.38498600	-2.79729900
C	-1.60416400	0.89576900	-2.60598900
H	-2.18979500	1.72832300	-3.00957300
H	-1.76966500	0.84804600	-1.53003000
C	-0.22120900	0.93103200	-4.54943400
H	-0.44317600	1.93471400	-4.92685400
H	0.70730800	0.60512200	-5.02480300
C	-1.41753500	-0.04566500	-4.79048400
H	-2.23715800	0.45348700	-5.31611300
H	-1.13632300	-0.92203100	-5.38336300
H	0.46024500	1.79864700	-2.60178400
H	-0.53460000	-2.14429200	-3.54459800
C	1.74857900	-0.84070800	-3.01382900
O	2.10745300	-1.99606500	-3.18710700
C	3.94004700	-0.11532100	-3.53603000
H	4.39293800	0.81831900	-3.87119100
H	4.44604000	-0.48121400	-2.63935800
H	3.98362100	-0.86936200	-4.32425300
C	3.45194100	2.61383700	-0.64357300
C	2.90568100	1.18941400	-0.44344300
O	1.64044700	1.09236100	-0.43289500
O	3.73623000	0.25161900	-0.26080300
C	1.85227500	2.81160100	1.75760700
C	0.57319000	3.22092200	1.36282400
C	1.92719200	1.76386200	2.68540200
C	-0.57446400	2.60031600	1.84370700

C	0.78855500	1.16427900	3.21098300
C	-0.46646600	1.57230200	2.77472700
F	3.11331500	1.26273500	3.05903000
F	0.89915400	0.15923000	4.09002800
F	-1.56877600	0.96102300	3.22101000
F	-1.78529500	2.96865900	1.39644300
F	0.41496000	4.19333000	0.45630200
C	4.94872300	2.61618400	-0.96942300
H	5.10227100	2.17794300	-1.96017400
H	5.33305300	3.64098500	-0.99235200
H	5.51456100	2.03152300	-0.24428200
C	2.64889400	3.37518900	-1.70218000
H	1.59957400	3.44843500	-1.42505800
H	3.05139300	4.38431200	-1.82423500
H	2.71976100	2.84443800	-2.65808400
S	3.33224800	3.49019900	1.04688100
Ag	2.93490600	-1.38299400	0.88501400
O	0.00538600	-1.15767200	1.57913800
C	0.53064900	-2.04035000	2.32247500
O	1.70563600	-2.51395600	2.20374700
C	-0.29659300	-2.58631900	3.46901800
H	0.20645800	-2.35628200	4.41094500
H	-1.29450400	-2.14707900	3.46774000
H	-0.35339400	-3.67316100	3.37428100
C	-4.01332900	0.88401000	0.62297700
C	-5.15560100	0.86540100	-0.18828600
C	-5.32112000	-0.15743300	-1.13178000
C	-4.34634400	-1.14001700	-1.27957000
C	-3.18328100	-1.10256600	-0.50009100
C	-3.04032300	-0.10007200	0.47254800
H	-3.87982700	1.66519400	1.36031100
H	-6.22198700	-0.16525000	-1.73605300
H	-4.48408100	-1.93893100	-2.00216800
H	-2.16118000	-0.10534900	1.10680700
C	-6.22872200	1.89371300	-0.08517900
O	-7.23684900	1.90802300	-0.76589600
O	-5.96221600	2.82484100	0.85849800
C	-6.95974000	3.84763900	1.00344200
H	-7.92248400	3.41013700	1.28171500
H	-6.59427200	4.50607500	1.79149600
H	-7.08460600	4.39905700	0.06753400

H	-3.11018400	-3.11008200	1.05279600
H	-2.88017100	-0.82375600	-3.31123200
O	2.57559300	0.21277900	-3.21496300
O	-1.35928400	-5.14072800	1.49164300
C	-2.54710000	-5.25879900	2.27197600
H	-2.40969400	-6.14868100	2.88700800
H	-2.68696600	-4.38765800	2.92260700
H	-3.43123200	-5.38649700	1.63597000

TS29

C	-2.86199300	-0.16775200	2.78874500
C	-1.66293300	-0.34007900	3.48924100
C	-0.52071400	-0.72925900	2.78850400
C	-0.56801000	-0.90429400	1.39834400
C	-1.76910000	-0.67423300	0.67489300
C	-2.93066500	-0.34081100	1.39388900
Pd	1.09799000	-0.46775300	0.26740200
H	0.07059900	-2.07425500	1.14834200
H	0.39247500	-0.92176600	3.34418200
C	-0.19007500	-0.81180800	-1.31511200
C	-0.03842300	0.37521100	-2.28377100
C	-2.19439900	0.51594400	-1.59927600
C	-1.68074900	-0.74983900	-0.83363700
C	-0.95403000	1.42698800	-1.62435900
H	-1.09083700	2.32119400	-2.24176400
H	-0.62746700	1.73128500	-0.62806300
C	-0.85275800	0.03570200	-3.56943800
H	-0.62655200	0.77631400	-4.34335000
H	-0.59724300	-0.94490300	-3.98004600
C	-2.33529300	0.13850800	-3.09147600
H	-2.87182000	0.92316500	-3.63390200
H	-2.89219300	-0.79348500	-3.22797500
H	0.99707400	0.65114300	-2.47822300
H	-2.20558800	-1.64030200	-1.19109300
C	0.21759300	-2.16285700	-1.83998900
O	-0.45064100	-3.17598000	-1.73503100
C	1.84499000	-3.40342000	-3.01321000
H	2.82808600	-3.21185400	-3.44285300
H	1.90387200	-4.15028500	-2.21824800
H	1.14889900	-3.74673200	-3.78334400
C	4.97847400	1.25244300	-0.92277400

C	3.97029700	0.14806900	-0.56023000
O	2.75228600	0.41546800	-0.79353900
O	4.42387600	-0.91319800	-0.03951100
C	3.25226300	3.05297300	0.50465800
C	2.83739000	4.10648700	-0.32051700
C	2.27740100	2.45988600	1.31694200
C	1.51085500	4.53143600	-0.36167300
C	0.95351200	2.88273500	1.30743600
C	0.56722600	3.91189000	0.45286100
F	2.58427600	1.40698000	2.09748700
F	0.03069100	2.26739200	2.05892600
F	-0.71495100	4.27914300	0.39618500
F	1.13715100	5.51801600	-1.18388500
F	3.70801000	4.72112500	-1.12801800
C	6.42089200	0.73710100	-0.93495500
H	6.51985400	-0.02173400	-1.71698600
H	7.11623400	1.55260300	-1.15403100
H	6.68924200	0.27187900	0.01472300
C	4.60889800	1.92457200	-2.24667600
H	3.58608000	2.30003300	-2.23064200
H	5.29291200	2.74897800	-2.45907300
H	4.68058500	1.18745800	-3.05508800
S	4.93650700	2.48551800	0.51710800
Ag	3.14842300	-2.59791200	0.24209500
O	0.14747700	-3.41224800	1.37093300
C	0.72961500	-4.33476700	0.72437800
O	1.91594500	-4.30474600	0.26464900
C	-0.06527000	-5.59529000	0.45835800
H	0.59370100	-6.45098100	0.30479600
H	-0.76635800	-5.78166100	1.27350700
H	-0.63755100	-5.41381000	-0.45718100
C	-6.25753600	1.16443200	0.36024800
C	-6.77548500	0.16224800	-0.47110500
C	-6.03698900	-1.01065300	-0.68071700
C	-4.79573300	-1.17517700	-0.07750200
C	-4.26012800	-0.17050000	0.74580100
C	-5.01427800	0.99455500	0.96300000
H	-6.82706100	2.07223100	0.52275400
H	-6.45805500	-1.78210400	-1.31661600
H	-4.23612200	-2.09208400	-0.23156100
H	-4.60473000	1.78053300	1.59085100

C	-8.09435000	0.28663700	-1.15042500
O	-8.57561000	-0.55725800	-1.88212500
O	-8.71461300	1.45609400	-0.86607200
C	-9.99340100	1.63413600	-1.49498700
H	-10.68669800	0.84604900	-1.18859000
H	-10.35093400	2.60984200	-1.16550600
H	-9.89461000	1.60756600	-2.58365400
H	-3.77640900	0.07840300	3.31538300
H	-3.09523000	0.94908400	-1.16898700
O	1.41021100	-2.13662800	-2.47653800
O	-1.51993400	-0.17977400	4.83534800
C	-2.65656000	0.20771200	5.59303900
H	-2.31521200	0.29240900	6.62573000
H	-3.05209100	1.17776200	5.26304800
H	-3.45616600	-0.54308800	5.53856400

int50

C	-2.99437100	-0.26231600	2.82152400
C	-1.78347600	-0.53891500	3.46494300
C	-0.59006800	-0.54983400	2.72606900
C	-0.60658700	-0.25703500	1.35871700
C	-1.82808100	0.03081700	0.70467500
C	-3.02283800	0.00675400	1.44221200
Pd	1.05303900	-0.20989400	0.29548200
H	-1.18705400	-2.33732400	0.84386600
H	0.33568600	-0.76880700	3.25296100
C	-0.25510100	0.21350700	-1.25757600
C	0.11452300	1.60681300	-1.80856400
C	-2.01473100	1.87380100	-1.07781900
C	-1.72849500	0.37317300	-0.75657300
C	-0.64307700	2.53468400	-0.83143800
H	-0.61180300	3.58567100	-1.13705600
H	-0.30453600	2.45937800	0.20429900
C	-0.69518700	1.83748400	-3.11950800
H	-0.32974800	2.74270600	-3.61565800
H	-0.58141900	1.01425700	-3.82865100
C	-2.16024100	2.01980700	-2.60863600
H	-2.54791700	3.01090700	-2.86505500
H	-2.85148800	1.28051600	-3.02624900
H	1.18783400	1.76301300	-1.92722300
H	-2.38558800	-0.26854400	-1.35001200

C	-0.01954600	-0.97502100	-2.13444800
O	-0.67165700	-2.01298100	-2.12015900
C	1.43009100	-1.95084100	-3.72248100
H	2.24551000	-1.61524800	-4.36314200
H	1.77881300	-2.74563400	-3.05423600
H	0.59856500	-2.33244200	-4.32043400
C	5.33889000	-0.50131700	-0.73045700
C	3.89779400	-0.99535300	-0.51095000
O	2.98730700	-0.14569200	-0.71717500
O	3.73375100	-2.19823800	-0.13381000
C	4.47909900	1.83664200	0.73555300
C	4.53740500	2.96342200	-0.09428900
C	3.34506200	1.70679500	1.54699800
C	3.50189200	3.89421300	-0.14638300
C	2.31343500	2.63898200	1.53273300
C	2.38508100	3.72827000	0.66884300
F	3.18020200	0.61852300	2.32281300
F	1.22563100	2.46887100	2.29719100
F	1.37890100	4.60394200	0.61585900
F	3.57127600	4.94295700	-0.97432200
F	5.58739700	3.16296400	-0.89912900
C	6.36581900	-1.63428800	-0.65482800
H	6.17283200	-2.34270600	-1.46580200
H	7.38049300	-1.24212100	-0.77246200
H	6.29170200	-2.17990300	0.28718300
C	5.44243900	0.26757000	-2.05068400
H	4.71462100	1.07658300	-2.09648500
H	6.44710200	0.67762700	-2.17616800
H	5.23513200	-0.41763800	-2.88169100
S	5.76415900	0.60814000	0.75058700
Ag	1.72763200	-2.98740700	0.00697100
O	-1.83023500	-2.99011500	0.48786900
C	-1.25049100	-3.99672500	-0.13000300
O	-0.04168600	-4.25516400	-0.08186000
C	-2.20485600	-4.82667000	-0.93305100
H	-1.79072800	-5.82005700	-1.10237700
H	-3.18240000	-4.88054500	-0.45089000
H	-2.31969300	-4.31398500	-1.89466600
C	-6.40837600	1.49686200	0.58433100
C	-6.84089900	0.63772400	-0.43482300
C	-6.02485500	-0.43227600	-0.82938200

C	-4.79121800	-0.63368900	-0.22225400
C	-4.34313000	0.23018900	0.79151800
C	-5.17239800	1.28912100	1.19193600
H	-7.03894100	2.32348100	0.89113700
H	-6.38192100	-1.09534100	-1.61034400
H	-4.16547900	-1.47185800	-0.51377500
H	-4.83131900	1.95943800	1.97559800
C	-8.14798200	0.80696600	-1.12548700
O	-8.56347200	0.07800200	-2.00653000
O	-8.84291600	1.87535500	-0.66687700
C	-10.11325800	2.09043500	-1.29996800
H	-10.77018800	1.22911500	-1.15018100
H	-10.53202300	2.97912900	-0.82731500
H	-9.98692800	2.24895200	-2.37449200
H	-3.93279000	-0.28182300	3.36237000
H	-2.85729700	2.27153800	-0.50893700
O	1.03433500	-0.80053300	-2.96505700
O	-1.66067200	-0.82260500	4.79539900
C	-2.83332900	-0.81606700	5.59429100
H	-2.50835600	-1.04780000	6.60991900
H	-3.32338300	0.16684500	5.58774000
H	-3.55463500	-1.57605600	5.26448900

int51

C	1.99575300	1.92064600	2.47127100
C	0.74117700	1.41779100	2.82805800
C	0.04149500	0.59065200	1.93854100
C	0.60360700	0.27037100	0.69994700
C	1.88149700	0.75847200	0.33133900
C	2.56668600	1.60081500	1.22654500
Pd	-0.31748000	-0.97516000	-0.55362800
H	-0.93720300	0.22700200	2.22511700
H	2.54427500	2.57790500	3.13510600
C	1.40099900	-0.64768100	-1.72391100
C	2.18636400	-1.94560500	-2.01296100
C	3.65880600	-0.71054900	-0.81628400
C	2.44089200	0.25543600	-0.97014500
C	2.98382500	-2.09308900	-0.69950700
H	3.70252100	-2.91996300	-0.72531100
H	2.34525000	-2.19861600	0.18192600
C	3.32645000	-1.65470800	-3.03065200

H	3.76757500	-2.59597200	-3.37672000
H	2.96337700	-1.12654000	-3.91551000
C	4.35051600	-0.82329700	-2.19256300
H	5.30623500	-1.34966200	-2.09973200
H	4.56116500	0.15974600	-2.62627600
H	1.55893700	-2.78957400	-2.29985700
H	2.72904600	1.09554200	-1.60881200
C	0.73406900	0.04563100	-2.84670500
O	0.41217200	1.24902000	-2.87223000
C	-0.34787300	-0.16213500	-4.94085200
H	-0.49663200	-0.95472600	-5.67425900
H	-1.30781400	0.18148700	-4.54396300
H	0.17162200	0.68671700	-5.39136900
C	-4.46433900	-0.44120000	1.01171100
C	-3.10314000	-0.22088400	0.31251100
O	-3.03329100	0.76228000	-0.47918600
O	-2.17662600	-1.04385800	0.58866900
C	-4.54267400	2.38163100	1.47847500
C	-3.31465200	3.01023700	1.24511600
C	-5.67567000	2.96663600	0.89946700
C	-3.20182700	4.11858200	0.41689200
C	-5.58683200	4.09902600	0.09066300
C	-4.34036900	4.66612200	-0.16753000
F	-6.88576000	2.42590600	1.07521500
F	-6.68498800	4.62853300	-0.46088500
F	-4.23740900	5.72432000	-0.97413200
F	-1.98397100	4.61115800	0.11564600
F	-2.18133500	2.51078300	1.75498700
C	-5.60462200	-0.31607500	-0.00221700
H	-5.51076500	-1.11573600	-0.74703500
H	-6.57363300	-0.40933900	0.49335700
H	-5.55661400	0.63555800	-0.53153300
C	-4.52255300	-1.77876300	1.75608100
H	-3.72079300	-1.86324100	2.49220100
H	-5.48865000	-1.90127100	2.25464200
H	-4.40098400	-2.59142700	1.03323500
S	-4.62505900	0.85666400	2.38617100
Ag	-1.00273000	1.70234500	-0.96493500
C	-0.43106600	-4.76697000	1.81633200
C	0.59804000	-5.67228100	1.52823400
C	0.98974500	-5.88553400	0.20050700

C	0.35913300	-5.19821600	-0.83693800
C	-0.66186400	-4.30474600	-0.51933100
C	-1.07289400	-4.07127300	0.79338300
H	-0.71299600	-4.60812100	2.85174000
H	1.78868500	-6.58393700	-0.01974400
H	0.67016200	-5.34943200	-1.86414300
H	-1.83868600	-3.33675500	1.01463100
I	-1.56178100	-3.14626000	-2.10354900
C	1.24502000	-6.37588300	2.67354800
O	0.92436700	-6.23013400	3.83657700
O	2.23719900	-7.20291400	2.27545600
C	2.90273500	-7.90948600	3.33573500
H	3.35954200	-7.20660800	4.03749900
H	2.19464500	-8.53888600	3.88141900
H	3.66476800	-8.51902800	2.85030100
H	4.32961000	-0.42451100	-0.00421900
O	0.44549600	-0.75085600	-3.89574300
C	6.25795600	2.43635200	1.48994800
C	6.46228200	3.20196300	0.33413400
C	5.38387700	3.45374600	-0.52571800
C	4.12458300	2.93974800	-0.24022600
C	3.91040600	2.15892600	0.90838600
C	4.99409400	1.92459300	1.77094900
H	7.09007600	2.24169300	2.15681100
H	5.55547700	4.05992300	-1.40893700
H	3.29044100	3.15204100	-0.90164000
H	4.83787600	1.31957100	2.65924200
C	7.78848900	3.77196800	-0.02572500
O	8.00866300	4.43744300	-1.02004000
O	8.74682000	3.47012400	0.88337200
C	10.04971200	3.99520100	0.58790700
H	10.02210800	5.08686600	0.53058000
H	10.69194600	3.66982100	1.40661600
H	10.41572300	3.60607100	-0.36631600
O	0.10634900	1.68303700	4.00830300
C	0.75300900	2.53089700	4.94306700
H	0.07940100	2.60718000	5.79817900
H	1.71247000	2.11252100	5.27680300
H	0.92649400	3.53418500	4.53035500

TS30

C	-1.58188500	0.87523500	2.73589600
C	-0.40583900	0.16426800	3.00339900
C	0.55568300	0.00297100	1.99726100
C	0.34411700	0.58964800	0.75695900
C	-0.78750200	1.37609100	0.48803100
C	-1.78108700	1.47075700	1.48080700
Pd	1.59623000	0.20804300	-0.74742200
H	1.42742000	-0.60548700	2.20113000
H	-2.36669700	0.96012800	3.47767500
C	0.49381700	1.85939200	-1.66327400
C	1.21599500	3.21435000	-1.78920700
C	-0.55068100	3.70545000	-0.46819200
C	-0.76737800	2.18773700	-0.77513800
C	0.98850100	3.80161400	-0.38201300
H	1.34684900	4.83215300	-0.28467200
H	1.42032100	3.19259200	0.41567300
C	0.36640300	4.19217100	-2.65635800
H	0.95830100	5.09016900	-2.86326200
H	0.08496800	3.76820100	-3.62161500
C	-0.85523100	4.51669800	-1.74287400
H	-0.91188800	5.58635800	-1.51718700
H	-1.81157400	4.22741500	-2.19076800
H	2.23851800	3.12668300	-2.15336600
H	-1.68340400	2.05074900	-1.35806100
C	0.18194000	1.18056500	-2.93664800
O	-0.73300000	0.33716100	-3.11420700
C	0.85811800	0.74322300	-5.16170200
H	1.54498300	1.20874700	-5.86699600
H	1.16555400	-0.28538700	-4.95195900
H	-0.16356900	0.75207100	-5.54566700
C	1.20994100	-4.00835200	1.15831400
C	1.07695000	-2.89573300	0.09675700
O	0.13968500	-3.07550100	-0.75047600
O	1.86514600	-1.91945000	0.15850800
C	-1.65397900	-3.96849500	1.41666600
C	-2.28467600	-2.88964500	0.78564100
C	-2.20304000	-5.23795000	1.19490800
C	-3.36386500	-3.06009800	-0.07132400
C	-3.30117500	-5.42904000	0.35705300
C	-3.87583700	-4.33635800	-0.29012500
F	-1.66259100	-6.32164900	1.76184800

F	-3.79562300	-6.65571800	0.15494800
F	-4.90742000	-4.51370300	-1.11752400
F	-3.87066900	-2.00275100	-0.73155200
F	-1.82234800	-1.64285600	0.93444600
C	1.11981000	-5.39449200	0.51758000
H	1.97430500	-5.53497400	-0.15487900
H	1.14185700	-6.17353500	1.28283400
H	0.21088900	-5.49620000	-0.07508900
C	2.48287200	-3.85431500	1.99541400
H	2.53033500	-2.87771300	2.48122400
H	2.53895900	-4.63858500	2.75550600
H	3.35326600	-3.94404100	1.33849900
S	-0.19627900	-3.72600600	2.40472200
Ag	-0.56942700	-1.40315700	-1.83168600
C	4.72526600	0.45320600	1.91142900
C	5.00628500	1.82470200	1.97217000
C	4.65637400	2.64943600	0.89322100
C	4.01017400	2.11946100	-0.22050800
C	3.66886400	0.76628200	-0.21400800
C	4.08306600	-0.09839800	0.80601400
H	5.02473700	-0.17894300	2.74113600
H	4.89691500	3.70616200	0.92135300
H	3.75941500	2.75116200	-1.05911200
H	3.86292700	-1.15584900	0.76129900
I	3.67773200	-0.30071300	-2.51675800
C	5.69627700	2.34100400	3.18357900
O	6.03509500	1.65538600	4.12953600
O	5.91091500	3.67706200	3.12633300
C	6.57267400	4.23457200	4.27236700
H	5.98318200	4.06542600	5.17765600
H	7.55788200	3.77997200	4.40784100
H	6.66657300	5.30142600	4.06889700
H	-1.10695600	4.03403600	0.41109600
O	0.95931300	1.53004900	-3.95852600
C	-4.65585500	3.94216000	1.72436500
C	-5.47584400	3.51552600	0.67105700
C	-5.09241000	2.40776200	-0.09881300
C	-3.89988800	1.74724000	0.17035100
C	-3.06113100	2.17940200	1.21261200
C	-3.46244100	3.27546000	1.99170100
H	-4.95355500	4.79609300	2.32201300

H	-5.74738800	2.08029500	-0.89932300
H	-3.61538600	0.87402900	-0.40984700
H	-2.81932900	3.61225300	2.79969700
C	-6.75585800	4.19196200	0.32649700
O	-7.49537800	3.85147400	-0.57735800
O	-7.01898300	5.24754500	1.13358500
C	-8.24057400	5.94354600	0.84262900
H	-9.09952300	5.27422900	0.94230100
H	-8.29903600	6.75399300	1.56946200
H	-8.22508100	6.34034500	-0.17623100
O	-0.12072000	-0.44353400	4.19128200
C	-1.10482000	-0.41892800	5.21250000
H	-0.68449200	-0.97760700	6.05015500
H	-1.32830800	0.60580400	5.53909300
H	-2.03631500	-0.90185400	4.88792800

int52

C	2.03136000	1.30077200	2.61877100
C	0.70346800	1.01161600	2.95159800
C	-0.06817200	0.20673900	2.10459600
C	0.49655000	-0.30879500	0.94510000
C	1.83462400	-0.05696600	0.60362700
C	2.59454900	0.78267000	1.44421500
Pd	-0.61437500	-1.22484200	-0.48311200
H	-1.10916400	0.05927400	2.36020400
H	2.64078600	1.94035800	3.24545200
C	1.31786300	-1.51146300	-1.44037100
C	1.89518000	-2.93437500	-1.54725800
C	3.41892600	-1.88534200	-0.24108000
C	2.40680200	-0.74970700	-0.59622500
C	2.50169600	-3.11767100	-0.13799000
H	3.05609800	-4.05664100	-0.03902100
H	1.77146900	-3.05113300	0.66849400
C	3.19837000	-2.92834700	-2.41001000
H	3.48871600	-3.96704500	-2.59782100
H	3.06930800	-2.45379200	-3.38198100
C	4.24253200	-2.20609700	-1.50312100
H	5.08353700	-2.86327700	-1.26048300
H	4.65787500	-1.30302400	-1.96285700
H	1.17775000	-3.67778800	-1.88541200
H	2.89908600	-0.01659700	-1.24061700

C	1.01121400	-0.78568100	-2.70839400
O	0.82791000	0.45633000	-2.77139700
C	0.55139000	-0.87928000	-5.02609000
H	0.61159800	-1.65623600	-5.78599900
H	-0.47829500	-0.53746500	-4.90576100
H	1.20933500	-0.04140900	-5.26491400
C	-4.14693100	0.97892600	1.21580000
C	-2.96691600	0.58169700	0.30901700
O	-2.63741100	1.44546900	-0.56611000
O	-2.41929400	-0.53233000	0.52909500
C	-3.02697600	3.61003300	1.42496700
C	-1.76049000	3.73532300	0.84106100
C	-3.97308100	4.59102900	1.09925000
C	-1.46717900	4.73562100	-0.07603400
C	-3.68794700	5.62309200	0.20585300
C	-2.43299900	5.68618300	-0.39674700
F	-5.20544100	4.54344800	1.61443500
F	-4.61618000	6.53810600	-0.09400100
F	-2.15887600	6.64921700	-1.27830000
F	-0.27172700	4.75113000	-0.69242400
F	-0.79017800	2.84714900	1.09671000
C	-5.28789400	1.58102100	0.39422900
H	-5.68986000	0.81174600	-0.27474100
H	-6.08683900	1.93236500	1.05070400
H	-4.93746700	2.40712900	-0.22465400
C	-4.62655400	-0.19125100	2.07899700
H	-3.82253000	-0.59720100	2.69616300
H	-5.45392500	0.12398700	2.72069500
H	-4.97294500	-0.99543900	1.42388600
S	-3.43967000	2.22628000	2.46305000
Ag	-0.82819200	1.31523600	-1.65889900
C	-1.08989200	-4.23106400	2.54338100
C	-1.16394100	-5.42166100	1.81345900
C	-1.03243000	-5.38152700	0.41984800
C	-0.81527000	-4.16952900	-0.23644500
C	-0.72690400	-2.99720900	0.51424400
C	-0.87477300	-3.01116500	1.89990400
H	-1.19695000	-4.26991200	3.62263600
H	-1.11476700	-6.29512300	-0.15803000
H	-0.75595000	-4.15276100	-1.31524900
H	-0.82151300	-2.10665900	2.48639800

I	-2.31707900	-1.87149800	-2.65159400
C	-1.39244300	-6.68776700	2.56222400
O	-1.51143900	-6.76303500	3.77033800
O	-1.45463100	-7.76625900	1.74661200
C	-1.68202400	-9.01846900	2.41149700
H	-0.87876300	-9.22881800	3.12300800
H	-2.63168900	-9.00010200	2.95320800
H	-1.70428900	-9.77118000	1.62328800
H	4.01832900	-1.64686800	0.63884400
O	0.98239800	-1.52006700	-3.80197900
C	6.36806800	1.05457800	1.73149600
C	6.69531100	1.73274700	0.55003700
C	5.67541900	2.11471000	-0.33266500
C	4.34977500	1.81206300	-0.04405900
C	4.01199000	1.11819500	1.13009300
C	5.03816000	0.75495500	2.01640100
H	7.15563200	0.76102900	2.41595600
H	5.94531400	2.65270600	-1.23523300
H	3.56128600	2.12514500	-0.72230100
H	4.78401900	0.21872100	2.92605800
C	8.09756000	2.07497200	0.18368500
O	8.42101500	2.65859200	-0.83316900
O	8.99058600	1.66252000	1.11321100
C	10.36274000	1.96399400	0.81388500
H	10.50804400	3.04354100	0.71912200
H	10.94041200	1.57036000	1.65031300
H	10.66645800	1.48767500	-0.12230100
O	0.06085600	1.48399600	4.05594300
C	0.75171400	2.38962000	4.90295400
H	0.04792900	2.65975000	5.69152900
H	1.63948100	1.92797700	5.35569900
H	1.05565100	3.29597900	4.36246500

int53

C	-4.02238900	-0.17362900	2.91734000
C	-2.80050900	0.22933100	3.47737900
C	-1.65753000	0.30260400	2.67148200
C	-1.78576500	-0.02241700	1.32101900
C	-2.97927800	-0.44845100	0.73977600
C	-4.12123900	-0.53180800	1.57228000
Pd	-0.14779700	-0.07600500	0.20643800

H	-0.69330200	0.60076200	3.06685700
C	-1.51313600	-0.60940800	-1.31572800
C	-1.70577500	0.30841700	-2.51789200
C	-3.79673600	0.12897000	-1.65729800
C	-2.94957600	-0.79187100	-0.72485400
C	-2.80392200	1.25909800	-1.99271200
H	-3.17551600	1.93821500	-2.76675100
H	-2.49500500	1.84412100	-1.12519500
C	-2.49184100	-0.48531200	-3.60929900
H	-2.47531700	0.08606200	-4.54277800
H	-2.04498000	-1.45856000	-3.81761900
C	-3.93659600	-0.57858700	-3.02161800
H	-4.65705200	-0.05157900	-3.65478400
H	-4.28938200	-1.60981000	-2.91718400
H	-0.78548700	0.76132600	-2.88525800
H	-3.25738900	-1.83393900	-0.86163500
C	-0.65769200	-1.82990200	-1.38854300
O	-0.42087200	-2.47203000	-0.35266600
C	1.04134200	-3.02071900	-2.50785000
H	1.39089100	-3.09212400	-3.53658700
H	1.82523900	-2.63531700	-1.85306900
H	0.68707600	-3.98821800	-2.14726300
C	-0.54137500	4.22112100	0.49122000
C	0.25094700	4.64520200	-0.58195500
C	0.87409500	3.69012000	-1.39461300
C	0.70724900	2.32910600	-1.14463800
C	-0.09418800	1.91641500	-0.07241000
C	-0.71791300	2.86006800	0.74789100
H	-1.02642000	4.95607800	1.12401400
H	1.49195400	4.02903000	-2.21995000
H	1.21563400	1.60446800	-1.76976900
H	-1.34317000	2.55457600	1.57575800
C	0.46570900	6.08251100	-0.90291100
O	1.14021800	6.48954600	-1.82951000
O	-0.17838800	6.90686700	-0.04283900
C	-0.00851400	8.30869500	-0.30336000
H	-0.57966800	8.82379800	0.46925700
H	1.04797900	8.58561100	-0.25054400
H	-0.38654300	8.56489900	-1.29694300
C	3.92187300	-0.31551100	0.75191000
C	2.40975200	-0.24143700	0.53824900

O	1.92289700	-0.37720400	-0.62828000
O	1.66353800	-0.00103000	1.53785000
C	6.29812400	-1.29939700	-0.41204000
C	7.28020800	-0.31430700	-0.58275900
C	6.72267300	-2.55071500	0.05676000
C	8.62283200	-0.55691600	-0.30052200
C	8.06017600	-2.81441700	0.34280100
C	9.01191000	-1.81302800	0.15987800
F	5.84049500	-3.53605600	0.25647600
F	8.43724400	-4.01704200	0.79221700
F	10.29578600	-2.05473900	0.43277800
F	9.53906900	0.40367500	-0.46761200
F	6.94961500	0.90818800	-1.01419000
C	4.43406600	1.11689700	0.98769700
H	3.98576600	1.51252300	1.90447200
H	5.52095700	1.12004800	1.09732300
H	4.17040500	1.77208600	0.15397300
C	4.24225100	-1.22268500	1.94645600
H	3.92178700	-2.25074500	1.76446300
H	5.31661900	-1.22190300	2.14873500
H	3.72155200	-0.84117600	2.82847900
S	4.59748000	-1.01456700	-0.86183100
H	-4.89063200	-0.23146600	3.56515700
O	-2.82798300	0.52408700	4.80687200
C	-1.61230300	0.91596500	5.43011900
H	-1.85517100	1.09332300	6.47880300
H	-0.85111400	0.12789600	5.36206200
H	-1.21150800	1.83915400	4.99053700
C	-6.83635800	-2.64774300	-0.03341800
C	-7.94036900	-1.78724300	0.03823900
C	-7.79463800	-0.52498300	0.62877400
C	-6.55643600	-0.12853600	1.12766900
C	-5.44121800	-0.97724100	1.04435600
C	-5.60243900	-2.24697100	0.46550000
H	-6.97083400	-3.62798100	-0.47829500
H	-8.64871000	0.13971500	0.68893000
H	-6.43920500	0.85362700	1.57582400
H	-4.75699600	-2.92671800	0.42753500
C	-9.23445100	-2.26672100	-0.52093500
O	-9.39898600	-3.35210300	-1.04455000
O	-10.22601500	-1.35537800	-0.38570700

C	-11.50095700	-1.76248600	-0.90692900
H	-11.43106800	-1.96956900	-1.97831400
H	-11.85433500	-2.66441600	-0.39976500
H	-12.17620600	-0.92730700	-0.72029400
O	-0.05175500	-2.06582300	-2.54681200
H	-4.74337000	0.42866500	-1.20602300

TS31

C	3.57872100	-0.15400200	-2.83599300
C	2.60372000	0.74142200	-3.29677800
C	1.64592300	1.23688800	-2.40616300
C	1.67907400	0.80264900	-1.07970700
C	2.63160300	-0.10804200	-0.59076000
C	3.59383000	-0.58803500	-1.50922400
Pd	0.01124900	0.90689600	0.09673600
H	0.89817400	1.95570600	-2.71472700
C	0.89727600	-0.68114100	1.13530400
C	0.89643900	-0.51290500	2.65481000
C	3.08722200	-0.33853100	2.09186100
C	2.38885000	-0.76698000	0.74758600
C	2.03138600	0.50383300	2.85019200
H	2.30218300	0.63645000	3.90310600
H	1.80827900	1.48068500	2.43147900
C	1.55157400	-1.79810800	3.26948200
H	1.34952400	-1.82324700	4.34437800
H	1.14202300	-2.71597600	2.84384600
C	3.07802100	-1.61029500	2.97343600
H	3.64139500	-1.44017300	3.89643200
H	3.52655500	-2.47083700	2.46815300
H	-0.08107000	-0.27242200	3.07188200
H	2.63043400	-1.82422700	0.58622100
C	0.02934200	-1.77009800	0.53299800
O	0.13959500	-2.17841100	-0.60993300
C	-1.85315800	-3.15450900	0.89286400
H	-2.35508400	-3.56755600	1.76739300
H	-2.57555400	-2.61564800	0.27612100
H	-1.36983200	-3.94133500	0.30976200
C	2.93104900	4.17236900	0.82148100
C	2.09706700	5.22014100	0.41076200
C	0.87940200	4.92061200	-0.21057400
C	0.48750600	3.59770800	-0.40698300

C	1.30418700	2.55234600	0.05771400
C	2.54655700	2.84732600	0.63226000
H	3.89120500	4.39481400	1.27301300
H	0.24466400	5.73674900	-0.53986500
H	-0.45843100	3.39249700	-0.89795200
H	3.23113500	2.05680500	0.90251500
C	2.46052500	6.65287500	0.58499600
O	1.77327700	7.58709300	0.21918400
O	3.65386900	6.81101500	1.20352800
C	4.05980100	8.17482400	1.40096000
H	5.02550800	8.12516400	1.90412200
H	4.15083600	8.69216900	0.44202400
H	3.33084100	8.70785800	2.01736200
C	-4.08750700	0.69928200	-0.37306400
C	-2.58541300	0.95811200	-0.21044600
O	-1.94448100	0.34148400	0.71743000
O	-2.01052400	1.73688000	-1.00903900
C	-6.17118300	-0.99403000	0.49989700
C	-7.34595900	-0.29350300	0.80187100
C	-6.30881800	-2.20245100	-0.19789700
C	-8.60181800	-0.76668300	0.42725500
C	-7.55414500	-2.69499100	-0.57943700
C	-8.70353400	-1.97339900	-0.26187300
F	-5.22897300	-2.92059300	-0.53553200
F	-7.65674400	-3.84906600	-1.24845500
F	-9.90184000	-2.43546700	-0.62457400
F	-9.70762200	-0.07443800	0.72369200
F	-7.29257900	0.87294600	1.45508900
C	-4.84569700	2.03290600	-0.29125900
H	-4.48960200	2.69600900	-1.08511900
H	-5.91903200	1.87285400	-0.41658000
H	-4.68491500	2.51939100	0.67386400
C	-4.30132100	0.02743800	-1.74028900
H	-3.80029700	-0.94214700	-1.79220300
H	-5.36755000	-0.11831400	-1.93208800
H	-3.89388700	0.67948200	-2.51744500
S	-4.56665100	-0.44473500	1.04325700
H	4.32121300	-0.51467300	-3.53972400
O	2.68349000	1.08206400	-4.61122000
C	1.70269900	1.96838800	-5.13496100
H	1.93682500	2.08355800	-6.19411100

H	0.69029900	1.55746100	-5.02918900
H	1.74563000	2.95089400	-4.64644800
C	5.52221300	-3.84493700	-1.36953500
C	6.43876200	-3.59356600	-0.34010400
C	6.43570100	-2.34632800	0.29966200
C	5.51936500	-1.37172500	-0.08360200
C	4.58980400	-1.61818000	-1.10608700
C	4.60957000	-2.86640900	-1.74999300
H	5.53933300	-4.81550300	-1.85378400
H	7.15295100	-2.14646100	1.08728300
H	5.53048000	-0.40011300	0.39779800
H	3.88942900	-3.06592500	-2.53748100
C	7.38954600	-4.67925200	0.02830100
O	7.42853100	-5.77179300	-0.50411200
O	8.22043600	-4.31928800	1.03464600
C	9.16375000	-5.32659300	1.43290000
H	8.64503000	-6.22392400	1.78115000
H	9.81100700	-5.60092500	0.59541700
H	9.74690400	-4.88219600	2.23959700
O	-0.87565400	-2.23126400	1.41119100
H	4.07229500	0.11240300	1.96527700

int54

C	0.81109000	0.26660400	2.24794500
C	-0.31547100	1.02725400	2.55582200
C	-1.57802100	0.54957300	2.19146900
C	-1.72637100	-0.61981300	1.43684200
C	-0.57592700	-1.35102200	0.97000000
C	0.70829500	-0.88917800	1.46846100
H	-2.47339200	1.08388000	2.48208200
C	-0.44101900	3.61187700	-2.71682200
C	-0.42549900	2.25334100	-2.01459400
O	-0.60851600	2.21274900	-0.75813500
O	-0.19922300	1.19506000	-2.68843700
C	1.55768500	4.18203300	-0.71397100
C	1.05052100	5.09027900	0.22391800
C	2.32462400	3.11895600	-0.21832700
C	1.28876300	4.94732100	1.58766800
C	2.60831700	2.98800800	1.13655400
C	2.07791200	3.89682300	2.04594600
F	2.79785500	2.17202300	-1.04047400

F	3.36932400	1.97361800	1.58037400
F	2.31476800	3.75794500	3.34978000
F	0.75035500	5.80367800	2.47128300
F	0.29314100	6.12249900	-0.16677800
C	-0.57426000	3.47080600	-4.23634400
H	-1.55375100	3.04116000	-4.46832900
H	-0.50560200	4.44845100	-4.72388100
H	0.18860800	2.80426700	-4.64057500
C	-1.53061000	4.51274100	-2.12962400
H	-1.42001500	4.61523200	-1.05131500
H	-1.49262100	5.50398500	-2.58800200
H	-2.51323300	4.06916900	-2.33082900
S	1.27835700	4.36926300	-2.45926900
C	-5.34236900	-0.48000400	0.31090300
C	-5.88959700	-1.58290900	0.98056800
C	-5.06851100	-2.38021800	1.78865700
C	-3.71398300	-2.08939600	1.91261700
C	-3.15406900	-1.00334700	1.22450100
C	-3.98745300	-0.18904000	0.44267300
H	-5.97920200	0.14160600	-0.30778100
H	-5.51332300	-3.21897400	2.31328100
H	-3.08156700	-2.70092000	2.54935400
H	-3.55284500	0.66142300	-0.07534000
C	-7.33084100	-1.94804400	0.87981700
O	-7.84225200	-2.89251000	1.45007100
O	-8.02163700	-1.10788000	0.07600000
C	-9.41942500	-1.41019400	-0.06266800
H	-9.91970700	-1.37088400	0.90873200
H	-9.82032600	-0.64981000	-0.73287800
H	-9.55670200	-2.40880100	-0.48613700
Pd	-0.18870200	-0.05853800	-0.87347200
C	-0.00864400	-2.02510100	-1.33614200
C	-1.03873500	-2.45840600	-2.40972800
C	-1.85722500	-3.29158300	-0.46522600
C	-0.55728900	-2.59406100	0.01015800
C	-2.35924700	-2.39521600	-1.61882400
H	-3.19881300	-2.84146800	-2.16221700
H	-2.63784700	-1.38513400	-1.32293300
C	-0.91241300	-3.99307600	-2.61902800
H	-1.56807000	-4.29528600	-3.44249600
H	0.09954300	-4.31984600	-2.86216900

C	-1.41368100	-4.55866300	-1.25291900
H	-2.26740900	-5.22959900	-1.38787900
H	-0.63158600	-5.11531700	-0.72894300
H	-0.97630600	-1.86701200	-3.32554600
H	0.12260100	-3.33684000	0.42608800
C	1.39698700	-2.43062300	-1.70499300
O	1.91137100	-3.48295400	-1.37728700
C	3.28450000	-1.91513000	-3.02102300
H	3.20981800	-2.81876400	-3.63233200
H	3.62105700	-1.07070200	-3.62137900
H	3.97127500	-2.10367500	-2.19340100
O	-0.09270900	2.18759800	3.21287400
C	-1.14139100	3.15619700	3.26595600
H	-0.67218000	4.07581200	3.61529000
H	-1.56854300	3.32035700	2.26975600
H	-1.93092400	2.85436400	3.96444900
H	1.78114500	0.60880100	2.58368100
C	3.39278800	-3.57062300	1.64005100
C	4.43905000	-2.95864400	0.93876200
C	4.26742800	-1.66682600	0.42730400
C	3.05481700	-1.00588300	0.58278100
C	1.99285200	-1.62655800	1.25807500
C	2.18316800	-2.90370900	1.80312200
H	3.52996200	-4.56531500	2.04724200
H	5.09369700	-1.20085500	-0.09896800
H	2.91886300	-0.01442500	0.16816400
H	1.37603500	-3.37745200	2.35431500
C	5.74135100	-3.63554000	0.68942500
O	6.64388900	-3.16473700	0.02312500
O	5.81820300	-4.84840900	1.28331100
C	7.04603800	-5.55848700	1.05877800
H	7.19641100	-5.73902300	-0.00912300
H	7.89697100	-4.98698800	1.43942200
H	6.94436100	-6.50101000	1.59694700
H	-2.57198300	-3.51445500	0.32239700
O	1.98692200	-1.53921700	-2.52397600

TS32

C	0.56224500	-1.86737800	3.45562200
C	-0.65666800	-1.80864300	4.14132500
C	-1.82844900	-1.54166300	3.42871300

C	-1.80033400	-1.35863600	2.03799400
C	-0.57697700	-1.46012900	1.31785800
C	0.61384400	-1.69169000	2.07645000
H	-2.77853300	-1.43701000	3.93820900
C	-0.84460300	3.41604400	-1.88731600
C	-0.62016200	2.01029300	-1.32579400
O	-0.55389500	1.84226200	-0.06642800
O	-0.50730800	1.02335900	-2.12142400
C	1.58121900	4.10123100	-0.54686400
C	1.41928500	5.13726400	0.38151400
C	2.36462600	3.00736200	-0.15672100
C	2.00410800	5.08879300	1.64484900
C	2.96470000	2.94440900	1.09629600
C	2.78042900	3.98851900	2.00034300
F	2.54184300	1.96826200	-0.98527000
F	3.71046800	1.88825500	1.44542600
F	3.34842400	3.93360300	3.20669500
F	1.82796500	6.08956300	2.51583300
F	0.67519200	6.20810700	0.08378500
C	-1.47648300	3.35926100	-3.28355600
H	-2.47443600	2.91614000	-3.20542900
H	-1.57946100	4.36568200	-3.70042800
H	-0.88701000	2.73903800	-3.96036600
C	-1.67443800	4.26425000	-0.92128500
H	-1.21219400	4.30888500	0.06457300
H	-1.79347400	5.27806100	-1.31038800
H	-2.66600800	3.81139300	-0.80225200
S	0.85900000	4.18013200	-2.16841600
C	-4.50308200	0.52662200	0.14854100
C	-5.57028300	-0.37891400	0.20834600
C	-5.41474400	-1.58340800	0.90800500
C	-4.20015500	-1.88751700	1.51227500
C	-3.10656600	-1.01200500	1.40834900
C	-3.28454600	0.21573100	0.74786400
H	-4.62985900	1.47212100	-0.36641600
H	-6.25587900	-2.26651700	0.95957100
H	-4.08048100	-2.82462600	2.04817500
H	-2.47074200	0.93076000	0.71227200
C	-6.88685500	-0.11365100	-0.43532700
O	-7.83812900	-0.87074200	-0.39527900
O	-6.91633200	1.07432800	-1.08207800

C	-8.16249500	1.38601700	-1.72482300
H	-8.97409700	1.42492300	-0.99312700
H	-8.01818600	2.36072300	-2.19096600
H	-8.40684600	0.63115300	-2.47715600
Pd	-0.40541600	-0.39675600	-0.51407900
C	-0.20458400	-2.19697400	-1.46259400
C	-1.34359300	-2.53161900	-2.44434700
C	-1.92249300	-3.46929000	-0.46276200
C	-0.57262200	-2.81683800	-0.20416400
C	-2.57197500	-2.54352900	-1.51376300
H	-3.44892700	-3.00234800	-1.98113800
H	-2.84594400	-1.55921800	-1.13811600
C	-1.19577700	-4.05686700	-2.73661900
H	-1.90977200	-4.35353400	-3.51108200
H	-0.19568300	-4.32992000	-3.08191200
C	-1.54903400	-4.70130800	-1.35874300
H	-2.41491000	-5.36581200	-1.43264900
H	-0.72081900	-5.28164900	-0.94208900
H	-1.38142500	-1.88753900	-3.32277600
H	0.18487100	-3.39795000	0.30735600
C	1.20009800	-2.37655600	-1.97606300
O	1.93047600	-3.29248300	-1.64842200
C	2.81528400	-1.58247100	-3.50495300
H	2.94345500	-2.58305100	-3.92641500
H	2.84314700	-0.82568000	-4.28794600
H	3.60274300	-1.39924800	-2.77130400
O	-0.59197200	-2.00078600	5.48410400
C	-1.79529000	-1.92498100	6.23887700
H	-1.51111700	-2.11214800	7.27517100
H	-2.25619700	-0.93188500	6.16300600
H	-2.52068700	-2.68423800	5.91917300
H	1.47184300	-2.03396500	4.02296700
C	3.92613000	-3.08070100	0.87813600
C	4.37916700	-2.04186100	0.05427200
C	3.64017000	-0.85777000	-0.04190600
C	2.43236900	-0.73424000	0.63340200
C	1.94007000	-1.79116400	1.41506300
C	2.71839300	-2.95094800	1.55569800
H	4.50479500	-3.99361900	0.95560700
H	4.01082200	-0.04314000	-0.65184200
H	1.87621900	0.19249800	0.57205800

H	2.34821400	-3.76789200	2.16840600
C	5.60503500	-2.16426200	-0.77675100
O	5.90507300	-1.39644200	-1.67429200
O	6.35651900	-3.23826900	-0.44756400
C	7.52920500	-3.43188800	-1.25389600
H	7.25636900	-3.56412400	-2.30454200
H	8.19900600	-2.57154900	-1.17271300
H	8.00896700	-4.33035600	-0.86555300
H	-2.50319800	-3.72037500	0.42264200
O	1.51188000	-1.45608000	-2.90083600

int55

C	0.82694700	-1.75964700	3.58187700
C	-0.34322900	-1.71554000	4.34343200
C	-1.55029600	-1.39045900	3.72403300
C	-1.58457200	-1.10215700	2.34719300
C	-0.40301600	-1.13846200	1.58226200
C	0.81527300	-1.48566900	2.20800800
H	-2.47562100	-1.33518900	4.28507700
C	-1.05163300	3.10601500	-1.87155800
C	-0.70236500	1.70770900	-1.36453900
O	-0.37859100	1.55277700	-0.13374500
O	-0.77798500	0.70179100	-2.13111400
C	1.43372400	4.01275100	-0.78566700
C	1.26899200	5.06231000	0.12692300
C	2.35352000	3.00984100	-0.45470600
C	1.98137400	5.11078400	1.32272100
C	3.08353900	3.04575200	0.72881300
C	2.89184600	4.09937100	1.62085900
F	2.53970100	1.96842400	-1.27630200
F	3.96050000	2.08005000	1.02378700
F	3.58253800	4.13950400	2.76117300
F	1.80147000	6.12048300	2.18202500
F	0.40095300	6.04991600	-0.12049000
C	-1.83621000	3.02973200	-3.18708400
H	-2.78795800	2.52094900	-3.00651900
H	-2.04638400	4.03492800	-3.56376100
H	-1.29273300	2.46116300	-3.94355400
C	-1.81867200	3.88696300	-0.80011500
H	-1.26009500	3.93266600	0.13488700
H	-2.02655400	4.90176400	-1.14560100

H	-2.77018500	3.38133400	-0.59572300
S	0.55900500	3.97108400	-2.33014700
C	-4.37077400	0.65054600	0.44074700
C	-5.40620800	-0.28932500	0.53584400
C	-5.20358500	-1.46400600	1.27293400
C	-3.97302100	-1.70942200	1.87408500
C	-2.91351000	-0.79551300	1.74525800
C	-3.14180700	0.40276000	1.04569800
H	-4.53532100	1.57396000	-0.10336400
H	-6.01904200	-2.17564800	1.34897700
H	-3.81022700	-2.63206100	2.42362900
H	-2.35298200	1.14372800	0.98872900
C	-6.73061800	-0.09277400	-0.11376000
O	-7.65495800	-0.88092100	-0.04921200
O	-6.80178800	1.07165900	-0.80110500
C	-8.05850800	1.31768800	-1.45139500
H	-8.87111900	1.34853100	-0.72049700
H	-7.95049400	2.28268700	-1.94678200
H	-8.27519200	0.53231900	-2.18074100
Pd	-0.53840700	-0.61834100	-0.36069000
C	-0.37324400	-2.40684700	-1.62154600
C	-1.30227100	-2.31929700	-2.83269100
C	-2.56502800	-3.02040600	-1.08471400
C	-1.16041000	-2.80496900	-0.54332900
C	-2.65560500	-1.94763600	-2.18768000
H	-3.49919800	-2.11189700	-2.86557000
H	-2.69729800	-0.92640500	-1.80674000
C	-1.56671300	-3.82652900	-3.17450000
H	-2.12823200	-3.89408100	-4.11087800
H	-0.64117700	-4.39446700	-3.30457800
C	-2.41819900	-4.31612300	-1.95868900
H	-3.40875400	-4.65844700	-2.27316900
H	-1.94376400	-5.13514500	-1.41050300
H	-0.93941600	-1.70442800	-3.65290400
H	-0.76958000	-3.33633100	0.31575400
C	1.08166400	-2.73073100	-1.77035100
O	1.69084800	-3.49017700	-1.04626200
C	2.96417600	-2.38553300	-3.18798700
H	3.24429900	-3.39369000	-2.87646100
H	3.03641200	-2.27582100	-4.27045900
H	3.61136500	-1.65970100	-2.69440300

O	-0.19927800	-1.99721300	5.67155800
C	-1.35511900	-1.95108400	6.49357900
H	-1.01917600	-2.19962800	7.50156000
H	-1.80851200	-0.95074900	6.50084800
H	-2.11032600	-2.68249300	6.17515900
H	1.75966200	-1.99204500	4.08514700
C	4.14204400	-2.80639400	0.97343800
C	4.50654000	-1.82834500	0.03893800
C	3.68202800	-0.71281200	-0.15178900
C	2.49585300	-0.58814400	0.56092400
C	2.09923900	-1.58446700	1.46752800
C	2.94883500	-2.68326700	1.67465800
H	4.77815000	-3.67159700	1.11999900
H	3.98420700	0.05658100	-0.85114800
H	1.88171700	0.29393600	0.42707700
H	2.64452500	-3.46752000	2.36042300
C	5.72099100	-1.94925600	-0.80498600
O	5.94717400	-1.26715400	-1.79030400
O	6.56033400	-2.92269600	-0.38180300
C	7.73295100	-3.10910800	-1.18860300
H	7.45874900	-3.36864400	-2.21507500
H	8.33567100	-2.19706600	-1.20986800
H	8.28627100	-3.92393100	-0.72133200
H	-3.36259000	-3.04953600	-0.34579200
O	1.58518600	-2.12017500	-2.85724600

int56

C	-0.98381200	-2.89629700	-2.14431700
C	0.22601800	-3.30837000	-2.71646000
C	1.42887500	-2.84103400	-2.18430500
C	1.42304400	-1.96322700	-1.08483400
C	0.21240700	-1.50641300	-0.51197600
C	-0.99774500	-2.00013100	-1.07434300
H	2.38251400	-3.16372100	-2.58476100
C	1.73543700	2.66150000	1.09723600
C	0.89477400	2.42673800	2.39699900
O	0.93151200	3.33130200	3.22111200
O	0.30936500	1.28172900	2.54535200
C	-0.17918000	2.20141700	-1.14009600
C	-1.27636000	2.81418600	-0.52250000
C	-0.24432600	1.99637100	-2.52381600

C	-2.39666600	3.20208900	-1.25171500
C	-1.35785700	2.37829800	-3.26810900
C	-2.43784200	2.98341000	-2.62817200
F	0.75800400	1.38055300	-3.16300100
F	-1.39692400	2.16109600	-4.58506000
F	-3.51141400	3.34381600	-3.32858400
F	-3.45197400	3.73474000	-0.63086500
F	-1.30208800	2.99189500	0.79869900
C	1.68099500	4.10807800	0.62074700
H	2.03084000	4.72760300	1.44943000
H	2.32148500	4.26759000	-0.25253600
H	0.66331900	4.42477900	0.38932600
C	3.18105200	2.22655200	1.40276000
H	3.23766900	1.17129600	1.68103500
H	3.84677000	2.40244200	0.55248200
H	3.52249600	2.82052200	2.25496400
S	1.21923700	1.47433600	-0.29020200
C	4.30509100	-1.34232800	1.31367100
C	5.22585700	-0.69082200	0.48149300
C	4.90873800	-0.47971300	-0.86694300
C	3.68246200	-0.90739400	-1.36950800
C	2.74323900	-1.53868100	-0.53910800
C	3.07766200	-1.75733900	0.80897900
H	4.56823400	-1.50587000	2.35324800
H	5.61874400	0.02665500	-1.51063400
H	3.42672600	-0.72306200	-2.40860200
H	2.37372500	-2.26550900	1.46000600
C	6.50809000	-0.23434800	1.08533100
O	6.82515300	-0.41416600	2.24524700
O	7.29378800	0.41935300	0.19783500
C	8.54209600	0.89443900	0.72726900
H	9.14425900	0.06166500	1.10053200
H	9.04479700	1.39067300	-0.10297300
H	8.36963400	1.59555200	1.54836000
Pd	0.22039000	-0.13705300	1.01828100
C	-1.62802100	-3.31733100	3.60069700
H	-1.19780600	-4.28956600	3.84573200
H	-2.64788700	-3.47041400	3.23064500
H	-1.66801500	-2.66829200	4.47509900
C	-0.84967000	-2.64542300	2.51039700
O	-0.77478900	-1.41604600	2.43708000

O	-0.29628500	-3.47436400	1.64067300
H	0.06267900	-2.94738900	0.88369800
O	0.12104700	-4.16871700	-3.76726200
C	1.31565800	-4.61073400	-4.39660600
H	1.00235600	-5.26887400	-5.20829500
H	1.88846300	-3.77125900	-4.81228700
H	1.95543500	-5.17232500	-3.70306200
C	-4.36163200	-2.17377100	0.67864700
C	-4.75274900	-0.82740600	0.66574200
C	-3.93342400	0.12501000	0.04501800
C	-2.73217600	-0.26741400	-0.53256000
C	-2.31611800	-1.60555800	-0.50120200
C	-3.15623600	-2.55847200	0.09369300
H	-5.00495800	-2.91087100	1.14603100
H	-4.25098600	1.16275800	0.02959100
H	-2.10376000	0.45642900	-1.03021400
H	-2.84690100	-3.59955400	0.11297400
C	-6.02537800	-0.35690300	1.28031600
O	-6.42549000	0.78997800	1.24023200
O	-6.70149200	-1.35445100	1.89770100
C	-7.93877500	-0.95827600	2.51114100
H	-8.62585200	-0.55081400	1.76451000
H	-8.34977400	-1.86374600	2.95791800
H	-7.76236600	-0.19673700	3.27554000
H	-1.91161400	-3.27495700	-2.56134100

TS33

C	-1.31665500	1.43032700	-2.25760600
C	-0.13460100	1.98548100	-2.77114000
C	1.08325200	1.31561700	-2.60633700
C	1.13834200	0.14232400	-1.84523900
C	-0.03177000	-0.38792400	-1.22626500
C	-1.27763700	0.26479100	-1.49973000
H	1.98838200	1.69966700	-3.05861700
C	1.74060600	0.72456200	3.11130300
C	0.84840700	-0.42787200	3.66644200
O	0.68370400	-0.45498700	4.87659400
O	0.43657200	-1.34266800	2.83697900
C	0.28359800	2.26878100	1.01612300
C	-1.00688600	2.26289500	1.55453000
C	0.61216300	3.29639300	0.12630700

C	-1.95127000	3.21852500	1.19763800
C	-0.31970200	4.26043400	-0.24665700
C	-1.60496300	4.21888800	0.28735900
F	1.83416500	3.36441300	-0.42528000
F	0.01393200	5.21333500	-1.12312700
F	-2.50403600	5.13411400	-0.06796400
F	-3.18060500	3.18277700	1.71168300
F	-1.36097600	1.31202700	2.42772600
C	1.52873400	2.02789600	3.86995700
H	1.75773200	1.83050300	4.91939300
H	2.18261600	2.82193100	3.49598400
H	0.48977500	2.35812600	3.82236300
C	3.20235100	0.24481400	3.19306900
H	3.36729200	-0.64725600	2.58071200
H	3.89803400	1.02810900	2.87778400
H	3.40575800	-0.01770900	4.23509000
S	1.46372800	0.95085500	1.25047500
C	3.81971000	-2.51240100	-1.41994700
C	4.95402200	-1.72876700	-1.16765300
C	4.83815400	-0.33244300	-1.15871800
C	3.60430700	0.26453800	-1.39668200
C	2.45836600	-0.51329000	-1.64087600
C	2.58630200	-1.91429100	-1.65049700
H	3.92631500	-3.59182900	-1.42990300
H	5.71141700	0.27655500	-0.95521700
H	3.51254700	1.34462900	-1.34377100
H	1.71870400	-2.53473200	-1.84361300
C	6.24460900	-2.42843300	-0.91600300
O	6.38975500	-3.63521300	-0.94036200
O	7.25631900	-1.56840000	-0.65180000
C	8.52721000	-2.18758300	-0.39623900
H	8.85524100	-2.76621400	-1.26410600
H	9.21915200	-1.36935500	-0.19615500
H	8.46239600	-2.85756700	0.46533700
Pd	0.28298200	-1.00131700	0.82754400
C	-1.76777600	-4.65185400	-0.36821700
H	-1.55873400	-5.26485000	-1.24575700
H	-2.82786900	-4.37477100	-0.37923000
H	-1.56228200	-5.19574900	0.55410400
C	-0.97003300	-3.37254300	-0.41301600
O	-0.68552200	-2.82468000	0.69175300

O	-0.67193000	-2.89233000	-1.55695300
H	-0.24431500	-1.71686400	-1.36178200
O	-0.27786700	3.17065400	-3.41029200
C	0.89623900	3.88114300	-3.80321800
H	0.54592100	4.83728800	-4.19236900
H	1.55201900	4.05502200	-2.94374700
H	1.44409100	3.34750600	-4.58894300
C	-4.72054700	-1.26361700	-1.78867500
C	-5.03265100	-1.56558200	-0.45556900
C	-4.12224700	-1.23750500	0.55671100
C	-2.91097900	-0.62831200	0.24246300
C	-2.57983300	-0.33834900	-1.08994100
C	-3.51024200	-0.65179900	-2.09708600
H	-5.42269200	-1.51666700	-2.57450600
H	-4.37634300	-1.46817300	1.58565000
H	-2.22047900	-0.38190300	1.03957100
H	-3.26093800	-0.43850900	-3.13202500
C	-6.30805800	-2.22787900	-0.06193800
O	-6.61429000	-2.51001900	1.08006400
O	-7.10380300	-2.48979100	-1.12559300
C	-8.34937100	-3.13088700	-0.80786300
H	-8.94440900	-2.50527700	-0.13700800
H	-8.86153400	-3.26880500	-1.76023000
H	-8.17355200	-4.09422100	-0.32141600
H	-2.25380700	1.94100300	-2.45344100

int57

C	0.63453900	3.64884900	-0.15271100
C	-0.03416400	3.88716800	-1.35802300
C	-0.53880100	2.82666900	-2.10668700
C	-0.37681200	1.51382600	-1.64167300
C	0.26758900	1.25983400	-0.43039800
C	0.78640200	2.33596400	0.31044100
Pd	0.22549400	-0.59601400	0.36048600
H	-0.73757200	0.67889400	-2.23853700
H	-0.15112600	4.90928200	-1.70615900
H	-1.04816300	3.00888000	-3.04855900
O	1.41533300	2.00823200	1.48932600
C	1.90864900	3.05735600	2.30782300
H	2.34627000	2.57401200	3.18276000
H	2.68439800	3.64147300	1.79556400

H	1.10393500	3.73132100	2.62914500
H	1.02497500	4.48584300	0.41469600
C	1.23317900	-1.96856900	-1.11339600
C	2.17875900	-2.96965400	-0.45988000
C	3.30996700	-0.98540800	-0.58632000
C	1.93706000	-0.78234000	-1.20788800
C	2.99642300	-2.06606200	0.48170700
H	3.89671300	-2.56330100	0.85545200
H	2.41895300	-1.68345300	1.32822900
C	3.24768300	-3.23937000	-1.57552700
H	3.90715200	-4.05275900	-1.25829100
H	2.79035200	-3.53549200	-2.52362800
C	4.02014700	-1.88365500	-1.66838900
H	5.07580200	-2.00898400	-1.41087100
H	3.97524900	-1.43720200	-2.66530300
H	1.71805500	-3.85497300	-0.02792300
H	1.73140400	-0.03309400	-1.95812500
C	0.04061700	-2.29991700	-1.97412100
O	-0.23486800	-1.63729300	-2.97767400
N	-0.68004900	-3.37122100	-1.55426200
H	-0.58531700	-3.61856300	-0.57228300
C	-1.92413700	-3.71063900	-2.22925900
H	-1.72876600	-3.90887700	-3.28583700
H	-2.34124900	-4.60376500	-1.76170200
H	-2.65277000	-2.89551000	-2.16563400
C	4.00478100	0.29767400	-0.11806000
C	5.32826700	0.04429600	0.62739100
C	4.22361900	1.31467100	-1.25625500
H	3.31245200	0.76065400	0.59898400
C	5.92455100	1.35535300	1.16384600
H	6.05331400	-0.42706900	-0.05090700
H	5.16995100	-0.65628800	1.45536800
C	4.82795000	2.62591600	-0.73173500
H	4.89675100	0.87988400	-2.00902400
H	3.27648500	1.53111800	-1.76171900
C	6.13256700	2.37834600	0.03846600
H	6.87075400	1.15739200	1.68150700
H	5.23895500	1.77776200	1.91288800
H	4.99834600	3.32144800	-1.56197800
H	4.09694400	3.10775400	-0.06699700
H	6.52371100	3.31949700	0.44360000

H	6.89302300	1.99597600	-0.65759200
C	-1.87736000	-1.46826300	2.68717200
C	-1.35429000	-2.65884200	1.82078500
O	-0.20413300	-2.49564400	1.23824200
O	-2.00620700	-3.69550300	1.81748300
C	-2.66980700	0.65686500	0.74896600
C	-3.18558100	-0.20035000	-0.22592900
C	-2.99582500	2.01319800	0.65862400
C	-3.99840700	0.26091900	-1.25250500
C	-3.80337000	2.49797300	-0.36745300
C	-4.30846500	1.61924100	-1.32254200
F	-2.48716300	2.89110800	1.53003600
F	-4.08400500	3.80100600	-0.44495000
F	-5.08101600	2.07645000	-2.30785800
F	-4.46143000	-0.58489700	-2.17713100
F	-2.86436000	-1.50159800	-0.21203600
C	-3.37779600	-1.54420700	2.94120400
H	-3.58006500	-2.48945100	3.44954400
H	-3.71900100	-0.71370700	3.56654300
H	-3.94310100	-1.55527800	2.00891500
C	-1.07416400	-1.48073600	4.00179300
H	-0.00296600	-1.36239000	3.81449300
H	-1.41145500	-0.69634600	4.68590200
H	-1.22562200	-2.45350800	4.47983100
S	-1.39693600	0.19315200	1.91479800

TS34

C	0.95668400	3.09988900	0.61559200
C	0.35436800	3.60480500	-0.54021100
C	-0.07323500	2.74570100	-1.55381800
C	0.12542500	1.37262400	-1.41215100
C	0.73368600	0.83119500	-0.26375000
C	1.14018300	1.71916900	0.76135500
Pd	-0.09647300	-0.95939000	0.44788100
H	-0.16342400	0.69072100	-2.20901100
H	0.21323300	4.67723300	-0.63708600
H	-0.54414100	3.14046400	-2.44874400
O	1.63718100	1.14200000	1.89602800
C	2.08512000	1.98080400	2.95355300
H	2.45680900	1.30836100	3.72746000
H	2.89878300	2.64084700	2.62549900

H	1.26478900	2.58493400	3.35961000
H	1.25332000	3.78399000	1.40135200
C	1.19804900	-1.90727700	-0.84600300
C	2.14216600	-2.86519700	-0.11192800
C	3.30128200	-0.89924100	-0.34903200
C	1.93976500	-0.67877000	-1.00306700
C	2.94315500	-1.89297100	0.78387800
H	3.82478200	-2.36857000	1.22422800
H	2.35203700	-1.42265800	1.57476800
C	3.22200800	-3.24134400	-1.16607400
H	3.89770100	-3.99898600	-0.75593500
H	2.78205100	-3.64788400	-2.08039400
C	3.96254000	-1.89026600	-1.39196200
H	5.02847800	-1.98145900	-1.17175100
H	3.87406100	-1.52358000	-2.41845100
H	1.65831600	-3.70967900	0.37868000
H	1.91114700	-0.19889600	-1.97076400
C	0.28246400	-2.32240000	-1.97495100
O	0.19484800	-1.64863400	-3.00811000
N	-0.42539200	-3.46393500	-1.75344500
H	-0.57908100	-3.69064300	-0.77111000
C	-1.50215300	-3.82456800	-2.66518200
H	-1.15523500	-3.71303700	-3.69340600
H	-1.79118300	-4.86173600	-2.48432500
H	-2.37941000	-3.17994400	-2.52492300
C	4.11682800	0.35090200	0.00573700
C	5.51401000	0.04462100	0.57976700
C	4.23389500	1.35345200	-1.15977000
H	3.56338700	0.84965500	0.80568800
C	6.21365000	1.33275500	1.04167800
H	6.13771100	-0.43913300	-0.18396700
H	5.43607500	-0.65966300	1.41619300
C	4.94287100	2.64179800	-0.71572200
H	4.79417500	0.89190700	-1.98543200
H	3.24067400	1.60346800	-1.54756500
C	6.32029200	2.35041600	-0.10352400
H	7.20772400	1.10111100	1.44214400
H	5.63876500	1.77726200	1.86752500
H	5.03799400	3.33186800	-1.56232200
H	4.31245000	3.14842100	0.02985800
H	6.78688000	3.27771500	0.25003800

H	6.98078800	1.94366900	-0.88258300
C	-2.76179900	-1.54513400	2.22651600
C	-2.27818600	-2.74693200	1.34624500
O	-1.03113600	-2.75594600	0.97266100
O	-3.07383100	-3.65876700	1.16603600
C	-2.67739900	0.92539900	0.55961900
C	-3.11020800	0.34071900	-0.63617500
C	-2.76163600	2.31763400	0.66171800
C	-3.62246200	1.10103400	-1.68086100
C	-3.25441500	3.09793500	-0.38067100
C	-3.69280900	2.48768100	-1.55187500
F	-2.30805800	2.94690100	1.75353500
F	-3.28271800	4.42995600	-0.26846600
F	-4.15785800	3.22909900	-2.55914800
F	-4.02073100	0.51501000	-2.81244300
F	-3.01026000	-0.98444200	-0.81555300
C	-4.26792700	-1.32781500	2.12530200
H	-4.75874400	-2.25721800	2.42069100
H	-4.59578700	-0.51577500	2.78132700
H	-4.57545300	-1.11252600	1.10130400
C	-2.33817100	-1.86922900	3.67315400
H	-1.25131700	-1.96209000	3.76073900
H	-2.69283800	-1.10738900	4.37370800
H	-2.78051400	-2.83283800	3.94308500
S	-1.81235000	0.05183200	1.85355500

int58

C	0.04968000	-2.71105700	0.30826000
C	0.84821700	-2.76932700	-0.83583700
C	0.65570400	-1.86904500	-1.87701200
C	-0.36333300	-0.91959800	-1.77112000
C	-1.24588600	-0.84994700	-0.65438300
C	-0.98028400	-1.76587600	0.42035900
Pd	-0.00880900	0.87071300	0.16349900
H	-0.55007500	-0.22991400	-2.58986900
H	1.63658400	-3.51486700	-0.89168200
H	1.29257900	-1.88282600	-2.75509600
O	-1.75986100	-1.67893100	1.52440900
C	-1.44761500	-2.45475900	2.67642100
H	-2.16799500	-2.14866500	3.43554800
H	-1.56071600	-3.52796300	2.48190300

H	-0.43071900	-2.24734500	3.03053600
H	0.23664500	-3.40407500	1.11822900
C	-1.80256000	1.53048000	-0.56136900
C	-2.71126900	2.17026600	0.49911600
C	-3.72277500	0.16735000	0.00867300
C	-2.42981300	0.15713100	-0.86128100
C	-3.25038400	0.94710000	1.26755000
H	-4.07639200	1.21996900	1.93265700
H	-2.49052900	0.42299000	1.84621100
C	-3.99175100	2.61965300	-0.25016400
H	-4.64363000	3.17125400	0.43601900
H	-3.77954100	3.27551800	-1.09796800
C	-4.62627000	1.26059200	-0.66710500
H	-5.65328100	1.17601200	-0.30161200
H	-4.66014100	1.13831200	-1.75328400
H	-2.23111000	2.94765700	1.09525800
H	-2.69221500	0.07722000	-1.91790200
C	-1.39129600	2.35558200	-1.75925700
O	-1.45772200	1.92039100	-2.91529300
N	-0.95143300	3.61428200	-1.46738600
H	-0.65231300	3.77255000	-0.50939200
C	-0.34989000	4.43978500	-2.50065700
H	-0.92008300	4.32521900	-3.42352600
H	-0.36938300	5.48586700	-2.18614100
H	0.68980600	4.14897300	-2.70545100
C	-4.42280300	-1.19586200	0.16581700
C	-5.51651500	-1.20463200	1.25185000
C	-4.99413200	-1.72330300	-1.16734800
H	-3.67011400	-1.91847900	0.49113800
C	-6.14047900	-2.60002000	1.41330600
H	-6.30743900	-0.48628900	0.99517400
H	-5.09400100	-0.87612400	2.20819900
C	-5.60564200	-3.12273700	-1.00369100
H	-5.76869500	-1.03757000	-1.53550700
H	-4.20860200	-1.74651200	-1.93243700
C	-6.69098100	-3.13135500	0.08228000
H	-6.93143400	-2.57479100	2.17266100
H	-5.37207200	-3.29403100	1.78477600
H	-6.01696700	-3.47080100	-1.95878200
H	-4.81253600	-3.83242000	-0.72623700
H	-7.09734000	-4.14173700	0.21207700

H	-7.52740600	-2.49492900	-0.24073700
C	2.68095500	2.00608900	1.69615600
C	1.49382500	3.03056500	1.63582500
O	0.40612500	2.72667200	0.98961100
O	1.70686500	4.11701900	2.15575800
C	3.24474300	-0.55599000	0.36913100
C	3.32193700	-0.37435800	-1.01734900
C	4.09847700	-1.50606900	0.94317100
C	4.17779000	-1.13397300	-1.80713700
C	4.97185400	-2.26831600	0.17004400
C	5.00675400	-2.08346700	-1.21082100
F	4.08440000	-1.71987600	2.26312600
F	5.77179900	-3.17293400	0.74240900
F	5.83152900	-2.81370400	-1.96098100
F	4.19383500	-0.97220800	-3.13399700
F	2.54703700	0.52432700	-1.63673900
C	3.68280100	2.43833800	0.61792300
H	3.97570300	3.46724500	0.84295800
H	4.57903600	1.81108300	0.62835800
H	3.23768500	2.41298700	-0.37815700
C	3.32421600	2.00713600	3.08593300
H	2.61345600	1.68891800	3.85339400
H	4.18866000	1.33624500	3.11325500
H	3.64202300	3.02572500	3.31919400
S	2.02484200	0.24618100	1.38456600

int59

C	2.65585200	1.17311200	-3.12207900
C	1.44864000	0.59919600	-3.54039800
C	0.65007200	-0.07548800	-2.62738800
C	1.02539100	-0.08413700	-1.27428200
C	2.16417100	0.59852700	-0.80114400
C	3.03227600	1.13924300	-1.77452500
Pd	-0.28589800	-0.53326600	0.51407500
H	0.73145100	-1.07982800	-0.78375100
H	1.17883300	0.63296800	-4.59145700
H	-0.20996400	-0.65761100	-2.93819900
O	4.23414400	1.59437500	-1.31039500
C	5.12668700	2.22259300	-2.22064300
H	6.00007300	2.50707000	-1.63257500
H	5.43680200	1.53847600	-3.02032000

H	4.67883400	3.12228500	-2.66321800
H	3.30496500	1.62979300	-3.85914300
C	1.47465400	-0.12105600	1.56714400
C	1.12590100	0.80424300	2.74582700
C	2.22312700	2.21791700	1.31956300
C	2.42384100	0.74491500	0.67494200
C	0.84358400	2.11405000	2.00573700
H	0.65679300	2.95920500	2.67781700
H	0.00597400	2.03427000	1.31172300
C	2.44422000	1.13290700	3.50395200
H	2.21604700	1.56513500	4.48326500
H	3.05290600	0.24096700	3.68126600
C	3.14251600	2.17250800	2.57499800
H	3.16444400	3.14660300	3.06732100
H	4.17468900	1.90903000	2.32402100
H	0.32447300	0.43057400	3.38202800
H	3.46400900	0.45436700	0.85366600
C	1.99604700	-1.47516400	1.93935200
O	3.03999200	-1.97216000	1.41251300
N	1.32525600	-2.15838000	2.88010900
H	0.39899200	-1.80660800	3.12064400
C	1.63323000	-3.55007600	3.16966700
H	1.04320100	-3.86736500	4.03057700
H	1.39695400	-4.19433100	2.31194800
H	2.69588800	-3.65893900	3.39354300
C	2.39816000	3.43654700	0.38181700
C	1.17049200	3.66487200	-0.53258600
C	2.71122300	4.76415200	1.10762600
H	3.26254000	3.23877500	-0.25586800
C	1.42995500	4.77097500	-1.56322900
H	0.31612000	3.96379900	0.09011800
H	0.87502800	2.74184200	-1.03692200
C	2.95498700	5.90480400	0.10360700
H	1.87857900	5.03010000	1.77455600
H	3.60021700	4.66075400	1.73731400
C	1.78118500	6.09231300	-0.86658300
H	0.55350200	4.89919300	-2.20992600
H	2.25985100	4.46717700	-2.21846500
H	3.15969200	6.83862600	0.64097700
H	3.86165400	5.67311000	-0.47466600
H	2.01515600	6.87057400	-1.60314100

H	0.90260100	6.44300800	-0.30647900
C	-2.92069900	-2.24717400	0.94971100
C	-2.34050500	-1.71711000	2.29498300
O	-1.23890600	-1.00764800	2.27878000
O	-2.90000800	-2.06609000	3.32397500
C	-3.57148600	0.19937600	-0.45109000
C	-4.73756100	0.11606600	-1.22654100
C	-3.38508900	1.36855700	0.29620300
C	-5.67129600	1.14752200	-1.26724200
C	-4.30436200	2.41450800	0.26435100
C	-5.45085600	2.30252700	-0.51900600
F	-2.30903700	1.52995100	1.07629100
F	-4.09302800	3.52058800	0.98272700
F	-6.33650800	3.29720800	-0.55133900
F	-6.77363500	1.03637200	-2.01338000
F	-4.99082800	-0.98158100	-1.94822500
C	-2.25921700	-3.60960600	0.66037700
H	-2.43455100	-4.25334800	1.52775000
H	-2.70293900	-4.07499100	-0.22376400
H	-1.18429900	-3.51955000	0.48580000
C	-4.44128500	-2.37055300	1.02193900
H	-4.91133500	-1.41433200	1.26430200
H	-4.84844300	-2.74046800	0.07741300
H	-4.68592300	-3.06577800	1.82718900
S	-2.41501000	-1.16340600	-0.52555900
O	0.08495200	-3.04312000	-1.56935800
C	0.82112800	-3.52653800	-2.45668100
O	2.09458000	-3.69560200	-2.35045500
C	0.22597800	-3.91245600	-3.80301600
H	0.35473700	-3.06828700	-4.49027300
H	0.74723900	-4.77177700	-4.22931000
H	-0.84107600	-4.11802500	-3.70308000
Ag	2.71711700	-2.91545400	-0.48147400

TS35

C	2.61676700	0.96283200	-3.04271200
C	1.30071500	0.67163700	-3.41936600
C	0.39657600	0.16673700	-2.49121500
C	0.78216600	0.00618700	-1.14601300
C	2.06552500	0.43163100	-0.72608800
C	3.00345700	0.82194800	-1.70657000

Pd	-0.41627000	-0.61613700	0.40947400
H	0.40272200	-1.43432200	-0.89674400
H	1.00420600	0.80163300	-4.45643900
H	-0.58622300	-0.16481900	-2.81066700
O	4.27838200	1.04049900	-1.25512700
C	5.25545700	1.50336800	-2.17684200
H	6.17687400	1.61665900	-1.60409800
H	5.41997600	0.78255000	-2.98780000
H	4.97366200	2.47429700	-2.60542600
H	3.32401500	1.29404800	-3.79302300
C	1.29719000	-0.29244500	1.56719900
C	0.87433800	0.67921800	2.69316700
C	2.26808100	1.97046900	1.41489700
C	2.35714200	0.50998700	0.74658000
C	0.81443600	2.01296800	1.93568200
H	0.63573900	2.87053500	2.59469100
H	0.06435100	2.02240400	1.14346700
C	2.09984100	0.89783300	3.61979100
H	1.78629400	1.40969800	4.53558900
H	2.56963700	-0.04176300	3.92426700
C	3.03364900	1.80356600	2.76257500
H	3.15778700	2.76960700	3.25448900
H	4.03320000	1.38089700	2.61784200
H	-0.03343700	0.38054200	3.21772500
H	3.36575900	0.13187500	0.93553400
C	1.74577000	-1.64386100	2.03747200
O	2.82460600	-2.19347700	1.64202300
N	0.98614700	-2.26926300	2.94653500
H	0.04033900	-1.90380400	3.07445800
C	1.25965800	-3.63891500	3.35365800
H	0.56876900	-3.90755300	4.15404500
H	1.13079200	-4.33622600	2.51633000
H	2.28695200	-3.72672400	3.71276700
C	2.71326100	3.15690900	0.52281700
C	1.61024900	3.61367900	-0.46275700
C	3.21055100	4.39699500	1.29889400
H	3.56861900	2.81260200	-0.06702700
C	2.12736700	4.67649500	-1.44073200
H	0.77847700	4.04232200	0.11377200
H	1.19944800	2.76661800	-1.01608900
C	3.71516800	5.49345500	0.34572100

H	2.39827000	4.79535000	1.92443900
H	4.02615200	4.12599000	1.97625000
C	2.65782300	5.90324000	-0.68764700
H	1.33206100	4.96763200	-2.13764800
H	2.93299400	4.24166500	-2.05078300
H	4.04615900	6.36630600	0.92160700
H	4.60235800	5.11515600	-0.18319200
H	3.07101000	6.64129100	-1.38608400
H	1.81987600	6.39303100	-0.17129700
C	-3.16131700	-2.26441900	0.63775100
C	-2.58650000	-1.91145100	2.04650900
O	-1.47885100	-1.22875300	2.11376600
O	-3.17519400	-2.37508100	3.01431900
C	-3.65466000	0.35388900	-0.51293900
C	-4.82298000	0.39946300	-1.28811000
C	-3.40568800	1.44321000	0.33125000
C	-5.70286200	1.47631400	-1.23297600
C	-4.27107800	2.53305400	0.39570200
C	-5.42298900	2.54832500	-0.38735300
F	-2.31989800	1.48604300	1.11223900
F	-4.00197600	3.56026800	1.20564000
F	-6.25681000	3.58570200	-0.32769800
F	-6.80999200	1.48757700	-1.98052700
F	-5.13035100	-0.61444100	-2.10529100
C	-2.54983300	-3.61348900	0.21011000
H	-2.77363600	-4.34171700	0.99524200
H	-2.98921100	-3.95913800	-0.73022100
H	-1.46590100	-3.55161400	0.08028500
C	-4.68657500	-2.32895200	0.66890900
H	-5.12190000	-1.37780500	0.98548000
H	-5.09115700	-2.59892600	-0.30995000
H	-4.97381400	-3.07872000	1.40844000
S	-2.57375200	-1.05708000	-0.70408100
O	0.21636200	-2.70827700	-1.62991700
C	1.01894000	-3.05133000	-2.55927100
O	2.28102300	-3.12005600	-2.44394700
C	0.41910800	-3.37292900	-3.91133000
H	0.17400200	-2.42287900	-4.39889700
H	1.12110500	-3.92507700	-4.53669700
H	-0.51146200	-3.93034300	-3.78463300
Ag	2.88912000	-2.61956900	-0.45542700

int60

C	-1.13308400	2.48402000	-2.62856800
C	-0.57714100	1.30778200	-3.14196500
C	0.08416500	0.40472600	-2.31112300
C	0.16744600	0.63337200	-0.92244400
C	-0.46541600	1.78604100	-0.38261100
C	-1.06631900	2.72972200	-1.25197700
Pd	1.11332200	-0.52772600	0.41167000
H	2.70461800	0.15432000	-1.20144800
H	-0.65039300	1.11145900	-4.20883800
H	0.53237100	-0.48169800	-2.74861400
O	-1.56365500	3.85885500	-0.65407600
C	-2.28689400	4.78563500	-1.45077600
H	-2.61925900	5.57078600	-0.77019000
H	-1.65644800	5.22904200	-2.23260500
H	-3.16231700	4.31475000	-1.91704200
H	-1.61538400	3.18591900	-3.29764000
C	0.54466300	0.97372100	1.76791500
C	-0.21200300	0.29467800	2.92978900
C	-1.88426300	1.40791500	1.82730100
C	-0.53414700	1.89677000	1.11728000
C	-1.54553200	-0.03964400	2.25244800
H	-2.29170700	-0.46030300	2.93600200
H	-1.42053900	-0.71928500	1.41203900
C	-0.64026400	1.39748800	3.93860600
H	-0.95967000	0.94283400	4.88201200
H	0.17993500	2.08217800	4.17438900
C	-1.83605600	2.09999900	3.21979600
H	-2.76003100	1.91537200	3.77277400
H	-1.71415500	3.18543700	3.13996700
H	0.31559900	-0.54759800	3.37715200
H	-0.37706900	2.94108900	1.40704600
C	1.84098700	1.62015200	2.10057900
O	2.21504700	2.73295900	1.60488500
N	2.64936200	0.98409800	2.97212600
H	2.44716500	-0.00417400	3.11707500
C	4.02516900	1.41301700	3.16772100
H	4.45346800	0.84898500	3.99815700
H	4.63218100	1.24270100	2.26811300
H	4.05329600	2.47864400	3.40012200

C	-3.18130000	1.58466700	0.99740200
C	-3.38462900	0.42875500	-0.00861300
C	-4.47132000	1.73067900	1.83200000
H	-3.08240000	2.51553900	0.42895000
C	-4.58476600	0.65993400	-0.93386100
H	-3.56576700	-0.49206200	0.56069300
H	-2.48087600	0.26303600	-0.59926600
C	-5.70034700	1.95015300	0.93149400
H	-4.62005800	0.82914100	2.44413800
H	-4.38730800	2.57319800	2.52623400
C	-5.86876200	0.83892400	-0.11384600
H	-4.68887400	-0.18205100	-1.62855000
H	-4.40372700	1.55579400	-1.54544900
H	-6.60440900	2.03584600	1.54673900
H	-5.58532200	2.91279100	0.41150900
H	-6.72280500	1.05585600	-0.76708900
H	-6.09523900	-0.10827900	0.39633000
C	2.22720000	-3.62397900	0.49256100
C	2.19893000	-2.93205500	1.90205300
O	2.04567200	-1.64647200	1.95022800
O	2.44155400	-3.66090200	2.85649900
C	-0.36708000	-2.93871700	-0.86288700
C	-1.03001300	-2.83724000	-2.09156900
C	-1.16186900	-3.03622800	0.28464500
C	-2.41855800	-2.77416100	-2.17516700
C	-2.54924000	-2.98921700	0.21893200
C	-3.18087800	-2.84717700	-1.01392400
F	-0.59907900	-3.10294500	1.49952000
F	-3.27705900	-2.99730700	1.34004600
F	-4.50999200	-2.73626000	-1.07418600
F	-3.01824000	-2.61837800	-3.35928500
F	-0.32897400	-2.72090200	-3.23076800
C	3.70505800	-3.62020300	0.04747700
H	4.28360200	-4.12196200	0.82800200
H	3.84160000	-4.15384700	-0.89791600
H	4.09080300	-2.60102700	-0.05844200
C	1.67102000	-5.04478900	0.53603200
H	0.62111600	-5.05783600	0.83100700
H	1.78167900	-5.54288800	-0.43200500
H	2.22971300	-5.59291200	1.29731400
S	1.39317900	-2.61312800	-0.86919100

O	3.31622000	-0.01356700	-1.96836100
C	3.49461800	1.03815900	-2.74955400
O	3.12624300	2.18640400	-2.48769300
C	4.20089300	0.69779800	-4.03120600
H	3.52050000	0.11080300	-4.65674800
H	4.48754600	1.60963100	-4.55298400
H	5.07552700	0.07634300	-3.82421500
Ag	2.09858900	2.75661500	-0.58733700

int61

C	-0.47812800	3.44371000	-1.91148400
C	0.20562400	2.36404500	-2.47646900
C	0.26370800	1.13317900	-1.82494300
C	-0.40934500	0.98072400	-0.60463400
C	-1.18131000	2.01869100	-0.05649900
C	-1.15630100	3.27388900	-0.69908700
Pd	-0.19069900	-0.66478200	0.47331600
H	0.84806300	0.32344000	-2.24373400
O	-1.81348100	4.28590200	-0.05040400
C	-1.82845400	5.57603000	-0.63721700
H	-2.41327400	6.20523100	0.03601500
H	-0.81597700	5.98978500	-0.73280300
H	-2.30846700	5.56817200	-1.62462900
H	-0.47350900	4.40224600	-2.41580600
C	-1.40400600	0.39153500	1.82933400
C	-2.67812000	-0.40599400	2.15468000
C	-3.50345800	1.43041100	1.07346000
C	-1.93851600	1.73104400	1.20660500
C	-3.52002700	-0.10693200	0.90844300
H	-4.52831100	-0.52621700	0.97468500
H	-3.05414400	-0.45242200	-0.01680300
C	-3.49069300	0.31688300	3.26368300
H	-4.28661900	-0.33542100	3.64082000
H	-2.86904300	0.59694200	4.11928100
C	-4.07668000	1.54993600	2.51398600
H	-5.17029100	1.49932300	2.48581000
H	-3.80835400	2.49974400	2.98504400
H	-2.51123500	-1.46826400	2.35767300
H	-1.80344700	2.56775800	1.90168800
C	-0.37008300	0.55471400	2.88397700
O	0.50070300	1.48111800	2.87798100

C	0.81074700	-0.46826700	4.78006400
H	0.56014100	-1.14788700	5.59682900
H	1.70104900	-0.84540000	4.25743500
H	1.04869500	0.51603200	5.18595200
C	3.46691000	-2.00370300	-1.77387700
C	2.54476800	-1.38424500	-0.70025600
O	3.12502400	-0.71394600	0.20629500
O	1.30217700	-1.58760100	-0.82538500
C	4.97793400	0.43291700	-1.83581000
C	4.40042400	1.48283200	-1.11295600
C	6.33945500	0.18556100	-1.61753900
C	5.11391300	2.20505800	-0.16542200
C	7.08101200	0.91872200	-0.69243800
C	6.46056900	1.92266100	0.04868000
F	6.96604700	-0.79869900	-2.27141500
F	8.37736500	0.65120000	-0.49549700
F	7.15354500	2.60868400	0.95977700
F	4.49068800	3.13272300	0.58137800
F	3.10597200	1.79115800	-1.26635600
C	4.67351100	-2.68419700	-1.12432100
H	4.32508700	-3.53819900	-0.53137100
H	5.37012700	-3.04423300	-1.88444300
H	5.19145500	-2.00256200	-0.44953300
C	2.71375400	-2.96237900	-2.70096500
H	1.87472900	-2.46867100	-3.19572600
H	3.38840800	-3.37585700	-3.45610300
H	2.30892200	-3.78617000	-2.10575000
S	4.00216900	-0.58532800	-2.91726800
Ag	2.03576700	0.82939000	1.36075800
C	-2.53734000	-2.61277300	-2.18292400
C	-3.88494500	-2.60695500	-1.80369000
C	-4.25467400	-3.06049600	-0.53198700
C	-3.28009100	-3.46526200	0.37975900
C	-1.94233100	-3.40383600	-0.00414300
C	-1.54880100	-3.01054600	-1.28428100
H	-2.26971200	-2.26036100	-3.17314000
H	-5.29927200	-3.06176200	-0.24390800
H	-3.56126800	-3.77796500	1.37856100
H	-0.50171800	-2.95706800	-1.55721900
I	-0.41155800	-3.72809900	1.48756500
C	-4.87487500	-2.04927900	-2.76923900

O	-4.61942500	-1.74679800	-3.91763300
O	-6.09451300	-1.88101000	-2.20931800
C	-7.08398400	-1.29313800	-3.07169100
H	-6.75680500	-0.30597600	-3.40693600
H	-7.25653000	-1.92580500	-3.94636400
H	-7.98812200	-1.21291800	-2.46848200
C	-4.27690100	2.23350500	0.00505900
C	-5.49873600	1.48381900	-0.57173700
C	-4.73435000	3.62106400	0.50289900
H	-3.59382600	2.39306800	-0.83935500
C	-6.17083600	2.29121700	-1.69450100
H	-6.22889000	1.29421800	0.22927800
H	-5.20597800	0.50413900	-0.96306900
C	-5.36601800	4.44119800	-0.63019800
H	-5.48352300	3.49052700	1.29608200
H	-3.89099900	4.15577100	0.94272800
C	-6.56682600	3.70219400	-1.23751500
H	-7.05107100	1.75389500	-2.06973100
H	-5.46922300	2.37095800	-2.53739600
H	-5.67232600	5.42885100	-0.26330100
H	-4.61288400	4.61464600	-1.41197500
H	-6.98912900	4.27046500	-2.07542300
H	-7.35862100	3.62552300	-0.47824400
N	-0.32669400	-0.36565300	3.88055800
H	-0.97886500	-1.13401800	3.83620500
H	0.72511900	2.49700000	-3.42169700

TS36

C	-0.20921200	2.65108100	-2.69140500
C	0.15036300	1.33349800	-2.98947600
C	-0.00434200	0.32125400	-2.04610600
C	-0.57994300	0.63492300	-0.80855000
C	-1.05502000	1.92398100	-0.51994900
C	-0.78986700	2.94860000	-1.45419500
Pd	-0.52046800	-0.70710400	0.66723300
H	0.35711700	-0.67858600	-2.25198400
O	-1.12321700	4.21511000	-1.05721900
C	-0.85466100	5.29772600	-1.93347300
H	-1.19881600	6.19447000	-1.41572800
H	0.21860800	5.38846200	-2.14534900
H	-1.40243400	5.19984800	-2.87962900

H	-0.02899700	3.43143800	-3.42043000
C	-1.53251300	0.88499900	1.71209500
C	-2.93866300	0.49555900	2.17928700
C	-3.36285200	2.21330500	0.73041100
C	-1.76963800	2.13238000	0.78104700
C	-3.74502100	0.72148000	0.88982600
H	-4.81879300	0.57184500	1.03984900
H	-3.41279600	0.10277900	0.05426000
C	-3.52198700	1.60058300	3.10253800
H	-4.44293400	1.23883400	3.57288000
H	-2.83929500	1.88480900	3.90726300
C	-3.81064300	2.76480500	2.11338000
H	-4.87992200	2.99858300	2.09477500
H	-3.28364300	3.68607300	2.37713600
H	-2.99460800	-0.50257700	2.62081400
H	-1.38620700	3.04004000	1.25975700
C	-0.48706600	1.11145100	2.75403500
O	0.52113500	1.86385000	2.55696200
C	0.48692300	0.41301500	4.89101100
H	0.10375300	0.08499500	5.85875300
H	1.24529300	-0.30090600	4.54121600
H	0.95288900	1.39293600	4.99546400
C	3.38797800	-2.48933900	-1.21033100
C	2.46804500	-1.64756300	-0.29906600
O	3.06821000	-0.79953200	0.43949900
O	1.23010600	-1.84887400	-0.37063200
C	4.78835500	-0.08130600	-1.87476500
C	4.15557000	1.07802500	-1.41054600
C	6.16209300	-0.19859400	-1.62702100
C	4.83477500	2.04621600	-0.68244500
C	6.86740800	0.77459100	-0.92082200
C	6.19673300	1.89506100	-0.43432900
F	6.83726300	-1.27863500	-2.03445500
F	8.17749600	0.63074000	-0.68869800
F	6.85616500	2.81761900	0.26948800
F	4.16841800	3.09535600	-0.17209800
F	2.84352600	1.26524700	-1.59932800
C	4.62268000	-2.97217800	-0.44644100
H	4.30449600	-3.64903500	0.35518800
H	5.30196500	-3.50937100	-1.11218600
H	5.15180700	-2.13856500	0.01543800

C	2.63706000	-3.65531000	-1.85997000
H	1.77856000	-3.30813300	-2.43869900
H	3.30422200	-4.22717300	-2.51109700
H	2.26385800	-4.31907000	-1.07424600
S	3.86769300	-1.37606100	-2.67047000
Ag	1.92919100	0.77130600	1.31627900
C	-2.24848000	-3.60836400	-1.70445200
C	-3.63047300	-3.46988000	-1.51812500
C	-4.11016700	-2.90829100	-0.32683100
C	-3.22514000	-2.46028100	0.65032800
C	-1.85308600	-2.52615200	0.39657600
C	-1.34669300	-3.17222900	-0.73761400
H	-1.88804900	-4.07126000	-2.61741300
H	-5.17825200	-2.83021300	-0.15805200
H	-3.60521000	-2.05338500	1.57561600
H	-0.28116600	-3.28219600	-0.88240700
I	-0.51331800	-2.83716000	2.49212400
C	-4.53240000	-3.95905300	-2.59357500
O	-4.15543300	-4.47760100	-3.62737200
O	-5.84011800	-3.76137600	-2.30120500
C	-6.76092500	-4.20856400	-3.30833100
H	-6.58233900	-3.68640200	-4.25229600
H	-6.65417300	-5.28338700	-3.47869300
H	-7.75432700	-3.97735200	-2.92349600
C	-3.97747000	2.95821000	-0.47517900
C	-5.38175100	2.44878400	-0.86437100
C	-4.03898100	4.48746800	-0.27094400
H	-3.33440500	2.76426000	-1.34270300
C	-5.91431800	3.16779700	-2.11520500
H	-6.07822900	2.60572500	-0.02738200
H	-5.35696300	1.37095700	-1.05679100
C	-4.52798700	5.20201600	-1.53808000
H	-4.74023800	4.71385100	0.54373800
H	-3.06115400	4.86517000	0.03297500
C	-5.91685000	4.69378300	-1.94928000
H	-6.92206900	2.80743800	-2.35538200
H	-5.27563000	2.90289300	-2.97005400
H	-4.54860500	6.28755900	-1.38046400
H	-3.81732500	5.01449900	-2.35536600
H	-6.24854000	5.17758900	-2.87610800
H	-6.64301900	4.97174600	-1.17177700

N	-0.61683100	0.49904400	3.94701600
H	-1.35520700	-0.18452600	4.03114500
H	0.59865800	1.10741100	-3.95291300

int62

C	-0.34218000	2.96259900	-2.69893700
C	0.22650600	1.72622700	-3.01348900
C	0.11383300	0.64628600	-2.14259400
C	-0.61285800	0.80682100	-0.95780100
C	-1.26507900	2.00581800	-0.64736100
C	-1.06139500	3.10785500	-1.50948900
Pd	-0.45929100	-0.53962100	0.54123100
H	0.62687900	-0.28057100	-2.36538700
O	-1.59177300	4.29282300	-1.08528100
C	-1.43136300	5.44556400	-1.89833700
H	-1.94261900	6.25424300	-1.37408900
H	-0.37252700	5.70468600	-2.02486600
H	-1.89304300	5.31113200	-2.88466600
H	-0.20767300	3.80043800	-3.37164600
C	-1.67769000	0.91528600	1.58340400
C	-3.03890700	0.41559900	2.07460000
C	-3.63540200	2.04079600	0.57053000
C	-2.04366900	2.10999500	0.63017600
C	-3.88199800	0.53206100	0.79043600
H	-4.93576100	0.29853400	0.96981400
H	-3.52437500	-0.08300300	-0.03238400
C	-3.72266800	1.50320000	2.95910800
H	-4.59915500	1.06352600	3.44613700
H	-3.07723500	1.89265200	3.74889100
C	-4.13485100	2.59621300	1.93224000
H	-5.22258400	2.71473400	1.91032600
H	-3.70786900	3.57686600	2.16096100
H	-3.00669500	-0.56626000	2.54941700
H	-1.76070900	3.05384400	1.10921600
C	-0.62787000	1.31998300	2.58290800
O	0.37446000	2.02386800	2.22121900
C	0.35744400	1.12303300	4.80559900
H	-0.00993100	0.92336400	5.81296300
H	1.16377200	0.41904200	4.56684900
H	0.73684000	2.14354300	4.74700700
C	3.17396900	-2.47192800	-1.32864600

C	2.28413800	-1.57019700	-0.45311100
O	2.90642300	-0.75293200	0.29941500
O	1.03678800	-1.69609900	-0.57679800
C	4.78480800	-0.17557500	-1.91810500
C	4.23554200	1.02032100	-1.44029000
C	6.13799600	-0.40873200	-1.64051200
C	4.96925800	1.91072700	-0.66800600
C	6.90029900	0.48780100	-0.89258600
C	6.30823900	1.64543600	-0.39147300
F	6.73449700	-1.52953300	-2.05808900
F	8.18773400	0.23396300	-0.63347900
F	7.01938500	2.49426700	0.35295800
F	4.37344300	2.99547800	-0.14248900
F	2.94758000	1.32008900	-1.65723700
C	4.33878600	-3.03888800	-0.51513100
H	3.93862300	-3.69351600	0.26742800
H	5.00632100	-3.61803800	-1.15689200
H	4.90360500	-2.24588700	-0.02469600
C	2.36823700	-3.58034200	-2.01174800
H	1.55931400	-3.17535300	-2.62284600
H	3.02206200	-4.19864000	-2.63309800
H	1.91193200	-4.20940900	-1.24240800
S	3.78322600	-1.37965200	-2.75935800
Ag	1.89342100	0.82634900	1.27709000
C	-2.75274800	-2.97762200	-2.13615800
C	-3.57019800	-3.73272000	-1.28907200
C	-3.52123300	-3.50592400	0.09215000
C	-2.67399900	-2.53134100	0.61927400
C	-1.87332300	-1.78268000	-0.24378600
C	-1.89756300	-2.00241900	-1.62069700
H	-2.79557800	-3.16002100	-3.20514200
H	-4.13599400	-4.09878600	0.75997800
H	-2.63403900	-2.38801700	1.68903800
H	-1.27302400	-1.43619500	-2.29485900
I	0.23405200	-2.16990300	2.77150600
C	-4.45655700	-4.75850900	-1.90296500
O	-4.52902700	-4.98410400	-3.09599400
O	-5.18775900	-5.42796500	-0.98077100
C	-6.05586000	-6.44051400	-1.51217400
H	-6.78530000	-6.00210000	-2.19890800
H	-5.48006800	-7.19727800	-2.05195600

H	-6.55680200	-6.88171700	-0.65029800
C	-4.29881800	2.68205100	-0.66922000
C	-5.61042000	1.99209500	-1.10325300
C	-4.56660200	4.19338000	-0.49891400
H	-3.60373200	2.56198900	-1.51024800
C	-6.16519200	2.61383900	-2.39565600
H	-6.35783000	2.08062600	-0.30099800
H	-5.44491000	0.92155400	-1.26380400
C	-5.07556400	4.81977500	-1.80357700
H	-5.33257900	4.33828800	0.27502500
H	-3.66387200	4.69972800	-0.15334500
C	-6.36551800	4.13077600	-2.27176500
H	-7.10733200	2.12570800	-2.67257800
H	-5.45769600	2.41205700	-3.21279400
H	-5.24315700	5.89589400	-1.67126600
H	-4.30462400	4.71290700	-2.58012000
H	-6.70446000	4.54952200	-3.22709400
H	-7.16153300	4.33119500	-1.54026900
N	-0.74381200	0.95951100	3.86389900
H	-1.43110000	0.24907300	4.07456400
H	0.79755200	1.61652200	-3.93094700

int63

C	4.12773800	-1.00757700	-3.19278300
C	3.42191300	0.03587100	-3.79885800
C	2.17412000	0.43015800	-3.31747800
C	1.63585700	-0.23119300	-2.21072800
C	2.33390700	-1.26266800	-1.55760700
C	3.57464000	-1.66812000	-2.09168100
Pd	-0.16326900	0.26328900	-1.45646200
H	3.85729600	0.54558100	-4.65392800
H	1.63789900	1.24914400	-3.78740100
O	4.16248500	-2.72802000	-1.45816500
C	5.44223200	-3.16049700	-1.89573200
H	5.71666700	-3.99095300	-1.24338700
H	5.41826000	-3.50987300	-2.93572500
H	6.18969500	-2.36261000	-1.79855400
H	5.09066500	-1.30319600	-3.59093900
C	0.15142900	-1.59489000	-0.49378400
C	-0.29186200	-1.56238200	0.95854300
C	1.93898800	-2.12433600	1.08105700

C	1.62222900	-2.05350000	-0.48190900
C	0.97944300	-1.05722800	1.66993200
H	0.89136400	-1.13342200	2.75877100
H	1.22782400	-0.02916200	1.41482500
C	-0.32700700	-3.05837600	1.39967100
H	-0.84136800	-3.12788800	2.36141400
H	-0.87193700	-3.69268600	0.69822800
C	1.17969900	-3.42288000	1.51886900
H	1.41184700	-3.67448300	2.55367400
H	1.46042700	-4.28321700	0.90431300
H	-1.21656800	-1.01370400	1.13686600
H	1.64235900	-3.08782900	-0.84194100
C	-0.66351800	-2.31208800	-1.56764800
O	-0.37256300	-3.39091900	-2.04443800
N	-1.62772500	-1.46533800	-2.11786600
H	-2.22173900	-0.98387500	-1.44367400
C	-2.29649500	-1.84495700	-3.36281900
H	-2.83091000	-0.97049200	-3.73467000
H	-1.54208500	-2.16006000	-4.08471000
H	-2.99555800	-2.66891200	-3.19486400
C	2.65194700	2.93901000	0.53219300
C	1.96238900	4.15465000	0.44478100
C	0.72409800	4.19081600	-0.20623600
C	0.16250900	3.02797000	-0.73386400
C	0.84001900	1.80475400	-0.61326200
C	2.09853400	1.77960700	-0.00829400
H	3.62497800	2.90166700	1.00956700
H	0.20651500	5.14107400	-0.29120400
H	-0.78297800	3.09764200	-1.25508700
H	2.66340900	0.86408900	0.02766900
C	2.49740900	5.42563400	1.00295000
O	1.93203200	6.50087400	0.94018500
O	3.70138900	5.26160700	1.60200600
C	4.26781000	6.45615100	2.16138100
H	5.22254900	6.15594700	2.59375900
H	4.41705800	7.21255700	1.38591700
H	3.61061400	6.87134900	2.93052800
C	3.42409400	-2.11565400	1.51257600
C	4.17214200	-0.81073000	1.17494800
C	3.64059100	-2.41141700	3.01656800
H	3.90727500	-2.92283200	0.94724400

C	5.66899600	-0.89670700	1.50552800
H	3.72928700	0.01148800	1.75424900
H	4.05379400	-0.56089500	0.12087200
C	5.13368400	-2.49578000	3.37569200
H	3.16785800	-1.61888100	3.61423200
H	3.16315600	-3.35064700	3.30840900
C	5.89303600	-1.22197500	2.98661600
H	6.16569100	0.04362500	1.23735700
H	6.12610900	-1.68164900	0.88562700
H	5.24717200	-2.69854300	4.44744500
H	5.57603800	-3.35252500	2.84701400
H	6.96245100	-1.32932300	3.20466800
H	5.52871800	-0.38295800	3.59657400
C	-3.87535300	2.31573800	-0.72286500
C	-2.66350300	1.52685800	-1.25512300
O	-2.08046700	0.73675900	-0.41820900
O	-2.23388700	1.71832100	-2.41075500
C	-4.71478100	-0.09638800	0.64451900
C	-4.31109400	-1.33880400	0.14425400
C	-4.61298500	0.09065500	2.02809600
C	-3.78732500	-2.33580200	0.95794400
C	-4.08965000	-0.89379900	2.86557800
C	-3.67811300	-2.11102900	2.32799100
F	-4.99497700	1.24057700	2.59169400
F	-3.98479100	-0.68062800	4.18128000
F	-3.16063700	-3.05284600	3.12308500
F	-3.35165700	-3.48716200	0.42575900
F	-4.36452900	-1.58783900	-1.17586900
C	-3.48128300	3.02482700	0.57846000
H	-2.65838300	3.72014100	0.37551700
H	-4.32766400	3.58759700	0.97903700
H	-3.13404000	2.31394500	1.32691700
C	-4.39082500	3.31008600	-1.76892200
H	-4.64342400	2.81011400	-2.70571100
H	-5.26556800	3.84911000	-1.39275200
H	-3.60215700	4.03555500	-1.98557100
S	-5.34091800	1.15025700	-0.45675700

TS37

C	4.33281400	-0.82186400	-3.03080700
C	3.71152700	0.28158200	-3.62439300

C	2.51743000	0.77510500	-3.11855300
C	1.91889100	0.15928800	-2.00347900
C	2.49919400	-0.99349400	-1.41579100
C	3.71765200	-1.46474500	-1.95385600
Pd	-0.08267800	0.33277700	-1.47435000
H	4.18060600	0.76505600	-4.47615100
H	2.06753500	1.65717000	-3.55889200
O	4.21253100	-2.58936100	-1.35872900
C	5.38460200	-3.19091600	-1.89113900
H	5.55929700	-4.08473300	-1.29071000
H	5.24791400	-3.47912500	-2.94084100
H	6.25297100	-2.52507400	-1.80644100
H	5.27469900	-1.18098900	-3.42687800
C	0.19544800	-1.55416700	-0.69645100
C	-0.41068300	-1.67972800	0.70694400
C	1.80983300	-2.17800100	1.02935800
C	1.67977000	-1.91187600	-0.53155100
C	0.74289600	-1.21889500	1.61865500
H	0.53544500	-1.42144300	2.67503700
H	0.96731600	-0.15951500	1.51252500
C	-0.44678300	-3.20217400	1.01560000
H	-1.01734200	-3.36439800	1.93408300
H	-0.93152600	-3.78664800	0.23055300
C	1.05822800	-3.54637700	1.20553500
H	1.22125800	-3.95354400	2.20362800
H	1.41531200	-4.29145900	0.48906000
H	-1.36599500	-1.17238300	0.83064000
H	1.82211500	-2.88247400	-1.01604400
C	-0.49007000	-2.36159700	-1.82211000
O	0.11886800	-3.23534000	-2.43608600
N	-1.79792700	-2.06735700	-2.04347700
H	-2.22946100	-1.31598900	-1.51758600
C	-2.60580100	-2.79087400	-3.01062800
H	-3.16443800	-2.08603700	-3.63202900
H	-1.94216300	-3.38881000	-3.63481900
H	-3.31593200	-3.44731700	-2.49817500
C	2.30882300	3.01924000	0.93851700
C	1.87475600	4.20713900	0.33717900
C	1.19056100	4.14491600	-0.88491000
C	0.93186800	2.92114400	-1.49380600
C	1.32117000	1.72994400	-0.85091700

C	2.04116600	1.78892300	0.34304000
H	2.86403900	3.05701800	1.86905000
H	0.86914400	5.07002700	-1.35190200
H	0.39683000	2.90228600	-2.43690300
H	2.41276200	0.88636300	0.79395300
C	2.12029800	5.54720700	0.93248400
O	1.76047500	6.59840300	0.43706600
O	2.79484500	5.47645500	2.10441200
C	3.05900500	6.74174000	2.73042000
H	3.59791200	6.50951700	3.64912000
H	3.66538200	7.37561300	2.07761800
H	2.12454100	7.26388900	2.95338200
C	3.23468100	-2.20373200	1.62684000
C	4.01567900	-0.88151400	1.48959500
C	3.28655800	-2.62142100	3.11607300
H	3.78380000	-2.96197800	1.05241800
C	5.47324100	-1.02320600	1.94959600
H	3.52798400	-0.11994300	2.11555200
H	3.99392900	-0.51667300	0.46205600
C	4.73365300	-2.76700600	3.61631000
H	2.76573900	-1.86479700	3.72031300
H	2.76511100	-3.56724800	3.28459500
C	5.54869500	-1.48385600	3.41019000
H	6.00287100	-0.07193900	1.81801700
H	5.97833900	-1.75682600	1.30509700
H	4.73511100	-3.05523100	4.67440900
H	5.21452900	-3.58978800	3.06790500
H	6.59050000	-1.63663200	3.71675900
H	5.14320500	-0.69147900	4.05572100
C	-3.57381500	2.40156300	-0.64736400
C	-2.46763200	1.57246000	-1.31926600
O	-2.09095000	0.49700700	-0.70479900
O	-1.87590700	2.00274300	-2.32686700
C	-4.60484200	0.00751400	0.63524000
C	-4.38971100	-1.24112000	0.04035100
C	-4.39783200	0.09633500	2.01627800
C	-3.94713900	-2.34146200	0.76478000
C	-3.95242100	-0.99331700	2.76371400
C	-3.73147500	-2.21574800	2.13503200
F	-4.59602300	1.24956500	2.66466300
F	-3.74150500	-0.87432600	4.07973700

F	-3.28753500	-3.26103800	2.84111500
F	-3.68569100	-3.50457900	0.15111800
F	-4.54899600	-1.39726600	-1.28194500
C	-2.99266600	2.94804700	0.66706600
H	-2.11669100	3.56774000	0.43985100
H	-3.73314400	3.55826500	1.18919100
H	-2.67165300	2.13864100	1.32323600
C	-4.04490200	3.54029000	-1.55932900
H	-4.43594000	3.16037200	-2.50600900
H	-4.81568900	4.13767200	-1.06341000
H	-3.19220000	4.18359000	-1.78751300
S	-5.13703000	1.38877700	-0.34961700

int64

C	5.79581200	0.89356500	-0.48206300
C	5.51119200	2.15278800	0.04352800
C	4.19370400	2.55433300	0.19135900
C	3.12494400	1.69680100	-0.14790800
C	3.38239100	0.39436600	-0.61038600
C	4.74453200	0.04125400	-0.81855500
Pd	-0.08373200	1.03428700	-0.23760500
H	6.32133000	2.82439800	0.31072700
H	3.97191100	3.55674600	0.54185400
O	4.94847400	-1.20262800	-1.35605400
C	6.27573900	-1.66158800	-1.55210500
H	6.18446800	-2.65937100	-1.98378900
H	6.83055400	-1.01766800	-2.24624200
H	6.82364100	-1.72774400	-0.60259700
H	6.82484100	0.59053200	-0.62746100
C	0.90701600	-0.47550600	-1.23626200
C	0.24578300	-1.77532600	-0.73880900
C	2.32782400	-1.93889400	0.17294800
C	2.38950300	-0.71793600	-0.88424500
C	0.86142100	-1.89301700	0.65883400
H	0.56897000	-2.81010000	1.18321300
H	0.62139100	-1.04091600	1.29644200
C	0.87831900	-2.99015000	-1.48190600
H	0.22732800	-3.86398700	-1.37546000
H	0.98644800	-2.80172400	-2.55403700
C	2.24435700	-3.18778700	-0.75282200
H	2.21939900	-4.10816200	-0.16411800

H	3.09763100	-3.24968700	-1.43376300
H	-0.83824700	-1.76745800	-0.77292300
H	2.78779900	-1.14943600	-1.80681000
C	0.69794200	-0.10765300	-2.69860200
O	1.61201400	0.34347100	-3.39583800
N	-0.56118400	-0.29588000	-3.18122900
H	-1.28575700	-0.61038700	-2.55639800
C	-0.94963200	0.08373200	-4.52623900
H	-1.44923100	1.06081200	-4.54190900
H	-0.05052500	0.14238100	-5.14044200
H	-1.63011800	-0.66661900	-4.93840300
C	0.47137400	4.06377600	1.09598400
C	-0.21703800	4.37046100	-0.10545400
C	0.08863100	3.68540600	-1.27022600
C	1.07336500	2.66420700	-1.26889300
C	1.78706300	2.35779000	-0.06736800
C	1.44670700	3.09056400	1.11532900
H	0.21227500	4.59854800	2.00146900
H	-0.43572100	3.93693200	-2.18530400
H	1.43562600	2.26251100	-2.20939900
H	1.99147300	2.87461400	2.02843000
C	-1.31302000	5.37769200	-0.15846400
O	-1.95863400	5.63878300	-1.15464300
O	-1.51679300	5.97739500	1.03560000
C	-2.58675600	6.93520300	1.05905700
H	-2.61509500	7.32085000	2.07820200
H	-2.39777400	7.74204300	0.34577300
H	-3.53499300	6.45545000	0.80187900
C	3.39498000	-1.96203000	1.28941300
C	3.13120800	-0.89987600	2.37970300
C	3.57075600	-3.33675800	1.96922400
H	4.36338100	-1.73025800	0.83554300
C	4.27616400	-0.83872700	3.39936200
H	2.20330300	-1.15417500	2.91000900
H	2.97593500	0.08291600	1.92833300
C	4.69444300	-3.30312300	3.02034900
H	2.62698200	-3.63709400	2.44689700
H	3.80678000	-4.10550700	1.22662700
C	4.47941600	-2.20423300	4.06958900
H	4.07238100	-0.06862700	4.15344300
H	5.19989500	-0.53822400	2.88439700

H	4.78405600	-4.28302600	3.50494400
H	5.64955800	-3.12127400	2.50574400
H	5.32501300	-2.17320400	4.76753800
H	3.58773900	-2.44505000	4.66617500
C	-3.61954700	0.66618800	1.85756500
C	-2.32971500	0.90910400	1.06718600
O	-1.72273900	-0.11205600	0.57946400
O	-1.85274800	2.06388700	0.93670200
C	-4.28453700	-1.51729300	0.10571700
C	-3.57648100	-1.59194300	-1.09843300
C	-4.42038500	-2.70574400	0.83487600
C	-3.00270200	-2.77642500	-1.54314300
C	-3.83973200	-3.90160800	0.41329000
C	-3.11628900	-3.93215300	-0.77630800
F	-5.09101100	-2.72140800	1.99173700
F	-3.96377000	-5.01298700	1.14734200
F	-2.51843600	-5.05695900	-1.17605600
F	-2.27074500	-2.79192100	-2.66990100
F	-3.36904500	-0.49595700	-1.84535300
C	-3.34324000	-0.33366700	2.98654900
H	-2.61449300	0.10269700	3.68004300
H	-4.26069600	-0.55990800	3.53394900
H	-2.91823000	-1.25934700	2.59680500
C	-4.19411700	1.98172400	2.39340000
H	-4.39127400	2.68882800	1.58473200
H	-5.11599500	1.79946400	2.95335900
H	-3.46053000	2.44201800	3.06038800
S	-4.95558500	0.02489800	0.68052400

TS38

C	5.79581200	0.89356500	-0.48206300
C	5.51119200	2.15278800	0.04352800
C	4.19370400	2.55433300	0.19135900
C	3.12494400	1.69680100	-0.14790800
C	3.38239100	0.39436600	-0.61038600
C	4.74453200	0.04125400	-0.81855500
Pd	-0.08373200	1.03428700	-0.23760500
H	6.32133000	2.82439800	0.31072700
H	3.97191100	3.55674600	0.54185400
O	4.94847400	-1.20262800	-1.35605400
C	6.27573900	-1.66158800	-1.55210500

H	6.18446800	-2.65937100	-1.98378900
H	6.83055400	-1.01766800	-2.24624200
H	6.82364100	-1.72774400	-0.60259700
H	6.82484100	0.59053200	-0.62746100
C	0.90701600	-0.47550600	-1.23626200
C	0.24578300	-1.77532600	-0.73880900
C	2.32782400	-1.93889400	0.17294800
C	2.38950300	-0.71793600	-0.88424500
C	0.86142100	-1.89301700	0.65883400
H	0.56897000	-2.81010000	1.18321300
H	0.62139100	-1.04091600	1.29644200
C	0.87831900	-2.99015000	-1.48190600
H	0.22732800	-3.86398700	-1.37546000
H	0.98644800	-2.80172400	-2.55403700
C	2.24435700	-3.18778700	-0.75282200
H	2.21939900	-4.10816200	-0.16411800
H	3.09763100	-3.24968700	-1.43376300
H	-0.83824700	-1.76745800	-0.77292300
H	2.78779900	-1.14943600	-1.80681000
C	0.69794200	-0.10765300	-2.69860200
O	1.61201400	0.34347100	-3.39583800
N	-0.56118400	-0.29588000	-3.18122900
H	-1.28575700	-0.61038700	-2.55639800
C	-0.94963200	0.08373200	-4.52623900
H	-1.44923100	1.06081200	-4.54190900
H	-0.05052500	0.14238100	-5.14044200
H	-1.63011800	-0.66661900	-4.93840300
C	0.47137400	4.06377600	1.09598400
C	-0.21703800	4.37046100	-0.10545400
C	0.08863100	3.68540600	-1.27022600
C	1.07336500	2.66420700	-1.26889300
C	1.78706300	2.35779000	-0.06736800
C	1.44670700	3.09056400	1.11532900
H	0.21227500	4.59854800	2.00146900
H	-0.43572100	3.93693200	-2.18530400
H	1.43562600	2.26251100	-2.20939900
H	1.99147300	2.87461400	2.02843000
C	-1.31302000	5.37769200	-0.15846400
O	-1.95863400	5.63878300	-1.15464300
O	-1.51679300	5.97739500	1.03560000
C	-2.58675600	6.93520300	1.05905700

H	-2.61509500	7.32085000	2.07820200
H	-2.39777400	7.74204300	0.34577300
H	-3.53499300	6.45545000	0.80187900
C	3.39498000	-1.96203000	1.28941300
C	3.13120800	-0.89987600	2.37970300
C	3.57075600	-3.33675800	1.96922400
H	4.36338100	-1.73025800	0.83554300
C	4.27616400	-0.83872700	3.39936200
H	2.20330300	-1.15417500	2.91000900
H	2.97593500	0.08291600	1.92833300
C	4.69444300	-3.30312300	3.02034900
H	2.62698200	-3.63709400	2.44689700
H	3.80678000	-4.10550700	1.22662700
C	4.47941600	-2.20423300	4.06958900
H	4.07238100	-0.06862700	4.15344300
H	5.19989500	-0.53822400	2.88439700
H	4.78405600	-4.28302600	3.50494400
H	5.64955800	-3.12127400	2.50574400
H	5.32501300	-2.17320400	4.76753800
H	3.58773900	-2.44505000	4.66617500
C	-3.61954700	0.66618800	1.85756500
C	-2.32971500	0.90910400	1.06718600
O	-1.72273900	-0.11205600	0.57946400
O	-1.85274800	2.06388700	0.93670200
C	-4.28453700	-1.51729300	0.10571700
C	-3.57648100	-1.59194300	-1.09843300
C	-4.42038500	-2.70574400	0.83487600
C	-3.00270200	-2.77642500	-1.54314300
C	-3.83973200	-3.90160800	0.41329000
C	-3.11628900	-3.93215300	-0.77630800
F	-5.09101100	-2.72140800	1.99173700
F	-3.96377000	-5.01298700	1.14734200
F	-2.51843600	-5.05695900	-1.17605600
F	-2.27074500	-2.79192100	-2.66990100
F	-3.36904500	-0.49595700	-1.84535300
C	-3.34324000	-0.33366700	2.98654900
H	-2.61449300	0.10269700	3.68004300
H	-4.26069600	-0.55990800	3.53394900
H	-2.91823000	-1.25934700	2.59680500
C	-4.19411700	1.98172400	2.39340000
H	-4.39127400	2.68882800	1.58473200

H	-5.11599500	1.79946400	2.95335900
H	-3.46053000	2.44201800	3.06038800
S	-4.95558500	0.02489800	0.68052400

int65

C	5.17267100	0.48417700	-2.03773200
C	4.93502600	1.74560300	-2.59567600
C	3.64493800	2.26003000	-2.66926300
C	2.57589400	1.49564700	-2.17656500
C	2.79777000	0.24035100	-1.58515900
C	4.10901600	-0.26573000	-1.51841300
Pd	1.12889100	-0.64874000	-0.90177900
H	5.77145800	2.31784000	-2.98584600
H	3.45234400	3.22825000	-3.12219000
O	4.25067300	-1.47797400	-0.91564300
C	5.55275000	-1.93282200	-0.55836200
H	5.38793600	-2.79161400	0.09096600
H	6.13021400	-2.22132800	-1.44558500
H	6.10118600	-1.16358900	-0.00033000
H	6.18323400	0.09329500	-2.00721700
C	1.72228900	-1.50584300	1.13353200
C	0.58249400	-1.38896700	2.14388800
C	1.50559600	0.69730200	1.97809500
C	2.27095400	-0.22084500	1.04611400
C	0.10240100	0.06223900	1.94845000
H	-0.49919500	0.40302000	2.79002900
H	-0.44441400	0.23132300	1.01757500
C	1.33179400	-1.22620200	3.51433300
H	0.58617200	-1.24308700	4.31395900
H	2.05557400	-2.02348600	3.69016100
C	2.00212400	0.17670000	3.38496400
H	1.66197600	0.86100300	4.16745600
H	3.09243700	0.12294700	3.44031200
H	-0.15866400	-2.18414100	2.11905000
H	3.31526500	-0.06248200	0.82604800
C	2.57363100	-2.75639300	1.05787600
O	3.60237700	-2.79753100	1.74521700
C	2.83569000	-5.01702800	0.21066700
H	2.14830100	-5.80446700	-0.10487100
H	3.64912300	-4.94497200	-0.52277000
H	3.27210600	-5.27457500	1.17856600

C	-2.47624700	-2.99077000	-1.74236800
C	-1.06380700	-2.66977500	-1.18311500
O	-0.88445500	-1.45793000	-0.77808300
O	-0.19973600	-3.56166000	-1.21457100
C	-3.51546000	-1.70684900	0.66551600
C	-2.90942500	-1.82972300	1.92137800
C	-3.97291500	-0.43330600	0.29946900
C	-2.76267900	-0.74363900	2.77559100
C	-3.76884800	0.67754500	1.11375500
C	-3.16427900	0.51989300	2.35688400
F	-4.60959100	-0.24112300	-0.85787300
F	-4.14902900	1.90219100	0.71517300
F	-2.91396500	1.58624200	3.12624900
F	-2.13419600	-0.88504400	3.95359900
F	-2.40775000	-3.00185700	2.33034600
C	-2.90861900	-1.92008700	-2.74799100
H	-2.18222800	-1.88351700	-3.57040300
H	-3.89012800	-2.15952700	-3.16493200
H	-2.96164300	-0.93802600	-2.28739000
C	-2.49839400	-4.38360800	-2.38590100
H	-1.82010500	-4.38740800	-3.24366500
H	-2.15570900	-5.14922600	-1.68909000
H	-3.50462400	-4.63041700	-2.74003400
S	-3.73462700	-3.15115400	-0.34293900
C	-0.63130300	3.47338800	-1.69691300
C	-1.58502700	2.53813300	-2.13489100
C	-1.16033100	1.32533300	-2.67838900
C	0.20057600	1.02085000	-2.73542900
C	1.16405100	1.93469600	-2.24958100
C	0.72626400	3.17896600	-1.76741300
H	-0.96540000	4.41971800	-1.28645500
H	-1.89993300	0.62979500	-3.05010900
H	0.53339200	0.11903100	-3.25191800
H	1.45754400	3.89007500	-1.39832300
C	-3.05500100	2.77996700	-2.05896700
O	-3.89189100	2.01763400	-2.50079100
O	-3.35562700	3.94154500	-1.44230300
C	-4.76285600	4.21670300	-1.32041500
H	-4.83077100	5.15679300	-0.77310500
H	-5.22039700	4.31196200	-2.30882100
H	-5.25795700	3.41180800	-0.77450600

C	1.60573200	2.19566600	1.68158400
C	0.65459800	3.05280300	2.53942500
C	3.04831900	2.73113600	1.78050600
H	1.28279600	2.31477100	0.63876800
C	0.73076500	4.53474200	2.14177100
H	0.92171800	2.95283100	3.60092100
H	-0.37679200	2.69589600	2.44178600
C	3.13318200	4.21764700	1.40386400
H	3.41101600	2.59699700	2.80924000
H	3.71437000	2.15185500	1.13052800
C	2.16682300	5.06929800	2.23921700
H	0.05730000	5.12916800	2.77023900
H	0.37267100	4.64404100	1.10796000
H	4.16206900	4.57739900	1.52268100
H	2.88861800	4.32882700	0.33810200
H	2.20850500	6.11799100	1.92123600
H	2.48675500	5.04688600	3.29083800
N	2.10356400	-3.76876600	0.31790400
H	1.26308000	-3.62951200	-0.25940800

int66

C	-1.97760800	-2.63262100	1.58172100
C	-1.31671900	-3.75028800	2.10893600
C	0.08023400	-3.81719100	2.04627600
C	0.80535400	-2.76486600	1.47041300
C	0.15387400	-1.63498500	0.97012900
C	-1.24621800	-1.59118100	1.01539300
Pd	1.29216600	-0.11135400	0.28879000
H	1.88454800	-2.86055300	1.38707200
H	0.61763100	-4.67771500	2.42756600
H	-3.06223000	-2.60338100	1.61830300
C	2.20971600	-0.89932300	-1.63280500
C	2.30805500	0.12288400	-2.76040800
C	0.13248900	-0.57012300	-2.69801900
C	0.90133900	-1.34840500	-1.63417100
C	0.91630800	0.76633600	-2.73348500
H	0.71130800	1.34671300	-3.63793500
H	0.74896100	1.39554000	-1.86126600
C	2.17565400	-0.75940300	-4.05306500
H	2.37779100	-0.14311700	-4.93411300
H	2.88272700	-1.59349500	-4.06179300

C	0.68341200	-1.22942000	-4.01754700
H	0.12714600	-0.85189100	-4.88047700
H	0.58161800	-2.31790700	-4.00989500
H	3.16605600	0.79097200	-2.73620800
H	0.60858700	-2.33054600	-1.29171400
C	3.37649800	-1.63967700	-1.03860200
O	3.34551900	-2.84901500	-0.81326300
N	4.44944600	-0.83686200	-0.78615000
H	4.25715700	0.16029300	-0.73532000
C	5.61197700	-1.35056000	-0.08305200
H	5.77028800	-2.38787500	-0.38094200
H	6.49073000	-0.75601800	-0.34434200
H	5.47678600	-1.32540300	1.00670900
C	-1.38241800	-0.47022600	-2.48168400
C	-2.08540600	0.46679900	-3.48338500
C	-2.08421300	-1.84013400	-2.43426400
H	-1.50372000	-0.00971000	-1.48863200
C	-3.58766100	0.59817700	-3.18512300
H	-1.95483100	0.07911200	-4.50311900
H	-1.62211800	1.45903800	-3.45780400
C	-3.58055500	-1.69665300	-2.12153500
H	-1.96068400	-2.34159600	-3.40471800
H	-1.61573900	-2.48007400	-1.67969700
C	-4.27756700	-0.77129200	-3.12805800
H	-4.06201600	1.23565500	-3.94049500
H	-3.72489900	1.11149800	-2.22461800
H	-4.05894600	-2.68277700	-2.10783400
H	-3.69385000	-1.28229700	-1.10882800
H	-5.33736000	-0.65405900	-2.87242000
H	-4.24288300	-1.23464400	-4.12447100
C	1.97505100	2.57677600	1.99458900
C	2.66033600	2.58185100	0.58530600
O	2.64101300	1.48788700	-0.11099200
O	3.26423600	3.60464400	0.28977900
C	-0.87364600	1.79327500	1.55234700
C	-2.03147900	1.36547000	2.21314600
C	-1.03739600	2.47065900	0.33819200
C	-3.29875600	1.55618600	1.66234400
C	-2.29086300	2.66551200	-0.22777500
C	-3.42600400	2.19839100	0.43389200
F	0.02828200	2.92121000	-0.33669000

F	-2.41100500	3.26330400	-1.41694600
F	-4.62708700	2.35040800	-0.12464100
F	-4.38272700	1.10217800	2.29514900
F	-1.94418600	0.69353300	3.36347600
C	3.06626100	2.16719300	3.00521200
H	3.89298100	2.87470300	2.89797800
H	2.69683100	2.20264000	4.03427400
H	3.45092400	1.16293600	2.79877300
C	1.37644000	3.93478700	2.34883500
H	0.59526000	4.22752200	1.64611800
H	0.97178100	3.94026500	3.36537600
H	2.17773400	4.67250700	2.26977900
S	0.69213900	1.20195400	2.19179100
O	-2.12250800	-4.71681200	2.64396300
C	-1.50715000	-5.87422800	3.18554700
H	-2.31824400	-6.50142100	3.55966800
H	-0.94385900	-6.43071900	2.42410700
H	-0.83213300	-5.62559400	4.01578000
H	-1.78490500	-0.75120100	0.59034000

TS39

C	2.39493200	-1.30968100	1.42451200
C	2.59013900	-0.98060400	2.77627900
C	1.83282300	0.04862100	3.35751400
C	0.89289900	0.73328500	2.58609200
C	0.67254000	0.40695900	1.23693000
C	1.46142000	-0.61388700	0.66805800
Pd	-1.25734400	0.60063200	0.48549300
H	0.32551200	1.54560100	3.03416400
H	1.96944100	0.32508300	4.39613200
H	2.97999500	-2.11890600	0.99869300
C	-0.78611200	2.53998100	-0.09749000
C	-0.85447300	2.70553700	-1.62044700
C	1.35414300	2.34027500	-1.11247300
C	0.59115200	2.30916800	0.20745600
C	0.28951800	1.78232100	-2.09038400
H	0.54947400	1.94420500	-3.14051600
H	0.08466400	0.71849200	-1.93498000
C	-0.22141700	4.10048600	-1.88436600
H	-0.28989400	4.34824800	-2.94844900
H	-0.72450400	4.89317700	-1.32494400

C	1.25920900	3.88803500	-1.45173800
H	1.94701800	4.11943800	-2.26749500
H	1.54619400	4.50899900	-0.59860800
H	-1.83482500	2.53769000	-2.06449600
H	1.01288800	2.76550500	1.09145300
C	-1.60588600	3.36063900	0.86819800
O	-1.12069200	3.80563300	1.91229800
N	-2.89503200	3.56999700	0.47726700
H	-3.27144800	2.87762600	-0.16652400
C	-3.83614400	4.20539100	1.38512000
H	-3.32949200	5.01712900	1.90871200
H	-4.67697000	4.60603500	0.81402600
H	-4.21914100	3.50162400	2.13640800
C	2.76249500	1.73059500	-1.14360400
C	3.49659400	1.92769500	-2.48416700
C	3.65034100	2.19541600	0.02719500
H	2.63359000	0.64956700	-1.02416800
C	4.84351900	1.18824900	-2.49166900
H	3.68528900	2.99566200	-2.65499800
H	2.87168500	1.58079200	-3.31540800
C	5.00965800	1.47924200	0.01826000
H	3.80376500	3.28208000	-0.04023700
H	3.14689700	2.00026100	0.97988300
C	5.73213500	1.64552000	-1.32582800
H	5.35477300	1.34726500	-3.44845100
H	4.66376900	0.10676100	-2.40798800
H	5.63557800	1.85042700	0.83841800
H	4.84260400	0.41026900	0.21177800
H	6.67673600	1.08870600	-1.32361600
H	5.99151000	2.70459200	-1.46768400
C	-3.75789000	-1.48854600	0.27739900
C	-3.95245300	-0.19326100	-0.58164200
O	-3.15199100	0.80834300	-0.37722600
O	-4.93112200	-0.17688100	-1.31662800
C	-1.01379100	-2.53561400	-0.22107600
C	-0.07049100	-3.44736500	0.26612900
C	-0.95523700	-2.21660600	-1.58277800
C	0.90373600	-4.00336100	-0.56015600
C	-0.00211600	-2.77553900	-2.42716400
C	0.93536900	-3.67125100	-1.91159000
F	-1.79845100	-1.31531900	-2.10430400

F	0.03628500	-2.44082200	-3.72003800
F	1.86492100	-4.19738200	-2.70984300
F	1.82525100	-4.82816700	-0.05339900
F	-0.03006700	-3.74977700	1.56729700
C	-4.61595100	-1.29667800	1.54512100
H	-5.64243600	-1.10158200	1.22225000
H	-4.60360200	-2.18990000	2.17667800
H	-4.27818100	-0.43797800	2.13426100
C	-4.17505800	-2.74371100	-0.48393500
H	-3.58180400	-2.88209200	-1.38898500
H	-4.09202200	-3.63538500	0.14460000
H	-5.21302600	-2.60976500	-0.79473200
S	-2.00933500	-1.66684900	0.97862600
O	3.53721600	-1.70831400	3.42518800
C	3.78191200	-1.43176700	4.79807900
H	4.56182200	-2.12780600	5.10986600
H	4.13514800	-0.40296200	4.94551600
H	2.88502500	-1.59571300	5.40915300
H	1.31252000	-0.89691100	-0.36876900

int67

C	0.43173300	2.20516300	1.04772000
C	0.99159800	1.76562600	2.26797600
C	0.44845500	0.66015400	2.91774300
C	-0.64957900	-0.01230100	2.34206500
C	-1.24552000	0.42435900	1.12898300
C	-0.64120800	1.54661900	0.48608500
Pd	-0.00464300	-1.28924600	0.29792000
H	-1.12317300	-0.82717800	2.88429900
H	0.86189200	0.29067900	3.84750500
H	0.88914200	3.05509900	0.55245500
C	-2.00887100	-1.62930000	0.08506700
C	-2.49460800	-1.65156200	-1.37058600
C	-3.39551700	0.27030900	-0.49067000
C	-2.53476500	-0.30653700	0.67390200
C	-2.55292100	-0.15185500	-1.72999000
H	-3.07350100	0.02057400	-2.67693900
H	-1.56564600	0.31279900	-1.79236800
C	-4.00677100	-1.98491800	-1.31402900
H	-4.39638600	-2.10242500	-2.33102600
H	-4.21243100	-2.91233900	-0.77435000

C	-4.60153800	-0.72425300	-0.62143300
H	-5.39642700	-0.28033600	-1.22610900
H	-5.03226800	-0.95588900	0.35683500
H	-1.90591100	-2.28490400	-2.03511800
H	-3.14012500	-0.48728500	1.56506500
C	-2.16777000	-2.85340000	0.95206400
O	-2.54500300	-2.78159700	2.12777800
N	-1.85918100	-4.03720300	0.34144200
H	-1.27581300	-3.96823500	-0.48657500
C	-1.77046900	-5.26251800	1.11691600
H	-2.57052400	-5.26915700	1.85816100
H	-1.88077700	-6.12319200	0.45273100
H	-0.81272000	-5.34538100	1.64952300
C	-3.82743300	1.74249200	-0.33751800
C	-4.44189100	2.34303200	-1.61823000
C	-4.78038300	1.95151500	0.85916600
H	-2.93645500	2.34321400	-0.11928100
C	-4.81088800	3.82306500	-1.42920500
H	-5.34527800	1.78303500	-1.89495800
H	-3.74242100	2.24125000	-2.45570400
C	-5.14029400	3.43270300	1.04778200
H	-5.70281500	1.37876300	0.69574100
H	-4.32531200	1.55638200	1.77514100
C	-5.74985700	4.02315900	-0.23136300
H	-5.26872800	4.21544500	-2.34509700
H	-3.89200100	4.40451900	-1.26532600
H	-5.83155100	3.54822900	1.89107000
H	-4.23186000	3.99526800	1.30757700
H	-5.97367400	5.08786700	-0.09453100
H	-6.70750800	3.52364100	-0.43708500
C	2.86857800	-2.52312100	-0.64474900
C	1.65497100	-2.95027100	-1.53471200
O	0.45251100	-2.78356300	-1.06092600
O	1.91602700	-3.53526600	-2.57616600
C	2.88966300	0.40913700	-0.31088300
C	3.75425300	1.30789400	0.32238900
C	2.30322900	0.81702600	-1.51459800
C	4.00004600	2.57655100	-0.19631900
C	2.54686800	2.07285600	-2.05772300
C	3.39798600	2.95733300	-1.39296500
F	1.45809900	0.00485200	-2.16329800

F	1.96090600	2.44431600	-3.19965500
F	3.63147700	4.16652400	-1.90403300
F	4.81051000	3.42234200	0.44501700
F	4.34632700	0.98283000	1.47911300
C	3.14080900	-3.70411700	0.30816300
H	3.30970300	-4.59666700	-0.30156500
H	4.02538400	-3.52158300	0.92527600
H	2.28325000	-3.89818500	0.96019200
C	4.09552200	-2.19267500	-1.48874000
H	3.90072300	-1.36516800	-2.17411500
H	4.95415400	-1.94264400	-0.85829400
H	4.32948700	-3.06824600	-2.09701400
S	2.45728600	-1.09685600	0.53377300
O	2.06977600	2.47556800	2.68841800
C	2.76790900	2.02562700	3.84664900
H	3.62225000	2.69401400	3.95529200
H	2.13717200	2.08760600	4.74177800
H	3.12647600	0.99885500	3.71484100
H	-1.02544700	1.89134800	-0.46368900

int68

C	-2.12817700	1.56161400	3.34753100
C	-1.13410300	0.60025800	3.60876100
C	-0.64711500	-0.16684300	2.55281300
C	-1.10935100	0.09012100	1.25010300
C	-2.02984900	1.11302400	0.95180500
C	-2.56888900	1.80125600	2.05252400
Pd	-0.02832400	-0.40283200	-0.66819300
H	-1.11165500	-0.87355900	0.63867800
H	0.00492900	-1.01788700	2.69787400
C	-1.73340600	0.46541200	-1.52037200
C	-1.29989700	1.38833600	-2.67116000
C	-1.99047100	2.87511600	-1.07430600
C	-2.39742600	1.43033800	-0.48059200
C	-0.71498300	2.56811600	-1.89095800
H	-0.42544500	3.40839300	-2.53197100
H	0.14422000	2.28559700	-1.28201200
C	-2.58254500	2.01014400	-3.29120500
H	-2.34590000	2.47334400	-4.25436800
H	-3.35872700	1.26198000	-3.47886800
C	-3.00427800	3.08016900	-2.23944000

H	-2.89540000	4.07772700	-2.66837000
H	-4.04338600	2.97872400	-1.90986600
H	-0.63502900	0.91733500	-3.39398500
H	-3.48853100	1.34963200	-0.55487700
C	-2.54381900	-0.73040800	-1.90834800
O	-3.59774100	-1.06521300	-1.28320800
N	-2.12180200	-1.44895900	-2.96263700
H	-1.17549700	-1.25788000	-3.28861800
C	-2.71319100	-2.73672500	-3.28879300
H	-2.31410100	-3.07456400	-4.24620300
H	-2.48256700	-3.48584900	-2.51828900
H	-3.79809600	-2.64150600	-3.35699700
C	-1.86297700	4.04169700	-0.06585400
C	-0.52705500	3.99924600	0.71355600
C	-2.01867100	5.44848700	-0.68663600
H	-2.67880200	3.95472300	0.66221400
C	-0.46785700	5.06939900	1.81038000
H	0.29275900	4.18069500	0.00558300
H	-0.35262300	3.00851000	1.14002700
C	-1.93534100	6.55083600	0.38361200
H	-1.23541700	5.60604200	-1.44206200
H	-2.97871400	5.53780900	-1.20414200
C	-0.64519300	6.47040400	1.21009000
H	0.48368100	5.00164100	2.35134700
H	-1.26115300	4.87919000	2.54745200
H	-2.02569000	7.53560400	-0.09038000
H	-2.79765600	6.45064000	1.05884600
H	-0.64867600	7.23379900	1.99729700
H	0.21413800	6.69087200	0.56067900
C	2.17351900	-2.54397600	-1.48109800
C	1.61344100	-1.78170100	-2.71920100
O	0.68902600	-0.87050500	-2.54417500
O	2.00742900	-2.13651300	-3.82054900
C	3.39565200	-0.42754400	0.08068600
C	4.58093700	-0.83940600	0.70837300
C	3.38967600	0.84999600	-0.49162200
C	5.70671200	-0.02331900	0.76817700
C	4.50314200	1.68526700	-0.43605000
C	5.66527200	1.24619100	0.19414500
F	2.30534200	1.32699700	-1.11581300
F	4.46124400	2.90197600	-0.98533100

F	6.73521000	2.03800100	0.24823500
F	6.82162000	-0.44815200	1.36873900
F	4.66275700	-2.05363800	1.26499600
C	1.27925500	-3.77807500	-1.24878300
H	1.26056000	-4.35376500	-2.17914600
H	1.68348300	-4.40383700	-0.44877600
H	0.25937000	-3.50159900	-0.97166200
C	3.62937300	-2.94780300	-1.70299900
H	4.26331900	-2.07967200	-1.89923900
H	4.02120100	-3.48986900	-0.83887000
H	3.67016700	-3.58508400	-2.58835700
S	1.99428800	-1.54008500	0.12188600
O	-0.64380100	-3.02440500	1.28766400
C	-1.41121500	-3.58587100	2.09710200
O	-2.69874600	-3.57562000	2.02886600
C	-0.84437800	-4.33911100	3.29341500
H	-1.24962400	-5.35435800	3.32083500
H	0.24512400	-4.37120000	3.24969100
H	-1.16476400	-3.84264100	4.21564800
Ag	-3.29234300	-2.37883100	0.38712800
H	-3.34801100	2.53867000	1.89783700
H	-2.55252700	2.09992800	4.18894000
O	-0.76767800	0.45752400	4.91093100
C	0.17104000	-0.56394100	5.22504700
H	0.33164800	-0.50472200	6.30223100
H	-0.21591500	-1.55869100	4.96855000
H	1.12584900	-0.40781300	4.70558800

TS40

C	-2.41405300	1.35896100	3.07694200
C	-1.11753800	0.91276800	3.38029900
C	-0.35925900	0.27887600	2.39298200
C	-0.86752000	0.13168100	1.08733100
C	-2.11843900	0.70357900	0.74876800
C	-2.89941000	1.25432600	1.77944400
Pd	0.14256700	-0.64188500	-0.53182000
H	-0.66792700	-1.34878000	0.88698000
H	0.59119300	-0.17953700	2.63660700
C	-1.60389600	-0.14873200	-1.57912100
C	-1.16528500	0.75239600	-2.75742000
C	-2.31568500	2.20764500	-1.41609200

C	-2.50614900	0.78029700	-0.70323200
C	-0.90817300	2.08468800	-2.04125900
H	-0.68827700	2.90598400	-2.73314600
H	-0.10472600	2.02513300	-1.30590400
C	-2.42738100	1.08578600	-3.59801100
H	-2.13159000	1.54201100	-4.54844800
H	-3.01722500	0.19734900	-3.84076800
C	-3.19190700	2.10452400	-2.70052200
H	-3.24675400	3.07049500	-3.20544500
H	-4.21848500	1.79608000	-2.47627700
H	-0.33604500	0.34953700	-3.33908100
H	-3.56263400	0.50839200	-0.80975200
C	-2.22438300	-1.45020600	-1.98762300
O	-3.32669400	-1.87465200	-1.50860600
N	-1.60061900	-2.16742600	-2.93195100
H	-0.63253200	-1.90863000	-3.13241200
C	-2.04766500	-3.50300900	-3.29638900
H	-1.90751900	-4.21069100	-2.46944100
H	-3.10857200	-3.48624200	-3.55276600
H	-1.46865400	-3.84004100	-4.15741700
C	-2.56283800	3.44408900	-0.51567600
C	-1.32982400	3.80065000	0.34770200
C	-3.01580200	4.71485400	-1.26791800
H	-3.38493500	3.19731400	0.16941200
C	-1.62997400	4.93086400	1.34026200
H	-0.52085000	4.12622800	-0.32084700
H	-0.95767300	2.92309900	0.88062300
C	-3.30248600	5.87519800	-0.29877600
H	-2.23642400	5.01574200	-1.98302100
H	-3.91994700	4.51538500	-1.85140600
C	-2.10456500	6.19121700	0.60595900
H	-0.73939800	5.14913900	1.94210700
H	-2.40729000	4.59688500	2.04205600
H	-3.60208100	6.76620300	-0.86381400
H	-4.16207500	5.60208300	0.33045000
H	-2.36405400	6.98298100	1.31913100
H	-1.27973800	6.57923400	-0.00901600
C	2.68702800	-2.55634600	-0.90478600
C	2.05100100	-2.17317800	-2.27948700
O	1.01783000	-1.37959700	-2.28984200
O	2.52037400	-2.71547000	-3.27137000

C	3.51112200	0.01817900	0.16238100
C	4.72272300	-0.04047200	0.86736200
C	3.31916500	1.11495800	-0.68724500
C	5.69739200	0.94494400	0.74221900
C	4.28035900	2.11468500	-0.82102300
C	5.47238900	2.02828200	-0.10543800
F	2.19915800	1.25212900	-1.40570700
F	4.06452000	3.15261100	-1.63295400
F	6.39650600	2.97946300	-0.23089500
F	6.84236700	0.85837400	1.42500200
F	4.97882900	-1.06941000	1.68428700
C	1.98147500	-3.83177700	-0.40343500
H	2.07205800	-4.58998600	-1.18675900
H	2.45481100	-4.20574200	0.50918800
H	0.92173000	-3.65933300	-0.19604900
C	4.19357100	-2.76696900	-1.03678000
H	4.69224700	-1.87137700	-1.41571400
H	4.63857100	-3.04522100	-0.07794500
H	4.35809600	-3.56218400	-1.76626900
S	2.31156800	-1.27638700	0.44634700
O	-0.53396100	-2.58211800	1.64346200
C	-1.32534900	-2.84239400	2.60977600
O	-2.59110300	-2.81060700	2.54475400
C	-0.71296800	-3.17964400	3.95276700
H	-1.33678700	-3.89005300	4.49755400
H	0.30099200	-3.56263400	3.82941000
H	-0.66890500	-2.25232200	4.53566200
Ag	-3.26280400	-2.28524500	0.58815500
H	-3.89554900	1.62561100	1.55810000
O	-0.71064700	1.09674800	4.67068000
C	0.62136400	0.73981500	5.00860300
H	0.79342200	-0.34071600	4.91315100
H	1.35221800	1.27112100	4.38412700
H	0.75705900	1.03097700	6.05129200
H	-3.01384200	1.78776100	3.87280300

int69

C	0.86353600	2.41774800	2.72579200
C	0.67205000	1.07922500	3.08981400
C	0.16074200	0.16371700	2.16082300
C	-0.16046800	0.55967900	0.85016000

C	0.12933300	1.89474000	0.45829000
C	0.59823400	2.81374600	1.41697000
Pd	-1.05892300	-0.57687000	-0.53494400
H	-2.53600800	-0.34179600	1.62932800
H	-0.03376800	-0.85255800	2.47874200
C	-0.93175100	1.16842400	-1.70287600
C	-0.16578500	0.80900900	-2.99597000
C	1.32345100	2.14990300	-1.88715700
C	-0.00831100	2.21823800	-1.00489700
C	1.27208200	0.72014100	-2.47138700
H	2.01600200	0.56062700	-3.26001500
H	1.38777100	-0.05614300	-1.71852600
C	-0.09648500	2.08024500	-3.88651300
H	0.22921100	1.81571900	-4.89788900
H	-1.06890200	2.57221200	-3.98192800
C	0.97063000	2.96357000	-3.16681100
H	1.84991700	3.07366800	-3.80506600
H	0.61007000	3.97114700	-2.93274300
H	-0.53965000	-0.07944500	-3.50531200
H	-0.41623500	3.23108700	-1.11511000
C	-2.35708900	1.55448700	-1.86200400
O	-2.91150600	2.49019600	-1.19131700
N	-3.09096800	0.88354900	-2.76924300
H	-2.70945600	-0.01603800	-3.06060300
C	-4.53585300	1.03996200	-2.83228800
H	-5.02480300	0.63766800	-1.93498400
H	-4.79274600	2.09710900	-2.91474000
H	-4.90679900	0.50677000	-3.70930000
C	2.62613100	2.54348500	-1.14733400
C	3.20992900	1.36813500	-0.32718800
C	3.74149600	3.10517600	-2.05466400
H	2.37875000	3.34664500	-0.43866800
C	4.42588400	1.78316600	0.50929700
H	3.52577700	0.58379400	-1.02737500
H	2.44576800	0.92728100	0.31704500
C	4.97951400	3.51979200	-1.24103200
H	4.02647700	2.34439800	-2.79578000
H	3.38102700	3.97310200	-2.61645300
C	5.52641200	2.36994900	-0.38408900
H	4.80600300	0.91661600	1.06366900
H	4.11480900	2.52776200	1.25547900

H	5.75826700	3.89950100	-1.91365900
H	4.70267100	4.35538100	-0.58162300
H	6.37561400	2.71350200	0.21912200
H	5.90838300	1.57714200	-1.04333400
C	-1.55336000	-3.80241400	-1.02753600
C	-1.79997700	-2.92217500	-2.30366300
O	-1.94728000	-1.64549000	-2.14059000
O	-1.95141100	-3.53432800	-3.35396600
C	0.95552800	-2.79101600	0.28464800
C	1.68007300	-2.76010100	1.48055200
C	1.66064000	-2.50942500	-0.89126800
C	3.01852100	-2.38141200	1.52282900
C	3.00145700	-2.14371900	-0.87075900
C	3.68058300	-2.05839700	0.34302800
F	1.03470000	-2.51117900	-2.07564300
F	3.62181500	-1.79921700	-2.00319400
F	4.94868800	-1.64477600	0.37248900
F	3.65374500	-2.29168500	2.69888900
F	1.06771700	-3.01151600	2.65100800
C	-2.95095700	-4.19427600	-0.50492700
H	-3.47885600	-4.69535400	-1.32109400
H	-2.88510500	-4.87479500	0.34925400
H	-3.53314100	-3.31256200	-0.21779300
C	-0.71270500	-5.03929000	-1.33189500
H	0.28510700	-4.77174800	-1.68196000
H	-0.62767100	-5.68641700	-0.45363500
H	-1.20735100	-5.58039600	-2.14093300
S	-0.82887200	-2.83605600	0.42758400
O	-2.70627000	-0.59810900	2.56666200
C	-2.73577900	0.44896800	3.37805300
O	-2.85940300	1.62036100	3.00771600
C	-2.56583600	0.10423700	4.82653700
H	-3.18639200	0.76024300	5.43831200
H	-2.78875500	-0.94510200	5.01971700
H	-1.51551200	0.30592200	5.07084600
Ag	-2.62565700	2.31269900	0.94045100
H	0.77326800	3.84714100	1.12903000
O	0.94912100	0.76001500	4.39763400
C	1.23995900	-0.60272000	4.69835300
H	0.35245400	-1.24380300	4.62372500
H	2.01580500	-1.00298100	4.03756500

H	1.59705400	-0.61192900	5.72987500
H	1.22902300	3.11728100	3.46999800

int70

C	0.49243400	3.74779200	0.99669900
C	-0.21515800	2.81682000	1.76572400
C	-0.25095700	1.46957300	1.37412500
C	0.43018000	1.06470600	0.22876100
C	1.19958100	1.97402100	-0.52927900
C	1.18881100	3.31544500	-0.13704900
Pd	0.26789300	-0.79007100	-0.43570900
H	-0.84617800	0.78063500	1.96048700
C	1.48655700	-0.05109700	-1.98467300
C	2.79781100	-0.85271800	-2.08973000
C	3.52899600	1.23537700	-1.52665300
C	1.95709600	1.41996700	-1.70325400
C	3.61879500	-0.20140500	-0.96896300
H	4.64547100	-0.57750200	-0.93191800
H	3.16511200	-0.31137200	0.01785500
C	3.58959100	-0.40868300	-3.34999300
H	4.42824800	-1.09037000	-3.53175600
H	2.97090300	-0.40709400	-4.25210100
C	4.09225100	1.01417300	-2.95985900
H	5.18665500	1.05006300	-2.94595900
H	3.75314000	1.78603500	-3.65714400
H	2.67920000	-1.93783300	-2.00473900
H	1.77443700	2.05378300	-2.57983900
C	0.46730200	-0.18893000	-3.05541800
O	-0.41588700	0.69101600	-3.30256700
C	-0.68472300	-1.69249900	-4.61670300
H	-0.44434900	-2.59861200	-5.17584900
H	-1.58689700	-1.86681000	-4.01461000
H	-0.89605300	-0.88029000	-5.31433000
C	-3.40297700	-1.67708500	1.98420900
C	-2.46713400	-1.27692900	0.82355800
O	-3.03515800	-0.81958000	-0.21325300
O	-1.22370400	-1.42843700	1.01103500
C	-4.93597700	0.69623300	1.50694000
C	-4.35422900	1.59686900	0.60725400
C	-6.28443600	0.37635000	1.30161400
C	-5.04935400	2.09847700	-0.48557300

C	-7.00791400	0.89190700	0.22742600
C	-6.38202300	1.74485400	-0.67960300
F	-6.91470000	-0.47476400	2.11890300
F	-8.29144300	0.55704800	0.04889500
F	-7.05595200	2.21873700	-1.72968800
F	-4.41897700	2.87459000	-1.38454900
F	-3.07167600	1.96086600	0.73207500
C	-4.58557200	-2.49824800	1.46638700
H	-4.21299700	-3.45214500	1.07424400
H	-5.29651700	-2.70132300	2.27005900
H	-5.09550600	-1.98303200	0.65217800
C	-2.65767000	-2.41035100	3.10351600
H	-1.83721200	-1.80903000	3.50064900
H	-3.34374400	-2.66959600	3.91494700
H	-2.22791600	-3.33213600	2.70012900
S	-3.97774600	-0.06107000	2.79766000
Ag	-1.94991000	0.47357600	-1.65183100
C	2.65328500	-1.67228700	2.65580000
C	4.01465900	-1.70062900	2.33051900
C	4.46672000	-2.52162500	1.29028000
C	3.55807700	-3.26319000	0.53581700
C	2.20210000	-3.16875500	0.84232500
C	1.73018100	-2.40784300	1.91350200
H	2.32001100	-1.03363200	3.46664300
H	5.52208500	-2.54942400	1.04597500
H	3.90183000	-3.86610400	-0.29661900
H	0.67098300	-2.34317500	2.13349900
I	0.76471700	-4.07654000	-0.49071100
C	4.92584300	-0.78603100	3.07610500
O	4.60193000	-0.13351400	4.04798900
O	6.15976600	-0.73115600	2.52247300
C	7.07320200	0.17757700	3.16158500
H	6.68278900	1.19733200	3.12366200
H	7.22930800	-0.10518100	4.20590000
H	8.00280800	0.10296700	2.59764300
C	4.24259400	2.32419200	-0.70793200
C	5.61071400	1.89192900	-0.13845300
C	4.41118100	3.64065700	-1.49349800
H	3.60764400	2.53662600	0.16219600
C	6.22070100	2.99813800	0.73891300
H	6.30179000	1.65627900	-0.96088400

H	5.50756200	0.97826100	0.45619300
C	4.98595500	4.75456600	-0.60803300
H	5.09339200	3.46979400	-2.33751700
H	3.45728800	3.95153500	-1.93400000
C	6.33710600	4.33308600	-0.01140200
H	7.20485500	2.68554500	1.11012900
H	5.58134200	3.13843800	1.62262000
H	5.09621100	5.68249600	-1.18223700
H	4.27817100	4.96768800	0.20565800
H	6.72447700	5.11320400	0.65514600
H	7.06751300	4.22387300	-0.82602000
N	0.44709800	-1.34096100	-3.77402900
H	1.11372800	-2.05868100	-3.53260100
H	1.73271600	4.05159200	-0.72084900
H	0.51255900	4.79767400	1.26298800
O	-0.92412400	3.11642000	2.89607000
C	-0.95609600	4.46591100	3.32645800
H	-1.56720700	4.48120600	4.23070200
H	0.04826500	4.84239400	3.56500300
H	-1.41185800	5.12338800	2.57308300

TS41

C	-0.09093300	2.47502200	-2.73623000
C	0.26078700	1.13303100	-2.92700100
C	0.03919400	0.20445700	-1.90076600
C	-0.55245900	0.61818900	-0.71230600
C	-0.99108000	1.94533900	-0.52604700
C	-0.70861000	2.86332300	-1.54395100
Pd	-0.63972700	-0.65080500	0.82403700
H	0.38983500	-0.80995500	-2.04353300
C	-1.64184700	1.03498900	1.73488400
C	-3.10833500	0.76355900	2.10628000
C	-3.28187200	2.51059000	0.64551300
C	-1.71533500	2.26366300	0.75160600
C	-3.81352400	1.06328400	0.77051800
H	-4.90351200	1.00861800	0.85561300
H	-3.48555300	0.42124900	-0.05010300
C	-3.65859600	1.91096800	2.99574800
H	-4.65699900	1.64224400	3.35840400
H	-3.03878500	2.10929000	3.87318400
C	-3.72115300	3.11226200	2.01183100

H	-4.73782200	3.51149400	1.94607900
H	-3.07195100	3.93797700	2.31783300
H	-3.28137800	-0.22596000	2.53708900
H	-1.24874300	3.13655900	1.22219400
C	-0.66541700	1.22799800	2.84805500
O	0.39203600	1.92628000	2.71414000
C	0.12545800	0.51211700	5.05401100
H	-0.33879900	0.23186400	6.00107300
H	0.85572300	-0.25709900	4.76734100
H	0.64639300	1.46250600	5.16935000
C	3.27781400	-2.51369800	-0.90677200
C	2.36473400	-1.66854300	0.00765700
O	2.96721400	-0.79943600	0.71969100
O	1.12768600	-1.88553800	-0.03812900
C	4.67746300	-0.11922900	-1.62691300
C	4.07793700	1.05984400	-1.16810500
C	6.05533400	-0.25504900	-1.41279100
C	4.79203300	2.02847600	-0.47439000
C	6.79537900	0.71713100	-0.74179600
C	6.15723400	1.85783500	-0.25871700
F	6.70250000	-1.35222100	-1.82067600
F	8.10870900	0.55469300	-0.54191800
F	6.85105300	2.78141500	0.40999600
F	4.15819900	3.10001100	0.02962900
F	2.76582900	1.27169600	-1.33030400
C	4.52708200	-2.97965700	-0.15699500
H	4.22702600	-3.65722500	0.65103500
H	5.20421000	-3.51141900	-0.82907700
H	5.05202600	-2.13796300	0.29495200
C	2.52618300	-3.69090800	-1.53555700
H	1.65795600	-3.35508200	-2.10665600
H	3.18912100	-4.26292200	-2.19075000
H	2.16820500	-4.35088500	-0.73965100
S	3.71661600	-1.40800500	-2.38458200
Ag	1.82148200	0.78392100	1.55523000
C	-2.27035300	-3.53657000	-1.63417700
C	-3.64716500	-3.27521100	-1.63196800
C	-4.21928400	-2.61201500	-0.53728100
C	-3.42674400	-2.18830900	0.52606000
C	-2.04528400	-2.38177600	0.45319000
C	-1.46087800	-3.12564600	-0.57889300

H	-1.84162400	-4.07607600	-2.47251900
H	-5.28880900	-2.43649100	-0.51101000
H	-3.88010700	-1.70321900	1.37761000
H	-0.39969900	-3.32988900	-0.58056900
I	-0.98795300	-2.71724400	2.69782600
C	-4.44993600	-3.74872800	-2.78972300
O	-3.99645500	-4.35119800	-3.74415600
O	-5.76228200	-3.43373400	-2.67185500
C	-6.58956700	-3.86395700	-3.76380300
H	-6.25682100	-3.41010600	-4.70133400
H	-6.55256700	-4.95157700	-3.87061000
H	-7.59939700	-3.53652300	-3.51582100
C	-3.74464600	3.32129700	-0.57636900
C	-5.25012100	3.19450000	-0.88921700
C	-3.37742600	4.81622200	-0.45661400
H	-3.21982500	2.91710200	-1.45120800
C	-5.62129000	3.97245900	-2.16314700
H	-5.84292200	3.57526000	-0.04517800
H	-5.52324600	2.14148600	-1.01658400
C	-3.71677800	5.58684100	-1.73929500
H	-3.93794200	5.25716500	0.37869300
H	-2.31793300	4.93702300	-0.20431700
C	-5.20825900	5.44895100	-2.07719200
H	-6.69782100	3.88815100	-2.35501000
H	-5.11314600	3.50829600	-3.02035800
H	-3.44494800	6.64394400	-1.63248600
H	-3.11641200	5.18848700	-2.56993100
H	-5.44013900	5.96515400	-3.01654700
H	-5.79875300	5.94329000	-1.29229800
N	-0.90868000	0.64636100	4.03891400
H	-1.68178300	-0.00223000	4.07887800
H	-0.97515500	3.90755700	-1.41971900
H	0.10494300	3.22023400	-3.49772400
O	0.85511200	0.63473400	-4.05065300
C	1.20328200	1.54178300	-5.08266200
H	1.68313100	0.94522200	-5.86029600
H	0.31943000	2.03913500	-5.50524400
H	1.90758600	2.30731100	-4.72905000
int71			
C	0.26710600	3.08392900	2.55782200

C	-0.33927300	1.85662700	2.85405600
C	-0.16956800	0.77098400	1.98371000
C	0.60111200	0.91619200	0.83599800
C	1.25256800	2.12508400	0.53451900
C	1.04264700	3.20253600	1.40388700
Pd	0.57181700	-0.49071200	-0.61520600
H	-0.69759200	-0.14568000	2.21385500
C	1.77252000	0.98207600	-1.66023800
C	3.17545100	0.53067800	-2.08310900
C	3.63213200	2.25297700	-0.64583100
C	2.04667900	2.22409400	-0.73599500
C	3.97139200	0.75335600	-0.78215500
H	5.04036900	0.56742600	-0.92258500
H	3.61959700	0.16186300	0.06122400
C	3.83480900	1.60755800	-2.99820400
H	4.76104900	1.19719100	-3.41361900
H	3.20980200	1.90926900	-3.84079300
C	4.12657700	2.78199200	-2.02018300
H	5.19827300	3.00007200	-1.97980000
H	3.62049800	3.70729600	-2.31125400
H	3.21003200	-0.47345000	-2.50818900
H	1.71600100	3.12931700	-1.25874000
C	0.74876000	1.29931000	-2.71568100
O	-0.29135000	1.98322900	-2.42846800
C	-0.14785000	0.94665400	-4.95610500
H	0.25861600	0.69002600	-5.93506800
H	-0.94381500	0.23826600	-4.69686800
H	-0.55483800	1.95799600	-4.97913500
C	-3.04106000	-2.47748900	1.21169700
C	-2.15417900	-1.58394600	0.32561200
O	-2.77806200	-0.80736400	-0.46779200
O	-0.90693400	-1.67299800	0.48346500
C	-4.73237600	-0.21600500	1.69438800
C	-4.22758900	0.98273400	1.17603100
C	-6.07291700	-0.51287300	1.41523600
C	-4.98977600	1.81270600	0.36452200
C	-6.86372300	0.32235800	0.62718100
C	-6.31423100	1.48342200	0.08724400
F	-6.62911700	-1.63936800	1.87186400
F	-8.13735200	0.00629300	0.36768000
F	-7.05186600	2.27429400	-0.69447400

F	-4.43378200	2.90158400	-0.19498900
F	-2.95595300	1.34539500	1.39057700
C	-4.17594000	-3.09811500	0.39593000
H	-3.74668800	-3.77489500	-0.35155700
H	-4.84695700	-3.66427700	1.04545700
H	-4.74369400	-2.33563200	-0.13736800
C	-2.22450800	-3.54375800	1.94743400
H	-1.43900800	-3.10045400	2.56245700
H	-2.87781200	-4.15659300	2.57461300
H	-1.73705900	-4.18651900	1.20898300
S	-3.69487700	-1.34754000	2.59152100
Ag	-1.79394400	0.77323300	-1.47224300
C	2.87298700	-2.67090900	2.27150200
C	3.77261800	-3.41104200	1.49758500
C	3.76789600	-3.25679700	0.10558900
C	2.88592500	-2.36445600	-0.50455100
C	2.00897100	-1.62266000	0.28777000
C	1.98384800	-1.77683200	1.67356600
H	2.87908100	-2.79974800	3.34906700
H	4.44484400	-3.84263800	-0.50598400
H	2.87881300	-2.28101400	-1.58162500
H	1.29632400	-1.22107000	2.29314600
I	0.04893100	-2.23945100	-2.79470800
C	4.69637500	-4.34300000	2.19972100
O	4.72926600	-4.50502700	3.40476800
O	5.51344200	-5.00312600	1.34533000
C	6.42435000	-5.92309600	1.96620400
H	7.08371400	-5.40068500	2.66485900
H	5.87805600	-6.69562900	2.51429000
H	6.99926500	-6.36418500	1.15175200
C	4.21057800	2.98956700	0.57501200
C	5.65799300	2.58327900	0.92022800
C	4.13756300	4.52446500	0.42861600
H	3.59993700	2.70718000	1.44293400
C	6.15171100	3.29744200	2.18970700
H	6.32438100	2.82741100	0.08025300
H	5.72134100	1.50019600	1.06862400
C	4.59339700	5.23566000	1.71013800
H	4.78980000	4.83633100	-0.39817000
H	3.12672800	4.84192400	0.14886600
C	6.02604800	4.82342400	2.07866400

H	7.18992000	3.01416900	2.40005700
H	5.55374400	2.95002900	3.04420100
H	4.52847600	6.32333900	1.58597400
H	3.91318700	4.96995700	2.53212900
H	6.33454600	5.30080800	3.01635700
H	6.71256800	5.18633600	1.30017500
N	0.92431800	0.87600100	-3.97055200
H	1.64005300	0.17693100	-4.11464000
H	1.49037000	4.16474100	1.17949300
H	0.13908000	3.94507500	3.20229600
O	-1.12719900	1.61669200	3.93990700
C	-1.41508500	2.69641600	4.81417000
H	-2.07589200	2.29316000	5.58304400
H	-0.50654200	3.08871200	5.29078700
H	-1.92660600	3.51546100	4.29076400

int72

C	4.76114600	-1.75435200	-2.05770900
C	3.85551700	-1.35103300	-3.05239600
C	2.51808900	-1.09681700	-2.71457000
C	2.13140800	-1.22216500	-1.38043300
C	3.01870700	-1.59160700	-0.36833600
C	4.33951300	-1.89029000	-0.74129700
Pd	0.20289300	-1.20832100	-0.91733300
H	1.78527500	-0.82670400	-3.46695300
C	0.91451400	-1.67923100	1.01296900
C	0.54643500	-0.76705400	2.17343100
C	2.83013400	-0.58528600	2.10231900
C	2.47629300	-1.70972300	1.02759900
C	1.59718300	0.34655200	2.03431700
H	1.56896600	1.06043900	2.86478000
H	1.51068200	0.89516700	1.10053900
C	1.01727400	-1.46528700	3.49130600
H	0.55404600	-0.96407100	4.34643700
H	0.73843900	-2.52045400	3.54581500
C	2.56311900	-1.26615900	3.47471600
H	2.85826900	-0.60858100	4.29427600
H	3.11707200	-2.20323500	3.59299200
H	-0.49753000	-0.45674100	2.19553200
H	2.80972500	-2.67271900	1.43804400
C	0.19789300	-2.97534300	0.76066500

O	0.39412400	-3.50617300	-0.36650700
N	-0.71814000	-3.46435000	1.61115400
H	-1.00606200	-2.89510800	2.39346900
C	-1.59723600	-4.55410100	1.19044800
H	-2.14026500	-4.27069600	0.28582700
H	-1.00871500	-5.45103700	0.98682800
H	-2.30572300	-4.75415200	1.99405000
C	0.68791800	3.04404900	-1.53378700
C	-0.35303600	3.57183400	-0.76071600
C	-1.17177800	2.70260200	-0.02809300
C	-0.95007200	1.32863200	-0.07090200
C	0.09206400	0.80185700	-0.84634100
C	0.91268400	1.66642200	-1.57736800
H	1.32741400	3.71271700	-2.09945800
H	-1.97868800	3.11909400	0.56575900
H	-1.59486600	0.66865200	0.49174000
H	1.73037600	1.28521400	-2.17466800
C	-0.63490200	5.02994500	-0.67926700
O	-1.52760700	5.52487400	-0.01775300
O	0.21859700	5.76601200	-1.43122300
C	-0.00824300	7.18299200	-1.39376200
H	0.75121300	7.62092200	-2.04186300
H	-1.01076300	7.42299500	-1.75862800
H	0.09070000	7.56314500	-0.37322700
C	4.21439300	0.07988200	1.91821200
C	4.20105100	1.17425000	0.82560700
C	4.81707400	0.67645300	3.20835700
H	4.91432000	-0.70183500	1.59103200
C	5.60614600	1.72579600	0.55412400
H	3.55816900	1.99864600	1.16339000
H	3.75950100	0.79374200	-0.09778000
C	6.21794100	1.26183200	2.96179400
H	4.15141000	1.46301400	3.59297700
H	4.88809200	-0.08697000	3.98991600
C	6.22459900	2.30283300	1.83452100
H	5.56344300	2.49146100	-0.22969000
H	6.24238900	0.91711100	0.16739100
H	6.60698100	1.69866800	3.88948300
H	6.89932300	0.44115400	2.69450100
H	7.24599700	2.65602100	1.64832900
H	5.64044800	3.17953100	2.14927200

C	-3.63183500	-0.77053500	-2.34477600
C	-2.21470800	-1.14526900	-1.88091700
O	-1.97815200	-1.41079200	-0.65970900
O	-1.27641900	-1.07134800	-2.72681100
C	-4.37486400	-0.41436000	0.43968400
C	-3.76568700	-1.21572600	1.41540000
C	-4.44121600	0.95866400	0.70109300
C	-3.17875000	-0.66973400	2.54825200
C	-3.87752700	1.52109500	1.84754700
C	-3.22146300	0.70561600	2.76437600
F	-5.01298600	1.79455300	-0.17105500
F	-3.91079400	2.84624300	2.03823700
F	-2.62193500	1.23249900	3.83420000
F	-2.50598800	-1.46069600	3.41333700
F	-3.68344000	-2.53904600	1.26695100
C	-3.60802800	0.72682100	-2.70521700
H	-2.88212700	0.88447000	-3.50788800
H	-4.59711700	1.05117300	-3.03687300
H	-3.30688600	1.34032100	-1.85467600
C	-4.02597500	-1.61793200	-3.56615700
H	-4.05202300	-2.68408300	-3.32384400
H	-5.00655300	-1.31683000	-3.94724500
H	-3.28007400	-1.46030000	-4.34883000
S	-4.97100200	-1.14645700	-1.07116600
H	5.04724200	-2.23562000	0.00706000
H	5.78319200	-1.97170300	-2.34892500
O	4.36445900	-1.25076700	-4.31326200
C	3.48215900	-0.88486900	-5.36425800
H	4.08571300	-0.86879300	-6.27312000
H	2.66869600	-1.61275300	-5.48229900
H	3.04895000	0.11128800	-5.20110500

TS42

C	4.88591900	-0.30240200	-2.32039700
C	4.22934800	0.82358800	-2.84479700
C	2.90940900	1.08154800	-2.47691900
C	2.23485100	0.22209300	-1.58734900
C	2.86667500	-0.95557300	-1.10906400
C	4.19625100	-1.18363700	-1.50371400
Pd	0.16451900	0.08282600	-1.40397000
H	2.40870800	1.97029100	-2.83438700

C	0.56720400	-1.86144100	-0.83118400
C	-0.16920000	-2.26238600	0.44957000
C	2.04307000	-2.56546900	0.98847000
C	2.05264100	-2.09022100	-0.52176600
C	0.80632800	-1.81966900	1.55869500
H	0.50471600	-2.19129800	2.54428100
H	0.90674800	-0.73904600	1.61745800
C	-0.04928100	-3.80784400	0.54530000
H	-0.71298400	-4.16032400	1.33955500
H	-0.34683900	-4.31415700	-0.37552600
C	1.44880200	-4.01414600	0.91296000
H	1.52077100	-4.50747400	1.88253600
H	1.98632200	-4.63650400	0.19071800
H	-1.18829600	-1.89484600	0.51718100
H	2.36598400	-2.95041100	-1.12230900
C	0.12773300	-2.51471700	-2.15935600
O	0.94732200	-3.00684700	-2.93465600
N	-1.20981300	-2.55187500	-2.39388300
H	-1.83357400	-2.01520800	-1.80294000
C	-1.73105700	-3.10362200	-3.63210000
H	-1.51118600	-2.45210400	-4.48684900
H	-1.27300500	-4.07608200	-3.82668800
H	-2.81229600	-3.21822600	-3.53552700
C	1.76767500	2.69918400	1.67543400
C	1.30117700	3.90128900	1.13157900
C	0.83092500	3.91457400	-0.18902700
C	0.82041500	2.75281800	-0.95257500
C	1.25038400	1.53699400	-0.38261100
C	1.75018400	1.52800000	0.92025000
H	2.15566100	2.67907000	2.68766900
H	0.47650200	4.85066100	-0.60798600
H	0.44316000	2.79274600	-1.96835700
H	2.15253000	0.62486500	1.34034700
C	1.29329400	5.18003600	1.88978900
O	0.90677300	6.24377400	1.44355900
O	1.76756100	5.03676100	3.14975600
C	1.78193600	6.24004100	3.93376900
H	2.18602900	5.95444300	4.90508000
H	2.41166900	6.99966600	3.46259500
H	0.77081000	6.64233800	4.04035400
C	3.40844200	-2.48785300	1.71394300

C	3.86030600	-1.04694200	2.02547900
C	3.48735800	-3.31812800	3.01625600
H	4.14913300	-2.92006300	1.02127000
C	5.26067300	-0.98413500	2.65094600
H	3.14257600	-0.60326600	2.73076000
H	3.84507700	-0.44095300	1.11825200
C	4.87957100	-3.25445100	3.66588300
H	2.73276900	-2.94649100	3.72476800
H	3.24761400	-4.36695700	2.82363500
C	5.32959100	-1.81463900	3.93719400
H	5.53277100	0.05962300	2.84811200
H	5.99450500	-1.36756700	1.92779800
H	4.88143500	-3.83985500	4.59314100
H	5.60482000	-3.73450200	2.99301200
H	6.34323200	-1.80087000	4.35507300
H	4.66996300	-1.36432300	4.69287800
C	-3.81863700	1.28905700	-1.93973100
C	-2.34134900	0.86056900	-1.91167100
O	-1.97482800	-0.11004400	-1.15201400
O	-1.51725500	1.52910500	-2.57439700
C	-4.58457900	-0.42398000	0.27251100
C	-3.85961000	-1.57230400	0.61521200
C	-5.01081200	0.39225800	1.32865900
C	-3.52436200	-1.86721200	1.93221000
C	-4.68155900	0.11735900	2.65504400
C	-3.92964000	-1.01497900	2.95668300
F	-5.74499300	1.48615200	1.09364700
F	-5.08924900	0.92819900	3.63792800
F	-3.60458900	-1.28829300	4.22204700
F	-2.79477900	-2.95543100	2.22202300
F	-3.44790600	-2.43465700	-0.32471000
C	-3.93916100	2.53796500	-1.04921800
H	-3.28575800	3.31757200	-1.45247600
H	-4.96936400	2.89876700	-1.03041100
H	-3.62470400	2.32956500	-0.02423900
C	-4.24484300	1.61278400	-3.38227000
H	-4.19237800	0.72970700	-4.02633000
H	-5.26541500	2.00537200	-3.40286700
H	-3.56286700	2.36463500	-3.78416900
S	-4.99795200	-0.07756100	-1.42306300
H	4.68623400	-2.09880800	-1.18298200

H	5.91864900	-0.47895300	-2.60177300
O	4.96830900	1.60415400	-3.68082900
C	4.35007000	2.74895100	-4.25192100
H	5.10307400	3.20947000	-4.89298700
H	3.47634400	2.47575400	-4.85816200
H	4.04260700	3.46874200	-3.48145700

int73

C	1.68337200	-4.52903200	-1.12129700
C	2.42551900	-3.90594200	-2.12580300
C	2.61925200	-2.51412900	-2.07165000
C	2.11585900	-1.72026000	-1.03355600
C	1.41642500	-2.35376600	0.06346100
C	1.20194800	-3.76649200	-0.06285300
Pd	-0.63462800	-2.04208100	-0.69090500
H	3.13844400	-2.00722900	-2.87501800
H	1.50821600	-5.59787300	-1.16995800
C	-0.57485700	-1.69896700	1.32017400
C	-0.90094600	-0.26732600	1.74593200
C	1.35149900	-0.48986200	2.12493800
C	0.94448200	-1.84283600	1.48179600
C	0.39464000	0.50285800	1.42419300
H	0.41783800	1.48556000	1.89615500
H	0.57929200	0.63300500	0.36457000
C	-0.82152400	-0.27385200	3.29924400
H	-1.14724500	0.70496100	3.66675900
H	-1.46351900	-1.02873600	3.75834300
C	0.69514000	-0.51350500	3.55261300
H	1.12225100	0.28547900	4.16476500
H	0.88179100	-1.45740100	4.07214800
H	-1.83691600	0.11521000	1.34234200
H	1.17418400	-2.66243200	2.16419100
C	-1.41843600	-2.84353900	1.87464500
O	-0.88691300	-3.83941100	2.38447900
C	-3.65772100	-3.71068800	2.24811100
H	-4.67508600	-3.31527800	2.24625200
H	-3.61439600	-4.59386800	1.59793900
H	-3.39111800	-4.02970100	3.25903700
C	-4.24022800	0.04557600	-2.18200300
C	-3.37145300	-0.64981200	-1.10412100
O	-2.25080600	-1.09735900	-1.54896900

O	-3.80041100	-0.75016100	0.05529000
C	-3.51511900	2.19604200	-0.36364300
C	-3.89469200	2.20628700	0.98692500
C	-2.19936200	2.57140200	-0.66583300
C	-3.01256500	2.60580200	1.98839500
C	-1.31212800	2.99059600	0.32041600
C	-1.72724200	3.01230900	1.64871000
F	-1.75051900	2.52366600	-1.93070300
F	-0.05226300	3.33232800	0.01779600
F	-0.86285800	3.35823800	2.61124700
F	-3.37488700	2.57158000	3.27716400
F	-5.11741200	1.83216800	1.35734900
C	-3.54016400	0.14823000	-3.53981800
H	-3.30350300	-0.85302800	-3.91215200
H	-4.19243400	0.64744700	-4.26276400
H	-2.61195300	0.71419900	-3.45736700
C	-5.56952500	-0.72141000	-2.28823200
H	-5.37869800	-1.72151800	-2.69470600
H	-6.03110800	-0.81902700	-1.30466300
H	-6.26336000	-0.21137800	-2.96450400
S	-4.70856800	1.79156000	-1.61224800
C	3.84752100	1.64933900	-1.38186000
C	2.80059500	2.46455400	-1.83033500
C	1.53459000	1.90694100	-2.04354600
C	1.31029200	0.56092900	-1.77561100
C	2.33710200	-0.25269000	-1.26642300
C	3.61715200	0.30110500	-1.11865800
H	4.83323700	2.07442700	-1.23342200
H	0.72882400	2.54276700	-2.38905400
H	0.32060000	0.14294300	-1.93674200
H	4.43310300	-0.32565600	-0.77238600
C	2.97292000	3.92224300	-2.08685700
O	2.09492400	4.65750500	-2.49302400
O	4.22691200	4.34920900	-1.80941800
C	4.45171500	5.75189500	-2.02374400
H	5.49253400	5.92870100	-1.75236800
H	4.27586500	6.01474700	-3.07044200
H	3.78303000	6.34816000	-1.39706100
H	0.69435100	-4.26908600	0.75605800
O	2.89438400	-4.70321400	-3.11288800
C	3.66311700	-4.12415700	-4.16403600

H	4.56893000	-3.63978700	-3.77910000
H	3.94510300	-4.95171100	-4.81559300
H	3.07579500	-3.39597000	-4.73686900
C	2.86198500	-0.20528900	2.13729600
C	3.19779500	1.28739700	2.31685400
C	3.62250800	-1.06325900	3.16999100
H	3.25370800	-0.49474400	1.15913600
C	4.71360400	1.53791800	2.28384400
H	2.79008500	1.64644900	3.27242700
H	2.71552700	1.87353300	1.52695800
C	5.13696000	-0.81792100	3.09829600
H	3.27529700	-0.81970200	4.18232400
H	3.40222300	-2.12624600	3.01138300
C	5.46295200	0.66820800	3.30235000
H	4.92243600	2.60043500	2.45642400
H	5.08573700	1.30750600	1.27601400
H	5.65526600	-1.43141000	3.84477500
H	5.51092900	-1.13857600	2.11468300
H	6.54383800	0.83822600	3.22796000
H	5.16739000	0.96392800	4.31924300
N	-2.75314400	-2.66891000	1.79695900
H	-3.12563600	-1.90796000	1.21390900

TS43

C	4.26810100	-2.85288800	-1.23585900
C	4.89205200	-1.73264400	-1.81522400
C	4.19034200	-0.52363600	-1.92932200
C	2.88857800	-0.41388800	-1.42858700
C	2.27962400	-1.51355700	-0.74847000
C	2.99640000	-2.73482200	-0.70351000
Pd	0.19442300	-1.46061200	-0.89881100
H	4.61493100	0.32267300	-2.45647800
H	4.81713600	-3.78756300	-1.19326000
C	0.20966500	-1.66472700	1.13912400
C	-0.46381500	-0.45963000	1.78994800
C	1.77984000	-0.04062100	1.90307700
C	1.62997700	-1.38851200	1.20021000
C	0.49708700	0.69612400	1.44001900
H	0.28363200	1.59304800	2.02760600
H	0.50234400	0.96236400	0.38347600
C	-0.18754400	-0.60549900	3.31109100

H	-0.72209700	0.17931500	3.85498700
H	-0.52068400	-1.56933000	3.70344700
C	1.35505400	-0.41077700	3.38441000
H	1.62612100	0.41711800	4.04487000
H	1.87629800	-1.30015600	3.74858600
H	-1.50075600	-0.32942300	1.50876800
H	2.27739400	-2.19950400	1.50223600
C	-0.24690700	-3.08972100	1.35491500
O	0.56472400	-4.01682400	1.41143400
C	-2.21477800	-4.55186800	1.42623400
H	-3.12965000	-4.55676800	2.02458700
H	-2.45151500	-4.79733200	0.38549000
H	-1.51473800	-5.28663100	1.82385800
C	-4.00547800	-1.54567900	-2.02387500
C	-2.63481500	-2.03059500	-1.49090200
O	-1.86247100	-1.07152900	-1.08618900
O	-2.34298900	-3.22729900	-1.53824700
C	-4.01133000	0.31979000	0.36237800
C	-4.07425700	0.09148400	1.74687000
C	-3.22756200	1.40448000	-0.06028700
C	-3.40650800	0.90047600	2.66575400
C	-2.52660200	2.19765000	0.84185300
C	-2.62130500	1.95156100	2.20848200
F	-3.12220400	1.71298800	-1.35427100
F	-1.73085200	3.19106400	0.41106600
F	-1.88928100	2.66925800	3.07142500
F	-3.44349200	0.61941400	3.97555600
F	-4.77044700	-0.94238400	2.23776500
C	-3.77698800	-0.63488400	-3.23892000
H	-3.27969900	-1.21429900	-4.02674000
H	-4.72972500	-0.26839700	-3.63134000
H	-3.15046500	0.21478500	-2.98105800
C	-4.89450900	-2.73825600	-2.40059200
H	-4.41193700	-3.28774500	-3.21260200
H	-5.01578300	-3.42392000	-1.56082200
H	-5.87932300	-2.40324700	-2.74342300
S	-5.04195600	-0.67201300	-0.69455800
C	1.55382300	3.15004700	-1.45092700
C	0.29553900	2.95135700	-2.03719400
C	-0.03877900	1.69420800	-2.54972100
C	0.84960900	0.63171200	-2.40602100

C	2.08055900	0.79680400	-1.73468000
C	2.44374800	2.08583800	-1.32095800
H	1.81710600	4.13119800	-1.07302000
H	-1.00293900	1.55600400	-3.02359900
H	0.62144500	-0.32273100	-2.88955600
H	3.39972900	2.24078400	-0.83246300
C	-0.73487900	4.02557700	-2.11781900
O	-1.77188900	3.93492500	-2.74254800
O	-0.39668400	5.11110000	-1.38755200
C	-1.40893100	6.12788600	-1.31562300
H	-0.97724000	6.93309200	-0.72112700
H	-1.67636300	6.48302500	-2.31402600
H	-2.30322100	5.72786000	-0.82989700
H	2.53977500	-3.58138900	-0.19583200
O	6.15793300	-1.92808400	-2.25703800
C	6.86565500	-0.82552700	-2.81305000
H	6.94480800	0.00220600	-2.09666200
H	7.86340900	-1.19806800	-3.04745100
H	6.38946700	-0.46387800	-3.73314000
C	3.14588400	0.63919300	1.76655100
C	3.17512000	2.08373100	2.29946900
C	4.29099400	-0.19101400	2.38139600
H	3.35590700	0.69398400	0.69569600
C	4.54530900	2.73974300	2.06470300
H	2.95502400	2.09122000	3.37582600
H	2.39257100	2.67658300	1.81294500
C	5.65456900	0.46559400	2.12266300
H	4.13617800	-0.28922800	3.46438000
H	4.28758500	-1.20513100	1.96583500
C	5.68789500	1.90371100	2.65860500
H	4.55311400	3.75332500	2.48236600
H	4.71174800	2.84903800	0.98283100
H	6.45453000	-0.13184600	2.57515400
H	5.84365500	0.47576800	1.03903400
H	6.65534400	2.37273200	2.44317900
H	5.58620600	1.88089900	3.75300000
N	-1.59172700	-3.23688600	1.49975100
H	-2.15450900	-2.46255200	1.17432300

int74

C	1.23504000	-5.05476000	-0.85286300

C	2.36759700	-4.68951500	-1.59280400
C	2.64384100	-3.33835000	-1.80502800
C	1.78798100	-2.33097600	-1.30922800
C	0.63426600	-2.71662600	-0.60630800
C	0.38509900	-4.07255400	-0.35523700
Pd	-0.81057200	-1.43815200	-0.09940700
H	3.51640800	-3.03154700	-2.36921000
H	1.04306600	-6.10754900	-0.67309700
C	-1.18799500	-1.64472900	2.02479700
C	-1.62828000	-0.32449600	2.65351800
C	0.65583200	-0.27207100	2.55962300
C	0.20241300	-1.59817900	1.94770600
C	-0.52906000	0.64151000	2.18375600
H	-0.53958100	1.57450200	2.74962700
H	-0.56403400	0.86542600	1.11404300
C	-1.21658200	-0.49337400	4.15430900
H	-1.59040400	0.36092700	4.72636700
H	-1.63130700	-1.40121600	4.60076600
C	0.34230900	-0.50089300	4.08970800
H	0.76998500	0.31349000	4.68072700
H	0.77252400	-1.43561300	4.45784700
H	-2.66156600	-0.02338100	2.48530400
H	0.82401400	-2.48420700	1.93267000
C	-2.01543200	-2.90185400	2.06705400
O	-1.53385500	-3.99505600	2.35878400
C	-4.24384900	-3.82921400	1.64046800
H	-5.26513700	-3.50159600	1.84902900
H	-4.20571700	-4.26598100	0.63406500
H	-3.95391200	-4.59865300	2.35689000
C	-3.67084200	0.15159400	-2.55173400
C	-2.65064200	-0.45086900	-1.58532300
O	-2.79094400	-0.35406300	-0.32578000
O	-1.66595100	-1.09077600	-2.07830800
C	-3.02887200	2.45629000	-0.88069000
C	-3.26036500	2.53496800	0.50017500
C	-1.79858300	2.93263900	-1.35022500
C	-2.32960100	3.10026900	1.36350900
C	-0.84667500	3.48754200	-0.49643100
C	-1.12192700	3.57684000	0.86406100
F	-1.48514100	2.84418300	-2.65199900
F	0.32410000	3.92449400	-0.96748200

F	-0.19796500	4.05381300	1.70609900
F	-2.54328500	3.10149200	2.68746500
F	-4.37319400	2.03366300	1.04131700
C	-3.08809200	0.29726700	-3.96250300
H	-2.77309600	-0.68047700	-4.33635600
H	-3.84409200	0.71064200	-4.63560800
H	-2.22393000	0.96190300	-3.96077800
C	-4.90690800	-0.77272100	-2.55342900
H	-4.62584900	-1.74935900	-2.96187600
H	-5.29766700	-0.90459300	-1.54226700
H	-5.69726900	-0.35617800	-3.18576200
S	-4.30189500	1.82554900	-1.94519300
C	3.91624100	0.79491700	-1.27198400
C	3.02283600	1.77236300	-1.73031800
C	1.73158300	1.39322800	-2.12124000
C	1.32447600	0.06687700	-2.00990900
C	2.19809600	-0.91455900	-1.50637400
C	3.50772900	-0.53074100	-1.17134600
H	4.91928600	1.08202300	-0.97843600
H	1.05598600	2.14890900	-2.50508000
H	0.33350300	-0.21624000	-2.34333900
H	4.19468500	-1.27817800	-0.78698800
C	3.39948000	3.20831400	-1.81667900
O	2.75680300	4.06546400	-2.38954300
O	4.55563600	3.47157600	-1.15626500
C	4.96880300	4.84619100	-1.18023900
H	5.89183100	4.88685900	-0.60165200
H	5.14217000	5.17997300	-2.20703900
H	4.20370200	5.48481000	-0.73047900
H	-0.46062600	-4.37230300	0.25599500
O	3.13824000	-5.72093600	-2.04889900
C	4.31015100	-5.40801900	-2.78414300
H	5.02009000	-4.81926500	-2.18710000
H	4.76832500	-6.36367700	-3.04430700
H	4.07786600	-4.85721600	-3.70570200
C	2.06146700	0.22332200	2.19375600
C	2.30624700	1.68278300	2.63366200
C	3.16530100	-0.70133200	2.74622300
H	2.12413000	0.20203000	1.09777500
C	3.71864800	2.16959400	2.27640200
H	2.16849000	1.76607400	3.72130200

H	1.56663900	2.34559100	2.17358400
C	4.57604600	-0.20489300	2.39619700
H	3.07191400	-0.75696600	3.83977200
H	3.02568300	-1.72111100	2.36692600
C	4.79494200	1.24264400	2.85685800
H	3.85903900	3.19360100	2.64349200
H	3.82485700	2.21419000	1.18555600
H	5.32604600	-0.86859900	2.84309700
H	4.71417700	-0.25661700	1.31008000
H	5.79447400	1.58775500	2.56577700
H	4.75511500	1.28328100	3.95526200
N	-3.33377400	-2.70382000	1.77604800
H	-3.57317900	-1.83754900	1.30759700

int75

C	-0.48101800	3.42185500	-0.08243600
C	-1.11433900	3.46522300	-1.33030200
C	-1.10272800	2.32296000	-2.13707700
C	-0.50490100	1.13656300	-1.70995500
C	0.10034700	1.09487300	-0.44280400
C	0.15279200	2.24249200	0.34641000
Pd	0.46861000	-0.71167900	0.37273900
H	-0.51402300	0.25798900	-2.34960000
H	-1.61032600	4.36404100	-1.67546700
H	-1.58058600	2.35940100	-3.11297400
C	1.78978900	-1.83961100	-1.05921000
C	2.89214600	-2.63922400	-0.37676600
C	3.58955400	-0.46071600	-0.41025000
C	2.23538000	-0.52999400	-1.10072300
C	3.46114600	-1.61376600	0.62020400
H	4.42713500	-1.92386500	1.02988800
H	2.77824500	-1.38516100	1.44329000
C	4.04112300	-2.64710700	-1.44552600
H	4.83962000	-3.31797200	-1.11481800
H	3.69567700	-2.99906500	-2.42137200
C	4.52155700	-1.15932300	-1.47063300
H	5.56712600	-1.07552100	-1.16112200
H	4.43321900	-0.70169200	-2.45957900
H	2.60691500	-3.61376400	0.01316000
H	1.92582700	0.17428100	-1.85885400
C	0.73427800	-2.40077900	-1.98002200

O	0.42706700	-1.82977200	-3.02963900
N	0.17461200	-3.56031600	-1.55374600
H	0.26436100	-3.76998200	-0.56186400
C	-0.96756300	-4.11845200	-2.26170100
H	-0.71869500	-4.25070600	-3.31690800
H	-1.21447300	-5.08321500	-1.81665900
H	-1.84043700	-3.45906100	-2.19578000
C	3.97411500	0.92352700	0.12507200
C	5.32303700	0.94332400	0.86860900
C	3.94715400	2.02362000	-0.95470700
H	3.19472400	1.17987200	0.86043600
C	5.60912600	2.32584100	1.47576600
H	6.13061800	0.68739500	0.16865500
H	5.33445800	0.18036900	1.65550000
C	4.23405000	3.40777900	-0.35391500
H	4.69875700	1.79400900	-1.72377600
H	2.97295100	2.04468800	-1.45345700
C	5.56704000	3.42727200	0.40684100
H	6.58108000	2.32068400	1.98336000
H	4.85391900	2.54126100	2.24525100
H	4.23224300	4.16799000	-1.14385700
H	3.41690300	3.66916100	0.33351500
H	5.73284800	4.40974500	0.86476400
H	6.39014800	3.26909400	-0.30501300
C	-1.56084600	-2.03501800	2.58242000
C	-0.80364600	-3.05105000	1.66871900
O	0.36744100	-2.67688400	1.24511900
O	-1.30668700	-4.15161900	1.47800100
C	-2.61609700	0.11947700	0.79530500
C	-2.98684200	-0.70754100	-0.26861000
C	-3.13621200	1.41709300	0.82088900
C	-3.85446500	-0.27759600	-1.26335100
C	-3.98139200	1.87671300	-0.18483900
C	-4.35001500	1.02579900	-1.22267100
F	-2.78243500	2.27776300	1.78153500
F	-4.41635300	3.14177400	-0.16564600
F	-5.15624400	1.46261900	-2.19035500
F	-4.17711800	-1.08733500	-2.27493000
F	-2.45357900	-1.93372600	-0.37831300
C	-3.04127900	-2.36098200	2.72933900
H	-3.11945900	-3.35758900	3.16947900

H	-3.54602600	-1.63833400	3.37755400
H	-3.54271000	-2.39840100	1.76237200
C	-0.84003800	-2.01851400	3.94285600
H	0.20782200	-1.72545100	3.83320500
H	-1.33459000	-1.34644800	4.65023500
H	-0.86199400	-3.03462200	4.34962200
S	-1.29850500	-0.26999400	1.93594900
H	0.60127000	2.24365200	1.33481500
O	-0.45613900	4.45967000	0.80382000
C	-1.40537900	5.50163000	0.61656600
H	-1.34621800	6.12964700	1.50718500
H	-1.17524900	6.11345500	-0.26569600
H	-2.42047200	5.09423500	0.51955300

TS44

C	-0.35802200	3.03744200	-0.09483200
C	0.30582600	3.25880400	1.11927900
C	0.47243700	2.19539300	2.01389000
C	-0.00870000	0.92415200	1.71753200
C	-0.67571400	0.69987900	0.49301700
C	-0.87272300	1.76566500	-0.39148000
Pd	-0.12179500	-1.10872600	-0.41327900
H	0.10295500	0.10920400	2.42736300
H	0.70502500	4.23498100	1.36570900
H	0.98593900	2.37083800	2.95534700
C	-1.57711900	-2.00962700	0.74238400
C	-2.57454100	-2.78700900	-0.12183600
C	-3.45962300	-0.68449500	0.11689800
C	-2.15599500	-0.70063900	0.91834400
C	-3.13884200	-1.67474100	-1.03019900
H	-4.03162600	-1.99456500	-1.57597000
H	-2.40854400	-1.27600500	-1.74310400
C	-3.79433600	-3.03895000	0.81315000
H	-4.52143500	-3.68586600	0.31199700
H	-3.50463700	-3.52567900	1.74807800
C	-4.36762700	-1.60508800	1.02607100
H	-5.40328500	-1.53936800	0.68517800
H	-4.34919400	-1.29165400	2.07337300
H	-2.17159700	-3.67430800	-0.60978300
H	-2.16593400	-0.28458800	1.91621800
C	-0.83180200	-2.63621000	1.89887500

O	-0.84173400	-2.12201300	3.02226900
N	-0.17135100	-3.78535700	1.59490100
H	0.07399900	-3.90785300	0.61171000
C	0.71989800	-4.38833900	2.57407300
H	0.23568700	-4.38300600	3.55182100
H	0.93640300	-5.41622900	2.27607400
H	1.66491300	-3.83581100	2.65643700
C	-4.03187900	0.68763900	-0.26033700
C	-5.39231700	0.62381800	-0.98249500
C	-4.11578900	1.66061800	0.93277200
H	-3.32749100	1.12402500	-0.97885000
C	-5.83546900	2.02001400	-1.44828100
H	-6.15589800	0.22050700	-0.30412800
H	-5.33849900	-0.05782400	-1.83911000
C	-4.56493500	3.05858000	0.48223400
H	-4.82632100	1.26439700	1.67236500
H	-3.14396800	1.73701500	1.43021900
C	-5.90066900	3.00629700	-0.27250400
H	-6.80834200	1.95807100	-1.95013100
H	-5.11994200	2.39405700	-2.19433500
H	-4.64135300	3.72604700	1.34873800
H	-3.79045800	3.48294600	-0.17266800
H	-6.17961000	4.00545900	-0.62774400
H	-6.69245500	2.68609400	0.42000400
C	2.41590500	-1.82175800	-2.33907300
C	1.88778500	-3.01345100	-1.47166200
O	0.65744100	-2.94813200	-1.04674400
O	2.62321100	-3.98263600	-1.34929800
C	2.64674200	0.60346200	-0.61610400
C	3.11917000	-0.04226100	0.53169000
C	2.84992000	1.98428700	-0.70502700
C	3.78915000	0.64521600	1.53710800
C	3.49230700	2.69390100	0.30394400
C	3.97170400	2.02322200	1.42449400
F	2.36468700	2.68097400	-1.74211400
F	3.60446600	4.02651200	0.21637100
F	4.57691300	2.69926400	2.40256700
F	4.22201700	0.00232200	2.62457400
F	2.90262600	-1.35395300	0.70210400
C	3.93778800	-1.73094200	-2.32177400
H	4.33336500	-2.67652900	-2.69785500

H	4.29299500	-0.90985200	-2.95166200
H	4.32030800	-1.60423200	-1.30835300
C	1.88212300	-2.05060700	-3.76706200
H	0.78818400	-2.04540300	-3.79124700
H	2.26124800	-1.29472000	-4.46100800
H	2.21986800	-3.03737300	-4.09817600
S	1.62039400	-0.17090700	-1.85034100
H	-1.34756200	1.62654600	-1.35497700
O	-0.53876200	3.98439200	-1.05777600
C	0.22941000	5.17973500	-0.96333400
H	0.05467300	5.72314400	-1.89303800
H	-0.09194400	5.80395900	-0.11936400
H	1.29825400	4.95400800	-0.86477800

int76

C	0.53914800	2.44160000	1.01621400
C	-0.13612400	3.10280100	-0.00147300
C	-0.04330200	2.60769100	-1.31731200
C	0.70103500	1.48339100	-1.62160500
C	1.42175100	0.80732700	-0.60144000
C	1.30784600	1.27781300	0.72744100
Pd	-0.03923600	-0.64304400	0.67230200
H	0.73157300	1.08122200	-2.62749200
H	-0.74180900	3.97648500	0.20081900
H	-0.58137600	3.12506200	-2.10680600
C	1.32045900	-1.60881800	-0.55882800
C	2.23718300	-2.57060500	0.19931800
C	3.58946500	-0.77494500	-0.27550200
C	2.22763200	-0.43731000	-0.97278000
C	3.15248100	-1.59992200	0.96960100
H	3.99620400	-2.11484700	1.43991800
H	2.63225800	-1.02751800	1.74136600
C	3.24028000	-3.14668900	-0.84160800
H	3.79974000	-3.97685600	-0.39825800
H	2.73430200	-3.53206600	-1.73047700
C	4.17274700	-1.93128200	-1.14802800
H	5.20276400	-2.14691900	-0.85061500
H	4.18860500	-1.67437000	-2.21077000
H	1.71198900	-3.32263800	0.78955600
H	2.35410800	-0.42067200	-2.05666800
C	0.43446900	-2.12128300	-1.68121000

O	0.37132000	-1.53629700	-2.76928900
N	-0.26229000	-3.26200300	-1.42390200
H	-0.42815700	-3.46830500	-0.44144800
C	-1.26479900	-3.71210700	-2.37848700
H	-0.80253900	-3.86441300	-3.35626700
H	-1.68662400	-4.65466900	-2.02480700
H	-2.07046900	-2.97740800	-2.49634200
C	4.52014600	0.42709200	-0.04488200
C	5.77512600	0.08702300	0.78357500
C	4.92407900	1.12280400	-1.36129900
H	3.95617800	1.16819300	0.53942100
C	6.63893800	1.33179400	1.03925900
H	6.37773900	-0.66091800	0.25072300
H	5.48794300	-0.36465800	1.73967500
C	5.79017800	2.36628100	-1.10731400
H	5.48565300	0.41463700	-1.98583300
H	4.02819000	1.40056800	-1.92922700
C	7.03278000	2.02163400	-0.27399600
H	7.53336600	1.05833300	1.61174200
H	6.07279400	2.03980300	1.66170300
H	6.08188400	2.82366400	-2.06028300
H	5.19230800	3.11637700	-0.56960800
H	7.62082000	2.92483000	-0.07142300
H	7.67975900	1.34821100	-0.85435700
C	-2.73379300	-1.37820400	2.37848100
C	-2.05975600	-2.59707000	1.67007200
O	-0.83927500	-2.46533100	1.22969800
O	-2.68029400	-3.65050700	1.66375400
C	-2.90850000	0.70521300	0.27523400
C	-3.11839000	-0.17490600	-0.79362900
C	-3.24299600	2.04730600	0.06421100
C	-3.60118300	0.25765900	-2.02344300
C	-3.71488600	2.50469600	-1.16243800
C	-3.89604800	1.60710400	-2.21195400
F	-3.07957500	2.95312600	1.04335600
F	-3.98615700	3.80302500	-1.33574800
F	-4.34894400	2.03729200	-3.38965400
F	-3.77177700	-0.61334100	-3.02002700
F	-2.84370700	-1.47890700	-0.66543300
C	-4.25451100	-1.42685300	2.25741700
H	-4.59357200	-2.38325400	2.65990200

H	-4.71970600	-0.60791600	2.81383000
H	-4.57533800	-1.38145300	1.21499000
C	-2.28333200	-1.43008100	3.85286900
H	-1.19682800	-1.33284700	3.94275300
H	-2.76529100	-0.64696500	4.44560500
H	-2.56949200	-2.40609000	4.25513800
S	-2.06904000	0.28821300	1.79766800
H	1.94829000	0.91019400	1.51997600
O	0.53903200	2.79907800	2.32465500
C	-0.24711300	3.92296700	2.71593600
H	-0.11865100	4.01527200	3.79464800
H	0.10293900	4.84154300	2.22812300
H	-1.30493300	3.76400200	2.48211700

int77

C	-2.57290800	1.51388000	2.94757200
C	-1.46095700	0.78539300	3.40791300
C	-0.77871300	-0.01929600	2.50471000
C	-1.13950200	-0.04348600	1.14748200
C	-2.20671100	0.75867900	0.66091800
C	-2.94809400	1.47362600	1.59443600
Pd	0.18799000	-0.53354200	-0.57444900
H	-0.96318500	-1.06995400	0.69736100
H	-1.17127000	0.79801900	4.45112600
H	0.00103200	-0.69560900	2.83883800
C	-1.55241000	-0.10878000	-1.66705000
C	-1.17692700	0.73285800	-2.89745600
C	-2.28383900	2.24146300	-1.57919400
C	-2.48181100	0.82619900	-0.82568100
C	-0.89778700	2.08991000	-2.24514500
H	-0.70406200	2.88645500	-2.97254400
H	-0.06730100	2.05616500	-1.53949000
C	-2.48044500	1.01734500	-3.69505500
H	-2.23564700	1.39841000	-4.69155800
H	-3.08483000	0.11622700	-3.83623800
C	-3.19455200	2.10435000	-2.83534600
H	-3.22629800	3.04603100	-3.38647400
H	-4.22583100	1.84409500	-2.57568500
H	-0.36630800	0.31470000	-3.49293000
H	-3.52800400	0.52979500	-0.96651700
C	-2.08192200	-1.47905500	-1.93389500

O	-3.09328400	-1.94000200	-1.31728000
N	-1.44689100	-2.21995200	-2.85977100
H	-0.52610500	-1.88640600	-3.14237400
C	-1.73656800	-3.63392100	-3.03362300
H	-1.23162800	-3.98873500	-3.93331400
H	-1.38730300	-4.22103700	-2.17188700
H	-2.81261200	-3.78313000	-3.13480800
C	-2.47262600	3.51977300	-0.73058800
C	-1.23886400	3.82649700	0.15128300
C	-2.81784700	4.79376000	-1.53373900
H	-3.32963900	3.36048000	-0.06583700
C	-1.51103000	4.98081200	1.12401100
H	-0.40552500	4.10992400	-0.50585400
H	-0.91115500	2.93859100	0.69714600
C	-3.06985500	5.98905300	-0.59657500
H	-1.99661900	5.02926500	-2.22555200
H	-3.71175800	4.63624200	-2.14484000
C	-1.89439400	6.25244500	0.35448600
H	-0.62841900	5.16461300	1.74882900
H	-2.32541300	4.69546900	1.80540900
H	-3.28954200	6.88575300	-1.18845700
H	-3.97054700	5.78112700	-0.00101200
H	-2.14148300	7.06663300	1.04640200
H	-1.02593700	6.58868500	-0.22978400
C	2.82205400	-2.27985600	-0.92961900
C	2.25380600	-1.79590700	-2.29767800
O	1.15467700	-1.08572900	-2.31456700
O	2.82336700	-2.18316700	-3.30800700
C	3.45217000	0.20284200	0.41460400
C	4.60307700	0.13927300	1.21427200
C	3.28255100	1.35235200	-0.36634300
C	5.53736800	1.17053200	1.24627100
C	4.20221700	2.39827200	-0.34362100
C	5.33316400	2.30598200	0.46436400
F	2.22235600	1.49488400	-1.17155600
F	4.00604600	3.48569000	-1.09437900
F	6.21934600	3.30068800	0.48834800
F	6.62487300	1.07785300	2.01665100
F	4.84130600	-0.93901000	1.96978000
C	2.16750600	-3.63826900	-0.60901000
H	2.36062800	-4.30588800	-1.45420500

H	2.59918400	-4.07285800	0.29641200
H	1.08963400	-3.54947200	-0.45371600
C	4.34415300	-2.39525200	-0.98062800
H	4.81092500	-1.44374300	-1.24675600
H	4.74302500	-2.73349700	-0.02078900
H	4.60217000	-3.11291700	-1.76164200
S	2.29171800	-1.15649700	0.50732800
O	-0.06288600	-2.98781900	1.66205500
C	-0.74317300	-3.72804400	2.40189100
O	-1.97778700	-4.04523900	2.19914300
C	-0.13387300	-4.31726100	3.66659400
H	-0.31640000	-5.39455800	3.70261300
H	0.93687400	-4.11353000	3.70883300
H	-0.62520600	-3.87711200	4.54056100
Ag	-2.65736900	-3.07595100	0.45021800
H	-3.81698600	2.05148800	1.30653400
O	-3.35449100	2.29551700	3.73184900
C	-3.05250100	2.39563200	5.11990900
H	-2.05186100	2.81459600	5.28317800
H	-3.79915700	3.07096900	5.53903500
H	-3.12453100	1.42068700	5.61761000

TS45

C	-2.81885900	1.29248200	2.65789500
C	-1.53917600	1.01513400	3.16153000
C	-0.61094900	0.38503100	2.33290500
C	-0.89862300	0.05221800	0.99549200
C	-2.15574700	0.48010200	0.46356100
C	-3.11874900	1.01598600	1.31555800
Pd	0.38710100	-0.67928700	-0.45057400
H	-0.58253100	-1.35973000	1.04978500
H	-1.27669400	1.24418600	4.18720200
H	0.34163200	0.07653100	2.75506100
C	-1.26015200	-0.44177300	-1.72188500
C	-0.77318000	0.42930900	-2.90437800
C	-2.20435400	1.83685600	-1.80544800
C	-2.35080900	0.43458200	-1.02852900
C	-0.72697200	1.81939900	-2.25576600
H	-0.50457900	2.61883100	-2.97230000
H	-0.01479200	1.88067500	-1.43194000
C	-1.94994900	0.58611400	-3.90424100

H	-1.58778900	1.01133000	-4.84609700
H	-2.42278900	-0.36982300	-4.14660800
C	-2.90512000	1.57687700	-3.17287900
H	-2.98089100	2.50379500	-3.74426900
H	-3.92136600	1.18752000	-3.05006400
H	0.15472700	0.08138000	-3.35856900
H	-3.35689700	0.05795100	-1.24618800
C	-1.69269200	-1.82468400	-2.09146600
O	-2.78118600	-2.35008000	-1.68169400
N	-0.90845400	-2.51971800	-2.92803400
H	0.04448700	-2.16915100	-3.04330700
C	-1.16181700	-3.92122500	-3.22377700
H	-0.47580800	-4.23973800	-4.01013100
H	-1.01001400	-4.55148900	-2.33814100
H	-2.19134700	-4.05237800	-3.56170800
C	-2.67440600	3.08768200	-1.02530700
C	-1.60600200	3.60255600	-0.03209000
C	-3.13350500	4.27488900	-1.90044300
H	-3.55670300	2.79873100	-0.43935000
C	-2.15494200	4.72219500	0.86076500
H	-0.75623600	3.99389900	-0.60850000
H	-1.21315000	2.79055900	0.58296100
C	-3.66360300	5.43507300	-1.03878800
H	-2.29376700	4.62384000	-2.51872100
H	-3.92485600	3.96443400	-2.58982700
C	-2.64644600	5.90189500	0.01122100
H	-1.38333300	5.05417200	1.56640700
H	-2.98414500	4.32627100	1.46475800
H	-3.95973400	6.27213300	-1.68267200
H	-4.57618200	5.09963700	-0.52501000
H	-3.08470100	6.68299200	0.64436100
H	-1.78447700	6.35603200	-0.49827000
C	3.11104300	-2.35566100	-0.37497000
C	2.61350300	-2.14311500	-1.84107800
O	1.52687500	-1.45405500	-2.03505300
O	3.24306900	-2.71453500	-2.72265900
C	3.56682000	0.35974500	0.55224200
C	4.67513800	0.47575100	1.40462800
C	3.39616400	1.36102100	-0.41247200
C	5.56940800	1.53802400	1.31315700
C	4.27764400	2.43537200	-0.51522800

C	5.36690100	2.52308900	0.34833400
F	2.37642100	1.33220100	-1.27664100
F	4.08337300	3.37965000	-1.43980900
F	6.21457200	3.54669400	0.25176600
F	6.61700100	1.61723200	2.13889500
F	4.90951900	-0.45525400	2.33709500
C	2.46892800	-3.65450300	0.15138400
H	2.72867400	-4.45803900	-0.54400100
H	2.85397100	-3.90506200	1.14430400
H	1.37978800	-3.57705200	0.21348100
C	4.63517800	-2.42483900	-0.31581000
H	5.09351000	-1.50910500	-0.69765800
H	4.98375300	-2.59932400	0.70564300
H	4.95769700	-3.24298300	-0.96255800
S	2.45833600	-1.02028900	0.80619900
O	-0.36603700	-2.49508300	1.82199400
C	-1.23605000	-2.84843500	2.69040100
O	-2.48262000	-2.91705600	2.48376100
C	-0.72360600	-3.18192900	4.07391100
H	-1.47662300	-3.71143400	4.65781700
H	0.19387700	-3.76990000	3.99834100
H	-0.47138400	-2.24095800	4.57517900
Ag	-2.97384200	-2.55465600	0.43139100
H	-4.10411700	1.28625700	0.95189100
O	-3.82911200	1.85130000	3.37636000
C	-3.59083000	2.18056500	4.73868800
H	-2.78930100	2.92371900	4.83876100
H	-4.52351500	2.60520800	5.11233800
H	-3.33569400	1.29141000	5.32957000

int78

C	2.09784900	2.29714500	2.43719900
C	1.46894800	1.20944900	3.05626600
C	0.49199300	0.49551100	2.35102400
C	0.15793100	0.79825500	1.00897400
C	0.85650300	1.88378600	0.38702400
C	1.76551600	2.64481300	1.11866400
Pd	-1.04763900	-0.27615200	-0.22154700
H	-3.41531800	0.11075900	0.08938400
H	1.70804300	0.92280300	4.07333000
H	0.00673100	-0.33837600	2.84938200

C	-0.67018600	1.30247200	-1.54808900
C	-0.22906100	0.70178800	-2.89747200
C	1.71168200	1.62814200	-2.11051300
C	0.58539900	2.10797800	-1.07429100
C	1.19537800	0.24369400	-2.56349000
H	1.74560900	-0.14219500	-3.42918900
H	1.21346000	-0.50899000	-1.77712500
C	0.03699800	1.87353300	-3.88426000
H	0.11153600	1.49649800	-4.90949200
H	-0.76950700	2.61213700	-3.87062900
C	1.40298700	2.44919300	-3.39636700
H	2.16971500	2.27388900	-4.15422200
H	1.37414000	3.52701300	-3.20482700
H	-0.89123200	-0.07369200	-3.28429400
H	0.42690000	3.18208800	-1.22970200
C	-1.96200100	2.06485300	-1.51912900
O	-2.14500900	3.05079400	-0.76438300
N	-2.94687500	1.60471500	-2.33585900
H	-2.81495800	0.67770700	-2.72490800
C	-4.29516400	2.14322400	-2.32304200
H	-4.65994300	2.27300200	-3.34642900
H	-4.98175200	1.47744600	-1.78690700
H	-4.27138900	3.11156600	-1.82248500
C	3.16789200	1.66958700	-1.59053800
C	3.50716700	0.44279100	-0.71154900
C	4.24929100	1.79145200	-2.68503600
H	3.27569700	2.56496200	-0.96436900
C	4.88946800	0.56493000	-0.05963000
H	3.50507800	-0.44889400	-1.35135300
H	2.74172300	0.28293100	0.05171400
C	5.65882200	1.88897200	-2.07426400
H	4.19473900	0.92046200	-3.35427200
H	4.07219700	2.67643600	-3.30459500
C	5.97514900	0.71780600	-1.13306500
H	5.09021800	-0.31702200	0.55958000
H	4.89859100	1.43598600	0.61092000
H	6.40768100	1.94943600	-2.87339700
H	5.73050100	2.82926000	-1.50856900
H	6.96140400	0.85502400	-0.67325900
H	6.02667800	-0.21226800	-1.71721500
C	-2.31553800	-3.32452900	-0.23918400

C	-2.50600100	-2.54411100	-1.58989100
O	-2.29962700	-1.26292900	-1.60576800
O	-2.95127500	-3.20449100	-2.52025100
C	0.47081000	-2.78277400	0.74603200
C	1.30526700	-2.76831900	1.86970900
C	1.09110200	-2.85722800	-0.50640600
C	2.69311500	-2.77378300	1.75735600
C	2.47439800	-2.88179000	-0.63761500
C	3.28016200	-2.82838000	0.49693300
F	0.36129500	-2.84071700	-1.63146300
F	3.03503900	-2.88512000	-1.85112600
F	4.60882600	-2.79865500	0.37134500
F	3.45870200	-2.70844400	2.85069500
F	0.77794200	-2.67290000	3.10054500
C	-3.70199100	-3.36183000	0.43835900
H	-4.39413100	-3.82981100	-0.26704500
H	-3.67917900	-3.94926100	1.36119500
H	-4.07770600	-2.35854600	0.65752600
C	-1.79281900	-4.74301400	-0.46037800
H	-0.80846900	-4.74782500	-0.92825900
H	-1.74929400	-5.29842200	0.48140000
H	-2.48155300	-5.24019900	-1.14651800
S	-1.25534500	-2.39453900	1.02199200
O	-4.39135700	0.07475700	0.24989600
C	-4.81114300	0.89928900	1.20120800
O	-4.08941600	1.65092300	1.85590100
C	-6.30032100	0.83254400	1.39645900
H	-6.59061800	1.44327400	2.24991000
H	-6.79291000	1.19968600	0.49047400
H	-6.61117200	-0.20566700	1.53959800
Ag	-1.84657200	1.88943500	1.46700900
H	2.26712000	3.50098700	0.68076200
O	3.04747700	3.07920500	3.02357700
C	3.46100700	2.76214600	4.34504300
H	3.88859800	1.75263700	4.40307100
H	4.22881500	3.49289100	4.60342600
H	2.63168300	2.84236500	5.06025800
int79			
C	0.63737800	3.67215200	1.16194700
C	-0.11913700	2.75600800	1.90152000

C	-0.23276900	1.43580100	1.44882900
C	0.41674700	1.02550200	0.28162000
C	1.22339700	1.93508300	-0.43861000
C	1.29697100	3.25875000	-0.00351800
Pd	0.20467400	-0.80401000	-0.43691200
H	-0.85065200	0.73967400	2.00425000
C	1.42229100	-0.04504900	-1.97217600
C	2.70430600	-0.88605100	-2.12599300
C	3.51484500	1.15125300	-1.48846800
C	1.94819300	1.39629200	-1.64115300
C	3.56031700	-0.30937900	-0.99083300
H	4.57436100	-0.71993500	-0.98233700
H	3.11476400	-0.44454300	-0.00359500
C	3.49662600	-0.41859300	-3.37752400
H	4.30782400	-1.12153000	-3.59864100
H	2.86761000	-0.35779300	-4.27032700
C	4.05441100	0.96835300	-2.93653700
H	5.14944800	0.96438300	-2.93278800
H	3.73691800	1.77960200	-3.59821200
H	2.54871400	-1.96906300	-2.08349900
H	1.77785600	2.07161400	-2.48845000
C	0.38964000	-0.10285000	-3.04055000
O	-0.45951000	0.81652200	-3.24813600
C	-0.82320200	-1.50253100	-4.65201000
H	-0.61881900	-2.39630000	-5.24445700
H	-1.73077300	-1.66289700	-4.05497800
H	-1.00270900	-0.65780100	-5.31938800
C	-3.47286700	-1.76899600	1.93175500
C	-2.52046600	-1.28454400	0.81605700
O	-3.06919700	-0.74574200	-0.18923900
O	-1.27961200	-1.45989500	1.00848900
C	-4.99571700	0.63718900	1.62151500
C	-4.39472000	1.59225300	0.79424700
C	-6.34343300	0.34385200	1.37629500
C	-5.06879700	2.17393000	-0.27128600
C	-7.04692800	0.93859400	0.32999200
C	-6.40113300	1.84563900	-0.50815500
F	-6.99122300	-0.55637800	2.12374900
F	-8.32992000	0.62779200	0.11105800
F	-7.05572400	2.39513400	-1.53287300
F	-4.41834400	3.00371600	-1.10565300

F	-3.11058800	1.93666000	0.96424800
C	-4.65236800	-2.54020800	1.33581100
H	-4.27811100	-3.46063000	0.87206300
H	-5.37346300	-2.80504800	2.11209000
H	-5.14989100	-1.95827400	0.55979800
C	-2.74610400	-2.59302300	2.99886700
H	-1.93008600	-2.02958500	3.45607000
H	-3.44430500	-2.91667500	3.77614300
H	-2.31155800	-3.47942800	2.52708000
S	-4.05887500	-0.22103700	2.86389800
Ag	-1.93596300	0.68337800	-1.50276600
C	2.58139700	-1.88599400	2.59166800
C	3.94017500	-1.93578900	2.25861500
C	4.36699900	-2.72788100	1.18577400
C	3.43707200	-3.41887900	0.40942500
C	2.08529800	-3.30367500	0.72732700
C	1.63743400	-2.57103400	1.82786000
H	2.26791800	-1.26978300	3.42735200
H	5.42018500	-2.77114800	0.93445500
H	3.76206000	-3.99856200	-0.44669900
H	0.58091400	-2.48899400	2.05400600
I	0.61688200	-4.12929100	-0.62490400
C	4.87724900	-1.07420000	3.03464000
O	4.56926400	-0.43968400	4.02365200
O	6.11555900	-1.04584900	2.48984400
C	7.05510100	-0.18568300	3.15801000
H	6.70095500	0.84780900	3.14271300
H	7.19298200	-0.49968700	4.19591500
H	7.98591700	-0.27882500	2.59886700
C	4.27599400	2.18051900	-0.63651100
C	5.63420500	1.67988900	-0.09996600
C	4.48430800	3.52086200	-1.37111400
H	3.66010700	2.38073200	0.24977700
C	6.28498400	2.72887600	0.81792100
H	6.31072700	1.45803700	-0.93812300
H	5.50754400	0.74573700	0.45736000
C	5.09718300	4.57931200	-0.44420500
H	5.15745400	3.36047300	-2.22460800
H	3.54021000	3.88006700	-1.79542800
C	6.43763200	4.09108500	0.12524600
H	7.26163900	2.37006600	1.16668100

H	5.65704400	2.85047600	1.71251200
H	5.23434000	5.52550100	-0.98145700
H	4.39894000	4.78204400	0.37998200
H	6.85212100	4.82900700	0.82278400
H	7.16046800	3.99502000	-0.69781200
N	0.32256200	-1.22695800	-3.79963800
H	0.96452000	-1.97659900	-3.59099500
H	-0.63699400	3.04926800	2.80690900
H	1.87178900	3.99992800	-0.54657500
O	0.80451100	4.99003200	1.49054600
C	0.14162800	5.47860200	2.64460400
H	0.47970400	4.96753800	3.55636100
H	0.39503300	6.53805000	2.71402700
H	-0.94894000	5.37350900	2.56249900

TS46

C	-0.31046500	2.87180100	-2.40274700
C	0.13018000	1.60186700	-2.79518600
C	0.01530100	0.53264900	-1.90279700
C	-0.56717500	0.71312500	-0.64628500
C	-1.07827700	1.97496900	-0.27502100
C	-0.90345200	3.05150800	-1.14643800
Pd	-0.57003000	-0.77098300	0.68443600
H	0.41235700	-0.43441900	-2.18843100
C	-1.58017200	0.73160300	1.86006300
C	-3.00840200	0.33986900	2.26990200
C	-3.35330000	2.22912700	1.03384300
C	-1.77128300	2.06996600	1.05417300
C	-3.79928100	0.74817300	1.01373200
H	-4.87903000	0.62258000	1.14295100
H	-3.48292900	0.22390600	0.10972100
C	-3.56631200	1.34606200	3.31343600
H	-4.52144700	0.97570500	3.70203200
H	-2.90237000	1.48685900	4.16949200
C	-3.76199100	2.64196100	2.47710800
H	-4.80668100	2.96692600	2.49875300
H	-3.15840900	3.47573700	2.84757000
H	-3.10397800	-0.69987400	2.59259200
H	-1.33951700	2.90478800	1.61777200
C	-0.55369000	0.84169100	2.94075700
O	0.46214800	1.60288000	2.84291000

C	0.37137300	-0.05778000	5.02301900
H	-0.02884300	-0.51428200	5.92979600
H	1.16391000	-0.69901700	4.61444500
H	0.80234700	0.91454400	5.26306200
C	3.32234700	-2.40436300	-1.31382700
C	2.40329300	-1.63971500	-0.33564000
O	3.00260500	-0.86484300	0.47766500
O	1.16400000	-1.82915100	-0.43120900
C	4.76212300	0.03890100	-1.73039700
C	4.13506800	1.16183600	-1.17778900
C	6.12922600	-0.11885700	-1.46873900
C	4.81089700	2.05248900	-0.35390200
C	6.83204500	0.77840600	-0.66611400
C	6.16576000	1.86084900	-0.09481500
F	6.79926900	-1.16761400	-1.95825200
F	8.13545900	0.59688600	-0.42357100
F	6.82256000	2.70808100	0.69987600
F	4.14694900	3.06045900	0.23538200
F	2.82939100	1.38347000	-1.37494200
C	4.53840300	-2.97795700	-0.58326900
H	4.19774300	-3.71934600	0.14915800
H	5.21688500	-3.46471700	-1.28756300
H	5.07581300	-2.20024200	-0.04068800
C	2.56466200	-3.49051600	-2.08280700
H	1.71838600	-3.07661200	-2.63523000
H	3.23290500	-4.00574400	-2.77856900
H	2.17222400	-4.22268000	-1.37065600
S	3.84114700	-1.16617700	-2.65567600
Ag	1.86336700	0.64708700	1.47228900
C	-2.26969400	-3.40048200	-2.02322700
C	-3.65152100	-3.20879000	-1.88916800
C	-4.16340100	-2.72662500	-0.67663500
C	-3.30840400	-2.40987800	0.37549300
C	-1.92947300	-2.52255800	0.18067400
C	-1.39825600	-3.09418900	-0.98202100
H	-1.88618600	-3.80307500	-2.95520200
H	-5.23375500	-2.60882600	-0.55071500
H	-3.71449100	-2.06548500	1.31474700
H	-0.33324900	-3.24303600	-1.08835200
I	-0.70066300	-3.07728400	2.28426900
C	-4.52053100	-3.56096300	-3.04222800

O	-4.11685300	-4.00488600	-4.10048600
O	-5.83146900	-3.33092300	-2.79062000
C	-6.72191600	-3.65076200	-3.87077000
H	-6.47830000	-3.06083400	-4.75860900
H	-6.65208400	-4.71152400	-4.12694900
H	-7.72177100	-3.40773000	-3.51069900
C	-3.91617200	3.14364900	-0.06718200
C	-5.41864700	2.94385100	-0.35456500
C	-3.65157800	4.63670500	0.22154400
H	-3.39687000	2.88743900	-0.99913200
C	-5.87920200	3.83229100	-1.52288700
H	-6.01012100	3.18375800	0.54065500
H	-5.62266000	1.89521600	-0.59625100
C	-4.07708000	5.52230600	-0.95693500
H	-4.21944800	4.93514000	1.11329500
H	-2.59698100	4.80346600	0.46740000
C	-5.56440200	5.31553200	-1.27934900
H	-6.95284200	3.69466300	-1.69987000
H	-5.36610800	3.50384800	-2.43791700
H	-3.87827700	6.57713100	-0.73245500
H	-3.47047500	5.26689500	-1.83734200
H	-5.85663700	5.91426400	-2.15042600
H	-6.16623900	5.67710400	-0.43296500
N	-0.70850700	0.11213000	4.06236300
H	-1.44904400	-0.57444200	4.06424800
H	0.59184600	1.43549500	-3.76094700
H	-1.23147300	4.05063000	-0.88603800
O	-0.21817500	3.99889600	-3.17005900
C	0.40386800	3.89379200	-4.44084800
H	-0.14115200	3.21046300	-5.10590600
H	0.38819900	4.89754700	-4.86905400
H	1.44473200	3.55335000	-4.35635200

int80

C	0.43918700	3.21022500	2.35997700
C	-0.20975900	2.03663300	2.76376800
C	-0.12497700	0.89785600	1.96003700
C	0.60629500	0.91571800	0.77204800
C	1.28631000	2.08117200	0.37468000
C	1.16741800	3.22672600	1.16476500
Pd	0.50661400	-0.59644400	-0.55966100

H	-0.66803600	0.01117400	2.26337100
C	1.70740300	0.76355500	-1.74651300
C	3.08813100	0.25163100	-2.17658200
C	3.62468000	2.06950900	-0.89169500
C	2.03634000	2.06542500	-0.92730300
C	3.93077400	0.55691400	-0.92279800
H	4.99088800	0.33818100	-1.08191100
H	3.59626000	0.04024300	-0.02520500
C	3.73769700	1.24119000	-3.19262300
H	4.64336000	0.78072700	-3.60091000
H	3.09323000	1.48910000	-4.03782500
C	4.07994500	2.48154100	-2.31900000
H	5.15534700	2.68327600	-2.32976200
H	3.57886700	3.39089400	-2.66400000
H	3.09254700	-0.78199400	-2.52594600
H	1.70145300	2.93742300	-1.50067300
C	0.65943400	1.02388300	-2.79502600
O	-0.35858900	1.74805800	-2.52901600
C	-0.30487700	0.53305200	-4.98184200
H	0.07556500	0.22038500	-5.95502800
H	-1.09968800	-0.15307100	-4.66579900
H	-0.70450800	1.54520600	-5.04998300
C	-3.09422700	-2.36504700	1.51188400
C	-2.21896300	-1.56161500	0.53221400
O	-2.85334500	-0.85550900	-0.31592400
O	-0.96968700	-1.64618500	0.67428800
C	-4.74544000	-0.04324000	1.81518400
C	-4.22061300	1.09327900	1.18858100
C	-6.09144300	-0.34134000	1.56567900
C	-4.96757200	1.85568100	0.30070100
C	-6.86790800	0.43034700	0.70227100
C	-6.29778400	1.52453100	0.05441100
F	-6.66544600	-1.41112800	2.12462900
F	-8.14702600	0.11413200	0.47304000
F	-7.02120300	2.24914800	-0.80079900
F	-4.39089800	2.87299100	-0.36244700
F	-2.94190200	1.45064700	1.37187500
C	-4.24770400	-3.04705800	0.77478600
H	-3.83428300	-3.77982700	0.07252300
H	-4.90242900	-3.56223900	1.48104500
H	-4.82918700	-2.32926300	0.19642400

C	-2.27276300	-3.36881400	2.32585800
H	-1.46237100	-2.88300000	2.87259200
H	-2.91635900	-3.90654400	3.02765900
H	-1.81781100	-4.08965200	1.64061300
S	-3.72154900	-1.11347800	2.79852800
Ag	-1.86208900	0.62652800	-1.46655500
C	2.82791900	-2.60476600	2.43377500
C	3.70175000	-3.41391700	1.70050200
C	3.67234700	-3.36155700	0.30136200
C	2.79296200	-2.50107600	-0.35650300
C	1.94183100	-1.68846400	0.39340500
C	1.94147000	-1.74240600	1.78761900
H	2.85290500	-2.65427100	3.51762900
H	4.32774300	-4.00221000	-0.27789200
H	2.76591500	-2.49809200	-1.43624900
H	1.27403600	-1.13293800	2.37717700
I	-0.09490900	-2.49673500	-2.57985900
C	4.62460000	-4.30639100	2.45306600
O	4.67599500	-4.38126100	3.66607100
O	5.41750100	-5.03879900	1.63577400
C	6.32690200	-5.92442200	2.30679400
H	7.00799100	-5.36187000	2.95138600
H	5.78039000	-6.64453400	2.92190800
H	6.87871700	-6.43465300	1.51712700
C	4.26027500	2.88670200	0.24678800
C	5.71306200	2.48378300	0.57262300
C	4.20636300	4.40699600	-0.01593600
H	3.67895500	2.68363600	1.15556800
C	6.25407300	3.28036600	1.77214700
H	6.35536800	2.65911300	-0.30260400
H	5.76857500	1.41321800	0.79617500
C	4.70764000	5.20403500	1.19579200
H	4.84013000	4.64224300	-0.88164700
H	3.19355200	4.72067600	-0.29218000
C	6.14408400	4.79647600	1.55528000
H	7.29470600	2.99796300	1.97168700
H	5.67803700	3.00369800	2.66658500
H	4.65600500	6.28016900	0.99149800
H	4.04492600	5.01319300	2.05183400
H	6.48424500	5.33435600	2.44821400
H	6.81433600	5.09290400	0.73549000

N	0.79019600	0.50699500	-4.02000100
H	1.49206500	-0.21073000	-4.13805700
H	-0.79985900	1.99625900	3.67121600
H	1.63487100	4.16000600	0.87577500
O	0.42087300	4.38630300	3.05055900
C	-0.32694300	4.44453700	4.25634000
H	0.05484900	3.73820500	5.00537700
H	-0.21296900	5.46231000	4.63279400
H	-1.39197300	4.24075700	4.08282600

int81

C	4.80710000	-1.45559400	-2.03537500
C	3.90156000	-1.11633100	-3.04859500
C	2.54737400	-0.94440200	-2.73103600
C	2.11962200	-1.07078200	-1.41548700
C	3.02359400	-1.38343500	-0.38854000
C	4.36002700	-1.61046600	-0.71583400
Pd	0.18898100	-1.17491000	-0.96973300
H	4.22299300	-1.00768500	-4.07742700
H	1.83667600	-0.72240700	-3.52339300
C	0.91011800	-1.56415700	0.97330700
C	0.47930000	-0.65146900	2.11202600
C	2.74896100	-0.33453500	2.05468400
C	2.47048400	-1.50411300	1.00384300
C	1.46322600	0.51928400	1.95622900
H	1.38509300	1.24739000	2.77094200
H	1.35360200	1.04231300	1.01049500
C	0.98019100	-1.29171800	3.44854900
H	0.47974000	-0.80211200	4.28925900
H	0.76617600	-2.36045200	3.52366400
C	2.51123100	-0.99937900	3.43981100
H	2.75899300	-0.30546800	4.24512000
H	3.12036000	-1.89754100	3.58487800
H	-0.58126700	-0.40289000	2.12041100
H	2.85780300	-2.43565900	1.43720100
C	0.28064300	-2.91003300	0.74581900
O	0.52547000	-3.45392700	-0.36465400
N	-0.60895200	-3.43880500	1.60095600
H	-0.94738300	-2.86976000	2.36309500
C	-1.40459000	-4.59860100	1.20200600
H	-2.08139500	-4.84928800	2.01878300

H	-1.98327200	-4.36878100	0.30426900
H	-0.74783500	-5.44585300	0.99530500
C	0.39974100	3.08686100	-1.65795900
C	-0.67695400	3.55874700	-0.89772100
C	-1.44276300	2.65042200	-0.15527800
C	-1.13330900	1.29299800	-0.17443700
C	-0.05455300	0.82303900	-0.93610800
C	0.71304900	1.72609900	-1.67810800
H	0.99788300	3.78606300	-2.23183100
H	-2.27852200	3.02384600	0.42715500
H	-1.73772800	0.60060300	0.39424300
H	1.55800000	1.38850400	-2.26323600
C	-1.05167400	4.99687800	-0.83972000
O	-1.97995100	5.44311800	-0.19260600
O	-0.23974400	5.77557300	-1.59484900
C	-0.55717500	7.17537000	-1.57992600
H	0.17959500	7.65226200	-2.22672700
H	-1.56899900	7.34569400	-1.95811300
H	-0.49387300	7.57504000	-0.56401000
C	4.09272700	0.40579200	1.86342400
C	4.02415100	1.46906500	0.74268600
C	4.65506200	1.06849400	3.13929300
H	4.83784500	-0.34201400	1.55953800
C	5.40143800	2.07939700	0.45605900
H	3.34107400	2.26926400	1.05935300
H	3.60163700	1.04383600	-0.17003700
C	6.02726600	1.71349800	2.87886800
H	3.94998400	1.83261500	3.49816600
H	4.75976200	0.33267800	3.94332100
C	5.98891100	2.71985800	1.72097600
H	5.32356200	2.82166000	-0.34749300
H	6.07563700	1.29130200	0.09149300
H	6.39146100	2.19617200	3.79384300
H	6.74781800	0.91863600	2.63765300
H	6.99372100	3.11389300	1.52643200
H	5.36477800	3.57789000	2.00959600
C	-3.65912900	-1.02361800	-2.42086400
C	-2.22238400	-1.28862300	-1.94193300
O	-1.97473500	-1.50750900	-0.71342700
O	-1.28673400	-1.17216100	-2.78530400
C	-4.44158900	-0.66225900	0.35325400

C	-3.78809300	-1.40086600	1.34960100
C	-4.59910700	0.70869500	0.58427500
C	-3.24562300	-0.79367300	2.47335000
C	-4.08124300	1.33110300	1.72133100
C	-3.37942100	0.58026000	2.65914900
F	-5.21846200	1.48625800	-0.30904500
F	-4.20265300	2.65493000	1.88329000
F	-2.82296800	1.16803900	3.72053500
F	-2.52875500	-1.52035000	3.35930800
F	-3.61962900	-2.71903500	1.23064400
C	-3.73696500	0.46277200	-2.81664200
H	-3.01965400	0.65062600	-3.62048800
H	-4.74429000	0.71016800	-3.15952100
H	-3.48341400	1.11595800	-1.98024100
C	-3.98590200	-1.92443900	-3.62384300
H	-3.93811800	-2.98397500	-3.35710400
H	-4.98318700	-1.70214500	-4.01560800
H	-3.24857200	-1.73241400	-4.40694100
S	-4.97687400	-1.46411700	-1.14487000
O	6.14436200	-1.66282800	-2.22529500
C	6.65934700	-1.55327400	-3.54278500
H	6.51912500	-0.54341800	-3.95160400
H	7.72766900	-1.76312400	-3.46801000
H	6.19566700	-2.28091600	-4.22231300
H	5.08535400	-1.90505000	0.03520600

TS47

C	4.89533600	-0.40835500	-2.17921000
C	4.16935400	0.48163700	-2.98510100
C	2.81861900	0.68516800	-2.72139500
C	2.16147500	0.02687000	-1.66990900
C	2.88681600	-0.93119800	-0.89746700
C	4.23686900	-1.12966200	-1.17426400
Pd	0.11830600	-0.18182800	-1.44667900
H	4.63991600	1.02121200	-3.79765800
H	2.27616300	1.40127600	-3.32847900
C	0.64243800	-1.88522800	-0.40420600
C	-0.08841900	-1.99497200	0.93681900
C	2.12924300	-2.00895600	1.53519200
C	2.13599700	-1.93438400	-0.04630200
C	0.83967200	-1.22435200	1.89569600

H	0.54649700	-1.35231100	2.94355700
H	0.87252300	-0.15994500	1.67765700
C	0.12458000	-3.45456300	1.42108300
H	-0.52788400	-3.63655600	2.27937200
H	-0.12638100	-4.19607700	0.65948300
C	1.62662700	-3.46551700	1.82828600
H	1.71163900	-3.69381200	2.89071700
H	2.21326200	-4.21377400	1.28634500
H	-1.12831700	-1.68538300	0.91007000
H	2.51532000	-2.89481200	-0.40932900
C	0.26374600	-2.88662200	-1.51626200
O	1.12175700	-3.51761300	-2.13333400
N	-1.06521300	-3.05737200	-1.73760800
H	-1.72827800	-2.43438700	-1.29250400
C	-1.53783900	-3.94791800	-2.78264200
H	-2.61749700	-4.06760200	-2.67560600
H	-1.31456900	-3.55044300	-3.78015500
H	-1.04870900	-4.92109200	-2.69383600
C	1.47217400	3.25241100	0.85096000
C	0.92751600	4.23529200	0.01578700
C	0.47456300	3.87185800	-1.25987200
C	0.55586000	2.55335900	-1.69553200
C	1.06192700	1.56378100	-0.82958400
C	1.54837800	1.92730100	0.42691800
H	1.84809700	3.52498000	1.83076200
H	0.06141000	4.63933500	-1.90615500
H	0.19253100	2.30028400	-2.68561800
H	2.00916700	1.19508200	1.06501800
C	0.81985500	5.66261000	0.41599300
O	0.36340700	6.54430800	-0.28717500
O	1.28968500	5.88591000	1.66656700
C	1.20973600	7.24929500	2.11015700
H	1.62282800	7.25613700	3.11896700
H	1.78849400	7.90351300	1.45231400
H	0.17145500	7.59222100	2.11679300
C	3.47042500	-1.65606400	2.22414000
C	3.80789700	-0.15174800	2.18458200
C	3.57472300	-2.14497600	3.68721700
H	4.25771800	-2.18224200	1.66052400
C	5.18240800	0.16440600	2.79224800
H	3.04049800	0.39221500	2.75428000

H	3.77627500	0.21709000	1.15816600
C	4.93897300	-1.82109400	4.31743600
H	2.77508000	-1.67664400	4.27955600
H	3.41888500	-3.22504800	3.74714900
C	5.27320000	-0.32776800	4.24105500
H	5.37373100	1.24269500	2.73617900
H	5.96171200	-0.32399900	2.19010700
H	4.95669800	-2.16744400	5.35772700
H	5.71652500	-2.38898600	3.78644400
H	6.27014400	-0.13470200	4.65479100
H	4.55965600	0.23641700	4.85872300
C	-3.95175500	0.51956300	-2.24102400
C	-2.44287100	0.24455200	-2.11684900
O	-2.00651100	-0.43560700	-1.11644600
O	-1.67116100	0.76439900	-2.95223000
C	-4.63603300	-0.64656900	0.32528400
C	-3.81166500	-1.58250400	0.96242100
C	-5.18388500	0.36219600	1.12917900
C	-3.49428100	-1.48845000	2.31303600
C	-4.87688800	0.47595000	2.48421800
C	-4.02289400	-0.45052500	3.07674000
F	-6.01851600	1.27174500	0.61229700
F	-5.40214800	1.46308400	3.21871000
F	-3.71814500	-0.35060600	4.37241700
F	-2.66844700	-2.37961300	2.88250100
F	-3.28358900	-2.61129400	0.28443600
C	-4.19768700	1.92522300	-1.66648200
H	-3.61926500	2.64688900	-2.25155100
H	-5.25756000	2.18118500	-1.71606200
H	-3.86994700	1.99393200	-0.62667400
C	-4.38418700	0.45489600	-3.71526200
H	-4.24451200	-0.54679600	-4.13302700
H	-5.43495600	0.73907000	-3.82072800
H	-3.76446100	1.14692800	-4.28863200
S	-5.01161200	-0.79032300	-1.40803800
O	6.22175500	-0.66734300	-2.31322300
C	6.93767100	-0.01916900	-3.35745600
H	6.92756600	1.07169300	-3.23674800
H	7.96467000	-0.37951500	-3.28504500
H	6.53209000	-0.27717200	-4.34401700
H	4.80207100	-1.88946000	-0.64404300

int82

C	-0.65413900	-1.58628500	2.48912300
C	-0.17112600	-0.54464200	3.27460600
C	0.90733900	0.20526100	2.80095700
C	1.47500700	0.02664700	1.53258800
C	0.97964200	-1.01000700	0.70985500
C	-0.06637800	-1.83695100	1.21661000
H	-0.60763800	-0.31368400	4.23706400
H	1.30089600	0.99975200	3.42726100
C	-5.49178400	-0.32723500	-0.67876900
C	-4.02761000	-0.73568300	-0.53352400
O	-3.58805200	-1.07483400	0.59862800
O	-3.24636500	-0.64909400	-1.54832300
C	-3.93306900	1.92339000	0.24304200
C	-3.63280900	1.69386900	1.59241100
C	-2.90257700	2.41684000	-0.56866200
C	-2.37393700	1.96435900	2.11747500
C	-1.63276700	2.67931300	-0.06191300
C	-1.37200700	2.46202500	1.28817100
F	-3.10914200	2.63161100	-1.87021600
F	-0.65433000	3.12467300	-0.86236800
F	-0.16311200	2.73722300	1.78335900
F	-2.12035900	1.73538600	3.41524700
F	-4.54764700	1.17712800	2.41962700
C	-6.02605600	-0.60632800	-2.08637000
H	-6.07497200	-1.68901600	-2.24788200
H	-7.03627500	-0.20206000	-2.20378600
H	-5.37502300	-0.16944800	-2.84380600
C	-6.35610000	-0.96624800	0.41148900
H	-5.96484200	-0.72839600	1.39992400
H	-7.38604200	-0.60615800	0.33626500
H	-6.35964600	-2.05535400	0.28915800
S	-5.53064700	1.57280600	-0.44857600
C	3.53042400	2.74082500	-0.16267900
C	4.75264500	2.61453800	0.51102600
C	4.89505800	1.64333800	1.51098000
C	3.82879600	0.80775500	1.82472200
C	2.60389700	0.92207200	1.14497800
C	2.46264400	1.90599900	0.15623700
H	3.41728000	3.49090000	-0.93642000

H	5.84768200	1.55717700	2.02260000
H	3.94135600	0.04584000	2.59095800
H	1.52725600	2.01180500	-0.37637900
C	5.92864900	3.47640400	0.20888600
O	7.00752800	3.39209300	0.76530000
O	5.67239300	4.38069600	-0.76497500
C	6.77286500	5.23771900	-1.10327800
H	7.62345200	4.65056000	-1.46049600
H	6.40337800	5.89567600	-1.89006100
H	7.09169900	5.81851100	-0.23326300
Pd	-1.47072000	-1.02133300	-0.30187000
C	0.13100100	-0.98001400	-1.60088700
C	0.11609700	-2.21932500	-2.53372700
C	1.95254300	-2.58222600	-1.21354900
C	1.40613800	-1.18828100	-0.74083200
C	0.66711200	-3.34466000	-1.64137900
H	0.90186800	-4.24292400	-2.22178500
H	0.00445800	-3.64605000	-0.82923000
C	1.30728700	-2.06470400	-3.52845000
H	1.22424300	-2.83235700	-4.30481200
H	1.32814500	-1.09249800	-4.02374000
C	2.55758200	-2.29980400	-2.62375500
H	3.13738900	-3.16117900	-2.96889100
H	3.22462600	-1.43455100	-2.61506500
H	-0.84398500	-2.39746100	-3.02365400
H	2.13495800	-0.41522900	-0.97705000
C	0.11268100	0.33894600	-2.37695900
O	1.13111000	1.02467100	-2.50492600
N	-1.04015500	0.65588500	-3.01679500
H	-1.89254800	0.15424200	-2.80054500
C	-1.10265600	1.83195800	-3.87080500
H	-0.33156700	1.77630500	-4.64433200
H	-2.08750900	1.87214500	-4.33796900
H	-0.94287900	2.74596100	-3.29336100
C	2.88546100	-3.25613200	-0.19737800
C	3.22659900	-4.72214600	-0.52789300
C	4.18275600	-2.45090300	0.01760200
H	2.35011400	-3.27128300	0.76550300
C	4.11149800	-5.35051000	0.56152800
H	3.75425100	-4.76941500	-1.49058000
H	2.30874900	-5.31007600	-0.64261600

C	5.06051700	-3.06860400	1.11412200
H	4.74803900	-2.42748400	-0.92410800
H	3.95139400	-1.41085700	0.26535300
C	5.39068700	-4.53431200	0.79733100
H	4.36158700	-6.38394300	0.29301600
H	3.53987500	-5.40098400	1.49959100
H	5.98020400	-2.48412900	1.23550400
H	4.52577500	-3.01660000	2.07408500
H	5.98323700	-4.97983700	1.60537700
H	6.01387400	-4.57230000	-0.10769500
H	-0.25171100	-2.81985100	0.79361300
O	-1.66905500	-2.40699200	2.82321000
C	-2.60229100	-1.94887300	3.80695400
H	-3.42891500	-2.65824700	3.78112600
H	-2.15586200	-1.94405100	4.80858600
H	-2.96867100	-0.94902200	3.55189700

TS48

C	3.13984100	-1.81645600	2.28929500
C	3.00655100	-0.86701300	3.30898800
C	2.20687700	0.25679000	3.09207600
C	1.53116500	0.47072400	1.88669700
C	1.68106800	-0.48970100	0.84458700
C	2.48432300	-1.61621200	1.06818800
H	3.51234900	-0.98584700	4.25924600
H	2.09809200	0.99000400	3.88634400
C	-2.64127900	-3.93853600	-1.07471900
C	-1.64159200	-2.82393100	-0.76049800
O	-1.05578700	-2.79793800	0.35468700
O	-1.41800400	-1.92062400	-1.64587000
C	-4.11978900	-1.78898300	0.14967100
C	-3.85097000	-1.90010500	1.52092300
C	-4.20291400	-0.49571800	-0.38342300
C	-3.67060400	-0.77952300	2.32744400
C	-4.07745900	0.63368400	0.41843100
C	-3.79984400	0.49282400	1.77532400
F	-4.40756600	-0.30306700	-1.69331300
F	-4.19706100	1.86085200	-0.11449800
F	-3.64209600	1.57481000	2.54009500
F	-3.38574400	-0.91463500	3.62650100
F	-3.75211200	-3.09956000	2.09858200

C	-2.52695500	-4.37378400	-2.54232400
H	-1.55716600	-4.85871900	-2.70046300
H	-3.30863500	-5.09861400	-2.79138300
H	-2.60331900	-3.51635600	-3.21115000
C	-2.47671400	-5.12164300	-0.11700600
H	-2.57349100	-4.80270800	0.91888900
H	-3.23031400	-5.88475900	-0.33098700
H	-1.48345700	-5.56438500	-0.24958500
S	-4.38463100	-3.20375300	-0.88913900
C	-1.26030500	2.85060400	0.94117800
C	-0.60835600	4.08386900	1.03867300
C	0.70708700	4.13980400	1.51502800
C	1.37876000	2.96650000	1.83995900
C	0.75329600	1.71573500	1.68470800
C	-0.58493100	1.67952300	1.26392500
H	-2.28488200	2.81810400	0.60186400
H	1.19241700	5.10680500	1.59291200
H	2.41343300	3.00370700	2.16896100
H	-1.08595300	0.72046700	1.17864300
C	-1.25987000	5.35300500	0.61832000
O	-0.78233800	6.46115300	0.76664300
O	-2.46019900	5.14028900	0.02487400
C	-3.13614600	6.32450200	-0.42295000
H	-2.52926100	6.85777800	-1.15967200
H	-4.06857200	5.97963300	-0.87023100
H	-3.33672600	6.99564100	0.41676900
Pd	0.14714800	-1.01276200	-0.47907100
C	0.87539000	0.35723300	-1.79876100
C	1.47221000	-0.27143800	-3.07243300
C	3.24742600	0.07941000	-1.66354500
C	1.99841900	0.54661700	-0.90541200
C	2.66418400	-1.07573700	-2.51532500
H	3.34384200	-1.40558900	-3.30651600
H	2.37167300	-1.94440800	-1.91828800
C	2.23062000	0.89076100	-3.77704700
H	2.64658100	0.52867300	-4.72287500
H	1.59284600	1.75005300	-3.98941900
C	3.35417500	1.22266000	-2.75626400
H	4.34137300	1.19113600	-3.22072300
H	3.22395400	2.21453800	-2.31653600
H	0.75610100	-0.80582000	-3.69846200

H	2.04138300	1.48325000	-0.36353200
C	-0.09690800	1.51226800	-1.99236500
O	0.30766800	2.67447500	-1.95047600
N	-1.37924900	1.18291700	-2.28317600
H	-1.65275800	0.20729900	-2.28261400
C	-2.36226100	2.21213800	-2.59079200
H	-2.21537600	2.61030700	-3.60159500
H	-3.35780500	1.77866200	-2.51090700
H	-2.26689500	3.03923200	-1.88312000
C	4.52592300	-0.18413900	-0.85570100
C	5.75380500	-0.53446500	-1.71971800
C	4.87119800	0.96001700	0.11805600
H	4.33219700	-1.06743900	-0.23916600
C	6.95283900	-0.91641800	-0.83747200
H	6.03611800	0.32477600	-2.34229200
H	5.51537400	-1.35614100	-2.40510100
C	6.07871500	0.59710200	0.99569300
H	5.08878100	1.87373200	-0.45323100
H	4.01306100	1.18093000	0.76064600
C	7.29859900	0.20946800	0.14836200
H	7.82033300	-1.15603700	-1.46376100
H	6.70882500	-1.82828300	-0.27391400
H	6.32464300	1.43169100	1.66307300
H	5.79964200	-0.24867400	1.64039200
H	8.13339200	-0.09021300	0.79332500
H	7.63818800	1.08934000	-0.41678300
H	2.62865000	-2.36704900	0.30016900
O	3.90643400	-2.94130900	2.36214300
C	4.61644800	-3.19327100	3.56680100
H	5.15237300	-4.13035600	3.40991200
H	5.33959600	-2.39569900	3.78394400
H	3.93629500	-3.30492300	4.42117200

int83

C	3.30142500	-1.00542600	2.71660800
C	3.13709500	0.11249300	3.54102400
C	2.14120800	1.03825800	3.23094500
C	1.30777700	0.89877300	2.11107600
C	1.50070500	-0.22851800	1.28269400
C	2.47336300	-1.17318900	1.59628800
H	3.76266700	0.27042600	4.41071200

H	1.99665600	1.89742200	3.88057400
C	-1.33045100	-4.18691700	-1.30606100
C	-0.72540500	-2.82666300	-0.97062900
O	-0.24651700	-2.62873200	0.19411600
O	-0.69877600	-1.89541100	-1.83942200
C	-3.40144700	-2.67901200	0.01081700
C	-3.19085900	-2.84790700	1.38631000
C	-3.80429900	-1.40945100	-0.42480300
C	-3.36234000	-1.80240600	2.28958800
C	-4.03436100	-0.37031900	0.47022400
C	-3.79712300	-0.56194900	1.82812400
F	-3.98092100	-1.15431200	-1.72946000
F	-4.46335600	0.82319600	0.03385900
F	-3.96736900	0.45000600	2.68026100
F	-3.12196900	-1.98065400	3.59143000
F	-2.80332000	-4.02904300	1.87439500
C	-1.06943800	-4.54704900	-2.77505600
H	0.00237200	-4.72181700	-2.91913700
H	-1.59831200	-5.46677900	-3.04416100
H	-1.38464000	-3.74159900	-3.43869800
C	-0.82617000	-5.27586000	-0.35465000
H	-1.02624100	-5.01744300	0.68313500
H	-1.31251300	-6.22713700	-0.58672800
H	0.25581200	-5.39763500	-0.47741200
S	-3.21475400	-4.00504500	-1.15529500
C	-1.96583500	2.56164700	1.17839800
C	-1.57633100	3.90249000	1.07980000
C	-0.26207400	4.26811900	1.39263200
C	0.66275400	3.29713600	1.75869200
C	0.29847300	1.94009700	1.80732500
C	-1.03441400	1.59274200	1.53339200
H	-2.98958800	2.28716300	0.96912300
H	0.02025200	5.31228100	1.31264400
H	1.69151900	3.57709600	1.96742200
H	-1.33039800	0.55224200	1.60961100
C	-2.50453100	4.96367300	0.61319500
O	-2.25377500	6.15296000	0.59816600
O	-3.68841100	4.45796200	0.17900100
C	-4.62143100	5.43274300	-0.30919900
H	-4.20091900	5.97363800	-1.16134600
H	-5.50554800	4.86988600	-0.60974000

H	-4.87187700	6.15418800	0.47337100
Pd	0.49972400	-0.68725300	-0.39446700
C	0.62501400	0.93715100	-1.90287900
C	1.15661500	0.44136700	-3.24739900
C	2.97706400	0.70013800	-1.88836700
C	1.73615700	1.08830500	-1.08391800
C	2.39377600	-0.37405000	-2.84212100
H	3.04715700	-0.58136200	-3.69463700
H	2.15748800	-1.31438400	-2.33497200
C	1.85143200	1.72373100	-3.82987200
H	2.16497600	1.52466100	-4.85926300
H	1.18412000	2.58802600	-3.83632400
C	3.08073000	1.91668600	-2.88659400
H	4.01845600	1.86574200	-3.44519000
H	3.05868000	2.87574100	-2.36245400
H	0.42495900	-0.03051100	-3.90305500
H	1.77198000	1.82395800	-0.29362500
C	-0.61411300	1.80235800	-1.88770700
O	-0.50983700	3.02293900	-1.78939000
N	-1.78832600	1.16503000	-2.11424400
H	-1.79502200	0.15680700	-2.20741900
C	-3.00973900	1.92546600	-2.34359200
H	-2.96092200	2.46011100	-3.29935500
H	-3.85129000	1.23571900	-2.35182400
H	-3.15173700	2.66034100	-1.54859200
C	4.22280100	0.30033700	-1.08590400
C	5.44621700	0.00464200	-1.97643400
C	4.60237500	1.30521200	0.02092400
H	3.95947100	-0.63764900	-0.57761700
C	6.64008300	-0.49995400	-1.15180400
H	5.74728900	0.92088700	-2.50217500
H	5.18749300	-0.73035200	-2.74767100
C	5.80642600	0.80954400	0.83859400
H	4.84094200	2.27729700	-0.43484800
H	3.75687800	1.46343000	0.69720700
C	7.01650900	0.50482100	-0.05372800
H	7.49683500	-0.69104200	-1.80901000
H	6.37794700	-1.46099100	-0.68695400
H	6.06659700	1.54959700	1.60490900
H	5.51580400	-0.10662500	1.36926400
H	7.84946100	0.12071900	0.54754700

H	7.36815800	1.43535700	-0.52224200
H	2.64545900	-2.04557400	0.97380000
O	4.25708900	-1.96625800	2.88474500
C	5.16710500	-1.82297700	3.96590400
H	5.84184000	-2.67838000	3.90734400
H	5.74969500	-0.89621200	3.87992800
H	4.65084300	-1.83618600	4.93464800

int84

C	-1.94423100	1.08458000	0.78788800
C	-2.60834100	0.50013500	-0.30612700
C	-1.84569300	-0.09164600	-1.32089400
C	-0.45070800	-0.12608200	-1.22733600
C	0.20798800	0.40280300	-0.11660500
C	-0.54955700	1.04591800	0.87790200
Pd	2.14049700	-0.07427600	0.19549100
H	0.13003100	-0.57120200	-2.03208900
H	-2.33806100	-0.51051900	-2.19326200
O	0.15858900	1.57208600	1.93080000
C	-0.56208300	2.04563800	3.05963600
H	0.19057200	2.35601300	3.78591900
H	-1.19289400	2.90795400	2.80723300
H	-1.18557800	1.25343500	3.49326800
H	-2.53445400	1.52832600	1.58059200
C	3.28029000	0.64952100	-1.61079200
C	4.63326900	1.26500600	-1.28009000
C	3.05817400	2.85015400	-0.79034200
C	2.33887900	1.62915900	-1.34391500
C	4.28402400	2.19247400	-0.10331400
H	5.08156300	2.91022700	0.11059300
H	4.02925800	1.65320200	0.81303700
C	4.82717500	2.32912800	-2.41859300
H	5.84036700	2.73829900	-2.36349800
H	4.69838800	1.89657300	-3.41453100
C	3.75428800	3.41700500	-2.08413800
H	4.22312200	4.38007100	-1.86369800
H	3.04232800	3.57613700	-2.89858100
H	5.45823400	0.56953300	-1.14331400
H	1.38968200	1.68849300	-1.85581200
C	3.04233400	-0.52071400	-2.53090900
O	2.10825300	-0.52713600	-3.33708600

N	3.92583900	-1.54023000	-2.38803800
H	4.44880000	-1.57705800	-1.51677700
C	3.70433700	-2.79459900	-3.09206200
H	3.64638100	-2.61162900	-4.16747700
H	4.53721500	-3.46474500	-2.87601700
H	2.76917100	-3.26948200	-2.77521800
C	2.19128800	3.77970200	0.06698500
C	2.96047900	4.98860000	0.63134800
C	0.91106200	4.25455600	-0.64966000
H	1.86462700	3.16879900	0.92122400
C	2.07869200	5.82444200	1.57215400
H	3.30286500	5.62627700	-0.19579800
H	3.85857800	4.65362200	1.16312600
C	0.02664400	5.09462200	0.28352400
H	1.18470800	4.85035900	-1.53245800
H	0.33486700	3.39553000	-1.00811600
C	0.79362800	6.28738200	0.87060300
H	2.64078400	6.68678600	1.94999800
H	1.81259800	5.21450200	2.44767100
H	-0.86737800	5.43720000	-0.25073000
H	-0.32344200	4.45060400	1.10272400
H	0.15796300	6.84779200	1.56679300
H	1.05732300	6.98034100	0.05866000
C	3.03248300	-2.55149800	2.13877000
C	3.96743500	-2.25587000	0.92391800
O	4.02997500	-1.01310800	0.54395000
O	4.63825400	-3.17102600	0.46192500
C	0.20885000	-2.47749000	1.13523900
C	0.42533700	-3.12407600	-0.08398700
C	-1.11153300	-2.34209100	1.57542800
C	-0.62426900	-3.62252100	-0.84477500
C	-2.17835700	-2.82273100	0.82149600
C	-1.93246500	-3.46154200	-0.38985000
F	-1.38621800	-1.68143500	2.70696300
F	-3.43398200	-2.63974000	1.23549200
F	-2.95767300	-3.87698700	-1.13749200
F	-0.38857900	-4.20190900	-2.02398800
F	1.66698900	-3.20533200	-0.58485700
C	2.72266700	-4.03349300	2.30198700
H	3.66907300	-4.55413900	2.46539600
H	2.06121400	-4.21125200	3.15524900

H	2.27919900	-4.45339200	1.39948000
C	3.70850100	-1.96379600	3.39095500
H	3.86675500	-0.88681700	3.28595500
H	3.11989600	-2.15967100	4.29199500
H	4.68920800	-2.43741300	3.50198900
S	1.44902000	-1.51688200	1.98567100
C	-6.21964800	1.63226000	-0.04002600
C	-6.90425500	0.49459500	-0.48943300
C	-6.17529200	-0.63804800	-0.87733100
C	-4.78718900	-0.63527500	-0.81854200
C	-4.08855600	0.50184200	-0.37166300
C	-4.82996600	1.63177300	0.01621500
H	-6.78006100	2.51280200	0.25255100
H	-6.71943200	-1.51463800	-1.21251300
H	-4.23829900	-1.53121400	-1.08885800
H	-4.30577200	2.52655400	0.33852800
C	-8.38799000	0.43309100	-0.57353400
O	-9.01994300	-0.53512300	-0.95191300
O	-8.97799300	1.58741000	-0.17868600
C	-10.41206100	1.58755900	-0.24137600
H	-10.82687600	0.80948700	0.40546400
H	-10.72252400	2.57560500	0.09924700
H	-10.75374100	1.40804200	-1.26450100

TS49

C	-1.65074800	0.89472300	0.83333600
C	-2.28619900	0.38501800	-0.31439800
C	-1.49615400	-0.00294700	-1.40839200
C	-0.11562500	0.16065300	-1.36481100
C	0.53833600	0.69315900	-0.23650000
C	-0.26224200	1.03849500	0.88103500
Pd	2.37463100	-0.19050800	0.23628800
H	0.48457000	-0.08359200	-2.23847300
H	-1.96555900	-0.38446000	-2.30917500
O	0.40888500	1.43008100	2.00332200
C	-0.33037000	1.68341400	3.19255700
H	0.40967700	1.94188000	3.95054800
H	-1.02572700	2.52297600	3.06398400
H	-0.88352200	0.79104100	3.50926500
H	-2.25461700	1.12696400	1.70116400
C	3.18368200	1.15662300	-1.09948100

C	4.24366900	2.03268800	-0.42064900
C	2.29066900	3.23399400	-0.33000500
C	1.96314800	1.92941900	-1.05214100
C	3.40715200	2.77891000	0.64294700
H	3.95302500	3.61884800	1.08387100
H	3.02467700	2.13804200	1.44294600
C	4.51175400	3.18361000	-1.43337000
H	5.33127300	3.81462900	-1.07424100
H	4.78990100	2.80765700	-2.42138800
C	3.16151100	3.96056800	-1.43328000
H	3.30550900	5.00422500	-1.14503100
H	2.67089400	3.95874600	-2.41067900
H	5.13111500	1.50291700	-0.07460200
H	1.37630700	1.98938900	-1.95759800
C	3.45209700	0.33662800	-2.33976300
O	2.68883400	0.37522700	-3.31144000
N	4.57773700	-0.42668100	-2.28929900
H	4.88923000	-0.68090600	-1.35183300
C	4.83707500	-1.39889700	-3.34093900
H	4.62383800	-0.94423700	-4.30937400
H	5.88546300	-1.70147700	-3.29904500
H	4.20577300	-2.29033200	-3.23243700
C	1.10794600	4.02861300	0.23914800
C	1.50276500	5.38446900	0.85625800
C	-0.03992300	4.22576000	-0.77184600
H	0.71402800	3.42373600	1.06054500
C	0.29555800	6.04977000	1.53588500
H	1.88071200	6.05837200	0.07582100
H	2.31546000	5.25184000	1.57976600
C	-1.25095800	4.90146800	-0.11105300
H	0.31309900	4.84143100	-1.61133200
H	-0.35041700	3.26264800	-1.18994300
C	-0.86759500	6.23311600	0.54979900
H	0.58745400	7.01508300	1.96614800
H	-0.03668900	5.42029700	2.37453300
H	-2.04841900	5.05359900	-0.84788200
H	-1.65660200	4.22041300	0.65198700
H	-1.73449500	6.67277700	1.05757500
H	-0.56576900	6.94646500	-0.23026400
C	3.10473800	-2.88791900	1.91156100
C	4.14376500	-2.47822400	0.81311900

O	4.18181800	-1.22346800	0.46383800
O	4.93248800	-3.33776400	0.44604600
C	0.31342100	-2.60921200	0.86503000
C	0.54033100	-3.10386100	-0.42381700
C	-1.00891400	-2.57339500	1.32025200
C	-0.49972500	-3.55817700	-1.22657800
C	-2.06482700	-3.01898700	0.53056600
C	-1.80664200	-3.51247300	-0.74446400
F	-1.29961300	-2.05297100	2.52088100
F	-3.32115300	-2.94418800	0.97802800
F	-2.82060700	-3.89578000	-1.52733200
F	-0.25911200	-4.00094100	-2.46282600
F	1.78003300	-3.11066400	-0.93370200
C	2.75167200	-4.36950700	1.84761600
H	3.67698600	-4.93671800	1.96694100
H	2.04999200	-4.64454700	2.64090500
H	2.33152800	-4.64111700	0.87879400
C	3.73914800	-2.51899000	3.26718200
H	3.93167400	-1.44414400	3.33813500
H	3.10341500	-2.82736500	4.10241700
H	4.69972300	-3.03779400	3.34084600
S	1.55041800	-1.79960200	1.86034300
C	-5.96396400	1.14219400	0.19950400
C	-6.56998200	0.04934300	-0.43507100
C	-5.76704100	-0.93247600	-1.03032800
C	-4.38256400	-0.82575400	-0.99416300
C	-3.76145400	0.26436600	-0.35726600
C	-4.57755900	1.24463100	0.23617300
H	-6.58233800	1.90943500	0.65093900
H	-6.24964900	-1.77750900	-1.50943700
H	-3.78111000	-1.61137900	-1.43673700
H	-4.11756700	2.11090400	0.70208600
C	-8.04754200	-0.11844900	-0.50925500
O	-8.60852500	-1.05170800	-1.05072100
O	-8.71410200	0.89161200	0.09726400
C	-10.14598900	0.78566600	0.05424500
H	-10.47951000	-0.13056400	0.54905100
H	-10.52270800	1.66438500	0.57792300
H	-10.50013600	0.77205300	-0.98013000

int85

C	0.02456600	2.19137500	-0.43195200
C	0.92510600	1.86059700	0.59784400
C	0.47009200	1.06256700	1.65104800
C	-0.84878700	0.60477000	1.66176500
C	-1.79739900	0.93441400	0.64853200
C	-1.29831500	1.73997700	-0.43148500
Pd	-1.28963100	-1.07634000	-0.22549400
H	-1.20853000	0.02733500	2.50932500
H	1.12722200	0.80468400	2.47383500
O	-2.15230500	2.01313500	-1.44823600
C	-1.69116400	2.72167900	-2.59297800
H	-2.55168700	2.78657900	-3.25952700
H	-1.35650200	3.73327700	-2.33347600
H	-0.87803400	2.18256200	-3.09407200
H	0.39220300	2.75484700	-1.27843300
C	-3.13763800	-1.09463600	0.63653700
C	-4.26979800	-1.37302800	-0.36256600
C	-4.51587700	0.84589700	0.18138100
C	-3.24016600	0.41042600	0.96052500
C	-4.40972400	-0.02520400	-1.10185400
H	-5.31658000	0.00854500	-1.71443600
H	-3.55272400	0.22660100	-1.72722400
C	-5.57934700	-1.37879900	0.46495900
H	-6.41931100	-1.66323700	-0.17829800
H	-5.55012400	-2.08506400	1.29816600
C	-5.68855800	0.10531100	0.91972000
H	-6.64827400	0.53849900	0.62513200
H	-5.60705300	0.20898200	2.00514200
H	-4.11303200	-2.25961800	-0.97906100
H	-3.38382000	0.56331800	2.03197100
C	-2.97177000	-2.02165100	1.82471500
O	-2.89824800	-1.59027200	2.98202200
N	-2.92101800	-3.34888200	1.52255300
H	-2.66213800	-3.58081600	0.56488900
C	-2.58317200	-4.31734700	2.55275400
H	-3.12611500	-4.07379200	3.46721400
H	-2.86637600	-5.31612400	2.21334500
H	-1.50893200	-4.31139000	2.78198300
C	-4.73286100	2.36730900	0.06594800
C	-5.79813900	2.75821900	-0.97692800
C	-5.05212400	3.02510100	1.42506800

H	-3.79587300	2.80938500	-0.28115700
C	-5.92877600	4.28439500	-1.10197500
H	-6.77320200	2.33599000	-0.69643200
H	-5.53986600	2.32885900	-1.95181500
C	-5.16845400	4.55134000	1.29744600
H	-5.99870800	2.62972900	1.81636200
H	-4.27932300	2.76763200	2.15960100
C	-6.22544900	4.94052100	0.25392700
H	-6.70838300	4.53961500	-1.82996200
H	-4.98602900	4.69129600	-1.49692500
H	-5.40978600	4.99566100	2.27047600
H	-4.19472700	4.96474000	0.99657300
H	-6.27827900	6.03084200	0.14802100
H	-7.21388600	4.61037700	0.60449100
C	0.37589600	-2.69011700	-2.47200500
C	-0.55904700	-3.59682000	-1.61001400
O	-1.53661300	-3.00197700	-0.98103600
O	-0.38720000	-4.80647300	-1.64752900
C	2.20183400	-1.56024500	-0.51326400
C	2.07184000	-2.18417400	0.73452800
C	3.49294000	-1.20958900	-0.92950200
C	3.17617200	-2.41990900	1.55033700
C	4.60723900	-1.43596600	-0.12728100
C	4.44639300	-2.03831500	1.11775700
F	3.68470100	-0.61512100	-2.11031600
F	5.82044800	-1.03577700	-0.51976500
F	5.50640200	-2.23859700	1.90059900
F	3.02713100	-3.00883200	2.73912700
F	0.87565000	-2.56904100	1.19366500
C	1.64002600	-3.42501800	-2.90255300
H	1.34937300	-4.28786500	-3.50539100
H	2.29455100	-2.77197500	-3.48758100
H	2.18947300	-3.80837600	-2.04049400
C	-0.43455200	-2.19241300	-3.68268500
H	-1.31149400	-1.61897300	-3.36856100
H	0.18295200	-1.57954100	-4.34640600
H	-0.78768000	-3.06543100	-4.24073300
S	0.82188100	-1.09939100	-1.54167500
C	4.70142200	1.80579500	0.87274000
C	5.05128900	3.02752300	0.28313800
C	4.04205800	3.88639300	-0.17191900

C	2.70525200	3.52354300	-0.05714000
C	2.34011600	2.29454500	0.52081700
C	3.36208800	1.45328700	0.99494800
H	5.47869200	1.12962500	1.20955800
H	4.32965000	4.83462600	-0.61332400
H	1.93414100	4.20674200	-0.39969700
H	3.10276300	0.49408000	1.42777800
C	6.46714500	3.45797400	0.11054900
O	6.80866500	4.50766400	-0.39958100
O	7.34312200	2.54480500	0.58539800
C	8.72907300	2.89589100	0.44117000
H	8.94881400	3.82226900	0.97867100
H	9.28935200	2.06265400	0.86505600
H	8.98241300	3.03451000	-0.61331300

int86

C	2.27403100	-2.55683300	0.64143300
C	2.54981200	-1.34120300	-0.01593500
C	1.47586300	-0.59602200	-0.50296000
C	0.16513700	-1.01622600	-0.24528300
C	-0.13038700	-2.15667900	0.52421800
C	0.96313200	-2.97813900	0.87427900
Pd	-1.71779900	0.24298700	-0.31621400
H	-0.52290800	-0.72993500	-1.11737900
H	1.62750500	0.27925000	-1.12302000
O	0.64211400	-4.18773000	1.42175000
C	1.69032500	-5.03573700	1.87226700
H	1.20178700	-5.91986800	2.28341500
H	2.34937900	-5.33673700	1.04847100
H	2.28590100	-4.55160600	2.65758600
H	3.10561000	-3.18719300	0.93040900
C	-2.61307900	-1.55653500	0.27969900
C	-3.61441500	-1.26017400	1.40815600
C	-1.88396400	-2.25311100	2.53135200
C	-1.53658100	-2.45884200	0.96134600
C	-2.65699900	-0.91502500	2.55094200
H	-3.16592600	-0.75445600	3.50811200
H	-2.04220600	-0.04021500	2.33893200
C	-4.21530600	-2.61511400	1.88528600
H	-5.11200500	-2.43678000	2.48690000
H	-4.51373100	-3.25285500	1.04722500

C	-3.07053700	-3.23644700	2.74518200
H	-3.36856200	-3.25501300	3.79562300
H	-2.81833300	-4.26186600	2.45743300
H	-4.35512200	-0.50163500	1.15781800
H	-1.73178500	-3.50980600	0.72460500
C	-3.19259900	-2.08533200	-0.99432200
O	-2.70251700	-3.09018500	-1.59707800
N	-4.27353500	-1.45954100	-1.48845000
H	-4.49120000	-0.55031700	-1.08253100
C	-4.77785400	-1.75761700	-2.81972700
H	-5.71712200	-1.22278200	-2.96721000
H	-4.06118400	-1.44835600	-3.59313500
H	-4.94738100	-2.83068200	-2.92282900
C	-0.71007600	-2.34224700	3.53527600
C	0.16539500	-1.06617200	3.53476200
C	-1.13399500	-2.63792700	4.99089400
H	-0.08102000	-3.18310400	3.23367700
C	1.41156900	-1.23233100	4.41333600
H	-0.42759300	-0.22985400	3.92913500
H	0.45515100	-0.78510500	2.51970500
C	0.09203200	-2.78492200	5.91033700
H	-1.78017800	-1.82965100	5.36252800
H	-1.72081500	-3.56030200	5.04227300
C	1.01452200	-1.55990200	5.85900800
H	2.02328600	-0.32259100	4.37961500
H	2.03495000	-2.04382000	4.00827500
H	-0.23382300	-2.97484000	6.94008800
H	0.66086700	-3.67243900	5.59562400
H	1.90343500	-1.72538400	6.47976600
H	0.48851600	-0.69444600	6.28653000
C	-2.56660300	2.85646600	-1.89649800
C	-3.75846300	2.24040800	-1.10434600
O	-3.56980100	1.13206200	-0.43013800
O	-4.85049000	2.77546900	-1.22317600
C	-0.70273400	3.55851300	0.21008000
C	0.00945900	4.74241500	-0.03298400
C	-1.17302300	3.35283400	1.51224200
C	0.25345900	5.67461600	0.97162700
C	-0.93392900	4.26959700	2.53296200
C	-0.21902900	5.43388700	2.26066500
F	-1.87432500	2.25720700	1.83077900

F	-1.38797700	4.03883400	3.76781400
F	0.01111200	6.31707800	3.23106400
F	0.93231200	6.79438700	0.70899400
F	0.46952600	5.01253600	-1.25952500
C	-2.53977700	2.19443300	-3.28905000
H	-3.52320100	2.34108300	-3.74607500
H	-1.77887000	2.65759600	-3.92259700
H	-2.32087700	1.12536700	-3.23358800
C	-2.70748400	4.37307700	-2.00423900
H	-2.75839800	4.84369600	-1.01936000
H	-1.87384300	4.80393700	-2.56468600
H	-3.64737100	4.59006000	-2.51541300
S	-0.88745400	2.39901100	-1.13950400
O	-0.07670800	0.02407700	-3.18637100
C	0.68033500	-0.67616000	-3.89103700
O	0.55977200	-1.94715800	-4.07286500
C	1.84782600	-0.03310200	-4.62839400
H	1.60793900	0.02662500	-5.69513100
H	2.03367700	0.97363000	-4.25035800
H	2.74364300	-0.65254000	-4.53357700
Ag	-1.06659200	-2.65568400	-2.91817100
C	6.23586200	-0.67536200	0.56423200
C	6.60835300	-0.07561000	-0.64640000
C	5.64643600	0.10787000	-1.64917300
C	4.33427900	-0.30226200	-1.44747000
C	3.94932500	-0.90631200	-0.23681800
C	4.92099100	-1.08394500	0.76337600
H	6.97568200	-0.80910000	1.34504000
H	5.95227700	0.56596800	-2.58370300
H	3.60496200	-0.17930900	-2.24162300
H	4.63350700	-1.52167900	1.71492300
C	7.99821900	0.38185200	-0.92116300
O	8.35831000	0.90836800	-1.95659000
O	8.83512000	0.14765200	0.11694300
C	10.19264800	0.56812300	-0.09112400
H	10.23890900	1.64552700	-0.27178300
H	10.72540900	0.30872100	0.82388100
H	10.62837000	0.05149200	-0.95063100
TS50			
C	1.91877500	-2.74129700	-0.00221400

C	2.29565700	-1.42402300	-0.32938700
C	1.29456900	-0.46262300	-0.49644300
C	-0.05453400	-0.77435700	-0.26085000
C	-0.40843800	-2.05284500	0.22966800
C	0.58407800	-3.05623700	0.25324500
Pd	-1.63793200	0.54374800	-0.30321300
H	-0.69959000	-0.30789300	-1.52710800
H	1.55414800	0.53251200	-0.84020100
O	0.14208700	-4.32115400	0.53603600
C	1.09933300	-5.36444700	0.65713700
H	0.53256600	-6.26293500	0.90448300
H	1.64200300	-5.52611600	-0.28276000
H	1.81803300	-5.15587300	1.46079200
H	2.67923800	-3.51102000	0.02698300
C	-2.74825900	-1.11157500	0.33896300
C	-3.45661600	-0.68776000	1.64698600
C	-1.91234600	-2.20690100	2.38881200
C	-1.78794500	-2.26070500	0.78391100
C	-2.29517000	-0.73316100	2.64801500
H	-2.61530700	-0.56645300	3.68312700
H	-1.50037000	-0.02377800	2.41362000
C	-4.33079500	-1.88054400	2.12226300
H	-5.01332400	-1.55111600	2.91248300
H	-4.94822100	-2.29310500	1.31921300
C	-3.28176100	-2.89348400	2.67192800
H	-3.42770600	-3.02600600	3.74550800
H	-3.35033400	-3.88304700	2.20850300
H	-3.99483500	0.25764600	1.57476100
H	-2.16680400	-3.23577600	0.46442000
C	-3.67262300	-1.45368100	-0.79052600
O	-3.56063000	-2.51809800	-1.48147000
N	-4.68239100	-0.61069600	-1.04400800
H	-4.61435400	0.31695100	-0.62138800
C	-5.54665700	-0.78183200	-2.20182800
H	-6.34341600	-0.03829000	-2.15281200
H	-4.98939700	-0.65205300	-3.13804800
H	-5.98095800	-1.78347200	-2.20191600
C	-0.69612500	-2.74803800	3.18266900
C	0.44555400	-1.71037300	3.30680300
C	-1.02580300	-3.27263700	4.59765100
H	-0.30861100	-3.61004200	2.63068600

C	1.70110700	-2.32076700	3.94267200
H	0.09965000	-0.88075500	3.93907200
H	0.69360500	-1.27599700	2.33653500
C	0.21841000	-3.87306100	5.27579400
H	-1.42601500	-2.45484100	5.21451700
H	-1.80163700	-4.04325300	4.55328600
C	1.39007200	-2.88438200	5.33516300
H	2.49906800	-1.57041300	4.00022200
H	2.07589500	-3.12626300	3.29328700
H	-0.03721600	-4.22376900	6.28304400
H	0.53025800	-4.76147600	4.70694100
H	2.27531200	-3.36675300	5.76746800
H	1.12720500	-2.05261000	6.00418400
C	-2.19324500	3.38352600	-1.68402800
C	-3.43713700	2.87931500	-0.88491500
O	-3.35682200	1.73919600	-0.25825900
O	-4.45434600	3.55488100	-0.96521300
C	-0.15599600	3.64347000	0.37038100
C	0.70140900	4.73648300	0.17581400
C	-0.59428200	3.39857200	1.67752000
C	1.11140900	5.54721800	1.23018100
C	-0.18955100	4.19414600	2.74675500
C	0.66453900	5.27148100	2.52135400
F	-1.42138600	2.38335200	1.95410600
F	-0.61781400	3.93030000	3.98390000
F	1.05283000	6.03866200	3.53876400
F	1.92454000	6.58429700	1.01318600
F	1.14340000	5.03680400	-1.05061900
C	-2.30944100	2.83350600	-3.11995700
H	-3.27854900	3.14852600	-3.51783700
H	-1.51629600	3.23611400	-3.75658700
H	-2.25225200	1.74164500	-3.14850000
C	-2.11721200	4.90855000	-1.67644500
H	-2.05263500	5.30126800	-0.65868100
H	-1.25823900	5.26372000	-2.25180500
H	-3.04055300	5.29223700	-2.11432100
S	-0.56965800	2.63619000	-1.04613300
O	-0.36574200	-0.08688400	-2.95640700
C	0.27839200	-0.94735700	-3.63785500
O	0.01656300	-2.18975600	-3.68739000
C	1.46798700	-0.47432500	-4.44867100

H	1.44960800	-0.92269700	-5.44447700
H	1.48488400	0.61390500	-4.51617000
H	2.38002900	-0.81965100	-3.95018100
Ag	-1.73032200	-2.68145000	-2.57157000
C	6.06140300	-1.35292400	0.10881600
C	6.44725900	-0.43206000	-0.87484800
C	5.46684400	0.16515700	-1.67861300
C	4.12581600	-0.15466300	-1.50531300
C	3.72476400	-1.08155100	-0.52493400
C	4.71782000	-1.66967700	0.27930800
H	6.81557200	-1.80687400	0.74137000
H	5.78012800	0.87256700	-2.43910500
H	3.38066100	0.30407800	-2.14706800
H	4.42654600	-2.35984700	1.06538400
C	7.86695200	-0.05036500	-1.10562200
O	8.23951600	0.74269300	-1.94935300
O	8.71719100	-0.68578600	-0.26499600
C	10.10344000	-0.35215300	-0.43703500
H	10.26529300	0.71693600	-0.27431100
H	10.64279000	-0.93980900	0.30602900
H	10.43881100	-0.60574900	-1.44640700

int87

C	1.91877500	-2.74129700	-0.00221400
C	2.29565700	-1.42402300	-0.32938700
C	1.29456900	-0.46262300	-0.49644300
C	-0.05453400	-0.77435700	-0.26085000
C	-0.40843800	-2.05284500	0.22966800
C	0.58407800	-3.05623700	0.25324500
Pd	-1.63793200	0.54374800	-0.30321300
H	-0.69959000	-0.30789300	-1.52710800
H	1.55414800	0.53251200	-0.84020100
O	0.14208700	-4.32115400	0.53603600
C	1.09933300	-5.36444700	0.65713700
H	0.53256600	-6.26293500	0.90448300
H	1.64200300	-5.52611600	-0.28276000
H	1.81803300	-5.15587300	1.46079200
H	2.67923800	-3.51102000	0.02698300
C	-2.74825900	-1.11157500	0.33896300
C	-3.45661600	-0.68776000	1.64698600
C	-1.91234600	-2.20690100	2.38881200

C	-1.78794500	-2.26070500	0.78391100
C	-2.29517000	-0.73316100	2.64801500
H	-2.61530700	-0.56645300	3.68312700
H	-1.50037000	-0.02377800	2.41362000
C	-4.33079500	-1.88054400	2.12226300
H	-5.01332400	-1.55111600	2.91248300
H	-4.94822100	-2.29310500	1.31921300
C	-3.28176100	-2.89348400	2.67192800
H	-3.42770600	-3.02600600	3.74550800
H	-3.35033400	-3.88304700	2.20850300
H	-3.99483500	0.25764600	1.57476100
H	-2.16680400	-3.23577600	0.46442000
C	-3.67262300	-1.45368100	-0.79052600
O	-3.56063000	-2.51809800	-1.48147000
N	-4.68239100	-0.61069600	-1.04400800
H	-4.61435400	0.31695100	-0.62138800
C	-5.54665700	-0.78183200	-2.20182800
H	-6.34341600	-0.03829000	-2.15281200
H	-4.98939700	-0.65205300	-3.13804800
H	-5.98095800	-1.78347200	-2.20191600
C	-0.69612500	-2.74803800	3.18266900
C	0.44555400	-1.71037300	3.30680300
C	-1.02580300	-3.27263700	4.59765100
H	-0.30861100	-3.61004200	2.63068600
C	1.70110700	-2.32076700	3.94267200
H	0.09965000	-0.88075500	3.93907200
H	0.69360500	-1.27599700	2.33653500
C	0.21841000	-3.87306100	5.27579400
H	-1.42601500	-2.45484100	5.21451700
H	-1.80163700	-4.04325300	4.55328600
C	1.39007200	-2.88438200	5.33516300
H	2.49906800	-1.57041300	4.00022200
H	2.07589500	-3.12626300	3.29328700
H	-0.03721600	-4.22376900	6.28304400
H	0.53025800	-4.76147600	4.70694100
H	2.27531200	-3.36675300	5.76746800
H	1.12720500	-2.05261000	6.00418400
C	-2.19324500	3.38352600	-1.68402800
C	-3.43713700	2.87931500	-0.88491500
O	-3.35682200	1.73919600	-0.25825900
O	-4.45434600	3.55488100	-0.96521300

C	-0.15599600	3.64347000	0.37038100
C	0.70140900	4.73648300	0.17581400
C	-0.59428200	3.39857200	1.67752000
C	1.11140900	5.54721800	1.23018100
C	-0.18955100	4.19414600	2.74675500
C	0.66453900	5.27148100	2.52135400
F	-1.42138600	2.38335200	1.95410600
F	-0.61781400	3.93030000	3.98390000
F	1.05283000	6.03866200	3.53876400
F	1.92454000	6.58429700	1.01318600
F	1.14340000	5.03680400	-1.05061900
C	-2.30944100	2.83350600	-3.11995700
H	-3.27854900	3.14852600	-3.51783700
H	-1.51629600	3.23611400	-3.75658700
H	-2.25225200	1.74164500	-3.14850000
C	-2.11721200	4.90855000	-1.67644500
H	-2.05263500	5.30126800	-0.65868100
H	-1.25823900	5.26372000	-2.25180500
H	-3.04055300	5.29223700	-2.11432100
S	-0.56965800	2.63619000	-1.04613300
O	-0.36574200	-0.08688400	-2.95640700
C	0.27839200	-0.94735700	-3.63785500
O	0.01656300	-2.18975600	-3.68739000
C	1.46798700	-0.47432500	-4.44867100
H	1.44960800	-0.92269700	-5.44447700
H	1.48488400	0.61390500	-4.51617000
H	2.38002900	-0.81965100	-3.95018100
Ag	-1.73032200	-2.68145000	-2.57157000
C	6.06140300	-1.35292400	0.10881600
C	6.44725900	-0.43206000	-0.87484800
C	5.46684400	0.16515700	-1.67861300
C	4.12581600	-0.15466300	-1.50531300
C	3.72476400	-1.08155100	-0.52493400
C	4.71782000	-1.66967700	0.27930800
H	6.81557200	-1.80687400	0.74137000
H	5.78012800	0.87256700	-2.43910500
H	3.38066100	0.30407800	-2.14706800
H	4.42654600	-2.35984700	1.06538400
C	7.86695200	-0.05036500	-1.10562200
O	8.23951600	0.74269300	-1.94935300
O	8.71719100	-0.68578600	-0.26499600

C	10.10344000	-0.35215300	-0.43703500
H	10.26529300	0.71693600	-0.27431100
H	10.64279000	-0.93980900	0.30602900
H	10.43881100	-0.60574900	-1.44640700

int88

C	1.91877500	-2.74129700	-0.00221400
C	2.29565700	-1.42402300	-0.32938700
C	1.29456900	-0.46262300	-0.49644300
C	-0.05453400	-0.77435700	-0.26085000
C	-0.40843800	-2.05284500	0.22966800
C	0.58407800	-3.05623700	0.25324500
Pd	-1.63793200	0.54374800	-0.30321300
H	-0.69959000	-0.30789300	-1.52710800
H	1.55414800	0.53251200	-0.84020100
O	0.14208700	-4.32115400	0.53603600
C	1.09933300	-5.36444700	0.65713700
H	0.53256600	-6.26293500	0.90448300
H	1.64200300	-5.52611600	-0.28276000
H	1.81803300	-5.15587300	1.46079200
H	2.67923800	-3.51102000	0.02698300
C	-2.74825900	-1.11157500	0.33896300
C	-3.45661600	-0.68776000	1.64698600
C	-1.91234600	-2.20690100	2.38881200
C	-1.78794500	-2.26070500	0.78391100
C	-2.29517000	-0.73316100	2.64801500
H	-2.61530700	-0.56645300	3.68312700
H	-1.50037000	-0.02377800	2.41362000
C	-4.33079500	-1.88054400	2.12226300
H	-5.01332400	-1.55111600	2.91248300
H	-4.94822100	-2.29310500	1.31921300
C	-3.28176100	-2.89348400	2.67192800
H	-3.42770600	-3.02600600	3.74550800
H	-3.35033400	-3.88304700	2.20850300
H	-3.99483500	0.25764600	1.57476100
H	-2.16680400	-3.23577600	0.46442000
C	-3.67262300	-1.45368100	-0.79052600
O	-3.56063000	-2.51809800	-1.48147000
N	-4.68239100	-0.61069600	-1.04400800
H	-4.61435400	0.31695100	-0.62138800
C	-5.54665700	-0.78183200	-2.20182800

H	-6.34341600	-0.03829000	-2.15281200
H	-4.98939700	-0.65205300	-3.13804800
H	-5.98095800	-1.78347200	-2.20191600
C	-0.69612500	-2.74803800	3.18266900
C	0.44555400	-1.71037300	3.30680300
C	-1.02580300	-3.27263700	4.59765100
H	-0.30861100	-3.61004200	2.63068600
C	1.70110700	-2.32076700	3.94267200
H	0.09965000	-0.88075500	3.93907200
H	0.69360500	-1.27599700	2.33653500
C	0.21841000	-3.87306100	5.27579400
H	-1.42601500	-2.45484100	5.21451700
H	-1.80163700	-4.04325300	4.55328600
C	1.39007200	-2.88438200	5.33516300
H	2.49906800	-1.57041300	4.00022200
H	2.07589500	-3.12626300	3.29328700
H	-0.03721600	-4.22376900	6.28304400
H	0.53025800	-4.76147600	4.70694100
H	2.27531200	-3.36675300	5.76746800
H	1.12720500	-2.05261000	6.00418400
C	-2.19324500	3.38352600	-1.68402800
C	-3.43713700	2.87931500	-0.88491500
O	-3.35682200	1.73919600	-0.25825900
O	-4.45434600	3.55488100	-0.96521300
C	-0.15599600	3.64347000	0.37038100
C	0.70140900	4.73648300	0.17581400
C	-0.59428200	3.39857200	1.67752000
C	1.11140900	5.54721800	1.23018100
C	-0.18955100	4.19414600	2.74675500
C	0.66453900	5.27148100	2.52135400
F	-1.42138600	2.38335200	1.95410600
F	-0.61781400	3.93030000	3.98390000
F	1.05283000	6.03866200	3.53876400
F	1.92454000	6.58429700	1.01318600
F	1.14340000	5.03680400	-1.05061900
C	-2.30944100	2.83350600	-3.11995700
H	-3.27854900	3.14852600	-3.51783700
H	-1.51629600	3.23611400	-3.75658700
H	-2.25225200	1.74164500	-3.14850000
C	-2.11721200	4.90855000	-1.67644500
H	-2.05263500	5.30126800	-0.65868100

H	-1.25823900	5.26372000	-2.25180500
H	-3.04055300	5.29223700	-2.11432100
S	-0.56965800	2.63619000	-1.04613300
O	-0.36574200	-0.08688400	-2.95640700
C	0.27839200	-0.94735700	-3.63785500
O	0.01656300	-2.18975600	-3.68739000
C	1.46798700	-0.47432500	-4.44867100
H	1.44960800	-0.92269700	-5.44447700
H	1.48488400	0.61390500	-4.51617000
H	2.38002900	-0.81965100	-3.95018100
Ag	-1.73032200	-2.68145000	-2.57157000
C	6.06140300	-1.35292400	0.10881600
C	6.44725900	-0.43206000	-0.87484800
C	5.46684400	0.16515700	-1.67861300
C	4.12581600	-0.15466300	-1.50531300
C	3.72476400	-1.08155100	-0.52493400
C	4.71782000	-1.66967700	0.27930800
H	6.81557200	-1.80687400	0.74137000
H	5.78012800	0.87256700	-2.43910500
H	3.38066100	0.30407800	-2.14706800
H	4.42654600	-2.35984700	1.06538400
C	7.86695200	-0.05036500	-1.10562200
O	8.23951600	0.74269300	-1.94935300
O	8.71719100	-0.68578600	-0.26499600
C	10.10344000	-0.35215300	-0.43703500
H	10.26529300	0.71693600	-0.27431100
H	10.64279000	-0.93980900	0.30602900
H	10.43881100	-0.60574900	-1.44640700

TS51

C	-0.11806700	2.26640200	-2.47583200
C	-0.63014500	2.30928600	-1.16605900
C	-0.20042800	1.35074400	-0.23843400
C	0.77149900	0.41670200	-0.60669800
C	1.38017600	0.43894900	-1.87068800
C	0.85766100	1.33379700	-2.82892600
Pd	1.16075200	-1.11715000	0.61057900
H	-0.62264000	1.33058100	0.75862500
O	1.35470400	1.20341300	-4.09604500
C	0.85418200	2.05168300	-5.11797200
H	1.39617200	1.77892600	-6.02470200

H	-0.22137700	1.90055000	-5.27598600
H	1.04132900	3.10991800	-4.89456700
H	-0.51430600	2.94988800	-3.21554700
C	2.53744100	-1.59725600	-0.98502200
C	3.99857600	-1.60689100	-0.52412400
C	3.98541900	0.07090600	-2.07834100
C	2.50320300	-0.51701700	-2.12803900
C	4.32771500	-0.10493600	-0.57941400
H	5.37962500	0.09990300	-0.35799500
H	3.69997000	0.50122200	0.07587700
C	4.91237000	-2.16192000	-1.65147200
H	5.91974800	-2.33477400	-1.25726800
H	4.55673900	-3.11274900	-2.05607600
C	4.90366200	-1.01713700	-2.70294900
H	5.91232100	-0.61675700	-2.84554300
H	4.54496900	-1.34454100	-3.68276200
H	4.15420300	-2.10710500	0.43508300
H	2.34807800	-0.99855900	-3.09972500
C	1.91426000	-2.89378400	-1.38844800
O	0.92682800	-2.95196400	-2.19063800
C	1.68609500	-5.29711600	-0.97516600
H	2.35186400	-6.11372100	-0.69135300
H	0.81500700	-5.29063900	-0.30523500
H	1.33765500	-5.44754200	-1.99719300
C	-3.15274000	-1.22690600	2.47821400
C	-1.96716900	-1.48092700	1.52046800
O	-2.20629800	-2.30704400	0.57984300
O	-0.89210600	-0.86583300	1.72862400
C	-4.73097700	-0.87922600	0.10952100
C	-3.93084900	-0.75162200	-1.03244800
C	-5.81112200	-1.76713400	0.03479700
C	-4.15622700	-1.50572900	-2.17620700
C	-6.06989900	-2.51369000	-1.11383600
C	-5.22928900	-2.39244400	-2.21847900
F	-6.61231800	-1.95326600	1.08861500
F	-7.10249700	-3.36325500	-1.15411300
F	-5.44582400	-3.12931500	-3.30963700
F	-3.29963800	-1.43503700	-3.20961600
F	-2.85717300	0.05047900	-1.03118000
C	-3.87198200	-2.53536300	2.81486700
H	-3.18141500	-3.19986300	3.34732600

H	-4.73754000	-2.34211300	3.45306600
H	-4.19760400	-3.05020100	1.91105900
C	-2.71576000	-0.48109200	3.74233300
H	-2.22957900	0.46651100	3.50203300
H	-3.57313800	-0.29169700	4.39464600
H	-1.99659200	-1.09942800	4.28824000
S	-4.33162600	-0.01913100	1.61149800
Ag	-0.84766100	-2.42413300	-1.05273600
C	1.84270100	1.35229100	3.86478300
C	3.20952200	1.65677800	3.81862200
C	4.08945900	0.77340100	3.17847900
C	3.61020000	-0.38212800	2.56689000
C	2.23288100	-0.61193500	2.55021300
C	1.34311400	0.20020400	3.26265900
H	1.17382200	2.02791600	4.38808700
H	5.15312200	0.98282900	3.16838600
H	4.29909800	-1.07127500	2.10167600
H	0.28862500	-0.03334100	3.30189300
I	1.68178100	-3.06358800	2.55271500
C	3.67053700	2.90161300	4.48880100
O	2.94462500	3.66894800	5.09150000
O	5.00372900	3.09723000	4.35426700
C	5.50769200	4.28838100	4.97911200
H	5.02728200	5.17597800	4.55861600
H	5.32038700	4.26732200	6.05618500
H	6.57854600	4.29784100	4.77540600
C	-3.61178000	4.00450900	0.45254900
C	-3.53465500	5.29577700	-0.08879300
C	-2.49640400	5.60538200	-0.97796800
C	-1.55672600	4.64137800	-1.32200900
C	-1.62846100	3.33977400	-0.79132700
C	-2.67113300	3.04182900	0.10396300
H	-4.41542300	3.75536100	1.13640400
H	-2.44079000	6.61164700	-1.37970700
H	-0.74090000	4.90283600	-1.98920200
H	-2.76430800	2.04104700	0.50661200
C	-4.51313600	6.36552600	0.24024300
O	-4.48107400	7.49627000	-0.20888700
O	-5.46667700	5.94762800	1.10782200
C	-6.44076600	6.93983500	1.46212400
H	-6.97556900	7.29067400	0.57502000

H	-7.12550900	6.44801600	2.15346600
H	-5.96161900	7.79840900	1.94098500
C	4.18423700	1.48206500	-2.67374700
C	5.34828400	2.26830600	-2.03290100
C	4.37597800	1.46589900	-4.20587800
H	3.27645700	2.05999000	-2.45908400
C	5.44718800	3.69147400	-2.60728700
H	6.29558800	1.73622100	-2.20596300
H	5.21500300	2.33024900	-0.94753500
C	4.42904100	2.88827200	-4.77834100
H	5.32330400	0.96361300	-4.44501000
H	3.57883600	0.88874200	-4.67798300
C	5.56912100	3.69246300	-4.13757300
H	6.29543200	4.22038800	-2.15594200
H	4.54379800	4.24893000	-2.32077900
H	4.54870400	2.85678400	-5.86842200
H	3.47334300	3.39368700	-4.57992100
H	5.58072100	4.72095000	-4.51830900
H	6.52947000	3.23977300	-4.42378400
N	2.41323100	-4.03956000	-0.88821600
H	3.12379100	-3.95791300	-0.17552600

int89

C	-0.20511600	2.72835800	-2.21254100
C	-0.78734100	2.55141500	-0.94471900
C	-0.34717500	1.48991400	-0.14291100
C	0.70918500	0.68441200	-0.57345900
C	1.37710800	0.91809400	-1.77957600
C	0.83895800	1.90727600	-2.63533700
Pd	1.13223600	-1.06063100	0.35185400
H	-0.82481600	1.30022900	0.80954200
O	1.39807900	1.97803100	-3.87809500
C	0.91535900	2.95080300	-4.79409500
H	1.51521800	2.83265300	-5.69746200
H	-0.14272600	2.78664400	-5.03366000
H	1.04719900	3.96904500	-4.40748700
H	-0.59938000	3.49334700	-2.86874100
C	2.59686000	-1.21563400	-1.23909800
C	4.05945400	-1.28499900	-0.79084200
C	4.01531500	0.66987500	-1.98965300
C	2.54920700	0.06346700	-2.15317400

C	4.37515600	0.20530600	-0.56165600
H	5.42940900	0.36452800	-0.31645400
H	3.76464200	0.67670000	0.20561700
C	4.98315100	-1.58000600	-2.01350100
H	5.99133900	-1.80017300	-1.64773300
H	4.66255800	-2.43702100	-2.60868100
C	4.95093600	-0.25085700	-2.81934100
H	5.95058000	0.19051500	-2.87885500
H	4.59646400	-0.38517500	-3.84541500
H	4.23736800	-1.95342300	0.05258600
H	2.41672700	-0.24010900	-3.19737400
C	1.97454200	-2.39564300	-1.93589300
O	0.89482700	-2.25661000	-2.60403600
C	1.88965500	-4.79973400	-2.35301600
H	2.61839200	-5.60974700	-2.40351200
H	1.08593700	-5.07628100	-1.66047700
H	1.47036500	-4.61889800	-3.34299200
C	-2.83802600	-1.37186800	2.50712100
C	-1.73528200	-1.46862800	1.43470400
O	-2.03987600	-2.15912800	0.40923800
O	-0.64881200	-0.86994400	1.65252300
C	-4.69107200	-1.00150700	0.34046100
C	-4.03062400	-0.75341800	-0.86924500
C	-5.70442200	-1.96777700	0.32522100
C	-4.31401900	-1.47163100	-2.02229300
C	-6.02659600	-2.67713500	-0.83154000
C	-5.31572100	-2.43924300	-2.00591200
F	-6.37270100	-2.26948000	1.44237300
F	-6.99214500	-3.60218900	-0.81465100
F	-5.58620800	-3.14034000	-3.10834900
F	-3.57108400	-1.28914500	-3.12918900
F	-3.02711200	0.13384400	-0.93597700
C	-3.41382400	-2.76034700	2.79783000
H	-2.62062800	-3.39933400	3.20235100
H	-4.22271100	-2.68946300	3.52867300
H	-3.78820400	-3.23160500	1.88875700
C	-2.33630600	-0.68491800	3.78009200
H	-1.94389200	0.31238000	3.57153200
H	-3.13968100	-0.61438200	4.51898100
H	-1.52064700	-1.27826300	4.20212700
S	-4.18343800	-0.20512800	1.84567300

Ag	-0.82184400	-2.21836600	-1.31483100
C	2.53686200	1.59895700	3.42376200
C	3.59893900	0.90058400	4.00655200
C	3.96247300	-0.34930000	3.49003800
C	3.28445900	-0.88787000	2.39644800
C	2.23715800	-0.16779600	1.81927300
C	1.84805400	1.06990700	2.33087300
H	2.25901900	2.56603700	3.83043100
H	4.76966600	-0.90990200	3.94793000
H	3.56212500	-1.86591900	2.03157100
H	1.03516500	1.63297800	1.89877200
I	1.30234600	-3.73524100	1.33695100
C	4.29726500	1.52479900	5.16355000
O	4.01199800	2.60672400	5.64001000
O	5.30260700	0.75202500	5.63765400
C	6.01391100	1.30053200	6.75804300
H	6.47237800	2.25716500	6.49272400
H	5.33827800	1.46015900	7.60281500
H	6.77786500	0.56521100	7.01110300
C	-3.87298300	3.89081200	0.81170100
C	-3.83671700	5.24635600	0.45636500
C	-2.79872900	5.71274200	-0.36138500
C	-1.81685700	4.84022400	-0.81516600
C	-1.84639600	3.47587600	-0.47006000
C	-2.89160900	3.01974500	0.35208100
H	-4.67410100	3.52064000	1.44150600
H	-2.77470700	6.76635300	-0.61884200
H	-0.99984900	5.22408900	-1.41844000
H	-2.95300200	1.97243000	0.61691400
C	-4.85715400	6.22633300	0.91593700
O	-4.86228500	7.40755300	0.62378400
O	-5.79825200	5.66046100	1.70847000
C	-6.80966500	6.55937900	2.18753200
H	-7.35824800	7.00392300	1.35245200
H	-7.47413900	5.95422500	2.80459400
H	-6.36246200	7.36398000	2.77778800
C	4.16784300	2.17740200	-2.29047200
C	5.28386100	2.86280800	-1.47317800
C	4.39618500	2.47393600	-3.78865000
H	3.23181300	2.66823100	-1.99388100
C	5.32840700	4.37574200	-1.74764900

H	6.25589800	2.41477000	-1.72702100
H	5.13023100	2.69841900	-0.40146800
C	4.38993600	3.98338200	-4.06444300
H	5.37324500	2.07174600	-4.08879900
H	3.64266700	1.96630100	-4.39322600
C	5.47614200	4.69184000	-3.24264700
H	6.14366900	4.83666100	-1.17729500
H	4.39597300	4.82603600	-1.37787200
H	4.53172700	4.17725700	-5.13481700
H	3.40635500	4.39496300	-3.79593700
H	5.44191300	5.77552900	-3.40747200
H	6.46282700	4.35228100	-3.58925700
N	2.56124100	-3.59347000	-1.88417800
H	3.30048700	-3.70827800	-1.20484500

int90

C	-3.58893200	1.56624700	-1.65826300
C	-3.68847500	0.22582600	-1.24434700
C	-2.52096600	-0.46682100	-0.89021100
C	-1.28735700	0.18006900	-0.94184000
C	-1.17379100	1.53120300	-1.31346800
C	-2.34797300	2.20167600	-1.71359300
Pd	0.41452300	-0.76825900	-0.43664100
H	-2.58724700	-1.48781200	-0.52806000
O	-2.16621900	3.48237900	-2.15384200
C	-3.30537400	4.24777800	-2.52163100
H	-2.92555300	5.22964200	-2.80781500
H	-3.83489900	3.80170600	-3.37282500
H	-4.00097500	4.36000100	-1.68012700
H	-4.48510700	2.08488000	-1.97399200
C	1.20289900	0.95009400	-1.38284400
C	2.40583700	1.49952500	-0.63574100
C	0.92718200	3.26596700	-0.66669300
C	0.20569600	2.11812400	-1.50764400
C	1.74677800	2.46076700	0.37503200
H	2.49009100	3.08209100	0.88566800
H	1.15307900	1.94704100	1.12788400
C	3.07208700	2.49967900	-1.62992700
H	4.05803800	2.77304000	-1.24521100
H	3.22304600	2.07192800	-2.62270100
C	2.08946100	3.70502100	-1.62222700

H	2.59729600	4.58553200	-1.22877700
H	1.72016100	3.96087800	-2.61967000
H	3.07479400	0.73746700	-0.23638100
H	0.21995400	2.45148800	-2.55114700
C	1.34761000	0.18408000	-2.69560200
O	1.08755500	0.64188100	-3.79054000
N	1.55560300	-1.17739600	-2.46473600
H	2.30228900	-1.40031300	-1.80793100
C	1.40483200	-2.12846900	-3.56662500
H	1.36548800	-3.13084700	-3.13962900
H	0.47725200	-1.90782500	-4.09606100
H	2.24150900	-2.05153300	-4.26647200
C	-1.17159600	0.78650500	3.31954700
C	-1.00556500	-0.32510600	4.15441600
C	-0.47114500	-1.50355200	3.62190600
C	-0.07780300	-1.56730100	2.28505600
C	-0.21460900	-0.44090100	1.45923900
C	-0.79157900	0.71955300	1.98029200
H	-1.60918100	1.69771200	3.71234700
H	-0.36649600	-2.36847100	4.26922200
H	0.30429100	-2.50351900	1.90101600
H	-0.96662200	1.57105800	1.34548500
C	-1.39022400	-0.31749300	5.59172700
O	-1.26816400	-1.26481500	6.34486400
O	-1.89836100	0.87486500	5.98483600
C	-2.29062700	0.94175900	7.36432600
H	-2.67347100	1.95151300	7.51381500
H	-3.06450100	0.20042800	7.58167900
H	-1.43469000	0.75359800	8.01835700
C	0.05747400	4.44948000	-0.18440000
C	-1.02921400	4.06059800	0.83883000
C	0.87228900	5.62202800	0.41375600
H	-0.45676800	4.82930500	-1.07658700
C	-1.94616800	5.24121700	1.18797900
H	-0.53990900	3.70835900	1.75766100
H	-1.63680500	3.23704500	0.46387400
C	-0.02440100	6.81661900	0.77771700
H	1.39905200	5.27489000	1.31417400
H	1.63918400	5.96932100	-0.28357800
C	-1.14437800	6.42233500	1.74753100
H	-2.71235800	4.92058100	1.90414300

H	-2.47759700	5.55897000	0.27915900
H	0.58525200	7.62306600	1.20255100
H	-0.47191300	7.21553200	-0.14404300
H	-1.80036000	7.27820600	1.94693700
H	-0.70286700	6.13143200	2.71138900
C	3.12418300	-3.79594100	0.94444400
C	2.09251300	-2.88357500	0.25648500
O	2.38009600	-1.62843000	0.19264800
O	1.00021400	-3.34113600	-0.14140800
C	5.19665900	-2.25054700	-0.37240600
C	4.92674800	-1.60863100	-1.58559400
C	5.89131500	-1.51112000	0.59233600
C	5.28022200	-0.28633000	-1.82400600
C	6.25350100	-0.18183800	0.37847400
C	5.94746000	0.43094100	-0.83448900
F	6.20896000	-2.05522600	1.77115400
F	6.89795700	0.50734700	1.32553200
F	6.27868900	1.70917300	-1.04134800
F	4.94568400	0.30813700	-2.97838700
F	4.24974500	-2.24746000	-2.55597000
C	3.43970400	-3.23172000	2.33531900
H	2.52324300	-3.22084300	2.93697100
H	4.18390900	-3.85216600	2.83983200
H	3.80643200	-2.20829100	2.27389100
C	2.61836100	-5.24018500	1.02945500
H	2.36900200	-5.63649500	0.04341100
H	3.36425900	-5.88408100	1.50518100
H	1.70644600	-5.25960500	1.63193800
S	4.68240500	-3.93261900	-0.11855100
C	-7.38931100	-0.35260400	-0.65859900
C	-7.52999900	-1.69678400	-1.02865000
C	-6.40634700	-2.41018300	-1.46872500
C	-5.16594400	-1.78490200	-1.53914900
C	-5.01263400	-0.43642800	-1.17078200
C	-6.14766300	0.26704500	-0.72767900
H	-8.26551300	0.18361800	-0.30985800
H	-6.51334900	-3.44805600	-1.76230300
H	-4.30692500	-2.33808100	-1.90614200
H	-6.04424700	1.29981800	-0.40914100
C	-8.88339500	-2.30772000	-0.93330000
O	-9.88134300	-1.71974500	-0.56094200

O	-8.89275100	-3.60825100	-1.30988900
C	-10.17395500	-4.25227000	-1.23706200
H	-10.55614000	-4.23578600	-0.21266500
H	-10.89596000	-3.74935100	-1.88632500
H	-10.00821600	-5.27748200	-1.56854500

TS52

C	-3.61355600	1.93260400	-1.14319800
C	-3.80784300	0.56003100	-0.90380900
C	-2.70913900	-0.22164000	-0.54153900
C	-1.42901000	0.34438400	-0.42552300
C	-1.21088200	1.71245800	-0.72397800
C	-2.33679400	2.48837300	-1.07894800
Pd	0.35203700	-0.72470100	-0.49846900
H	-2.86390500	-1.26191800	-0.28273800
O	-2.06420000	3.79080400	-1.37977800
C	-3.11824500	4.62998700	-1.83321400
H	-2.65966600	5.59812800	-2.03846100
H	-3.57485500	4.24162300	-2.75194100
H	-3.89274700	4.75330100	-1.06545300
H	-4.46221400	2.53920900	-1.43256100
C	1.09745100	1.02312700	-1.29397600
C	2.44055600	1.40470800	-0.65739900
C	1.09664900	3.21527000	-0.21161000
C	0.17576400	2.22680800	-1.04664200
C	2.01202200	2.23601700	0.56781800
H	2.86182900	2.74264700	1.03827900
H	1.50986500	1.63812600	1.32587800
C	3.04296400	2.50663600	-1.57237100
H	4.07358100	2.70069300	-1.26265000
H	3.07475500	2.21840100	-2.62538200
C	2.11789400	3.72509700	-1.29096200
H	2.70838600	4.55598700	-0.90427200
H	1.60395400	4.08271200	-2.18748500
H	3.10496700	0.56298100	-0.47020600
H	0.02078700	2.70620600	-2.01793800
C	1.12684800	0.59724100	-2.78016300
O	0.51314800	1.23588800	-3.63282700
N	1.89725000	-0.48334600	-3.06945900
H	2.35200400	-0.98104000	-2.31275100
C	2.09035700	-0.95894600	-4.42909600

H	1.94954900	-2.04217500	-4.46908700
H	1.36161000	-0.46682100	-5.07267000
H	3.10170700	-0.72297300	-4.77415400
C	-0.69928300	0.13671000	3.61897500
C	-1.06278600	-1.16802500	3.97364200
C	-1.26992000	-2.11856000	2.96443500
C	-1.11083300	-1.77965100	1.62488100
C	-0.69373800	-0.47879500	1.28174600
C	-0.52407600	0.48101800	2.28046700
H	-0.56195000	0.88690800	4.38964400
H	-1.56304800	-3.12458500	3.24577700
H	-1.27462200	-2.53664800	0.86603900
H	-0.28527000	1.49656800	2.02053500
C	-1.25577900	-1.59480800	5.38507800
O	-1.56259200	-2.72064100	5.72857400
O	-1.04997400	-0.58505700	6.26296100
C	-1.22144200	-0.93761900	7.64478300
H	-1.02526400	-0.02544400	8.20844900
H	-2.23916500	-1.29280800	7.82809600
H	-0.51990100	-1.72592200	7.93112900
C	0.39700500	4.37360300	0.53412900
C	-0.61738400	3.93115800	1.60731800
C	1.37293600	5.37318700	1.19960300
H	-0.16676700	4.92337600	-0.23193100
C	-1.39349300	5.12062200	2.19019500
H	-0.07059100	3.44097700	2.42605400
H	-1.32069200	3.20077500	1.20575800
C	0.63078600	6.57705100	1.80384600
H	1.93472900	4.85594500	1.99070800
H	2.11251700	5.74473600	0.48535400
C	-0.44097300	6.14789800	2.81366500
H	-2.11960800	4.76833300	2.93271400
H	-1.97132200	5.59554600	1.38441500
H	1.34857800	7.25918100	2.27508100
H	0.15256200	7.14066300	0.98987000
H	-0.99561500	7.02030200	3.17956000
H	0.04825600	5.69613600	3.68850100
C	2.92075200	-3.79524600	0.54345500
C	1.90190900	-2.89034000	-0.16639500
O	2.28422100	-1.68636800	-0.44921200
O	0.72410600	-3.26452000	-0.32598900

C	5.09435000	-2.29390000	-0.66169000
C	4.88377200	-1.63400900	-1.87776400
C	5.77166900	-1.58486500	0.33642500
C	5.27776300	-0.31745000	-2.08499900
C	6.17669400	-0.26346700	0.15194200
C	5.93024500	0.36918500	-1.06372500
F	6.02820500	-2.14958900	1.52173800
F	6.80298700	0.39888200	1.13131300
F	6.29920600	1.64187300	-1.24239000
F	4.99672500	0.30818600	-3.23727200
F	4.22511300	-2.24546600	-2.87322200
C	3.16778100	-3.19373300	1.93664600
H	2.21818100	-3.15978000	2.48435000
H	3.87854200	-3.80561400	2.49667100
H	3.55295900	-2.17642800	1.86626800
C	2.40409100	-5.23509900	0.64775500
H	2.20194800	-5.66095600	-0.33778400
H	3.12652600	-5.86664800	1.17326300
H	1.46558700	-5.23216900	1.20653600
S	4.52323100	-3.96304100	-0.43796300
C	-7.56285800	0.10068200	-0.65968800
C	-7.72867300	-1.17507000	-1.21479900
C	-6.60501500	-1.88167200	-1.66549400
C	-5.33834000	-1.31612700	-1.56351900
C	-5.16058500	-0.03663800	-1.00845700
C	-6.29545900	0.66118500	-0.55761300
H	-8.44130600	0.63033200	-0.30670500
H	-6.73170700	-2.86512600	-2.10312500
H	-4.47635300	-1.85723600	-1.94172200
H	-6.17543200	1.63792400	-0.09874200
C	-9.11000000	-1.72336700	-1.30071600
O	-10.10811700	-1.13881500	-0.92396800
O	-9.14294100	-2.95927200	-1.85118800
C	-10.45153400	-3.54053400	-1.96216100
H	-10.91336700	-3.64093400	-0.97616500
H	-11.09738900	-2.91875300	-2.58821000
H	-10.30177800	-4.51941400	-2.41784300
int91			
C	-4.19323000	1.88643000	-0.71997600
C	-4.55141300	0.54761200	-0.51051300

C	-3.53326500	-0.37600400	-0.28098700
C	-2.17761000	0.00046200	-0.23191500
C	-1.80686100	1.34506900	-0.41236000
C	-2.85505400	2.26621500	-0.68494700
Pd	0.94622500	-0.91478100	-0.39297200
H	-3.79538100	-1.40773500	-0.07454700
O	-2.45350400	3.55186100	-0.92762600
C	-3.42269800	4.52609700	-1.28317600
H	-2.86600400	5.44767400	-1.45836500
H	-3.95914800	4.24622000	-2.19827800
H	-4.14623800	4.69028300	-0.47387500
H	-4.96515300	2.61008300	-0.94636300
C	0.80337000	1.07067700	-0.88027000
C	1.97363100	1.77317400	-0.16786900
C	0.16015800	2.82752100	0.74860000
C	-0.40846800	1.92644400	-0.45674600
C	1.38569400	2.01335900	1.23286700
H	2.04811700	2.60552500	1.87395200
H	1.14385900	1.08728400	1.75705100
C	2.07618000	3.22647200	-0.72469900
H	3.04550700	3.65551000	-0.45913800
H	2.00507600	3.24895400	-1.81483900
C	0.90774900	3.96772100	-0.01014800
H	1.31361700	4.70247000	0.68816400
H	0.24002300	4.49729500	-0.69552400
H	2.91513000	1.22956600	-0.20668200
H	-0.50612500	2.61848100	-1.29704300
C	0.86401400	0.90860800	-2.40331000
O	-0.13101200	1.09645200	-3.10552300
N	2.08483200	0.59706100	-2.92486100
H	2.79342300	0.23201200	-2.30407400
C	2.26527700	0.37067300	-4.34742200
H	2.02996800	-0.66361700	-4.63041000
H	1.59729400	1.03515800	-4.89680600
H	3.30347500	0.58451800	-4.60739200
C	-0.04949000	-2.31802900	1.91367600
C	-0.23434000	-3.52295400	1.24880200
C	-0.93726700	-3.55524100	0.02134900
C	-1.43129600	-2.39224400	-0.53348600
C	-1.25390100	-1.12345800	0.11457400
C	-0.53338000	-1.11703400	1.34936500

H	0.48946400	-2.28990500	2.85260700
H	-1.04776600	-4.50856000	-0.48228400
H	-1.97624600	-2.41589200	-1.47108400
H	-0.51597200	-0.21208700	1.94053900
C	0.38760700	-4.79123600	1.72135700
O	0.18240300	-5.88103000	1.22641000
O	1.23620800	-4.59342200	2.75709000
C	1.90865000	-5.77503800	3.22276100
H	2.53255700	-5.44994300	4.05521100
H	1.18660700	-6.52746800	3.55043200
H	2.52309300	-6.20160500	2.42512700
C	-0.84371400	3.31227000	1.81998300
C	-1.42404200	2.17411700	2.68704800
C	-0.26436800	4.39471300	2.76080000
H	-1.68052900	3.77569600	1.28401800
C	-2.48539000	2.67864600	3.67507500
H	-0.60616200	1.70748600	3.25573000
H	-1.86586900	1.40172100	2.05615200
C	-1.30868500	4.90482600	3.76706900
H	0.59519000	3.97992800	3.30641100
H	0.11044300	5.24652200	2.18679100
C	-1.91653400	3.76561500	4.59406500
H	-2.87746200	1.84096400	4.26432300
H	-3.33384500	3.08610600	3.10682500
H	-0.85621100	5.65769400	4.42366200
H	-2.11201000	5.41401700	3.21506800
H	-2.69240800	4.14986300	5.26711400
H	-1.13626300	3.32470400	5.23108400
C	4.52778100	-2.88053100	0.05956900
C	3.18078300	-2.28468900	-0.37130400
O	3.10051900	-1.04301900	-0.68669200
O	2.14973800	-2.98766400	-0.25077800
C	5.88259500	-0.40537200	-0.65595400
C	5.40761000	0.39144700	-1.70508000
C	6.26352800	0.25339800	0.51766900
C	5.27214200	1.76943800	-1.58653800
C	6.13042700	1.63412300	0.66263900
C	5.63660400	2.39236600	-0.39496900
F	6.74557400	-0.43226900	1.56202000
F	6.48008900	2.23405100	1.80671500
F	5.48616100	3.71428800	-0.25840000

F	4.75037100	2.49056400	-2.58677600
F	4.99863200	-0.16704200	-2.85310800
C	4.62369800	-2.64851100	1.58038100
H	3.77253900	-3.14061600	2.06457800
H	5.55518100	-3.06485900	1.97116000
H	4.59140800	-1.58515600	1.82405400
C	4.58267600	-4.38254800	-0.25981700
H	4.50790700	-4.56735300	-1.33467000
H	5.51263700	-4.82219500	0.11303600
H	3.73586100	-4.87301400	0.22501200
S	6.00535900	-2.16905000	-0.85743200
C	-8.30462000	0.56461600	0.01933500
C	-8.67650700	-0.66721700	-0.53544400
C	-7.69148900	-1.49940300	-1.08516800
C	-6.35881800	-1.10154500	-1.07867500
C	-5.97311900	0.13110000	-0.52235800
C	-6.97156400	0.95665000	0.02607500
H	-9.07678900	1.19376800	0.44926700
H	-7.97750300	-2.44866500	-1.52326800
H	-5.60699800	-1.73966300	-1.53266800
H	-6.69162400	1.89953700	0.48601700
C	-10.11790600	-1.03668900	-0.51136900
O	-11.00036200	-0.34280900	-0.04259000
O	-10.35169500	-2.24570800	-1.07385900
C	-11.72736700	-2.65760400	-1.07939600
H	-12.11308800	-2.72690500	-0.05853500
H	-12.34118100	-1.94427200	-1.63620600
H	-11.74079500	-3.63489200	-1.56218400

TS53

C	3.61762400	-1.74912600	-0.79442600
C	4.05573500	-0.41714500	-0.87396000
C	3.11294000	0.61321000	-0.74273000
C	1.77901200	0.33751400	-0.43748400
C	1.34251100	-1.00530300	-0.21025400
C	2.28287300	-2.03638800	-0.50595700
Pd	-0.72390300	-1.22353200	-0.55487300
H	3.41657900	1.64699700	-0.87460800
O	1.78713600	-3.28727400	-0.42286100
C	2.65673100	-4.41211000	-0.33900000
H	2.01115800	-5.24654700	-0.06737300

H	3.14540100	-4.60940100	-1.30055100
H	3.41915300	-4.26628900	0.43652500
H	4.31840700	-2.55272200	-0.98552700
C	-0.81360100	-1.97709400	1.35857700
C	-1.55898900	-1.12027700	2.38738600
C	0.65430800	-0.59743800	2.65275300
C	0.59314800	-1.62591100	1.51613700
C	-0.69249000	0.14867700	2.46559600
H	-0.95575300	0.77290900	3.32404000
H	-0.73035500	0.75957400	1.56385700
C	-1.21848000	-1.78279300	3.75521100
H	-1.79083100	-1.28651300	4.54519700
H	-1.46470100	-2.84687600	3.78345700
C	0.30366400	-1.50674000	3.89727500
H	0.53188700	-0.95906200	4.81520300
H	0.89535100	-2.42589900	3.90948100
H	-2.61831700	-0.98669900	2.20880900
H	1.25967600	-2.47755300	1.55696100
C	-1.18739400	-3.44413500	1.20456400
O	-0.36875000	-4.34328300	1.39867500
C	-2.99009200	-4.94367500	0.47773100
H	-4.02343700	-5.07668200	0.80952100
H	-2.94498600	-5.02319100	-0.61483600
H	-2.36220400	-5.71592400	0.92291100
C	-4.43346700	-1.73217900	-2.69495900
C	-3.10353200	-2.04518000	-1.96175800
O	-2.76836800	-1.17118700	-1.05876200
O	-2.42747400	-3.01877000	-2.30378400
C	-5.52502700	-0.06054000	-0.61329400
C	-4.87577300	-0.07906100	0.62504800
C	-5.89809700	1.19184900	-1.11895300
C	-4.54377600	1.09015400	1.29839500
C	-5.60775500	2.37730200	-0.44408200
C	-4.90694300	2.32032800	0.75631900
F	-6.54420000	1.28954800	-2.28616400
F	-6.00074700	3.55513400	-0.93392400
F	-4.58531000	3.44821800	1.40496400
F	-3.87915900	1.04931900	2.46522900
F	-4.55491400	-1.24544900	1.20639000
C	-4.24163600	-0.44267700	-3.50456400
H	-3.44507500	-0.60223900	-4.24117100

H	-5.15855600	-0.16837500	-4.03082100
H	-3.94145500	0.38302100	-2.85649200
C	-4.84809200	-2.89973000	-3.59714300
H	-4.04220500	-3.09981900	-4.30645100
H	-5.00354500	-3.81453900	-3.01924200
H	-5.76274200	-2.65920900	-4.14677800
S	-5.87295600	-1.57181600	-1.48207500
C	-0.17827200	3.52737700	0.29766200
C	-1.28308800	3.34997900	-0.54789400
C	-1.33224100	2.24332800	-1.40214300
C	-0.30757100	1.30337100	-1.37556100
C	0.77979700	1.43729400	-0.48549500
C	0.84932600	2.58563100	0.31635100
H	-0.13803600	4.39501600	0.94630900
H	-2.17688900	2.13036900	-2.07202300
H	-0.30177800	0.50324500	-2.11897100
H	1.68665500	2.71451700	0.99445900
C	-2.42316900	4.30771900	-0.60940300
O	-3.33816000	4.21424700	-1.40585300
O	-2.34084200	5.28544100	0.31352900
C	-3.44770000	6.20774800	0.31399900
H	-3.27915700	6.86570200	1.16627400
H	-3.46627600	6.78034400	-0.61722900
H	-4.38827000	5.66425000	0.41703600
C	7.82930500	-0.56814200	-0.64466000
C	8.21085100	0.48713800	-1.48375100
C	7.22526300	1.24395900	-2.13219900
C	5.87969300	0.94788700	-1.94046400
C	5.48582000	-0.10924400	-1.10139700
C	6.48449100	-0.86270100	-0.45732300
H	8.60411800	-1.13785000	-0.14286600
H	7.51939700	2.05480100	-2.78849600
H	5.12406400	1.52352100	-2.46587600
H	6.19698400	-1.66348800	0.21695900
C	9.66681900	0.75685600	-1.64584400
O	10.54852900	0.12141000	-1.10014700
O	9.91051700	1.79784000	-2.47449900
C	11.30000600	2.10620300	-2.67133600
H	11.77471700	2.36544900	-1.72113100
H	11.82656100	1.25069300	-3.10288600
H	11.31960100	2.95470000	-3.35526000

C	1.95371200	0.20283900	2.78635100
C	1.90866700	1.30418000	3.86166900
C	3.19165600	-0.69519200	2.98801700
H	2.10352500	0.71429300	1.83372700
C	3.20550500	2.13038200	3.85845000
H	1.77193600	0.85786700	4.85595700
H	1.04857500	1.96129700	3.68975000
C	4.48672900	0.12999600	2.97933600
H	3.10550500	-1.22900700	3.94434700
H	3.23840100	-1.45543600	2.20090000
C	4.44512300	1.24139100	4.03759500
H	3.16630900	2.89630400	4.64184400
H	3.28761900	2.66695600	2.90140500
H	5.35282600	-0.52220300	3.14349400
H	4.61742500	0.57672200	1.98408100
H	5.35800300	1.84702000	3.99395000
H	4.41702900	0.78522800	5.03756100
N	-2.49760600	-3.64508900	0.90762500
H	-3.01868100	-2.83362600	0.59935800

int92

C	3.59547300	-1.56822700	-1.12720300
C	3.98143100	-0.22098300	-1.01129400
C	2.99226600	0.75030700	-0.83529700
C	1.63410700	0.39878100	-0.74273700
C	1.25570700	-0.95135000	-0.81698000
C	2.24894300	-1.92491000	-1.03929700
Pd	-0.67925400	-1.47496500	-0.65276500
H	3.26911700	1.79486800	-0.73041800
O	1.79850600	-3.21184400	-1.12838300
C	2.73852400	-4.27642000	-1.16302700
H	2.14545000	-5.19028100	-1.12264400
H	3.33306600	-4.26165900	-2.08553600
H	3.41535000	-4.24237200	-0.29855400
H	4.35320800	-2.32120400	-1.30698000
C	-1.09052400	-2.58018000	1.23053500
C	-1.82465400	-1.75654900	2.28420300
C	0.40634900	-1.31632500	2.53547300
C	0.25507000	-2.28253900	1.36950400
C	-0.91895100	-0.51655500	2.41951000
H	-1.14891800	0.06473700	3.31711700

H	-0.94084000	0.14696200	1.55070200
C	-1.47791900	-2.50274200	3.61444000
H	-2.04179100	-2.05411600	4.43779400
H	-1.73652400	-3.56425000	3.57467300
C	0.05064900	-2.24930000	3.76353800
H	0.28161200	-1.72690900	4.69579300
H	0.63373400	-3.17362900	3.75228100
H	-2.88442100	-1.58731300	2.12091300
H	1.02400000	-2.96897800	1.04480700
C	-1.55986900	-3.92931200	0.72863000
O	-0.77593000	-4.86658900	0.59157300
C	-3.46792400	-5.22960900	-0.05856000
H	-4.53810900	-5.26747000	0.15692500
H	-3.32014300	-5.26213500	-1.14614500
H	-2.97526900	-6.10027600	0.37630900
C	-3.85922500	-0.82117600	-3.10481200
C	-2.66133400	-1.11819700	-2.19817300
O	-2.81422300	-1.63341300	-1.04750300
O	-1.49088800	-0.85023400	-2.61666600
C	-5.25599500	0.27950800	-0.86286200
C	-4.88879000	-0.10288400	0.43577900
C	-5.49482600	1.64552200	-1.07761800
C	-4.65778400	0.83475100	1.43812600
C	-5.33494200	2.59268200	-0.06765800
C	-4.87848000	2.18628400	1.18314300
F	-5.89376000	2.08473300	-2.27515300
F	-5.62740200	3.87583700	-0.28414100
F	-4.67810100	3.09028000	2.14680600
F	-4.24615900	0.44267500	2.65296600
F	-4.77659400	-1.39443000	0.77691800
C	-3.67486300	0.54106300	-3.78714600
H	-2.74328600	0.53213100	-4.35901100
H	-4.51328500	0.74446100	-4.45640400
H	-3.61436100	1.34997500	-3.05676900
C	-3.95131700	-1.94941400	-4.15357700
H	-3.02971200	-1.95902700	-4.74210500
H	-4.07161900	-2.92780100	-3.67983000
H	-4.79445900	-1.77540600	-4.82863500
S	-5.47889900	-0.92043200	-2.16058700
C	-0.27387500	3.25486500	0.88710100
C	-1.29848100	3.47246400	-0.04285700

C	-1.33298700	2.71581800	-1.22122100
C	-0.38309500	1.72765000	-1.45021700
C	0.63309400	1.48192200	-0.51139300
C	0.69248600	2.28255500	0.64040100
H	-0.23636700	3.84939600	1.79306400
H	-2.11087800	2.92271800	-1.94847700
H	-0.42706500	1.13564200	-2.35509700
H	1.48831200	2.12349800	1.35825100
C	-2.35272700	4.50391100	0.14497500
O	-3.11888100	4.86191200	-0.73001800
O	-2.38715900	4.99401200	1.40346300
C	-3.42982500	5.95463400	1.64893100
H	-3.34629700	6.21320700	2.70449400
H	-3.29258800	6.84001800	1.02252100
H	-4.40448800	5.51287400	1.43382600
C	7.72542900	-0.29031000	-0.43112500
C	8.13952400	0.87581500	-1.08895000
C	7.18561600	1.68080300	-1.72735200
C	5.84201800	1.32136900	-1.70641300
C	5.41468600	0.15373600	-1.04979200
C	6.38234800	-0.64519900	-0.41261300
H	8.47348200	-0.89815300	0.06672500
H	7.50416300	2.57860000	-2.24449800
H	5.11317700	1.93662900	-2.22478800
H	6.06838600	-1.53467500	0.12461100
C	9.59005700	1.20576100	-1.07676400
O	10.44609100	0.53733200	-0.52840400
O	9.86751000	2.34698300	-1.75117100
C	11.25483500	2.71579100	-1.77588800
H	11.63111700	2.87095900	-0.76094800
H	11.85315500	1.93492400	-2.25341600
H	11.30396600	3.64165000	-2.34935100
C	1.73862600	-0.56396500	2.62766700
C	1.75683400	0.52451500	3.71768600
C	2.94668300	-1.50862800	2.79739300
H	1.87437600	-0.06149300	1.66661500
C	3.08562600	1.29794800	3.71705100
H	1.61426100	0.06688300	4.70628500
H	0.92091900	1.21802200	3.57054700
C	4.27223100	-0.73277900	2.79204600
H	2.85236100	-2.05966200	3.74334400

H	2.95674000	-2.25272800	1.99307200
C	4.28671700	0.35532400	3.87464800
H	3.08156700	2.05320500	4.51184100
H	3.18924800	1.84299500	2.76770600
H	5.11360100	-1.42239500	2.93150600
H	4.40777600	-0.26605700	1.80807500
H	5.22429100	0.92204700	3.83417800
H	4.24545700	-0.11808800	4.86624500
N	-2.90222400	-4.02574000	0.52664300
H	-3.40152300	-3.15929400	0.37004900

int93

C	-2.12311800	1.98340000	-2.15446800
C	-1.19812800	2.63884700	-2.97182100
C	0.16079200	2.31792300	-2.86439500
C	0.61044700	1.36241100	-1.94722400
C	-0.31297500	0.72944100	-1.08307900
C	-1.66530000	1.04745200	-1.21773500
Pd	0.26704100	-0.63072200	0.31525700
H	0.86229100	2.81401100	-3.52799000
H	-3.18384500	2.19499100	-2.21839700
C	1.48932600	0.42807900	1.95858400
C	0.94173300	0.16204800	3.35510100
C	-0.35238600	1.81071300	2.44403200
C	0.69863000	1.41580700	1.40720100
C	-0.55512600	0.46449800	3.18365500
H	-1.06657100	0.58072600	4.14362800
H	-1.08294800	-0.28036800	2.58212200
C	1.39561100	1.43835800	4.14586800
H	1.15974500	1.30990000	5.20658700
H	2.46942800	1.62028900	4.05777500
C	0.53741200	2.57193900	3.50425400
H	-0.10117300	3.05474300	4.24841300
H	1.14821200	3.34971200	3.03848000
H	1.21904900	-0.79346200	3.79496600
H	1.05439000	2.08949600	0.64019300
C	2.95685800	0.21473400	1.65660400
O	3.69167100	1.18082600	1.45160600
N	3.36893200	-1.07055800	1.74942700
H	2.64398400	-1.77890500	1.84459800
C	4.75640900	-1.45636900	1.56214700

H	5.02743800	-2.22891300	2.28761800
H	4.95071900	-1.82924400	0.55125000
H	5.38104700	-0.57574900	1.71966300
C	-1.60775300	2.52271600	1.92600700
C	-2.61628100	2.86145200	3.04188300
C	-1.29082000	3.77775400	1.08808900
H	-2.10471300	1.80729100	1.25761200
C	-3.89302900	3.50241300	2.47733900
H	-2.15941200	3.56101900	3.75471200
H	-2.87167100	1.95837400	3.60773800
C	-2.56593300	4.43981600	0.54361600
H	-0.74340600	4.49855800	1.71204900
H	-0.63772200	3.51666300	0.24900200
C	-3.56587300	4.76069900	1.66175700
H	-4.58658300	3.74104800	3.29232100
H	-4.40690200	2.77585900	1.83084500
H	-2.30637300	5.34717500	-0.01516100
H	-3.03498600	3.75441000	-0.17490100
H	-4.48148600	5.19664800	1.24408100
H	-3.13251300	5.51870400	2.32999500
C	-0.04184900	-3.83633200	-0.09845600
C	0.36191800	-3.47441700	1.36695400
O	0.76626300	-2.26121300	1.59830200
O	0.37920300	-4.39446700	2.17219600
C	-2.37811000	-2.15614400	-0.81360500
C	-3.17991700	-1.91815000	-1.93556900
C	-2.98152800	-2.07991800	0.44641600
C	-4.53082100	-1.60022800	-1.80859700
C	-4.32782400	-1.76547300	0.59246500
C	-5.10474600	-1.52497500	-0.54170700
F	-2.25898700	-2.28122700	1.55474300
F	-4.87705800	-1.68470500	1.80629400
F	-6.39482900	-1.22019800	-0.41007100
F	-5.27197800	-1.35779200	-2.89250100
F	-2.65327500	-1.94288800	-3.16198600
C	1.25950700	-4.23578800	-0.82360300
H	1.70715200	-5.06601700	-0.26991600
H	1.06465800	-4.55786100	-1.85071800
H	1.98090000	-3.41212500	-0.83703500
C	-1.08160700	-4.94964800	-0.15004700
H	-2.00339500	-4.66235300	0.35957200

H	-1.31148100	-5.23607200	-1.18076700
H	-0.66924900	-5.80675400	0.38631500
S	-0.62201600	-2.32634400	-1.07527500
C	4.35766200	1.76988000	-1.53085800
C	4.79260900	0.44153400	-1.59871200
C	3.86533400	-0.57833000	-1.85091400
C	2.51723900	-0.27647100	-1.99141000
C	2.06288700	1.05045700	-1.87815700
C	3.00570600	2.06786000	-1.67506500
H	5.07341500	2.55691600	-1.32700700
H	4.22217600	-1.60008900	-1.92706700
H	1.80627400	-1.06519000	-2.21081400
H	2.66473300	3.09494100	-1.58476900
C	6.20676600	0.05024900	-1.36808100
O	6.59727200	-1.10143600	-1.28267600
O	7.03064300	1.11413500	-1.24405000
C	8.40273100	0.79386700	-0.96941700
H	8.82863000	0.19357400	-1.77808500
H	8.91837700	1.75083200	-0.88838600
H	8.48681600	0.23121500	-0.03551300
O	-1.51113700	3.58992200	-3.90070700
C	-2.86808200	3.98848500	-4.01254000
H	-3.24759100	4.40177900	-3.06800900
H	-2.89369600	4.76399400	-4.77979800
H	-3.51342500	3.15542500	-4.32295000
H	-2.40084700	0.57904700	-0.57038600

TS54

C	2.24247100	1.73979500	1.63435500
C	1.50474200	2.11542000	2.76309000
C	0.12852000	1.84076100	2.81424700
C	-0.50581100	1.15204200	1.78191000
C	0.23633900	0.74490400	0.63528000
C	1.59867000	1.07840900	0.58860600
Pd	-0.22251700	-1.03432300	-0.36593400
H	-0.42449600	2.13604100	3.70019200
H	3.30440800	1.93964600	1.56480000
C	-1.35785100	0.05124800	-1.72441100
C	-0.75645000	0.06076300	-3.14058400
C	-0.07526100	2.01394200	-2.14818100
C	-0.89941400	1.26320700	-1.10490800

C	0.55950800	0.83593400	-2.92936700
H	1.01527300	1.14726800	-3.87359300
H	1.30152400	0.28548700	-2.34248500
C	-1.58624200	1.12748800	-3.90992500
H	-1.25336100	1.17141200	-4.95199900
H	-2.65741500	0.91594300	-3.90494700
C	-1.23375600	2.43620300	-3.14934500
H	-0.86370600	3.20810700	-3.82649000
H	-2.09611800	2.84546100	-2.61677700
H	-0.69049900	-0.91802100	-3.61538400
H	-1.59312900	1.80689700	-0.47697900
C	-2.83101500	-0.30444000	-1.57771700
O	-3.66912000	0.57724600	-1.37008000
N	-3.14863300	-1.60295800	-1.77221000
H	-2.39153300	-2.27878300	-1.85498800
C	-4.53333500	-2.04525700	-1.71480600
H	-4.99944100	-1.78106900	-0.76025800
H	-5.12190200	-1.57866500	-2.51189500
H	-4.55909200	-3.12901700	-1.84231100
C	0.83733400	3.15376100	-1.67693900
C	1.51120900	3.93141400	-2.82581700
C	0.14383200	4.13086400	-0.70698700
H	1.65189900	2.68986100	-1.11250400
C	2.51328500	4.96038200	-2.28047200
H	0.75401400	4.46151400	-3.41841100
H	2.01814500	3.23980900	-3.50888800
C	1.13121300	5.17816000	-0.16975300
H	-0.68606700	4.63402700	-1.22372600
H	-0.28814300	3.58004900	0.13503200
C	1.83413700	5.93390800	-1.30633000
H	2.97825900	5.50888600	-3.10811900
H	3.32458100	4.43289900	-1.75811700
H	0.61205900	5.87962100	0.49401300
H	1.88370100	4.66430000	0.44531800
H	2.56602800	6.64224700	-0.89995700
H	1.09151800	6.52991900	-1.85614100
C	0.66469800	-4.11648000	0.27578000
C	0.03907000	-3.92892700	-1.14861800
O	-0.56676500	-2.81074000	-1.41544200
O	0.06575400	-4.90989600	-1.87884700
C	2.69810000	-1.96639900	0.69276000

C	3.45429600	-1.31446200	1.67352000
C	3.19640400	-1.95556700	-0.61506800
C	4.64664700	-0.66604700	1.36512600
C	4.40075300	-1.33762600	-0.93611900
C	5.12746000	-0.68304600	0.05945700
F	2.48924800	-2.50413900	-1.61109400
F	4.84727100	-1.33793100	-2.19486200
F	6.26651400	-0.05938900	-0.24474800
F	5.30159400	0.02083700	2.31195100
F	2.99940300	-1.21413100	2.92702600
C	-0.45572800	-4.70589600	1.15839000
H	-0.80552700	-5.62421300	0.67880500
H	-0.09302900	-4.94264800	2.16287300
H	-1.30773500	-4.02258900	1.23801400
C	1.88481400	-5.03258000	0.24843500
H	2.68157500	-4.62327300	-0.37444100
H	2.26849300	-5.21262200	1.25710200
H	1.57632000	-5.97852100	-0.20094900
S	1.05422400	-2.48455800	1.14474300
C	-4.25642900	1.65555800	1.81086800
C	-4.71374000	0.33834800	1.68754500
C	-3.79858800	-0.71944100	1.72435000
C	-2.43754200	-0.46091600	1.81539100
C	-1.96175100	0.86034200	1.86718600
C	-2.89078900	1.91099800	1.90766900
H	-4.96761500	2.47293900	1.79158200
H	-4.17025700	-1.73551700	1.65038000
H	-1.73285800	-1.28447400	1.83714300
H	-2.53089000	2.93474200	1.95966700
C	-6.14455100	0.00468200	1.45990400
O	-6.55595600	-1.11289100	1.20317000
O	-6.95398800	1.08214900	1.55382100
C	-8.34186300	0.82595000	1.28786500
H	-8.74228900	0.09692000	1.99758000
H	-8.84539100	1.78647500	1.39797900
H	-8.47240700	0.43629200	0.27464600
O	2.03136500	2.73098000	3.85346200
C	3.44480600	2.89306700	3.90746500
H	3.79904900	3.59297700	3.13911200
H	3.66270300	3.30437200	4.89386100
H	3.96333300	1.93325700	3.78594200

H	2.19292000	0.77972800	-0.26840900
int94			
C	0.53918900	-2.58777200	-1.84081500
C	1.08001500	-1.53223900	-2.57300800
C	0.62418400	-0.21994500	-2.34264300
C	-0.37829300	0.05009400	-1.42380200
C	-0.97468500	-1.02200000	-0.66227000
C	-0.45878800	-2.32142600	-0.89181100
Pd	0.32842900	-0.95194900	1.20314400
H	1.06990100	0.58498600	-2.91710100
H	0.88026300	-3.60585100	-1.97814600
C	-1.59181600	-0.36581100	1.62542700
C	-2.27938200	-1.33000100	2.61617500
C	-3.22214600	-1.84573200	0.58919100
C	-2.19199900	-0.71897800	0.25236700
C	-2.52071600	-2.59163000	1.76078800
H	-3.18426700	-3.30306400	2.26256900
H	-1.60294200	-3.11899200	1.48909300
C	-3.74448900	-0.84647000	2.79069600
H	-4.23424800	-1.46029000	3.55458300
H	-3.82126200	0.19775300	3.09542100
C	-4.35265700	-1.09901600	1.38041800
H	-5.25022700	-1.71949400	1.44206800
H	-4.62578600	-0.16053300	0.89329200
H	-1.73201400	-1.46128100	3.55175600
H	-2.71097500	0.14426200	-0.15970200
C	-1.71196700	1.11378600	1.99811900
O	-2.63485000	1.78960100	1.53019400
N	-0.82413100	1.60066500	2.88960600
H	-0.08524600	0.98627200	3.23335500
C	-0.89674800	2.98137500	3.33346900
H	0.04238700	3.24202400	3.82533100
H	-1.06022400	3.64307800	2.47822800
H	-1.72338500	3.13676000	4.03701300
C	-3.72043000	-2.66073000	-0.61818400
C	-4.63718000	-3.84217600	-0.24056600
C	-4.40825100	-1.77009900	-1.67369500
H	-2.84669900	-3.10394400	-1.11375900
C	-5.06022900	-4.64821500	-1.47886500
H	-5.53825600	-3.46759400	0.26254900

H	-4.12856000	-4.49818000	0.47516700
C	-4.83403200	-2.57491800	-2.91013600
H	-5.29235400	-1.29571100	-1.22705300
H	-3.73683300	-0.95720000	-1.97404300
C	-5.73920500	-3.75346300	-2.52567200
H	-5.72676500	-5.46762100	-1.18436200
H	-4.17044700	-5.11405600	-1.92712100
H	-5.34100300	-1.92139000	-3.63012400
H	-3.93586500	-2.96020800	-3.41461000
H	-6.00624800	-4.33816300	-3.41411100
H	-6.67980400	-3.36403300	-2.11044400
C	3.25712000	-1.38693000	2.62994000
C	2.29822400	-0.40213600	3.36966000
O	1.02117400	-0.50426700	3.11360900
O	2.77597900	0.32611200	4.22649600
C	3.41263300	-0.45814700	-0.16419100
C	4.05750600	-0.83541300	-1.34561700
C	3.23381500	0.91136400	0.05553100
C	4.43806300	0.09698300	-2.30617000
C	3.62245200	1.86299700	-0.87899300
C	4.22114300	1.45233000	-2.07157400
F	2.63385100	1.34024400	1.17647900
F	3.40254600	3.16001900	-0.65119500
F	4.58022000	2.35644000	-2.98288400
F	5.00007400	-0.30783800	-3.44814500
F	4.27814100	-2.13069200	-1.61306800
C	4.70245300	-0.90105500	2.66145800
H	4.99680100	-0.78121600	3.70590800
H	5.37004200	-1.61664500	2.17240700
H	4.80819200	0.07503600	2.18436100
C	3.10414200	-2.75717400	3.31888300
H	2.07806200	-3.12895000	3.24140600
H	3.79028400	-3.49513000	2.89295600
H	3.33587600	-2.63153600	4.38098000
S	2.69787700	-1.72921500	0.85702000
C	-2.46455600	3.20593100	-1.69964600
C	-1.71439600	4.10228200	-0.92777500
C	-0.50964900	3.68315300	-0.35438100
C	-0.07187100	2.37473900	-0.52442400
C	-0.83152900	1.46535400	-1.27116600
C	-2.01982400	1.89956200	-1.87471700

H	-3.39464100	3.53361600	-2.14891900
H	0.06222400	4.39043200	0.23628200
H	0.83616400	2.04580000	-0.03890200
H	-2.60491700	1.20277300	-2.46832200
C	-2.15828800	5.49882500	-0.66409900
O	-1.55679100	6.29144500	0.03538300
O	-3.31998100	5.80046600	-1.28899300
C	-3.81110600	7.12807600	-1.04895700
H	-3.08915900	7.87437000	-1.39192400
H	-4.74097300	7.20522900	-1.61274900
H	-3.99362600	7.28356100	0.01785500
O	2.05143800	-1.64642400	-3.51192500
C	2.50120500	-2.95001700	-3.87767600
H	1.68479500	-3.53926800	-4.31233100
H	3.28085000	-2.79156700	-4.62278400
H	2.92673900	-3.47905300	-3.01997700
H	-0.88739500	-3.16370200	-0.36665500

int95

C	-2.08908200	0.49520100	2.74720800
C	-0.77930200	0.33045900	3.22472900
C	0.19485600	-0.15554100	2.35481700
C	-0.13684500	-0.32905400	1.00317000
C	-1.40651800	-0.01757500	0.47002100
C	-2.42750000	0.29717900	1.40472000
Pd	1.34441600	-0.52551200	-0.67769900
H	0.41171000	-1.25074700	0.58677200
H	1.16331700	-0.49900000	2.69311200
H	-2.86171400	0.73180800	3.47140200
C	-0.39799000	-0.60901300	-1.82674200
C	-0.21864000	0.32905500	-3.03294900
C	-1.69162900	1.48594700	-1.71991900
C	-1.57867300	0.02727600	-1.03026500
C	-0.29418200	1.69532100	-2.34167900
H	-0.28099200	2.53643400	-3.04403900
H	0.50285700	1.84567100	-1.61204200
C	-1.53829300	0.30647600	-3.85814100
H	-1.36935300	0.73766200	-4.84969600
H	-1.91247800	-0.71061900	-4.01106300
C	-2.50610600	1.19002400	-3.01307900
H	-2.71854100	2.11742900	-3.54871600

H	-3.46538600	0.70774500	-2.79980200
H	0.68016200	0.13499900	-3.61746000
H	-2.49390300	-0.50486900	-1.29009400
C	-0.55939700	-2.06508800	-2.13526700
O	-1.48119600	-2.76852400	-1.61146700
N	0.30073800	-2.61727500	-3.00349400
H	1.12743800	-2.06557400	-3.23177300
C	0.35165400	-4.05661700	-3.20856800
H	1.04348500	-4.27012200	-4.02439000
H	0.69289100	-4.57262500	-2.30074000
H	-0.64077400	-4.43377400	-3.46140600
C	-2.21021100	2.63365400	-0.82733700
C	-1.12502400	3.18619500	0.12703100
C	-2.83897500	3.81519600	-1.59827900
H	-3.01700500	2.22985600	-0.21179100
C	-1.69719600	4.21986000	1.10640300
H	-0.33956900	3.66854000	-0.47085400
H	-0.64096100	2.37651000	0.67961600
C	-3.40969200	4.86862100	-0.63374200
H	-2.08538600	4.27852000	-2.25168100
H	-3.64746300	3.46373800	-2.24661600
C	-2.35550300	5.38402900	0.35434000
H	-0.90540300	4.58891300	1.76961600
H	-2.44113800	3.73216700	1.75197700
H	-3.84062300	5.70146100	-1.20228800
H	-4.23689600	4.41289000	-0.07050300
H	-2.80518700	6.09524100	1.05776200
H	-1.58133700	5.93458400	-0.19894300
C	4.33757500	-1.56430100	-0.87548300
C	3.72942100	-1.27079200	-2.28040700
O	2.48693500	-0.86410700	-2.36252600
O	4.42199700	-1.52300800	-3.25521300
C	4.29759900	1.04343800	0.37935400
C	5.37992900	1.29929800	1.23417000
C	3.90471800	2.07627000	-0.48014100
C	6.03522800	2.52730900	1.24567600
C	4.54323600	3.31416200	-0.47971400
C	5.61179200	3.53912500	0.38561800
F	2.89388300	1.91260100	-1.34206200
F	4.13887200	4.28256000	-1.30554600
F	6.22948700	4.71928800	0.38961900

F	7.06494100	2.73960800	2.06952900
F	5.82350200	0.34831300	2.06431300
C	4.00457400	-3.02675400	-0.51846300
H	4.38584900	-3.65997800	-1.32535400
H	4.48645900	-3.31537200	0.41939300
H	2.93021400	-3.19013600	-0.40543000
C	5.84477000	-1.31928100	-0.86796000
H	6.08782900	-0.29231000	-1.15100400
H	6.26931400	-1.53001700	0.11721600
H	6.29703400	-1.97659600	-1.61300000
S	3.49777200	-0.55190500	0.49331300
O	1.50119700	-2.91409500	1.61053700
C	0.84465100	-3.55159100	2.46004300
O	-0.33247000	-4.04515800	2.27485900
C	1.41366900	-3.78151600	3.85398900
H	0.77066200	-3.28741000	4.59008500
H	1.40379400	-4.84960200	4.08834100
H	2.43015900	-3.39226300	3.92700800
Ag	-1.02543500	-3.51731300	0.34836600
C	-6.06113500	1.39475200	1.16338800
C	-6.61582300	0.35630200	0.40341600
C	-5.79956200	-0.70292600	-0.01513800
C	-4.44676500	-0.71638400	0.30516900
C	-3.87341900	0.33397100	1.04315700
C	-4.70691700	1.37658300	1.48216500
H	-6.69072200	2.21277700	1.49378600
H	-6.24712800	-1.50988700	-0.58551600
H	-3.82792500	-1.55264100	-0.00579600
H	-4.27896900	2.19352800	2.05494200
C	-8.05404400	0.32310600	0.01859700
O	-8.57089900	-0.56064700	-0.63756900
O	-8.73757200	1.39645400	0.47950400
C	-10.13223400	1.42130200	0.13632000
H	-10.64519500	0.54683900	0.54583700
H	-10.52726400	2.33836800	0.57358700
H	-10.26131000	1.42481400	-0.94941900
O	-0.59267600	0.57539800	4.54884700
C	0.68979000	0.29720800	5.09892400
H	1.47462400	0.89079900	4.61165600
H	0.63094800	0.57158200	6.15281500
H	0.94113700	-0.76781400	5.01354900

TS55

C	-1.95133400	0.74961100	2.63948200
C	-0.61572700	0.73752600	3.06005700
C	0.37325300	0.27869700	2.18866900
C	0.03180100	-0.09092000	0.87737800
C	-1.29589100	0.05823000	0.40073700
C	-2.31073700	0.40646100	1.33217900
Pd	1.38108500	-0.69415200	-0.54920400
H	0.67225000	-1.49235400	0.79761300
H	1.38826600	0.12510000	2.53229700
H	-2.71226300	1.00439900	3.36932000
C	-0.30683200	-0.77845500	-1.77835600
C	0.00654900	0.09283400	-3.01529900
C	-1.55491400	1.34499600	-1.90505800
C	-1.49767800	-0.04209100	-1.09092400
C	-0.10780900	1.50249800	-2.42058900
H	-0.02157400	2.29505500	-3.17277100
H	0.62179300	1.69376400	-1.63280300
C	-1.22908000	0.04270800	-3.95711000
H	-0.96525800	0.44538700	-4.94024600
H	-1.59112800	-0.97727800	-4.11674500
C	-2.26659000	0.95438500	-3.23432500
H	-2.45856300	1.84235900	-3.83956000
H	-3.22961500	0.46379600	-3.05969700
H	0.95077400	-0.14970400	-3.50295500
H	-2.42693900	-0.56767200	-1.31096100
C	-0.53007100	-2.23312600	-2.06716300
O	-1.52449400	-2.88641400	-1.61054300
N	0.34608200	-2.84665000	-2.87336600
H	1.22538500	-2.35532900	-3.04381700
C	0.30557800	-4.28464500	-3.09139400
H	1.03302100	-4.54002800	-3.86322600
H	0.54819100	-4.83275800	-2.17214900
H	-0.69215100	-4.58704400	-3.41455300
C	-2.14450500	2.55453500	-1.13972900
C	-1.10948300	3.22645400	-0.20766200
C	-2.78069800	3.63872200	-2.03598600
H	-2.95956000	2.17942000	-0.51454900
C	-1.73461200	4.33711000	0.64669200
H	-0.31458200	3.66755700	-0.82503000

H	-0.62796400	2.48789700	0.43682900
C	-3.40698800	4.76531600	-1.19565700
H	-2.01959700	4.05942500	-2.70967100
H	-3.55831300	3.20163200	-2.66980100
C	-2.39535700	5.40377900	-0.23493700
H	-0.97140400	4.78954900	1.29172200
H	-2.48678400	3.89817900	1.31680600
H	-3.84118000	5.52619200	-1.85551900
H	-4.23947800	4.34480200	-0.61312600
H	-2.88263300	6.16969000	0.38068400
H	-1.61791100	5.91673400	-0.81923500
C	4.36527000	-1.89139100	-0.51476600
C	3.81104100	-1.77294800	-1.97043400
O	2.60050400	-1.32040900	-2.13956300
O	4.52444800	-2.20011800	-2.86809500
C	4.38901200	0.86764500	0.39305200
C	5.47546500	1.18231100	1.22259300
C	4.03249700	1.81065200	-0.57851600
C	6.17208500	2.38107200	1.10075900
C	4.71292500	3.01869900	-0.71238000
C	5.78642600	3.30302800	0.12900100
F	3.01625800	1.58770500	-1.41980500
F	4.34348300	3.90181600	-1.64306900
F	6.44452300	4.45427100	0.00445000
F	7.20427300	2.65104400	1.90448500
F	5.88060300	0.31862700	2.16106200
C	3.95297300	-3.27386600	0.02804300
H	4.32634700	-4.02902200	-0.67001200
H	4.39292100	-3.45339900	1.01334900
H	2.86766700	-3.37367400	0.11330200
C	5.88077200	-1.70818500	-0.48342700
H	6.17621600	-0.73614800	-0.88604200
H	6.26812000	-1.80713900	0.53399200
H	6.32445300	-2.47217600	-1.12450600
S	3.52956800	-0.67226100	0.67667500
O	1.05618800	-2.59149600	1.74978600
C	0.27725100	-2.92821000	2.69894800
O	-0.94767100	-3.23395100	2.56389100
C	0.82779600	-2.93382100	4.11032300
H	0.48652800	-2.01546200	4.60137400
H	0.42966400	-3.77866300	4.67555900

H	1.91824000	-2.94962800	4.10233300
Ag	-1.54294200	-3.09940100	0.51920300
C	-5.95573100	1.45969400	1.10223900
C	-6.53039000	0.36879300	0.43676500
C	-5.72129000	-0.71444500	0.06973300
C	-4.36057500	-0.70067200	0.35173400
C	-3.76538400	0.39407100	1.00242900
C	-4.59297000	1.46550300	1.38299800
H	-6.57720900	2.29976700	1.39013300
H	-6.17990300	-1.56041100	-0.43125900
H	-3.75229800	-1.55503600	0.07133600
H	-4.15265700	2.32273000	1.88210100
C	-7.97898100	0.30387300	0.10064500
O	-8.51224400	-0.62632100	-0.47339100
O	-8.65387100	1.40552400	0.50497200
C	-10.05859400	1.40031600	0.20586000
H	-10.55332500	0.55615200	0.69399100
H	-10.44511300	2.34533000	0.58780200
H	-10.22240600	1.32426100	-0.87253400
O	-0.39440700	1.12323300	4.35007500
C	0.94982300	1.19115100	4.80509200
H	1.55264400	1.86428000	4.18095300
H	0.90445700	1.58413500	5.82178800
H	1.42589600	0.20195100	4.82378400

int96

C	-1.73628600	0.35247300	2.52837100
C	-0.41637000	0.49625600	2.96187000
C	0.63979200	0.19768800	2.09513700
C	0.39129800	-0.22858600	0.77954000
C	-0.95118000	-0.27014000	0.30484700
C	-2.02234600	-0.02832000	1.21053200
Pd	1.80131400	-0.86727300	-0.49671100
H	1.80900200	-2.29732700	1.70113300
H	1.65543000	0.24789000	2.46447100
H	-2.53750800	0.52974900	3.23771100
C	0.16654100	-1.13994200	-1.77947500
C	0.44297700	-0.33607300	-3.06991500
C	-1.23529800	0.86517600	-2.07924800
C	-1.10398700	-0.45742000	-1.18521800
C	0.20929800	1.09624400	-2.57529100

H	0.26153000	1.84933000	-3.36949600
H	0.89845600	1.37639800	-1.78123600
C	-0.76233000	-0.53979200	-4.03064000
H	-0.50627000	-0.19621500	-5.03811700
H	-1.04878800	-1.59235500	-4.11511800
C	-1.87895300	0.35035500	-3.39962000
H	-2.10466800	1.18543700	-4.06639000
H	-2.81591200	-0.18834300	-3.22297500
H	1.41681600	-0.53088900	-3.51960000
H	-1.98413100	-1.06484200	-1.40078100
C	0.10041000	-2.61854900	-1.91646600
O	-0.75010700	-3.34216700	-1.29293400
N	0.97541600	-3.21199100	-2.74730200
H	1.79100900	-2.65238100	-2.99535900
C	1.13145900	-4.65793800	-2.77378800
H	1.76079000	-4.92709000	-3.62382500
H	1.59865800	-5.02857500	-1.85143300
H	0.15572600	-5.13417600	-2.87805500
C	-1.92423200	2.06825300	-1.39065000
C	-0.94134700	2.89609400	-0.53042500
C	-2.67084700	3.02269500	-2.34588300
H	-2.69072700	1.66805100	-0.71988500
C	-1.64365400	4.01051200	0.25591700
H	-0.20170800	3.36067500	-1.19592900
H	-0.38791000	2.24723800	0.15334800
C	-3.38282800	4.14532100	-1.57245500
H	-1.96250000	3.46188100	-3.06382000
H	-3.41449700	2.47250100	-2.93133100
C	-2.41560300	4.94243000	-0.68750600
H	-0.90426100	4.57813700	0.83382800
H	-2.33663300	3.56210600	0.98181200
H	-3.89858800	4.81364700	-2.27273600
H	-4.16103000	3.69509000	-0.93915900
H	-2.95717900	5.70877700	-0.11958700
H	-1.69614000	5.47327600	-1.32739400
C	5.09485600	-0.70323200	-0.74688400
C	4.38047300	-1.14348700	-2.07244800
O	3.14749200	-1.53319300	-1.99702800
O	5.09006500	-1.19452300	-3.06975500
C	3.50389900	1.57007500	0.41081900
C	3.23615500	2.29317800	1.57746700

C	3.18006600	2.18384800	-0.80474800
C	2.59597200	3.52839000	1.54898700
C	2.55724900	3.42547600	-0.85442100
C	2.24420200	4.09367200	0.32770800
F	3.39847800	1.55008800	-1.96432800
F	2.18717800	3.94576200	-2.02793600
F	1.58652500	5.25364700	0.28595800
F	2.28650000	4.15077400	2.69431800
F	3.51266300	1.76226400	2.78180900
C	5.72014200	-1.98310300	-0.15408100
H	6.37952600	-2.40902500	-0.91541200
H	6.30485900	-1.76663600	0.74496800
H	4.95699000	-2.73065800	0.08622200
C	6.15778400	0.36528600	-0.98855200
H	5.72399700	1.28237000	-1.38920200
H	6.70511000	0.59432000	-0.06915400
H	6.84856900	-0.02327200	-1.73958900
S	3.89536800	-0.16451600	0.61243900
O	2.03331800	-2.38660900	2.65758000
C	0.97354800	-2.68044500	3.39594900
O	-0.09748900	-3.10034000	2.94755900
C	1.15784700	-2.41982900	4.86005400
H	0.70198800	-1.44191900	5.05921100
H	0.61849000	-3.16908700	5.44062900
H	2.21256400	-2.38951900	5.13389900
Ag	-0.71264400	-3.03002900	0.84573700
C	-5.70862300	0.78221500	0.81010800
C	-6.19325200	-0.36379700	0.16596400
C	-5.30950200	-1.40982000	-0.13142500
C	-3.96311600	-1.30731800	0.19894900
C	-3.45957300	-0.15775200	0.83299000
C	-4.36061900	0.87696000	1.14130500
H	-6.38776200	1.59453800	1.04193700
H	-5.69934900	-2.29684900	-0.61950200
H	-3.29519100	-2.13039500	-0.03716400
H	-3.98607500	1.77486100	1.62274100
C	-7.62177200	-0.52456700	-0.21893100
O	-8.08120500	-1.50438400	-0.77414100
O	-8.37208100	0.55115800	0.11786100
C	-9.76161200	0.45581100	-0.23144700
H	-10.22697500	-0.39851500	0.26781300

H	-10.21459100	1.38943100	0.10261200
H	-9.88017200	0.33507700	-1.31174500
O	-0.24833700	0.86374800	4.27432800
C	0.99867800	1.44840600	4.64297800
H	1.25918900	2.28657400	3.98840900
H	0.86863800	1.80900800	5.66493500
H	1.82002600	0.72128800	4.62350100

int97

C	1.20327200	2.01911500	2.16700300
C	0.14772100	1.24266400	2.64481100
C	-0.37326500	0.21566400	1.84511700
C	0.22422800	-0.06096900	0.62165100
C	1.38741600	0.61256600	0.17753300
C	1.81596600	1.72663700	0.93097500
Pd	-0.69656900	-1.26231300	-0.64743200
H	-1.27134000	-0.29095500	2.17546400
H	1.54103600	2.89021100	2.71432500
C	0.98704000	-0.83913400	-1.82355400
C	1.74118500	-2.13713800	-2.15354100
C	3.23849900	-0.99453500	-0.85681500
C	2.03453000	0.03899100	-1.05798200
C	2.50269700	-2.35434800	-0.83917200
H	3.18981000	-3.20373000	-0.89177000
H	1.84556000	-2.48604500	0.02240800
C	2.89923400	-1.83763900	-3.14328100
H	3.31625500	-2.77053000	-3.53902900
H	2.56901800	-1.24201900	-3.99974100
C	3.93179800	-1.08976700	-2.24807800
H	4.85717100	-1.66895900	-2.16437700
H	4.20114100	-0.10581900	-2.64242200
H	1.10126400	-2.97017100	-2.46252300
H	2.39577000	0.83650600	-1.70855600
C	0.25893900	-0.11929600	-2.89729300
O	-0.01744700	1.12228300	-2.83989100
C	-1.13351200	-0.28644900	-4.91409400
H	-1.22825400	-0.97075000	-5.75909300
H	-2.11830300	-0.15173300	-4.44596400
H	-0.79195400	0.68655700	-5.27073600
C	-4.69777000	-0.70980800	1.32201900
C	-3.51177500	-0.57684400	0.34172800

O	-3.58552200	0.38171800	-0.48581300
O	-2.57283100	-1.41789700	0.45742700
C	-4.67021700	2.13364300	1.68383200
C	-3.57207200	2.78388900	1.10973700
C	-5.93461600	2.68050300	1.42855700
C	-3.72007700	3.87710400	0.26599500
C	-6.10283400	3.79358800	0.60624500
C	-4.99097500	4.38496800	0.00935800
F	-7.03495600	2.12157600	1.94400300
F	-7.32481300	4.28461800	0.36901400
F	-5.14385400	5.43099000	-0.80497400
F	-2.64498000	4.40399700	-0.34542700
F	-2.32637400	2.33159700	1.30543700
C	-6.03092500	-0.55884100	0.58707500
H	-6.15462800	-1.40017000	-0.10520000
H	-6.86366500	-0.55869300	1.29358300
H	-6.05295000	0.35883800	-0.00082800
C	-4.64268300	-2.01222200	2.12601700
H	-3.70601800	-2.10280900	2.68002300
H	-5.48312800	-2.06745500	2.82373600
H	-4.70525000	-2.85983500	1.43712000
S	-4.46549600	0.64457900	2.63184500
Ag	-1.78683300	1.23423300	-1.43731700
C	0.11230300	-4.14890400	1.98028100
C	1.34673000	-4.76004700	1.73067000
C	1.60938500	-5.31383700	0.47184600
C	0.66708900	-5.21066900	-0.55133800
C	-0.53084000	-4.54843800	-0.29073700
C	-0.84139000	-4.03624000	0.97004700
H	-0.07521700	-3.72713900	2.96176400
H	2.56279800	-5.79294300	0.28281100
H	0.88485200	-5.60489200	-1.53709200
H	-1.77310900	-3.51329200	1.14905800
I	-1.88399000	-4.14474100	-1.92661100
C	2.36242900	-4.73977300	2.82190400
O	2.14656000	-4.35669800	3.95428200
O	3.57453300	-5.16737500	2.40053500
C	4.61478400	-5.12018700	3.39258800
H	4.75591500	-4.09596500	3.74578000
H	4.36355600	-5.75861100	4.24365400
H	5.51367600	-5.47956800	2.89200600

C	4.81928500	4.04944400	0.86949900
C	4.78327500	4.52427400	-0.44828300
C	3.75576900	4.10061700	-1.30401100
C	2.79592200	3.19999200	-0.85901000
C	2.84665200	2.68369400	0.44958800
C	3.85683600	3.14655000	1.30960300
H	5.60745800	4.37868300	1.53671100
H	3.72529000	4.49708500	-2.31341100
H	1.99008200	2.89544000	-1.51972400
H	3.90265800	2.76404500	2.32422200
C	5.79250600	5.47438000	-0.98599400
O	5.79736600	5.91020200	-2.12198800
O	6.72881900	5.81327000	-0.06603700
C	7.73175900	6.72797300	-0.53165700
H	7.27685400	7.66846500	-0.85484700
H	8.39639200	6.89474600	0.31640400
H	8.28271800	6.30092300	-1.37428100
C	4.20113800	-0.72757500	0.32089000
C	4.87838200	-2.01271400	0.84800900
C	5.28955300	0.31501600	-0.01446200
H	3.60171200	-0.32764300	1.15068200
C	5.79916800	-1.72740500	2.04464500
H	5.46824500	-2.47174000	0.04072500
H	4.12768200	-2.75274200	1.14307200
C	6.18291400	0.61851400	1.19565600
H	5.92559800	-0.07664500	-0.81963700
H	4.83720300	1.23354700	-0.39529200
C	6.85175200	-0.65865700	1.72001100
H	6.28621500	-2.65479000	2.37139500
H	5.18470100	-1.38162400	2.88888900
H	6.93543200	1.37033200	0.92916000
H	5.57364000	1.05894100	1.99550700
H	7.46199100	-0.44131200	2.60528400
H	7.53655500	-1.04861400	0.95299700
N	-0.17244600	-0.83088600	-3.96780600
H	-0.00024400	-1.82526000	-3.96927800
O	-0.49188800	1.44556200	3.83400600
C	-0.06874700	2.52764200	4.64577500
H	-0.20325400	3.49287200	4.13834500
H	-0.69758500	2.50110000	5.53729800
H	0.98384900	2.42629900	4.94380800

TS56

C	1.80488700	-0.17225600	2.44752700
C	0.49388300	0.10719900	2.83967100
C	-0.54872200	-0.04885500	1.91740200
C	-0.26725300	-0.56802700	0.66165900
C	1.02046800	-1.01910300	0.29757500
C	2.08326600	-0.71004500	1.17613100
Pd	-1.62703000	-0.35317400	-0.77927900
H	-1.53538600	0.31075600	2.18188200
H	2.63700800	0.07579600	3.09404600
C	-0.17338500	-1.52797600	-1.85924000
C	-0.69996500	-2.91533300	-2.23754600
C	1.03645000	-3.41009700	-0.83339500
C	1.09361900	-1.82004900	-0.97519100
C	-0.48758700	-3.67315300	-0.91568600
H	-0.73102900	-4.73639900	-1.00456400
H	-1.04315800	-3.24978500	-0.07696100
C	0.31025400	-3.63642900	-3.17037700
H	-0.14582600	-4.54595200	-3.57640200
H	0.61532000	-3.02193800	-4.02141200
C	1.48789000	-3.97147200	-2.21313100
H	1.63382800	-5.05415300	-2.14776000
H	2.43667400	-3.53772100	-2.54119900
H	-1.71760300	-2.90646700	-2.63641100
H	1.99235000	-1.57159800	-1.54061900
C	0.10010300	-0.55123300	-2.95379900
O	0.94785200	0.39411000	-2.82540000
C	-0.59348900	0.39020000	-5.10913900
H	-0.95390600	-0.01362700	-6.05670400
H	-1.25873400	1.20249000	-4.78537300
H	0.41097800	0.79192800	-5.24155100
C	-2.64163700	3.70166500	1.33380700
C	-2.08269600	2.72191300	0.27896500
O	-1.23663700	3.22779700	-0.53134400
O	-2.48075100	1.53158700	0.31045900
C	0.03602500	4.65723900	1.72493900
C	1.02247400	3.86958500	1.12015600
C	0.11518700	6.04045500	1.51947400
C	2.00202100	4.41296400	0.29944300
C	1.10487300	6.60934100	0.71914700

C	2.04388100	5.78998700	0.09518300
F	-0.78844500	6.86239400	2.06391100
F	1.14799700	7.93335200	0.52997700
F	2.97647500	6.32224800	-0.69704200
F	2.86648900	3.60795700	-0.34070600
F	1.01476000	2.53736300	1.26025100
C	-3.01625000	5.04066400	0.69578100
H	-3.83781700	4.88293200	-0.01293300
H	-3.34055200	5.75227800	1.45832800
H	-2.17701400	5.46122300	0.14200200
C	-3.81669000	3.09763500	2.10834000
H	-3.54026300	2.15695900	2.58903500
H	-4.17835300	3.79830000	2.86627900
H	-4.63328500	2.89002500	1.41019200
S	-1.28760500	3.91367600	2.64847200
Ag	0.05724200	1.92228500	-1.58381300
C	-4.61899000	-1.65920900	1.72986700
C	-4.61240100	-3.05451100	1.60210000
C	-4.13111900	-3.63457400	0.42003500
C	-3.63394700	-2.83702000	-0.60697100
C	-3.56696200	-1.45499700	-0.41335400
C	-4.13111600	-0.84293000	0.71292700
H	-5.02129500	-1.21926200	2.63667200
H	-4.15378500	-4.71166000	0.29874500
H	-3.28698000	-3.29116200	-1.52310500
H	-4.13757600	0.23310200	0.81571800
I	-3.79953600	-0.15676100	-2.53785800
C	-5.15141700	-3.86125700	2.72842700
O	-5.60856600	-3.39438100	3.75434600
O	-5.07694400	-5.19276000	2.49208900
C	-5.57968000	-6.02527800	3.54883500
H	-5.02143900	-5.85299000	4.47308400
H	-6.63647800	-5.81546500	3.73531100
H	-5.44642100	-7.05115300	3.20504600
C	5.80256300	-1.46718200	1.32420700
C	6.22872800	-1.03250900	0.06225600
C	5.29678600	-0.47058000	-0.82238800
C	3.95903800	-0.36650100	-0.46175100
C	3.51222700	-0.83671500	0.78809900
C	4.46185400	-1.36170600	1.68033000
H	6.52025900	-1.89681000	2.01346300

H	5.64521300	-0.11439400	-1.78611100
H	3.24972000	0.09109000	-1.14448300
H	4.13457000	-1.72125400	2.65054200
C	7.64318500	-1.13529300	-0.38565000
O	8.05300900	-0.77208600	-1.47199700
O	8.44645800	-1.68761300	0.55566300
C	9.82532400	-1.81400600	0.17728600
H	10.25575400	-0.83393800	-0.04630900
H	10.32619300	-2.26709400	1.03311600
H	9.92625400	-2.44824100	-0.70784600
C	1.78746300	-4.02402200	0.36926800
C	1.19016400	-5.37334200	0.82399800
C	3.29904800	-4.19942000	0.10154100
H	1.67770700	-3.33481900	1.21729300
C	1.93723100	-5.95468400	2.03457400
H	1.23238600	-6.09349600	-0.00648300
H	0.13253000	-5.25034500	1.08060600
C	4.04015900	-4.76055300	1.32260100
H	3.43643400	-4.90138700	-0.73119800
H	3.74582100	-3.25283900	-0.21313100
C	3.44002700	-6.10181900	1.76288800
H	1.49982900	-6.92048400	2.31558500
H	1.79361100	-5.28392500	2.89394300
H	5.10799700	-4.86611000	1.09649900
H	3.96791800	-4.04598600	2.15237100
H	3.95462400	-6.48226400	2.65364200
H	3.59342700	-6.84601800	0.96799600
N	-0.56217600	-0.67481800	-4.11797500
H	-1.29605300	-1.36749600	-4.15393100
O	0.13733700	0.61560800	4.05357200
C	1.16704900	0.98145100	4.95757400
H	1.82485900	1.74942700	4.52877800
H	0.66604200	1.38842500	5.83722500
H	1.77454200	0.11643000	5.25686000

int98

C	1.82936100	1.15775500	2.41282400
C	0.54478000	0.83858300	2.85667400
C	-0.28237700	0.04442100	2.05330700
C	0.21758900	-0.48293500	0.87201100
C	1.55862800	-0.30258300	0.47348600

C	2.33452700	0.61901000	1.21640700
Pd	-1.04306800	-1.06358300	-0.60145000
H	-1.32180400	-0.05023400	2.33979500
H	2.44003200	1.86892900	2.95453200
C	0.81219000	-1.47404400	-1.63443900
C	1.06736000	-2.94595200	-1.96996500
C	2.75188300	-2.48802000	-0.48563900
C	2.02869300	-1.08559000	-0.72249600
C	1.57456400	-3.47767200	-0.61436400
H	1.90483900	-4.51854800	-0.68290400
H	0.85255900	-3.39700900	0.19586500
C	2.36102000	-3.08669400	-2.82866300
H	2.42320300	-4.11075500	-3.21082000
H	2.38588500	-2.41952400	-3.69272400
C	3.50162500	-2.79110800	-1.81363300
H	4.14436700	-3.66785300	-1.68848100
H	4.14355300	-1.96226300	-2.12587800
H	0.20768900	-3.45999400	-2.40110400
H	2.71328700	-0.47100200	-1.30689800
C	0.65713900	-0.46766600	-2.74274000
O	0.80029600	0.78170100	-2.51134000
C	0.05035900	0.06052100	-5.04964400
H	0.09332300	-0.46294700	-6.00563200
H	-0.96319500	0.44517800	-4.88892800
H	0.75748200	0.89032800	-5.05249800
C	-4.31286700	1.40923100	1.28617900
C	-3.15661200	0.95691600	0.37497900
O	-2.70281400	1.84909200	-0.41306200
O	-2.75102900	-0.22883700	0.50084700
C	-2.94599500	3.89579500	1.70294300
C	-1.65173200	3.92938500	1.17064700
C	-3.77883700	4.98365100	1.40911800
C	-1.22539200	4.94890500	0.33026700
C	-3.35980800	6.03327600	0.59223200
C	-2.08167500	6.00760000	0.03776600
F	-5.02905800	5.02922900	1.87978600
F	-4.18231100	7.05225800	0.31984700
F	-1.68056500	6.99006300	-0.77086200
F	-0.01045800	4.88445400	-0.24226900
F	-0.78561900	2.93263400	1.40052900
C	-5.36816900	2.16867500	0.47994800

H	-5.82136000	1.48357700	-0.24560300
H	-6.14834100	2.55515700	1.13928000
H	-4.92313400	2.99303300	-0.07770900
C	-4.92631800	0.23723300	2.05771100
H	-4.18238000	-0.28362100	2.66400700
H	-5.73810700	0.58837700	2.70072800
H	-5.32817800	-0.48532400	1.34214000
S	-3.52964700	2.49714900	2.63209700
Ag	-0.89055900	1.61281500	-1.46835900
C	-2.07670300	-4.19295900	2.14231200
C	-2.33434200	-5.29527900	1.32130300
C	-2.17224800	-5.16998200	-0.06404600
C	-1.74441400	-3.96448800	-0.62073000
C	-1.47518100	-2.88161600	0.21738100
C	-1.65034600	-2.98099900	1.59701400
H	-2.20801700	-4.29554000	3.21470100
H	-2.39416200	-6.00992500	-0.71275200
H	-1.66044700	-3.87933200	-1.69441800
H	-1.45992800	-2.14740600	2.25504200
I	-2.81905500	-1.27001600	-2.80719500
C	-2.78204500	-6.55898600	1.96752600
O	-2.93291000	-6.70552400	3.16549900
O	-3.00738000	-7.54717000	1.06998600
C	-3.44941200	-8.79103000	1.63495800
H	-2.70045700	-9.18872400	2.32542400
H	-4.38790400	-8.65500700	2.17928200
H	-3.58967500	-9.46551900	0.79011000
C	5.97166200	1.70894700	1.22585700
C	6.13650500	2.15448700	-0.09218800
C	5.04678500	2.11615800	-0.97360100
C	3.81859600	1.61945400	-0.55312800
C	3.65359600	1.13201400	0.75686700
C	4.74082300	1.21171200	1.64246000
H	6.80961300	1.74288100	1.91238800
H	5.18336600	2.48928600	-1.98312500
H	2.97245200	1.61731900	-1.23388000
H	4.62426600	0.84600200	2.65739800
C	7.43070000	2.68046900	-0.60564600
O	7.61363300	3.07170400	-1.74275700
O	8.40175200	2.67730700	0.33778900
C	9.67644500	3.17239600	-0.10089900

H	9.59179200	4.20875600	-0.43911200
H	10.33395500	3.10352900	0.76587700
H	10.06188800	2.56697100	-0.92587900
C	3.62452100	-2.59403100	0.78253200
C	3.73964000	-4.03250700	1.33084100
C	5.04250700	-2.02046900	0.57225200
H	3.13699100	-2.00004700	1.56823000
C	4.58065800	-4.08286300	2.61727100
H	4.19969700	-4.67979300	0.56957700
H	2.74465000	-4.44304900	1.53393500
C	5.86332700	-2.04054800	1.86745000
H	5.56687000	-2.63146900	-0.17410300
H	4.99360100	-1.00829600	0.16476000
C	5.97344500	-3.46738300	2.42092700
H	4.66441000	-5.11805600	2.96926600
H	4.05248800	-3.52674000	3.40516900
H	6.85761200	-1.61318600	1.69065500
H	5.37741000	-1.40109100	2.61655400
H	6.52974200	-3.47459700	3.36605000
H	6.54575100	-4.08488900	1.71377100
N	0.40568100	-0.87437200	-3.98782600
H	0.12425300	-1.83822900	-4.10235000
O	-0.02512700	1.31579700	3.99629600
C	0.65818700	2.33051800	4.71681300
H	0.83834000	3.21305500	4.08882900
H	0.00299600	2.60393600	5.54506500
H	1.61550200	1.97264500	5.11855900

int99

C	3.44034900	0.67658200	-2.96271000
C	2.28088300	1.01007100	-3.67432900
C	1.02579200	0.70925300	-3.12994300
C	0.97760500	0.13742100	-1.86030900
C	2.11495100	-0.15652100	-1.10168400
C	3.37895600	0.06888500	-1.70520300
Pd	-0.74114900	-0.63707800	-1.24245700
H	0.10823300	0.88910300	-3.67902100
C	0.41078600	-1.23569500	0.41514200
C	-0.01016900	-0.79903300	1.81030000
C	2.02321100	0.22762300	1.55917400
C	1.87454500	-0.71659200	0.27648800

C	0.56198000	0.62521900	1.86762000
H	0.45810100	1.08439400	2.85671400
H	0.12139600	1.28757400	1.12902200
C	0.91500900	-1.53918900	2.83486900
H	0.48081000	-1.45498400	3.83552300
H	1.02962600	-2.60495400	2.62156500
C	2.26768700	-0.76984500	2.72628900
H	2.46115200	-0.23287200	3.65676100
H	3.12438900	-1.42657300	2.54353100
H	-1.07340700	-0.91111200	2.02199600
H	2.54715000	-1.56344600	0.43522800
C	0.13038800	-2.61630300	-0.10794900
O	0.28213400	-2.77854500	-1.34951600
N	-0.38912300	-3.58123800	0.66540100
H	-0.69000100	-3.34469500	1.59936800
C	-0.90008800	-4.81167900	0.06369000
H	-1.34998400	-5.41746000	0.84999000
H	-1.65255300	-4.57612800	-0.69206200
H	-0.08443800	-5.36566900	-0.40600400
C	-1.79413700	3.52011700	-0.68399600
C	-2.80190200	3.43702600	0.28417900
C	-3.15289900	2.18424400	0.80408400
C	-2.50402800	1.03489800	0.36062000
C	-1.49661900	1.12075200	-0.61015800
C	-1.14198100	2.36884500	-1.13077400
H	-1.51501300	4.48814900	-1.08523500
H	-3.93768600	2.12850000	1.55132100
H	-2.78723300	0.07292000	0.76393700
H	-0.35687800	2.46132300	-1.86959400
C	-3.52708200	4.63148600	0.79415500
O	-4.40804800	4.59850700	1.63206900
O	-3.09958800	5.78187900	0.22027700
C	-3.76627400	6.96969900	0.67365600
H	-3.30865600	7.79300400	0.12472400
H	-4.83789900	6.91510500	0.46283000
H	-3.62980200	7.10169400	1.75055800
C	3.03470300	1.38627700	1.41448900
C	2.45035400	2.58708100	0.63442600
C	3.62334500	1.89511000	2.74754900
H	3.88518400	1.00400500	0.84272000
C	3.50463800	3.67304900	0.38112000

H	1.62963900	3.02540800	1.21851800
H	2.01455200	2.25688200	-0.31155600
C	4.67834100	2.98840000	2.51045600
H	2.81759900	2.29058500	3.38370000
H	4.09014300	1.07329100	3.29982200
C	4.11951400	4.16381900	1.69858600
H	3.05743300	4.50926800	-0.16973800
H	4.29744900	3.26444100	-0.26035900
H	5.07485700	3.34006500	3.47061500
H	5.52389700	2.54444100	1.96547400
H	4.90524700	4.90468900	1.50699400
H	3.34319400	4.67282200	2.28786400
C	-4.68458200	-1.32707100	-2.18997000
C	-3.16682400	-1.24683300	-1.95962800
O	-2.64916100	-1.66526400	-0.87512200
O	-2.46694400	-0.64945600	-2.82796800
C	-5.01420100	-1.92556500	0.63091800
C	-4.01328000	-2.64741200	1.29555200
C	-5.48951900	-0.77251200	1.26501200
C	-3.45536600	-2.19859500	2.48434800
C	-4.95498300	-0.31924000	2.47212200
C	-3.91585900	-1.02305600	3.07289200
F	-6.45160000	-0.03190000	0.70644100
F	-5.39546600	0.81915800	3.02312100
F	-3.34950400	-0.57187500	4.19411200
F	-2.41988300	-2.86282500	3.04338700
F	-3.52130600	-3.77485700	0.77922900
C	-5.22572300	0.11366600	-2.12108400
H	-4.74798200	0.70648800	-2.90623300
H	-6.30843000	0.11754100	-2.26625800
H	-5.00053800	0.58344300	-1.16214800
C	-4.97588800	-1.95215600	-3.56469000
H	-4.59852200	-2.97665000	-3.62818700
H	-6.05089200	-1.95738100	-3.76886600
H	-4.47501300	-1.35253400	-4.32840100
S	-5.57979500	-2.45550400	-0.97288300
H	4.39910900	0.85815500	-3.43635000
O	2.47790900	1.58972800	-4.89134200
C	1.33558900	1.88787000	-5.68226000
H	1.71477300	2.33298800	-6.60333700
H	0.76475800	0.98219800	-5.92516600

H	0.67211700	2.60529600	-5.18093100
C	6.07260100	-2.04392300	-0.05491800
C	7.10440300	-1.11015700	0.10973300
C	6.92463100	0.20180200	-0.34934400
C	5.72102600	0.57290100	-0.94080100
C	4.66597200	-0.34556400	-1.07801300
C	4.87216400	-1.66695300	-0.64634800
H	6.23633500	-3.06221800	0.28147000
H	7.72410500	0.92455300	-0.23376800
H	5.57792400	1.59387000	-1.27989500
H	4.09154100	-2.40525800	-0.80030200
C	8.35916500	-1.56649700	0.76723700
O	8.54830300	-2.69315200	1.18513400
O	9.28412700	-0.58214000	0.85768900
C	10.51652600	-0.96299900	1.48889900
H	10.33641000	-1.30023100	2.51335000
H	10.99905700	-1.77297600	0.93511200
H	11.13989600	-0.06872600	1.48270300

TS57

C	3.35614900	1.98784000	-2.51611000
C	2.25831300	2.70720000	-3.00915800
C	0.98036800	2.39862700	-2.54970500
C	0.80617400	1.38515000	-1.59126200
C	1.89951100	0.61474000	-1.11364200
C	3.18464800	0.93158200	-1.62393500
Pd	-1.00219200	0.40948600	-1.32528200
H	0.12000000	2.95738500	-2.89053800
C	0.20921000	-1.15080400	-0.74099900
C	-0.30991600	-1.83540900	0.52622500
C	1.79205700	-1.11662500	1.12551600
C	1.63650600	-0.70448300	-0.40686500
C	0.33496400	-0.99983300	1.64954200
H	0.20400900	-1.46793900	2.63089700
H	-0.05813800	0.01396300	1.69949300
C	0.48140700	-3.16569300	0.64632000
H	0.02977700	-3.77095900	1.43668900
H	0.45600100	-3.75879500	-0.27101600
C	1.90770700	-2.68217100	1.03199800
H	2.19456900	-3.10861400	1.99292400
H	2.67378600	-2.97946000	0.31009900

H	-1.38918700	-1.95926200	0.56288600
H	2.27995500	-1.39531000	-0.94554400
C	0.15138300	-1.94378200	-2.06581600
O	1.14756700	-2.08511000	-2.77820800
N	-1.04402800	-2.50220600	-2.37723300
H	-1.85659800	-2.30213600	-1.80620400
C	-1.21489300	-3.26580000	-3.60089400
H	-1.10517500	-2.62744700	-4.48497800
H	-0.46111700	-4.05546400	-3.66359900
H	-2.21139100	-3.71047900	-3.59578100
C	-0.41367300	3.47858000	1.71492500
C	-1.36978800	4.38232700	1.23710300
C	-1.90920400	4.19229700	-0.04298400
C	-1.50966700	3.11960900	-0.83280000
C	-0.57939800	2.19079700	-0.32566100
C	-0.01601500	2.39631900	0.93288500
H	0.03084300	3.62756800	2.69267700
H	-2.64500600	4.90066800	-0.40936500
H	-1.95079300	2.99253000	-1.81512000
H	0.75249000	1.73677000	1.28998800
C	-1.83451500	5.55553300	2.02342500
O	-2.65374000	6.36595500	1.63332700
O	-1.24288800	5.63064900	3.23882000
C	-1.65335500	6.74537800	4.04605500
H	-1.09178800	6.65857000	4.97633100
H	-1.42430100	7.68949700	3.54426100
H	-2.72869900	6.70537500	4.23997000
C	2.95992800	-0.50940500	1.94148100
C	2.97218800	1.02908300	2.03640500
C	3.04406600	-1.06634100	3.38444800
H	3.88132100	-0.80912400	1.42103200
C	4.21139700	1.56196600	2.77332800
H	2.08357500	1.35033100	2.59717000
H	2.91106100	1.48119700	1.04384900
C	4.28248900	-0.55060000	4.13425900
H	2.14032400	-0.76756400	3.93447500
H	3.06376200	-2.15880000	3.38929700
C	4.31393400	0.98101800	4.18764500
H	4.18072700	2.65794400	2.80567100
H	5.10975400	1.28566500	2.20756300
H	4.30654500	-0.97224500	5.14627600

H	5.18491000	-0.91190900	3.62076500
H	5.22662900	1.33209400	4.68387400
H	3.46778200	1.33989000	4.79130600
C	-5.11364400	-0.19100100	-1.84688700
C	-3.59645100	0.05444600	-1.81807400
O	-2.85009100	-0.68800900	-1.07985700
O	-3.13539300	1.03326100	-2.44842500
C	-5.08904600	-2.25621400	0.18997000
C	-3.92983600	-2.97806500	0.50057100
C	-5.87019800	-1.82157500	1.26942200
C	-3.53435700	-3.20944900	1.81362100
C	-5.48978300	-2.03903300	2.59263400
C	-4.31328900	-2.73216500	2.86510400
F	-7.01516600	-1.16103800	1.06194300
F	-6.24969600	-1.59356500	3.59936500
F	-3.93630300	-2.94536300	4.12733300
F	-2.40040600	-3.87638500	2.07481100
F	-3.14531800	-3.47484700	-0.46588300
C	-5.74090900	0.78446600	-0.83601200
H	-5.49400400	1.80693100	-1.13855600
H	-6.82555600	0.66554300	-0.80871000
H	-5.34542700	0.62496400	0.16970000
C	-5.66812900	0.06208200	-3.25864700
H	-5.25464500	-0.64245100	-3.98672500
H	-6.75831700	-0.02267400	-3.26402200
H	-5.38415800	1.06964900	-3.56860400
S	-5.57354700	-1.97917900	-1.49955400
H	4.34508100	2.23829000	-2.88506600
O	2.54562500	3.68134600	-3.91495800
C	1.46568600	4.42791800	-4.46003600
H	1.91178200	5.13291600	-5.16277600
H	0.75819800	3.78117800	-4.99539200
H	0.92677800	4.98478100	-3.68192800
C	5.68247900	-1.90763600	-1.24804400
C	6.66936900	-1.30374200	-0.45571800
C	6.53431300	0.04157400	-0.08964700
C	5.40869200	0.75925800	-0.48695300
C	4.39731400	0.14919200	-1.24141600
C	4.56045200	-1.18774000	-1.64453200
H	5.81614400	-2.94260400	-1.54431400
H	7.30383000	0.51471900	0.50936000

H	5.29548100	1.79793600	-0.19294600
H	3.80336000	-1.65380500	-2.26924700
C	7.83463900	-2.13214800	-0.03946700
O	7.99098000	-3.30133600	-0.33482500
O	8.71618300	-1.43955200	0.71995200
C	9.86121800	-2.18822000	1.15668400
H	9.55355500	-3.04296900	1.76536400
H	10.43021300	-2.55787100	0.29926200
H	10.46090500	-1.49365400	1.74520200

int100

C	3.76917400	-2.91598300	1.36833600
C	2.78845300	-3.88463300	1.59276600
C	1.45131900	-3.52193200	1.46871100
C	1.08310300	-2.22290100	1.05822400
C	2.06078200	-1.25673400	0.76081700
C	3.42093600	-1.62173500	0.99133500
Pd	-1.28425700	0.04929100	0.88328900
H	0.66719100	-4.24224400	1.66294200
C	0.54662300	0.94303600	0.62231900
C	0.36024600	1.88632300	-0.58088400
C	1.98912100	0.46706500	-1.33769100
C	1.80082900	0.13763300	0.22308100
C	0.57777400	0.92460100	-1.76725900
H	0.58486200	1.43846000	-2.73107800
H	-0.16980100	0.13351900	-1.81725500
C	1.61894500	2.80115800	-0.69033900
H	1.39881900	3.64709400	-1.34853900
H	1.91035900	3.21132100	0.27957300
C	2.69304100	1.86161600	-1.31300600
H	2.92316700	2.19359200	-2.32694800
H	3.63276200	1.83991400	-0.75324800
H	-0.57442000	2.44872000	-0.57366200
H	2.58928400	0.71356600	0.70107400
C	0.71739000	1.52878700	2.02528200
O	1.43687000	0.97326200	2.86196200
N	0.08195900	2.70757000	2.28660800
H	-0.70125700	2.94702000	1.69289700
C	0.05250000	3.23386600	3.64195900
H	-0.22210600	4.29073900	3.61110600
H	-0.66615800	2.69449500	4.27337400

H	1.04213800	3.12640900	4.08748800
C	-2.41804300	-2.28380400	-0.45141400
C	-3.15006900	-2.71547400	0.64605300
C	-2.53196100	-2.81935300	1.91348000
C	-1.20036200	-2.49546500	2.07055100
C	-0.40281700	-2.05632100	0.95942100
C	-1.05845300	-1.92985300	-0.30152800
H	-2.88971800	-2.19825600	-1.42112600
H	-3.13786200	-3.13309300	2.75586900
H	-0.71789300	-2.58881600	3.03760800
H	-0.46629400	-1.74489400	-1.18605900
C	-4.61899200	-2.96178300	0.56659200
O	-5.29827500	-3.36723100	1.48888100
O	-5.10943300	-2.64888800	-0.64772300
C	-6.53306700	-2.74458000	-0.79600400
H	-6.74521300	-2.34107100	-1.78501600
H	-6.85880000	-3.78558500	-0.71878500
H	-7.03611700	-2.15551700	-0.02563000
C	2.70379000	-0.60295800	-2.19350900
C	1.84321100	-1.85395100	-2.46395400
C	3.24808300	-0.06845500	-3.53678100
H	3.57648800	-0.93406100	-1.62027600
C	2.61179500	-2.93827700	-3.23307600
H	0.95899500	-1.56273800	-3.04993300
H	1.48958500	-2.27544300	-1.52205100
C	4.00820800	-1.14955700	-4.32232800
H	2.41355800	0.31029900	-4.14472500
H	3.92361700	0.77421400	-3.36677000
C	3.15381500	-2.39963100	-4.56152000
H	1.96351600	-3.80643500	-3.40308500
H	3.44791100	-3.28930300	-2.61118100
H	4.36286300	-0.73716000	-5.27459700
H	4.90495900	-1.43280300	-3.75181200
H	3.73501800	-3.16880900	-5.08419700
H	2.30928700	-2.14177100	-5.21680900
C	-4.77042600	2.08774100	1.79603700
C	-3.51842600	1.27346200	1.46803700
O	-2.40690000	1.88431600	1.26909800
O	-3.58712800	0.02400700	1.36867400
C	-4.39525900	2.09823800	-1.05195700
C	-3.25251000	2.68862800	-1.60609400

C	-4.74405000	0.81797400	-1.50451600
C	-2.50117700	2.04958700	-2.58659100
C	-3.98574900	0.15404000	-2.46438800
C	-2.84871000	0.76438000	-2.98937700
F	-5.81975500	0.19587000	-1.01111900
F	-4.32258700	-1.07616300	-2.88084900
F	-2.08878400	0.11099000	-3.87393900
F	-1.42685800	2.65425600	-3.11083100
F	-2.82451800	3.88310400	-1.19135000
C	-5.90222800	1.18034200	2.28461900
H	-5.60796000	0.69233300	3.21970600
H	-6.80615400	1.76878200	2.46568500
H	-6.11954200	0.40567700	1.54999200
C	-4.44327800	3.19976400	2.80180900
H	-3.61160700	3.81064700	2.44901800
H	-5.31417100	3.84156300	2.96672200
H	-4.16919200	2.75061500	3.76331500
S	-5.32919200	2.95292000	0.19198600
H	4.80866100	-3.17982000	1.53040500
O	3.23504100	-5.12246800	1.94620800
C	2.27217800	-6.13101500	2.21572200
H	2.83835000	-7.02643000	2.47639000
H	1.62289000	-5.85686400	3.05784400
H	1.64841700	-6.34165800	1.33666500
C	5.66411100	1.36181000	1.69158500
C	6.69746700	1.16636900	0.76360000
C	6.66554900	0.04758600	-0.07847900
C	5.60313200	-0.84988900	-0.00084800
C	4.54954400	-0.64407600	0.90233000
C	4.60451000	0.46493400	1.76704700
H	5.71285900	2.22388400	2.34832500
H	7.46743900	-0.11202400	-0.79003000
H	5.57874600	-1.71590500	-0.65585000
H	3.80169700	0.62057400	2.48252300
C	7.79661700	2.16900600	0.72244100
O	7.86171600	3.15216900	1.43553300
O	8.73500000	1.87202300	-0.20836800
C	9.82181500	2.80620300	-0.29310800
H	9.45373600	3.80463000	-0.54490600
H	10.35713800	2.86253900	0.65875100
H	10.47557600	2.42821000	-1.07941000

TS58

C	-1.20504500	-2.24642900	2.96807600
C	-2.24413500	-1.53369000	3.57785900
C	-2.75474300	-0.39598000	2.94641400
C	-2.28531100	0.00175300	1.68628100
C	-1.27855800	-0.75842500	1.00583000
C	-0.71370600	-1.86647900	1.72387300
H	-3.50092200	0.22053000	3.43228400
C	2.45695700	3.60534100	-1.20172300
C	1.54081900	2.46292400	-0.73964500
O	1.35554400	2.25865400	0.48561600
O	0.99553400	1.73125700	-1.64341600
C	4.58293500	2.14272600	-0.01324300
C	5.32461600	2.87908100	0.91963800
C	4.21768000	0.83931000	0.34438700
C	5.68010600	2.34769000	2.15738000
C	4.55939200	0.29175100	1.57566100
C	5.29434300	1.04972100	2.48479100
F	3.50239800	0.07840600	-0.49839300
F	4.18289200	-0.95267100	1.89720800
F	5.62569200	0.53311200	3.66928600
F	6.38403300	3.07400400	3.03304500
F	5.70122600	4.13323100	0.65101200
C	1.98361400	4.19232400	-2.53782600
H	0.99592100	4.64377100	-2.39806900
H	2.67074500	4.97148700	-2.88122900
H	1.89322100	3.41969200	-3.30282500
C	2.58877800	4.68236000	-0.12524400
H	2.91037000	4.25480000	0.82443300
H	3.29822900	5.45195400	-0.43773900
H	1.60997700	5.14622100	0.04102000
S	4.13463400	2.82557700	-1.59094800
C	-2.53788000	3.53932000	0.31341200
C	-3.91817800	3.67033600	0.11979300
C	-4.76882100	2.62536300	0.50608200
C	-4.24154200	1.45352000	1.03499500
C	-2.85205400	1.28100100	1.16711900
C	-2.01283800	2.36264900	0.84408200
H	-1.87648300	4.35823000	0.05546000
H	-5.83833000	2.74854600	0.37279400

H	-4.90948300	0.64575700	1.31276400
H	-0.94646000	2.30535400	1.03725500
C	-4.53604200	4.89240800	-0.46624700
O	-5.73155900	5.05063000	-0.62449500
O	-3.61578400	5.82135400	-0.81232700
C	-4.15166000	7.02451400	-1.38571600
H	-4.82605700	7.51950300	-0.68165400
H	-3.29056700	7.65673900	-1.60237800
H	-4.70569600	6.80068700	-2.30140500
Pd	-0.09918600	0.40591300	-0.34400400
C	-0.74870300	-0.87362500	-1.78515200
C	-1.69381000	-0.24345600	-2.82811100
C	-3.04931300	-1.36407100	-1.35991200
C	-1.62673500	-1.54191800	-0.83325600
C	-2.96330500	0.04562300	-2.00184100
H	-3.82367500	0.27034400	-2.63880200
H	-2.84291600	0.84963900	-1.27835100
C	-2.19634500	-1.43604300	-3.69162600
H	-2.84098500	-1.05410700	-4.48992000
H	-1.38847500	-2.00896100	-4.14935200
C	-3.00248000	-2.27048300	-2.66018000
H	-4.02425100	-2.46314800	-2.99740200
H	-2.52741700	-3.23428500	-2.46289900
H	-1.26212000	0.58573700	-3.39032200
H	-1.32710400	-2.53688500	-0.53444000
C	0.43403200	-1.67672500	-2.32974400
O	0.34494800	-2.90206800	-2.43566400
N	1.50396700	-0.96205900	-2.74329800
H	1.52673600	0.03335800	-2.54452100
C	2.69272100	-1.60556300	-3.28124100
H	2.55888600	-1.87711300	-4.33477400
H	3.53031900	-0.91090300	-3.19574900
H	2.92536700	-2.51426900	-2.72176100
C	-4.18148800	-1.71009400	-0.38657500
C	-5.58162700	-1.32976300	-0.90149900
C	-4.14778400	-3.18594300	0.06138300
H	-4.01009800	-1.12165400	0.51650300
C	-6.66629100	-1.63333900	0.14493400
H	-5.80829700	-1.88523500	-1.82178800
H	-5.60572900	-0.26561900	-1.16113100
C	-5.22305000	-3.46985300	1.11994700

H	-4.31109300	-3.84065800	-0.80506700
H	-3.15939200	-3.43431000	0.46499900
C	-6.62019500	-3.09747500	0.60425600
H	-7.65615700	-1.38697800	-0.25676800
H	-6.51634800	-0.98336700	1.01974000
H	-5.19256500	-4.52462400	1.41760000
H	-4.99750500	-2.88245800	2.02229700
H	-7.37693800	-3.27913600	1.37683900
H	-6.87423100	-3.74873600	-0.24428400
O	-2.65978600	-2.00363600	4.77989100
C	-3.72470700	-1.33047300	5.44181500
H	-3.90995100	-1.89238500	6.35795800
H	-3.45161600	-0.29920900	5.69859200
H	-4.63591800	-1.32174600	4.83004200
H	-0.77794200	-3.09426700	3.49296500
C	1.16006200	-4.82215900	0.28343600
C	2.33441300	-4.20848200	-0.17196600
C	2.55163000	-2.85086200	0.08026600
C	1.57951900	-2.09515000	0.72322900
C	0.37487600	-2.68559300	1.13251900
C	0.19473700	-4.06614500	0.93920000
H	0.99763500	-5.87670900	0.09418200
H	3.47310000	-2.39046300	-0.25078800
H	1.75649700	-1.04351300	0.91177700
H	-0.73223500	-4.53112400	1.26317600
C	3.35905300	-4.93518500	-0.96716100
O	4.30114300	-4.40111200	-1.52480200
O	3.13013900	-6.26622800	-1.02402700
C	4.06373400	-7.01022400	-1.82215700
H	4.05450500	-6.65431400	-2.85600100
H	5.07760700	-6.90677700	-1.42598600
H	3.73488100	-8.04824500	-1.77001100

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C	-1.33432300	-2.22552700	3.14995500
C	-2.40611500	-1.50475300	3.68580200
C	-2.79909900	-0.30814600	3.08319000
C	-2.14060700	0.15727900	1.92998500
C	-1.08524400	-0.58918500	1.36610300
C	-0.67329400	-1.78495900	1.99926700
H	-3.60771200	0.28783100	3.48919100

C	1.98490000	3.43518500	-1.21973900
C	1.20401400	2.16811800	-0.87388200
O	1.07520500	1.81280900	0.33606900
O	0.68313000	1.47139500	-1.81035000
C	4.28949400	2.27418700	-0.02125500
C	4.92432100	3.11308800	0.90458800
C	4.11548500	0.93340500	0.34172700
C	5.36265000	2.64139700	2.13974400
C	4.54573000	0.44271200	1.56945900
C	5.17204200	1.30126600	2.47100700
F	3.50639900	0.07902800	-0.49260500
F	4.35892200	-0.84172100	1.89386300
F	5.58600500	0.84079000	3.65144600
F	5.96071700	3.46359600	3.00825800
F	5.11030900	4.40848100	0.63148800
C	1.47410200	4.05381400	-2.52705100
H	0.43144000	4.35882200	-2.39238300
H	2.06354500	4.93786400	-2.78588200
H	1.50881200	3.33770600	-3.34983600
C	1.95539100	4.43982700	-0.06733900
H	2.28798900	3.98378600	0.86542300
H	2.58778100	5.30035600	-0.29532800
H	0.92635000	4.78500800	0.08255100
S	3.74995200	2.87970200	-1.60187600
C	-2.20028200	3.67457800	0.48453300
C	-3.52753100	3.78171000	0.04912100
C	-4.41698200	2.72760800	0.29647800
C	-3.97423100	1.57234200	0.93136400
C	-2.63043200	1.42851700	1.31691600
C	-1.76186700	2.51558800	1.11913300
H	-1.51765300	4.50266100	0.33061100
H	-5.44823900	2.83018500	-0.02464000
H	-4.66883500	0.76010300	1.10882100
H	-0.73799600	2.45026200	1.46356200
C	-4.04514100	4.98316600	-0.65977700
O	-5.19533400	5.12634400	-1.02837400
O	-3.08534700	5.91782300	-0.86101500
C	-3.52579700	7.10452700	-1.53921600
H	-4.31699000	7.60205400	-0.97170500
H	-2.64673900	7.74488600	-1.61460200
H	-3.91072300	6.86025700	-2.53312400

Pd	-0.28211100	0.13187500	-0.34231500
C	-0.58494000	-1.20097200	-2.09089000
C	-1.47870100	-0.56084800	-3.15016400
C	-2.87198100	-1.49748800	-1.59688700
C	-1.44054100	-1.71648300	-1.12706800
C	-2.72214200	-0.14194300	-2.33378300
H	-3.57498200	0.08950500	-2.97895600
H	-2.54941200	0.69716400	-1.65258300
C	-2.05542100	-1.80361000	-3.91029600
H	-2.64037000	-1.45867100	-4.76835500
H	-1.27026900	-2.46844100	-4.27639600
C	-2.95802800	-2.47596200	-2.83429200
H	-3.99491000	-2.55518000	-3.17214600
H	-2.61408100	-3.48064700	-2.57733300
H	-1.00274500	0.19228800	-3.77778800
H	-1.15844700	-2.55605700	-0.50949900
C	0.73056100	-1.86575400	-2.45920100
O	0.75809800	-3.09303200	-2.55929100
N	1.77197100	-1.05429000	-2.73391900
H	1.65441400	-0.05758400	-2.58663800
C	3.07435900	-1.58111700	-3.11382700
H	3.13070400	-1.76825100	-4.19270800
H	3.83835500	-0.85342000	-2.83672500
H	3.26751600	-2.51937800	-2.59027700
C	-3.95321800	-1.66113200	-0.52374400
C	-5.35976500	-1.25390600	-1.00114600
C	-3.97710700	-3.08086500	0.08105200
H	-3.67681400	-0.98595900	0.28980600
C	-6.41033300	-1.39606800	0.11275400
H	-5.66075800	-1.88290500	-1.85005000
H	-5.34433400	-0.22010200	-1.36534700
C	-5.01163500	-3.19313200	1.20985900
H	-4.21635100	-3.81208100	-0.70366500
H	-2.98658500	-3.34219500	0.46873100
C	-6.41284500	-2.80655400	0.71788800
H	-7.40356700	-1.14066600	-0.27508900
H	-6.19647100	-0.67280900	0.91264300
H	-5.01506300	-4.21049200	1.61855500
H	-4.71250800	-2.52634200	2.03106000
H	-7.13988300	-2.86838500	1.53668600
H	-6.73769800	-3.52728900	-0.04623300

O	-2.99198800	-2.04818600	4.79238300
C	-4.12877600	-1.39494000	5.33572900
H	-4.45358500	-2.00579300	6.17947100
H	-3.88605900	-0.38574700	5.69452300
H	-4.94475800	-1.32747600	4.60324500
H	-1.02248200	-3.13763800	3.64838700
C	1.14895300	-4.75966200	0.52476000
C	2.32490800	-4.16019200	0.05671300
C	2.56677600	-2.80888500	0.32575300
C	1.61900000	-2.04757600	0.99805200
C	0.40815300	-2.62209700	1.41909000
C	0.20529600	-3.99656900	1.20554100
H	0.96370000	-5.80774500	0.32083900
H	3.49014200	-2.36043200	-0.01588900
H	1.81415900	-1.00057500	1.19658200
H	-0.72652600	-4.45181000	1.52907000
C	3.31737400	-4.88876600	-0.77413800
O	4.28348300	-4.37066200	-1.30711700
O	3.03296400	-6.20436100	-0.89573800
C	3.92693500	-6.94426300	-1.74061600
H	3.91819900	-6.53882500	-2.75612800
H	4.94909300	-6.89953200	-1.35483900
H	3.55816800	-7.97015700	-1.73376300
A			
C	3.23453900	1.68946500	0.92989000
C	3.12497200	1.64251500	2.31744900
C	1.92501800	1.94627700	2.97440900
C	0.81013900	2.26826800	2.21410600
C	0.86884300	2.33128300	0.79982600
C	2.10819500	2.02389600	0.16732800
H	0.36177100	3.52192500	0.36918700
Pd	-0.80608300	1.51111800	-0.15062300
C	0.02508400	-1.13688600	-1.04883700
O	0.77878300	-2.10860500	-1.21608000
O	0.25167800	-0.21891000	-0.17948400
C	-1.42471100	4.38137300	-0.10162200
O	-0.19341600	4.61419500	0.10302800
O	-1.94384900	3.22154900	-0.15596500
H	-0.13142800	2.49994200	2.70652100
H	3.99330700	1.34160300	2.89481400

H	1.86937300	1.91454900	4.05795200
O	2.10312000	2.08456200	-1.18265500
C	3.33573900	1.90299300	-1.88854400
H	3.09185000	2.05698400	-2.94061000
H	4.07692400	2.64868900	-1.57561400
H	3.72573300	0.89444900	-1.73774600
H	4.16123300	1.39234400	0.45806300
C	-1.17271100	-1.01407600	-2.02457500
C	-3.48509800	-0.70327700	-0.28236000
C	-4.61744500	-1.33087400	-0.82315700
C	-3.27769000	-0.82733600	1.09817600
C	-5.50631100	-2.05351700	-0.03392200
C	-4.16164300	-1.54300200	1.90417800
C	-5.27602500	-2.15698600	1.33708300
F	-2.22761400	-0.26407200	1.70124100
F	-3.94389600	-1.64338700	3.21695300
F	-6.12023600	-2.84414400	2.10366600
F	-6.57112400	-2.64641700	-0.57945000
F	-4.86432400	-1.25998700	-2.13656800
C	-0.63359900	-0.37996200	-3.32240700
H	0.16259700	-1.02514200	-3.70379100
H	-1.42173500	-0.30169900	-4.07632300
H	-0.20862800	0.61227500	-3.14001000
C	-1.81815900	-2.37187500	-2.29031400
H	-2.18280600	-2.83073600	-1.36799900
H	-2.64806600	-2.28005700	-2.99506000
H	-1.05314300	-3.03100000	-2.70533900
S	-2.44465800	0.24122100	-1.38957500
C	-2.33973600	5.56210700	-0.32241500
H	-2.24998100	5.87554400	-1.36792600
H	-3.37580600	5.28547000	-0.12607700
H	-2.03084200	6.39750100	0.30799600
C	4.09980000	-2.00953900	-0.19355500
H	3.86507900	-3.05683700	-0.42981800
C	5.46839000	-1.71746200	-0.81409300
C	4.14046800	-1.92270600	1.34396700
O	3.20331800	-1.10352500	-0.73429100
H	2.30043200	-1.50934800	-0.77907500
F	4.76310800	-2.99930400	1.86915400
F	4.79405200	-0.82451500	1.78464100
F	2.89017500	-1.88455800	1.83036100

F	5.79222200	-0.41005600	-0.71434100
F	5.45707200	-2.03224400	-2.12217600
F	6.44423900	-2.43305200	-0.22096300

B

C	3.18074400	-2.45018800	2.73675300
C	3.79919100	-3.66365400	2.43769100
C	3.69262400	-4.25073800	1.16964400
C	2.96343700	-3.59922000	0.18597000
C	2.31329500	-2.36475300	0.43757300
C	2.44968600	-1.79341600	1.73924300
H	1.03587300	-2.39362000	0.18708200
Pd	2.34140000	-0.98519100	-1.12993500
C	4.26818500	-0.16264300	-2.44743300
O	4.33746100	-1.17409600	-1.67176500
O	3.11994000	0.38300000	-2.62389100
C	5.49435900	0.40285600	-3.09098400
H	5.26782600	0.72655900	-4.10907100
H	5.79974500	1.28262200	-2.51377000
H	6.30408600	-0.32774900	-3.08409600
C	-0.46253400	-1.04524600	-0.28359300
O	-0.27924100	-2.20587300	0.17975900
O	0.42240200	-0.35402200	-0.87945400
H	2.86581400	-4.04435300	-0.80005900
H	4.37287100	-4.16288100	3.21380600
H	4.17284700	-5.20197300	0.96490800
O	1.80208100	-0.61956200	1.92867700
C	1.74130900	-0.05994300	3.24326100
H	1.15445900	0.85032800	3.14321800
H	1.25376300	-0.75237600	3.93870500
H	2.74049300	0.19886200	3.60631500
H	3.28305600	-2.02596800	3.72801100
C	-1.81132100	-0.35664300	-0.04093400
C	-4.59016200	-0.86438100	-0.09427000
C	-5.25174800	-0.44391100	1.06760200
C	-5.22015000	-0.60378200	-1.31996500
C	-6.48378800	0.20422800	1.01935800
C	-6.45225400	0.04213000	-1.38942700
C	-7.08564200	0.44297100	-0.21443600
F	-4.64016500	-0.95783900	-2.47070900
F	-7.03006000	0.28276200	-2.57126600

F	-8.26532200	1.06316600	-0.27148700
F	-7.09124200	0.59775900	2.14439300
F	-4.70383600	-0.64234600	2.27265300
C	-1.72101500	0.30533200	1.34956800
H	-0.98476500	1.11383600	1.32736000
H	-2.69021300	0.72843800	1.62188500
H	-1.43784400	-0.42535200	2.11005800
C	-2.12277800	0.67481200	-1.12788300
H	-2.22365400	0.20416300	-2.10758300
H	-3.05395200	1.19580200	-0.89212100
H	-1.31854200	1.41116600	-1.16586300
S	-3.06059500	-1.77109800	-0.01802400
C	2.16018100	2.31570400	0.00989300
H	1.78582500	1.29755600	0.16734500
C	3.54059600	2.37703700	0.67568900
C	1.14430800	3.24575500	0.67121600
O	2.25409000	2.68839400	-1.33007400
H	2.56109700	1.92513000	-1.85742100
F	0.97735700	2.92379800	1.98026300
F	1.49842700	4.53473100	0.60896100
F	-0.05780400	3.10988900	0.07579400
F	4.09248000	3.59568600	0.61813000
F	4.37335700	1.51613900	0.03556200
F	3.49606600	1.99843500	1.97253400
C			
C	-2.61181000	-3.22002700	1.69724400
C	-3.46417300	-2.68806500	2.66529500
C	-3.33552200	-1.36436100	3.10517800
C	-2.35101100	-0.56294000	2.53957100
C	-1.48052600	-1.04278000	1.52998600
C	-1.61552000	-2.40534100	1.13729200
H	-0.24170100	-0.69274400	1.72304900
Pd	-1.18091200	0.27521300	-0.13324500
C	-1.98177500	2.43320600	-1.97172300
O	-1.84103700	3.56954200	-2.39407200
O	-0.99842000	1.60755700	-1.71449100
C	1.52977900	-0.19444000	0.76037900
O	1.05790300	-0.46370500	1.90494100
O	0.83568200	-0.02188800	-0.28695200
H	-3.99380800	-0.97537300	3.87527800

H	-2.73249200	-4.25063900	1.38613400
C	-3.42195600	1.85542100	-1.80852700
C	-4.44770100	-0.49886700	-0.33493100
C	-5.70574200	-0.47817200	0.28184700
C	-4.04898100	-1.69156200	-0.95073500
C	-6.52370200	-1.60480400	0.31127400
C	-4.84686300	-2.82916000	-0.91708300
C	-6.08763600	-2.78677000	-0.28555200
F	-2.86759100	-1.79309200	-1.57063100
F	-4.41163200	-3.96899200	-1.46671900
F	-6.85396400	-3.87454400	-0.24815100
F	-7.71355200	-1.56174600	0.91387800
F	-6.14587400	0.63282500	0.87776700
C	-4.47109600	2.95799800	-1.70472400
H	-4.44364500	3.55116000	-2.62202500
H	-5.47146100	2.53237300	-1.57785300
H	-4.26071500	3.62840500	-0.86881800
C	-3.68120400	0.90580500	-2.98224900
H	-2.93151100	0.11564900	-3.02786300
H	-4.67953200	0.46268400	-2.92053600
H	-3.62711200	1.49154800	-3.90527200
S	-3.39817000	0.93371000	-0.14257100
C	3.05121800	-0.04666400	0.62925500
H	-4.23658500	-3.32407000	3.08965200
C	3.46937800	0.24853700	-0.80946000
H	2.99106200	1.17880800	-1.12336900
H	4.55295200	0.37877100	-0.86448500
H	3.16919800	-0.55100100	-1.48896400
C	3.53118300	1.05103200	1.59115000
H	3.19699400	0.84762800	2.60955800
H	4.62296300	1.09537500	1.58120800
H	3.13170400	2.01766300	1.27004500
S	3.65876500	-1.75122600	1.21920700
C	5.22092600	-1.87366100	0.38310000
C	5.33268500	-2.52273500	-0.85430000
C	6.39713000	-1.36088900	0.94700000
C	6.55833100	-2.66747300	-1.49945600
C	7.63211600	-1.49308400	0.31634100
C	7.71058900	-2.15266800	-0.90872000
F	8.74044600	-0.99467200	0.87565300
F	8.88934100	-2.28497700	-1.52025100

F	6.63766000	-3.28971200	-2.68147100
F	4.24840000	-3.00930300	-1.46778900
F	6.36401000	-0.71045800	2.11547300
H	-2.23801600	0.46742400	2.86603000
O	-0.73828800	-2.82585500	0.20317400
C	-0.87426200	-4.13450800	-0.34682000
H	-1.85452400	-4.25667500	-0.82228400
H	-0.08901900	-4.21850800	-1.09759600
H	-0.73114900	-4.90714100	0.41788600
C	0.75989100	4.01692300	-0.30620100
H	0.03872100	4.50977300	-0.97084800
C	0.04166700	3.79268700	1.04082500
C	1.96532900	4.95036600	-0.15419800
O	1.23420300	2.81192100	-0.81296300
H	0.50672400	2.36043200	-1.29987800
F	1.58153900	6.19194200	0.20221200
F	2.82700700	4.49912000	0.78433100
F	2.62776800	5.04101700	-1.31653800
F	0.71458500	2.94662300	1.83938300
F	-1.18529000	3.23765200	0.82134200
F	-0.16745800	4.93613200	1.71601900

D

C	0.60873200	3.66946300	-0.34478900
C	1.34454400	4.85599600	-0.41467100
C	2.28108800	5.13397300	0.58483700
C	2.47999200	4.26467100	1.66166500
C	1.73790900	3.08917100	1.72466600
H	1.85942300	2.40538900	2.55991600
C	0.78782600	2.75381400	0.72921500
H	-0.43245200	2.49201400	1.30022200
Pd	0.85886800	0.67938700	0.33371900
O	1.42970400	0.94330700	-1.63279600
C	0.70335800	0.75870200	-2.67029700
O	-0.54916800	0.64279200	-2.70729500
Ag	-1.71992600	0.86116900	-0.88160600
O	-2.50391400	0.71612700	1.15263100
C	-2.14739000	1.43294100	2.14723900
O	-1.44183700	2.48459100	2.05172300
C	-2.56097900	0.98628600	3.52552600
H	-1.71726400	0.42091700	3.94128200

H	-2.73271500	1.85252300	4.16648400
H	-3.44256900	0.34439700	3.49045700
C	1.47781500	0.62772500	-3.96744400
H	0.81615300	0.73785200	-4.82684000
H	2.28755300	1.35986700	-4.00317600
H	1.92901400	-0.37036100	-3.98647500
H	2.85534100	6.05453900	0.52115900
H	3.20160100	4.50651800	2.43557500
C	0.54586400	-2.12398100	1.84987100
C	0.56010300	-0.88951400	2.79646100
O	0.44453000	-1.10934000	3.99351400
O	0.56277100	0.31493600	2.28986500
C	2.80978100	-1.73371500	-0.08429700
C	3.72778100	-1.28524400	0.87089900
C	3.31023800	-2.10563000	-1.33728400
C	5.09316000	-1.24587900	0.60822700
C	4.67153800	-2.06016400	-1.62376600
C	5.56684700	-1.63807100	-0.64344300
F	2.47148600	-2.47276500	-2.31725300
F	5.11874100	-2.41322800	-2.83167800
F	6.87294500	-1.59759800	-0.90427100
F	5.94789300	-0.82058400	1.54109600
F	3.30553800	-0.84896800	2.06547000
C	1.38368400	-3.28050800	2.38609100
H	1.01143700	-3.51238300	3.38659400
H	1.28282500	-4.16358500	1.74848200
H	2.43749600	-3.01809000	2.48025200
C	-0.93502300	-2.52726000	1.70759400
H	-1.53903000	-1.71082500	1.31232700
H	-1.05931900	-3.40263000	1.06655600
H	-1.30934700	-2.75914100	2.70780500
S	1.02951700	-1.66933400	0.08029900
H	1.19819200	5.56215300	-1.22329200
O	-0.34638600	3.32750700	-1.24673900
C	-0.52089300	4.10741900	-2.42554900
H	0.41719300	4.18294600	-2.98835000
H	-1.25895000	3.57137800	-3.02257900
H	-0.89124800	5.11224000	-2.19058500
C	-4.74218900	-1.76620200	0.27209300
H	-5.55589900	-2.45301200	0.53043600
C	-5.41619100	-0.60413500	-0.48270300

C	-3.79641000	-2.57548900	-0.63491500
O	-4.11215800	-1.37285500	1.44107700
H	-3.52056300	-0.58960700	1.29541500
F	-4.37906400	-2.91138500	-1.79893600
F	-2.65930200	-1.89393000	-0.92630800
F	-3.42673400	-3.70625300	-0.00655400
F	-4.51950300	0.17463200	-1.14871400
F	-6.06787400	0.18717900	0.37945700
F	-6.29479200	-1.06190700	-1.39111400

E

C	4.40594200	2.60173500	1.07671300
C	4.95141700	1.84606800	0.03678100
C	4.15746200	1.01715100	-0.76082800
C	2.79021100	0.96751100	-0.52608900
C	2.18453000	1.70879400	0.51817700
C	3.02908200	2.53585300	1.31630100
H	1.51571900	0.88732900	1.33005600
Pd	0.26691500	2.46685300	0.18316300
Pd	-1.10908700	0.35489700	-1.28788700
C	0.49040500	2.39629800	-2.76741900
O	0.88172000	2.96966600	-1.70820700
O	-0.31470300	1.41514700	-2.86803900
C	1.07380100	2.90975400	-4.06573600
H	1.98656300	2.34094800	-4.27288700
H	0.37475100	2.75081600	-4.88790800
H	1.33634100	3.96424900	-3.97189400
C	-2.61429100	2.83247100	-0.70977900
O	-1.60899800	3.38922100	-0.20782400
O	-2.69033400	1.62894700	-1.15053900
C	-3.88240100	3.64750900	-0.85633800
H	-4.76242100	3.00789100	-0.76792400
H	-3.90428900	4.44484200	-0.11270100
H	-3.88911700	4.09797700	-1.85444400
C	-0.05449900	0.98781200	2.66741300
O	0.90244600	0.24228300	2.28321000
O	-0.45635700	2.02061100	2.05020800
H	2.17357000	0.30195700	-1.11817900
H	6.02329500	1.89312400	-0.13694100
H	4.60146300	0.37887700	-1.51461400
C	-0.86018300	-2.53090000	0.09764200

C	0.27301800	-2.19620800	-0.90863900
O	1.10313400	-3.08799900	-1.10772800
O	0.31360000	-1.05440200	-1.51318500
C	-3.52111500	-1.25939900	0.38375900
C	-4.23080100	-1.31513400	-0.82253900
C	-4.24486900	-1.39237500	1.57571500
C	-5.61237200	-1.47985200	-0.84151900
C	-5.62620400	-1.56309900	1.57505600
C	-6.30956800	-1.60410200	0.36040200
F	-3.61520200	-1.36284100	2.75807000
F	-6.29411100	-1.69087300	2.72314500
F	-7.62980600	-1.76940800	0.34711600
F	-6.27113600	-1.52981200	-1.99995500
F	-3.59908400	-1.22477800	-1.99596900
C	-1.78393000	-3.56716600	-0.54842200
H	-1.17453100	-4.44544300	-0.77629700
H	-2.58391800	-3.86391500	0.13532800
H	-2.22113400	-3.19951200	-1.47924900
C	-0.27103500	-3.02737500	1.42321800
H	0.35377300	-2.26439800	1.89134000
H	-1.07381800	-3.30922000	2.11183000
H	0.34955500	-3.90230100	1.21414700
S	-1.77948500	-0.90938500	0.50427200
C	-0.81147600	0.59259600	3.91259700
H	-0.17038900	0.01811100	4.58221200
H	-1.20473700	1.47938600	4.41175100
H	-1.65557900	-0.03531200	3.60889100
O	2.40632900	3.20463400	2.32067400
C	3.18239000	4.00091800	3.20759100
H	2.47689000	4.41379800	3.92939200
H	3.93443100	3.39957700	3.73374400
H	3.67987200	4.82216100	2.67698300
H	5.05318800	3.22550700	1.68143200
C	4.07008000	-2.75293900	-0.47729500
H	3.65688900	-3.76877500	-0.44713600
C	5.57087700	-2.89258100	-0.73765200
C	3.79808300	-2.16049400	0.92396400
O	3.53123700	-1.98527900	-1.50348600
H	2.60236600	-2.28791900	-1.61376900
F	3.91656600	-3.11959300	1.86709300
F	4.63293400	-1.15889800	1.25457400

F	2.53885800	-1.67763000	0.98977000
F	6.16046900	-1.70057100	-0.94071800
F	5.78110000	-3.64873700	-1.82967100
F	6.18619000	-3.49016700	0.30617200

G

C	0.00155300	-5.58279600	-0.04804400
C	-1.00676000	-5.30555800	0.87410600
C	-0.88656100	-4.26019500	1.79999300
C	0.26780000	-3.48619400	1.78611000
C	1.32123800	-3.72971000	0.87364100
C	1.16259100	-4.79566900	-0.05081800
H	2.53090000	-3.75121300	1.48358500
Pd	2.12851200	-1.95894700	-0.00321500
Pd	-2.54174700	1.16833000	-0.33555500
C	-4.34996400	2.75295100	-0.96411600
O	-4.54808900	1.50201700	-0.79784900
O	-3.16539200	3.19629400	-0.78124200
C	4.46991900	-3.16768400	1.29003100
O	3.67920900	-3.86041700	2.00002200
O	4.10431700	-2.39423500	0.35066900
H	0.36729500	-2.65937900	2.48413700
H	-1.90571100	-5.91732900	0.86699000
H	-1.69010800	-4.04567600	2.49630600
C	1.70430000	1.57054700	-0.10141700
C	0.27644400	1.37891300	-0.69192300
O	0.09154100	1.38637000	-1.90498300
O	-0.62943800	1.27485400	0.23510600
C	4.39195900	0.56622700	-0.47224700
C	5.25576200	1.07383300	-1.45374700
C	4.94485800	0.28710600	0.78450800
C	6.61247000	1.27618900	-1.20762300
C	6.29900800	0.46950100	1.04084700
C	7.13747200	0.96148600	0.04332100
F	4.19747200	-0.16706700	1.79684900
F	6.80334400	0.14675500	2.24065500
F	8.43553400	1.13725400	0.28879800
F	7.41011400	1.76196700	-2.16293100
F	4.79554000	1.37525100	-2.66981500
C	2.25397000	2.91451500	-0.59633100
H	1.64138800	3.71572900	-0.17764300

H	3.28639900	3.05490400	-0.26237900
H	2.20594300	2.97869700	-1.68447200
C	1.74510000	1.45756800	1.41871400
H	1.41546700	0.47395600	1.75577300
H	2.75042600	1.64952500	1.79528600
H	1.07213100	2.20848000	1.83378300
S	2.71604500	0.19428300	-0.96119600
C	-5.47202700	3.67421600	-1.32962900
H	-6.33936900	3.10436900	-1.66471300
H	-5.74554900	4.26574400	-0.44947600
H	-5.14170300	4.36524300	-2.10899300
C	5.94999600	-3.21945400	1.58490600
H	6.18458400	-4.05355500	2.24545600
H	6.50791400	-3.29912300	0.64924700
H	6.23659400	-2.27936800	2.06719100
O	2.19901600	-4.99153900	-0.89697400
C	1.96945700	-5.72939900	-2.09599400
H	2.87684300	-5.61595200	-2.69003900
H	1.80589500	-6.79502100	-1.89068700
H	1.11879800	-5.30605000	-2.63929600
H	-0.12847400	-6.38856100	-0.76047700
C	-1.82621800	-1.93594600	-1.69202400
C	-0.30715800	-2.18715500	-1.47909900
O	0.26396100	-2.93619400	-2.26390600
O	0.19828200	-1.53036900	-0.48370700
C	-4.10774100	-1.58830500	0.19126100
C	-5.14437900	-1.43700800	-0.73608000
C	-4.44889100	-2.06858300	1.46447100
C	-6.46236500	-1.74597500	-0.41617700
C	-5.76240300	-2.38079000	1.80364900
C	-6.77273100	-2.21737000	0.85816300
F	-3.51076600	-2.22218100	2.40779900
F	-6.05637100	-2.83251200	3.02557700
F	-8.03337100	-2.51429200	1.17011200
F	-7.43036700	-1.59313000	-1.32363700
F	-4.89794700	-1.00619400	-1.97689200
C	-1.97449300	-1.01236000	-2.90727600
H	-1.55963400	-1.55201000	-3.76439100
H	-3.01865000	-0.77851400	-3.10455700
H	-1.40386200	-0.09081900	-2.77585500
C	-2.55617400	-3.26787600	-1.87345600

H	-2.51795400	-3.88228900	-0.97066500
H	-3.59337100	-3.11283200	-2.17509800
H	-2.03298100	-3.80556800	-2.66716500
S	-2.39106300	-1.12945800	-0.04399300
C	-1.13741300	5.28761200	0.31961800
H	-2.19261500	5.55704700	0.19589400
C	-1.00851600	4.67890200	1.72521900
C	-0.32102800	6.57536400	0.16587900
O	-0.68294600	4.39617700	-0.65225500
H	-1.44486100	3.88573900	-0.96866600
F	-0.65326000	7.48134300	1.10735100
F	0.99967600	6.33944500	0.26118700
F	-0.56324400	7.12223500	-1.03774700
F	0.27503400	4.40676300	2.03801500
F	-1.70310100	3.52543500	1.79636800
F	-1.49881500	5.50780600	2.66694400

F-2

C	4.04741900	-1.73128500	-3.11913300
C	4.44665200	-0.41150500	-3.32529800
C	3.68621800	0.67126800	-2.86258500
C	2.52162200	0.41537900	-2.15359200
C	2.06525100	-0.90640400	-1.92049400
C	2.85778900	-1.98144400	-2.42244000
H	0.79580600	-1.14517600	-2.36976400
Pd	1.32115700	-1.28241100	-0.01430500
Pd	0.36031600	1.19986400	1.16238300
C	3.21595900	0.42044500	1.54782800
O	3.11011100	-0.53082700	0.69414000
O	2.27997900	1.16530700	1.94882600
C	4.59882800	0.66016700	2.09942000
H	5.20456900	1.10118600	1.30368900
H	4.55820900	1.34969900	2.94163200
H	5.04784900	-0.29113600	2.39169200
C	0.12476200	-1.23810200	2.79328700
O	0.83346700	-1.88117100	1.97533500
O	-0.29156900	-0.03772800	2.64865500
C	-0.25172400	-1.91715200	4.09090200
H	-0.34047500	-2.99366700	3.93812700
H	0.54746600	-1.73549600	4.81757300
H	-1.17783400	-1.50141900	4.49031600

C	-0.93172600	-2.03482100	-1.75970900
O	-0.33708400	-1.51576700	-2.75751700
O	-0.47598700	-2.07200300	-0.58348500
H	1.94830500	1.23816000	-1.73856100
H	5.37427400	-0.22301900	-3.85921700
H	4.02717700	1.68535200	-3.02867700
C	-1.39411500	2.53595500	-1.15410000
C	-0.06016400	3.25190500	-0.84774800
O	0.12894200	4.35085100	-1.36954800
O	0.85760000	2.62603800	-0.17049800
C	-2.82520200	1.85720900	1.34810700
C	-2.61826900	3.07052400	2.01183200
C	-3.95813700	1.11098800	1.68431500
C	-3.53096500	3.55256800	2.94339400
C	-4.89097200	1.58041900	2.60299600
C	-4.67572100	2.80592800	3.23153700
F	-4.16473600	-0.09877300	1.14376700
F	-5.97532400	0.85846500	2.88784900
F	-5.55817400	3.26245200	4.11611900
F	-3.32436800	4.71767600	3.55646600
F	-1.52477900	3.79753300	1.74842700
C	-2.55982500	3.51335500	-1.26388000
H	-2.33608900	4.18636400	-2.09455000
H	-3.49626900	2.99168600	-1.46599900
H	-2.66338600	4.12861800	-0.37040500
C	-1.19716800	1.74470500	-2.46085400
H	-0.39478900	1.00897500	-2.37946700
H	-2.11288900	1.22103700	-2.73995900
H	-0.92872900	2.45604000	-3.24738200
S	-1.69471900	1.17843900	0.15205600
O	2.35552200	-3.21559300	-2.20403900
C	3.18211100	-4.35587900	-2.44413900
H	2.60756900	-5.21108700	-2.09188700
H	3.40143200	-4.47033400	-3.51238400
H	4.10633800	-4.28209300	-1.86377400
H	4.66174500	-2.54404500	-3.48696200
C	-2.28297700	-2.72402500	-2.00457900
C	-4.84293400	-1.37897900	-2.16973000
C	-5.77927000	-2.42247800	-2.16035900
C	-5.19291000	-0.21413900	-1.48025000
C	-6.98672600	-2.32382000	-1.47550000

C	-6.38616000	-0.09593300	-0.77612800
C	-7.29094400	-1.15338900	-0.77863100
F	-4.35164700	0.83287200	-1.43666200
F	-6.64403000	1.01432900	-0.07222700
F	-8.43656900	-1.05682200	-0.10526400
F	-7.85077300	-3.34257800	-1.46957700
F	-5.50200700	-3.57921900	-2.77638600
C	-2.02758000	-3.96619000	-2.87623700
H	-1.37377100	-4.66304700	-2.33896900
H	-2.97745900	-4.46030000	-3.09170300
H	-1.54450000	-3.69316800	-3.81657200
C	-2.95655800	-3.09458000	-0.68443300
H	-3.18580500	-2.21332800	-0.08195900
H	-3.87001900	-3.66075400	-0.87064000
H	-2.27102300	-3.72281100	-0.11118100
S	-3.29977100	-1.48793300	-3.04072300
C	3.33244100	4.29503400	-1.18713600
H	2.71805300	3.43681500	-1.47574000
C	4.05053600	4.77921500	-2.45257100
C	4.30679400	3.76773400	-0.12795600
O	2.57957700	5.33795500	-0.66057700
H	1.64001200	5.11987600	-0.84496600
F	4.87309600	2.60052300	-0.54606600
F	5.30437800	4.62681200	0.14050800
F	3.66209800	3.50472400	1.01896500
F	4.77672100	5.88372000	-2.24183300
F	3.13693600	5.05014000	-3.40494600
F	4.88618800	3.82832400	-2.95168600
C	3.67458300	-3.50548300	1.55537400
H	2.94683600	-2.83035100	2.01651800
C	2.89550700	-4.76305100	1.16114600
C	4.75091000	-3.77996600	2.61100200
O	4.26705300	-2.96966100	0.40616400
H	4.07761000	-2.01042100	0.40415200
F	4.20588500	-4.18237000	3.77653200
F	5.63624500	-4.70807000	2.21792400
F	5.42991700	-2.63460500	2.85543600
F	3.66065600	-5.64131500	0.48565900
F	1.85835400	-4.43188800	0.36176800
F	2.39182100	-5.38941400	2.24216800

F-3

C	-0.10804800	-5.54777200	-2.40869200
C	1.12349200	-5.25633800	-2.99568900
C	1.73315500	-4.00449400	-2.84371300
C	1.10308900	-3.04365500	-2.06686900
C	-0.14946500	-3.28594200	-1.44356000
C	-0.73962100	-4.57325500	-1.62454300
H	-1.12402700	-2.44046000	-1.87596200
Pd	-0.43103500	-2.41966200	0.42314600
Pd	1.00431600	0.10654500	0.43667100
C	2.31425800	-2.49031700	1.38129700
O	1.36477700	-3.22343800	0.97678200
O	2.32863100	-1.21191700	1.39052200
C	3.56008800	-3.17356200	1.88612700
H	4.33471500	-3.04627200	1.12443900
H	3.89731800	-2.68719300	2.80486200
H	3.37462500	-4.23338900	2.05919600
C	-0.61681800	-0.48886800	2.80658200
O	-0.70497100	-1.70151800	2.43998200
O	-0.07370000	0.44309700	2.13408900
C	-1.18043800	-0.11968100	4.15690700
H	-2.16515000	-0.57403400	4.27956600
H	-0.52093000	-0.52944100	4.92900900
H	-1.23260300	0.96287000	4.27025200
C	-2.68233900	-1.32444500	-1.14508800
O	-2.13710400	-1.75428100	-2.20711000
O	-2.22827000	-1.51919000	0.02064700
H	1.57670800	-2.07837500	-1.93662000
H	1.61376300	-6.02428700	-3.58820400
H	2.68961200	-3.78919700	-3.30603500
C	0.72650600	1.55102800	-2.41091500
C	2.10335900	0.90219100	-2.15009100
O	3.05037800	1.14713000	-2.86981500
O	2.13367400	-0.02735700	-1.21084900
C	-0.02643800	3.13469800	-0.02510800
C	1.24228000	3.67913400	0.20070200
C	-1.13864300	3.83415500	0.45243800
C	1.40500000	4.88289200	0.87648600
C	-0.99843500	5.04564400	1.12074200
C	0.27731800	5.56803900	1.33257800
F	-2.37542000	3.33358800	0.30550800

F	-2.07376500	5.69786400	1.56643500
F	0.42032300	6.72310700	1.97727500
F	2.61948000	5.38399600	1.08805900
F	2.32559800	3.03425300	-0.23573200
C	0.84925800	2.94246400	-3.01964600
H	1.37324800	2.82893100	-3.97178900
H	-0.13125800	3.38529800	-3.19912200
H	1.44954900	3.60879900	-2.40142000
C	-0.05649200	0.59293000	-3.32748500
H	-0.16516300	-0.39747800	-2.88216400
H	-1.05178200	0.98487400	-3.54290200
H	0.50453700	0.48681200	-4.26082500
S	-0.29033600	1.55099000	-0.79364700
O	-1.94799500	-4.74027800	-1.04105200
C	-2.65406800	-5.96541600	-1.23503800
H	-3.59607100	-5.84410600	-0.70589800
H	-2.84251000	-6.14772600	-2.29965700
H	-2.10120100	-6.80932900	-0.80699800
H	-0.55294900	-6.52467700	-2.55362900
C	-4.02002300	-0.57591000	-1.24499600
C	-4.52030200	2.03292000	-2.37318100
C	-5.86430900	2.28670800	-2.06666500
C	-3.64286300	3.11906100	-2.29734700
C	-6.30674200	3.54684100	-1.67487500
C	-4.05563800	4.38314300	-1.89123600
C	-5.39609300	4.60056500	-1.58562800
F	-2.33849200	2.96602500	-2.58160800
F	-3.16321400	5.37318200	-1.76611100
F	-5.80717900	5.80616300	-1.19406900
F	-7.59127700	3.75226200	-1.37096700
F	-6.75820200	1.28954000	-2.08858200
C	-5.12432600	-1.64257300	-1.38735200
H	-5.14472900	-2.27583200	-0.49519100
H	-6.09084900	-1.14600300	-1.49443400
H	-4.95143500	-2.27115600	-2.26409600
C	-4.25387200	0.30164400	-0.01403800
H	-3.50537100	1.09144100	0.07628200
H	-5.24775700	0.74899400	-0.05465800
H	-4.20732600	-0.31591300	0.88178600
S	-3.93388100	0.42840000	-2.85966900
C	5.23379700	-1.12861000	-1.57860900

H	5.15742100	-0.05424100	-1.78399200
C	6.52301600	-1.36760900	-0.79484500
C	5.21387900	-1.84709700	-2.93359100
O	4.18134100	-1.60325600	-0.79636200
H	3.40776600	-1.01853000	-0.97667400
F	6.12794700	-1.34902600	-3.78411800
F	5.42870100	-3.17195600	-2.81372800
F	3.99142500	-1.69096700	-3.49635300
F	6.63576600	-2.65275900	-0.40450700
F	6.53540100	-0.60669400	0.32049100
F	7.60975200	-1.05305400	-1.52317100
C	-3.50191900	-3.10600100	2.54366300
H	-3.07764700	-2.57887300	1.68557600
C	-3.86685600	-4.50434000	2.04301400
C	-4.72278000	-2.29270100	2.97472900
O	-2.61596700	-3.20490600	3.61780300
H	-1.78532500	-2.77115900	3.33133400
F	-5.63289400	-2.19866500	1.97555400
F	-5.33614900	-2.79148400	4.05201000
F	-4.32728700	-1.02697000	3.26613900
F	-4.57238700	-5.21525800	2.93486300
F	-2.74516400	-5.19026000	1.75140100
F	-4.60291400	-4.42809500	0.90101100
C	4.66400700	1.42486400	1.97501900
H	5.36083400	0.73785300	2.47350700
C	5.50244900	2.61925300	1.50595100
C	3.61202200	1.81879400	3.02722500
O	4.06082300	0.87896400	0.84802400
H	3.78039900	-0.03700400	1.03159800
F	4.17486400	2.37340000	4.11524700
F	2.69770500	2.68715600	2.54423900
F	2.94380300	0.71389900	3.42431900
F	4.74322600	3.58782200	0.96434800
F	6.39051400	2.21627500	0.58418100
F	6.18368300	3.15412700	2.53954100

F-4

C	-4.60797000	-2.76135300	1.46776600
C	-4.15336500	-3.70543400	0.54606800
C	-2.84651600	-3.66939000	0.04808600
C	-1.98809400	-2.66964900	0.48682800

C	-2.40572100	-1.66600100	1.39767700
C	-3.73697600	-1.75362900	1.90314700
H	-2.38095000	-0.39112500	0.84164200
Pd	-0.92650200	-0.79896300	2.58487900
Pd	1.25762100	-0.53369000	0.64041600
C	1.14982500	-2.85719300	2.56023400
O	-0.06312800	-2.63239400	2.84375300
O	1.90678500	-2.11357600	1.85098500
C	1.77881600	-4.09444200	3.15177200
H	1.00936400	-4.82040200	3.41252300
H	2.48845900	-4.52516000	2.44611900
H	2.31489400	-3.80096700	4.06071500
C	1.43261300	0.79829900	3.29115500
O	0.57294000	0.04144300	3.81610700
O	1.68207900	0.90050400	2.03997800
C	2.28305300	1.66644400	4.18803100
H	1.90188400	1.65981900	5.20895700
H	3.30417600	1.27543600	4.16543000
H	2.30925500	2.68555400	3.79419300
C	-2.37149500	1.51751900	1.53224100
O	-2.63389300	0.80309800	0.50331200
O	-1.70789100	1.09577700	2.51307400
H	-0.96920400	-2.64457400	0.11693500
H	-4.83863000	-4.47576800	0.20551500
H	-2.50384000	-4.42017900	-0.65344600
C	0.28563200	-0.04524400	-2.34725000
C	1.04491000	-1.36852500	-2.12512300
O	1.36563600	-2.02842800	-3.11110000
O	1.14746100	-1.81594300	-0.90426400
C	1.96711400	2.04850100	-1.00154400
C	3.15668000	1.64499100	-1.61417700
C	1.94240200	3.30282800	-0.38490400
C	4.25011300	2.50251800	-1.69717300
C	3.01888600	4.17616000	-0.46248600
C	4.17766600	3.77273400	-1.12406000
F	0.86063800	3.69254500	0.31195100
F	2.94184500	5.38567400	0.09817200
F	5.21923700	4.59724000	-1.20322200
F	5.36577800	2.11958400	-2.31359000
F	3.26781000	0.41622700	-2.12599500
C	0.63449200	0.67568700	-3.64210200

H	0.44050900	-0.02448800	-4.45823500
H	0.00723900	1.55864500	-3.76655400
H	1.68398500	0.95751900	-3.69822700
C	-1.20734000	-0.42916500	-2.32965500
H	-1.50616000	-0.88412000	-1.38540000
H	-1.85249500	0.42276800	-2.52893200
H	-1.36391000	-1.17132900	-3.11634000
S	0.49748800	1.05461200	-0.81325200
O	-4.10355500	-0.76110200	2.75383900
C	-5.45421400	-0.70549900	3.21519600
H	-5.50937000	0.17823300	3.85093500
H	-6.15311600	-0.60131600	2.37971600
H	-5.70740500	-1.59313800	3.80620800
H	-5.62962900	-2.81085700	1.82137700
C	-2.95081400	2.93429000	1.69905400
C	-2.13133700	4.45173900	-0.62967400
C	-1.66338800	5.70199700	-0.19675500
C	-1.46719500	3.87137500	-1.71673200
C	-0.53613800	6.30205100	-0.75278900
C	-0.35302300	4.46556600	-2.30052700
C	0.12424700	5.67569700	-1.80624300
F	-1.88054500	2.70154900	-2.22201800
F	0.30098200	3.85627100	-3.30076600
F	1.22956600	6.21490200	-2.32217500
F	-0.08842700	7.46944100	-0.28564500
F	-2.28260100	6.35721000	0.78988400
C	-4.23432800	2.76287000	2.54702300
H	-3.96968300	2.27064800	3.48674800
H	-4.66518500	3.74327700	2.76427200
H	-4.97805800	2.15182300	2.03216200
C	-1.93897700	3.82642100	2.42841200
H	-1.00688000	3.91348300	1.86634900
H	-2.35765100	4.82045700	2.58254400
H	-1.70390900	3.37636800	3.39481300
S	-3.56598500	3.68016000	0.08994800
C	0.83711600	-4.80597600	-1.74386500
H	0.25813500	-3.88590500	-1.62871100
C	-0.12796100	-5.85795600	-2.29702500
C	1.32397000	-5.16364800	-0.33001200
O	1.90552800	-4.66205000	-2.61766500
H	1.93753700	-3.71006200	-2.85483800

F	0.34874700	-4.90112400	0.58354600
F	1.66342100	-6.45759800	-0.19427400
F	2.39645400	-4.42407300	0.00663200
F	0.47989100	-7.00778000	-2.60960100
F	-0.72820400	-5.38149700	-3.40371500
F	-1.10818700	-6.14011300	-1.39455900
C	-4.84565000	-0.38088900	-1.27612300
H	-4.27066600	-0.85412300	-0.47614300
C	-6.18704700	0.03499900	-0.65891100
C	-5.00232900	-1.44103800	-2.36706300
O	-4.21406600	0.73109100	-1.83577900
H	-3.69035300	1.15536400	-1.13322400
F	-5.71498500	-2.49401900	-1.91254000
F	-5.61187800	-0.96101100	-3.45843800
F	-3.78614100	-1.89885600	-2.72999400
F	-7.06034600	0.48579800	-1.56554900
F	-5.96673200	1.02906300	0.23912400
F	-6.76898400	-0.98249200	0.01809900
C	5.24465900	-1.50319600	0.77275700
H	5.70745800	-2.25198900	1.43194100
C	6.24407400	-1.25121000	-0.36361700
C	5.03019600	-0.24992600	1.64064200
O	4.06413800	-1.92863200	0.17610600
H	3.43141200	-2.26924700	0.83824200
F	6.18008900	0.20068200	2.17238500
F	4.46577700	0.76324600	0.95342000
F	4.20321600	-0.55797900	2.66878500
F	5.82940900	-0.26702400	-1.18253000
F	6.40098000	-2.36587400	-1.08938400
F	7.44890800	-0.89968500	0.13039200

F-5

C	4.21694800	2.99173200	-0.67031100
C	3.54876000	3.67541800	-1.68763700
C	2.18460200	3.47976400	-1.92258500
C	1.48010200	2.58833500	-1.12227900
C	2.11507700	1.84368400	-0.09475800
C	3.50065600	2.09617000	0.12802800
H	2.10330200	0.49557500	-0.36555800
Pd	0.93786100	1.17445100	1.49602100
Pd	-1.49310000	0.25400900	0.13675700

C	-1.32069100	3.00134700	1.40468400
O	-0.06143300	2.95792000	1.49457100
O	-2.07658800	2.01332000	1.08677100
C	-2.01159100	4.31538700	1.64882300
H	-2.21894400	4.75407200	0.66725400
H	-2.96146300	4.14515100	2.15930200
H	-1.37014300	4.98227100	2.22453600
C	-1.01807500	-0.44125200	2.96729500
O	-0.22976500	0.52562800	3.13154500
O	-1.43415100	-0.88419000	1.83900300
C	-1.56467500	-1.14478400	4.18583500
H	-0.93815700	-0.94575100	5.05542700
H	-2.57324800	-0.76158800	4.36801900
H	-1.63974900	-2.21768700	3.99648300
C	2.37074700	-1.23760200	0.67025200
O	2.39682700	-0.74562900	-0.50937800
O	1.84284400	-0.65159100	1.64931300
H	0.42005100	2.45024900	-1.30252800
H	4.11025400	4.36288900	-2.31273900
H	1.67928500	4.01677600	-2.71403500
C	-1.11926400	-0.72158100	-2.87046000
C	-1.98762400	0.54621500	-2.73921600
O	-2.56930300	0.99453400	-3.70799100
O	-1.92272100	1.18177000	-1.58314300
C	-2.30049700	-2.59685100	-0.82694800
C	-3.62029600	-2.35599000	-1.21655800
C	-2.06127000	-3.67884500	0.02562400
C	-4.65464900	-3.20271000	-0.83214500
C	-3.07565500	-4.54818900	0.40588800
C	-4.37917800	-4.30782800	-0.02625100
F	-0.83024500	-3.88961700	0.52131600
F	-2.80415600	-5.59086000	1.19365000
F	-5.36358600	-5.12338700	0.34292700
F	-5.90638900	-2.95106800	-1.21061000
F	-3.92251100	-1.27368000	-1.94093900
C	-1.61809900	-1.70362000	-3.92040600
H	-1.69030400	-1.15147900	-4.86083800
H	-0.91558500	-2.52917900	-4.03656800
H	-2.60913900	-2.09403400	-3.69376700
C	0.29575600	-0.21816200	-3.21529900
H	0.70738000	0.41536200	-2.42941600

H	0.98557900	-1.03681700	-3.40727400
H	0.21542300	0.39453800	-4.11608400
S	-0.90409100	-1.53482800	-1.16114000
O	4.07401300	1.35943700	1.12468400
C	5.50348600	1.37648500	1.27368100
H	5.70948500	0.69523600	2.09672800
H	5.98615600	1.03213800	0.35584300
H	5.85475400	2.37594000	1.54594000
H	5.27623300	3.15344400	-0.52063100
C	3.09271800	-2.55098400	1.02164200
C	2.06251800	-4.56830700	-0.78170300
C	1.78406600	-5.72875000	-0.04339400
C	1.18717000	-4.26025800	-1.83006700
C	0.64966900	-6.50093800	-0.28172700
C	0.05766000	-5.02806800	-2.09351200
C	-0.22033300	-6.14247600	-1.30797400
F	1.40495500	-3.19154700	-2.60800900
F	-0.79953900	-4.67246400	-3.06255100
F	-1.33583400	-6.84301300	-1.51825400
F	0.38963300	-7.57488500	0.46731500
F	2.60031600	-6.12400700	0.93837400
C	4.46919300	-2.12825900	1.59175500
H	4.31210400	-1.46846000	2.44844800
H	5.01689200	-3.01484600	1.92060500
H	5.06675100	-1.59813300	0.84722900
C	2.29023200	-3.31914800	2.07940100
H	1.29417200	-3.58048100	1.71587600
H	2.81774300	-4.23084900	2.35875300
H	2.16955600	-2.68258700	2.95821100
S	3.51766200	-3.58738900	-0.48247700
C	-2.31137900	4.13332300	-2.82760800
H	-2.98066300	3.37704500	-3.25445800
C	-3.07850500	5.45214300	-2.74423900
C	-1.10360300	4.20781300	-3.76888300
O	-1.88670400	3.80944000	-1.53597400
H	-1.98427800	2.83457400	-1.45154500
F	-1.47101200	4.36832200	-5.04990800
F	-0.25889700	5.20996400	-3.44580200
F	-0.39532000	3.05181700	-3.68486400
F	-2.36080800	6.40676600	-2.12531200
F	-4.21361500	5.27076300	-2.04447000

F	-3.41044200	5.90598200	-3.97015800
C	4.07689000	0.11449700	-2.91064500
H	3.61169900	0.73478200	-2.13993400
C	5.53434500	-0.09148700	-2.47967700
C	3.94871600	0.89972000	-4.21627100
O	3.45443400	-1.12215500	-3.08636300
H	3.12601900	-1.41081100	-2.21633600
F	4.62195500	2.06810800	-4.14116000
F	4.41431100	0.21512400	-5.26906900
F	2.65141200	1.19085900	-4.44131500
F	6.26551000	-0.72691100	-3.40081600
F	5.55129200	-0.83876100	-1.34414200
F	6.14738100	1.07804700	-2.18650000
C	-5.44690800	1.34560200	1.49386400
H	-6.49564500	1.65843900	1.44443100
C	-5.44839800	-0.15141500	1.13221500
C	-5.00729200	1.58469900	2.94969900
O	-4.72165200	2.09862900	0.58327300
H	-3.75750200	2.06417500	0.77859500
F	-5.87375800	1.03606300	3.81941300
F	-3.78264800	1.06939200	3.21117800
F	-4.94525900	2.90671700	3.19412900
F	-4.21203200	-0.70200700	1.21521500
F	-5.87598700	-0.32381700	-0.12869500
F	-6.25544000	-0.85663600	1.94924500
C	3.60502200	2.18094700	4.82221000
H	4.31982200	2.52058600	5.57731300
C	2.24233400	2.78940600	5.20343300
C	3.60925200	0.64494100	4.88510800
O	4.02826000	2.65796600	3.58304100
H	3.54560300	2.21351900	2.86370000
F	3.49685900	0.20256300	6.14699300
F	2.61321500	0.10352100	4.15693200
F	4.77405500	0.17047300	4.38106900
F	1.34963100	2.65113200	4.20696600
F	2.39406200	4.10354400	5.44136600
F	1.73292300	2.21693200	6.31104700

F-6

C	5.67333500	2.57587900	1.29098700
C	5.90351800	1.66119500	2.32035300

C	5.02572600	0.59929800	2.56486300
C	3.90774500	0.44634400	1.75447200
C	3.62311300	1.35108400	0.70154500
C	4.54504400	2.41431500	0.47818200
H	2.42954100	1.94528600	0.85824800
Pd	2.76294400	0.54236100	-1.02761600
Pd	1.42194300	-1.94015700	-0.18477100
C	4.29010100	-1.98821800	-1.01507200
O	4.37047600	-0.72162000	-1.08318600
O	3.25687000	-2.68931500	-0.79252300
C	5.58790000	-2.74793500	-1.18910300
H	5.98988900	-2.96521200	-0.19397600
H	5.40118100	-3.69778500	-1.69293400
H	6.31293900	-2.14892000	-1.74104000
C	1.24735900	-1.13048200	-3.03713400
O	2.09797300	-0.21550800	-2.88616100
O	0.74765200	-1.86900300	-2.12145800
C	0.76940300	-1.42760700	-4.44321900
H	0.98361900	-0.58782700	-5.10464400
H	1.29598800	-2.31537300	-4.80842200
H	-0.29917500	-1.65275400	-4.43726200
C	0.72925200	2.48993800	-0.15070000
O	1.34858200	2.62901400	0.95026500
O	1.11273400	1.76261000	-1.10830700
H	3.23402800	-0.38708100	1.92567200
H	6.78561300	1.78630600	2.94298600
H	5.21824400	-0.09947500	3.37268100
C	-0.18851300	-1.23079400	2.48086800
C	1.08032600	-2.09778100	2.70873000
O	1.27604000	-2.50666400	3.84052800
O	1.93515300	-2.24810900	1.72634300
C	-1.80736100	-2.13371200	0.16143100
C	-1.76870300	-3.50857900	0.41618600
C	-2.91149100	-1.63249500	-0.53321000
C	-2.81321900	-4.34673700	0.04066700
C	-3.97376000	-2.44947700	-0.90543100
C	-3.92333800	-3.81133500	-0.61489600
F	-2.96876900	-0.33921400	-0.88591800
F	-5.02533000	-1.93478600	-1.54645300
F	-4.93094500	-4.60594000	-0.97077000
F	-2.76365200	-5.65309500	0.30585500

F	-0.71519300	-4.04546200	1.04282200
C	-1.39904300	-1.80392700	3.21122000
H	-1.14687800	-1.81705500	4.27393800
H	-2.28677600	-1.18761200	3.05669500
H	-1.60575000	-2.83295300	2.91776200
C	0.13451000	0.19053700	2.97474500
H	0.95588900	0.64506000	2.41696100
H	-0.73597900	0.84222800	2.88896300
H	0.43587300	0.11199300	4.02301400
S	-0.50564400	-1.00180900	0.61128900
O	4.21872200	3.25536300	-0.53627500
C	5.03997800	4.39053200	-0.78715800
H	4.57225000	4.91691000	-1.61967300
H	5.08480800	5.05391600	0.08562800
H	6.05643300	4.09297900	-1.07218000
H	6.37237500	3.38766500	1.12965300
C	-0.54775200	3.31916100	-0.37134900
C	-3.16059200	2.80962800	0.76946700
C	-4.00033700	3.71709900	0.10886400
C	-3.69689300	1.54925000	1.05199400
C	-5.29253500	3.37852300	-0.28107400
C	-4.97806000	1.17987800	0.65615600
C	-5.78314000	2.10114100	-0.00670500
F	-2.96376200	0.61938500	1.68482600
F	-5.41784700	-0.06507800	0.88124200
F	-7.01286500	1.76165700	-0.39345300
F	-6.06278300	4.26071900	-0.92550600
F	-3.54839200	4.93645100	-0.21577300
C	-0.12096900	4.78353400	-0.58105700
H	0.50077300	4.85866700	-1.48085000
H	-1.00819400	5.40780900	-0.70732900
H	0.45419500	5.15038700	0.27181500
C	-1.34614800	2.79607800	-1.56453300
H	-1.70092700	1.77666000	-1.40274900
H	-2.19485900	3.45003200	-1.77039100
H	-0.69385500	2.78991500	-2.44048500
S	-1.50789300	3.22199300	1.27068200
TS3'			
C	3.63368100	3.70829600	-0.27078300
C	2.36136600	3.66151600	0.30958200

C	1.70463500	2.44866800	0.43919400
C	2.32692800	1.25018200	0.01232700
C	3.67866800	1.27337400	-0.44116900
C	4.28357900	2.52981400	-0.65666900
Pd	1.77052700	-0.67661600	0.67512200
H	1.39302700	0.69910500	-0.65322800
H	1.88034100	4.58504400	0.61770300
H	0.68148300	2.40852800	0.79613000
C	3.67441900	-1.15739400	0.18324800
C	4.54533000	-1.53732300	1.40707500
C	5.77358800	0.00858000	0.30167300
C	4.45505100	-0.02169300	-0.54776700
C	5.23206500	-0.19870700	1.73098700
H	6.02469200	-0.30162000	2.47971200
H	4.53613500	0.58134400	2.05220000
C	5.74835700	-2.36681300	0.87834100
H	6.33571100	-2.74188400	1.72322700
H	5.44140000	-3.23278500	0.28502000
C	6.54534900	-1.31112600	0.05034300
H	7.57586400	-1.22332900	0.40813900
H	6.58645700	-1.56103100	-1.01405900
H	3.99366300	-2.02945900	2.21166000
H	4.67084900	-0.27890900	-1.59067300
C	3.23133900	-2.31253000	-0.65100000
O	3.48073800	-2.58437000	-1.80168900
C	1.64661500	-4.11567500	-0.57168200
H	0.98915200	-4.57011500	0.16834800
H	1.06922900	-3.70653200	-1.40433700
H	2.36498300	-4.84412800	-0.95424100
O	0.02286000	0.63743700	-1.23630000
C	-0.75135600	0.23142200	-0.32191900
O	-0.37736800	-0.29728600	0.77227700
C	-2.25751500	0.44521100	-0.55822700
O	2.34337700	-3.05855600	0.12034900
H	6.36996500	0.90131500	0.13204900
O	5.51902400	2.50983100	-1.24227200
C	6.19132700	3.74023700	-1.46904800
H	5.62239600	4.39398800	-2.14265400
H	6.38928300	4.27411100	-0.53011800
H	7.13990600	3.47905200	-1.94024900
H	4.11268700	4.66932000	-0.41464100

C	-2.66010300	-0.20054600	-1.89184200
H	-3.71578800	-0.01188800	-2.10515200
H	-2.05827100	0.23818600	-2.69200200
H	-2.49799200	-1.28078700	-1.87584300
C	-2.52635100	1.95936900	-0.58041400
H	-3.58493900	2.15845900	-0.76449400
H	-2.25240100	2.42371000	0.37015100
H	-1.93842700	2.41216600	-1.38406000
S	-3.11644800	-0.37801100	0.89710100
C	-4.82407300	-0.13811800	0.43987300
C	-5.54013500	0.99830900	0.84048500
C	-5.53183600	-1.12016600	-0.26736700
C	-6.89390500	1.15646600	0.55171700
C	-6.88567800	-0.98226400	-0.56564000
C	-7.56757500	0.15970700	-0.15080400
F	-4.93197600	1.98513000	1.50925700
F	-7.55120000	2.25531100	0.94230000
F	-8.86495300	0.30223600	-0.43283600
F	-7.53472900	-1.93413800	-1.24722800
F	-4.91515900	-2.22837900	-0.69258200

int3'

C	0.50681800	-3.39591700	2.35851600
C	1.40973400	-4.05311600	1.51505000
C	1.62600900	-3.59016700	0.22136100
C	0.93804600	-2.45327600	-0.23038100
C	0.03171500	-1.77919200	0.58804900
C	-0.17752700	-2.26733000	1.89441900
Pd	-0.90484800	-0.06363100	0.04888000
H	1.12039400	-2.09984500	-1.24029600
H	1.93865900	-4.92868200	1.88062600
H	2.32205100	-4.09977500	-0.43900600
O	-1.09506900	-1.56807700	2.63311300
C	-1.41207000	-2.00804000	3.94359100
H	-2.17904600	-1.32250000	4.30521300
H	-1.80997000	-3.03194500	3.94095600
H	-0.53838900	-1.96601100	4.60767100
H	0.34594200	-3.76604600	3.36479300
C	-3.38321400	-0.53286900	-0.55764100
C	-3.77643600	-0.55840500	-2.03309100
C	-2.75098000	-2.52501400	-1.58125500

C	-2.76300300	-1.72247500	-0.27983400
C	-4.12212800	-2.06900500	-2.16100700
H	-4.29017800	-2.39483400	-3.19363700
H	-4.97441200	-2.36965800	-1.54387700
C	-2.48602500	-0.48288600	-2.90489200
H	-2.76008100	-0.39319000	-3.96044500
H	-1.87651000	0.38353200	-2.63967000
C	-1.79096600	-1.85024500	-2.61317700
H	-1.73591900	-2.46921100	-3.51427100
H	-0.77980800	-1.74454300	-2.22339500
H	-4.54231800	0.16813000	-2.29595500
H	-2.56878900	-2.11087200	0.71145000
C	-3.85697500	0.47015400	0.44497900
O	-3.65171600	0.39194500	1.64184700
C	-4.85503300	2.60528400	0.63546900
H	-5.66651200	3.11706200	0.11742900
H	-5.15654300	2.32246100	1.64594900
H	-3.95813200	3.23169600	0.65888000
C	0.41620900	2.89950200	0.29615800
C	-1.13474200	2.92506200	0.04928800
O	-1.68071000	1.85407800	-0.42369800
O	-1.69940700	3.99820700	0.23650700
C	2.39310600	0.73238000	0.09545800
C	2.48139900	0.27374400	-1.22382700
C	3.57832900	0.80168600	0.83823900
C	3.69051800	-0.13597700	-1.77369200
C	4.80098700	0.40567500	0.30069700
C	4.85429100	-0.06694300	-1.00880300
F	3.56220000	1.25320300	2.09575300
F	5.91759800	0.48107500	1.02889200
F	6.01758200	-0.44918200	-1.53287900
F	3.74238600	-0.59221800	-3.02815700
F	1.39248300	0.19384800	-2.00185100
C	1.08796600	3.23262100	-1.03949700
H	0.74403400	4.22778700	-1.33710800
H	2.17790100	3.26031400	-0.94788200
H	0.80589800	2.52311400	-1.81871700
C	0.83355300	3.86779800	1.40202200
H	0.36129500	3.61310300	2.35404900
H	1.92022300	3.86862600	1.53597100
H	0.49679300	4.86824100	1.12054500

S	0.86386300	1.15202600	0.90928300
H	-2.58481300	-3.59490100	-1.44965700
O	-4.56538600	1.43431300	-0.15647500
TS2'			
C	-0.74087900	-2.77275200	-2.37825800
C	-1.73293200	-3.34356900	-1.57406100
C	-1.72783400	-3.12887200	-0.19901800
C	-0.73482000	-2.32601000	0.37452500
C	0.25403200	-1.71137300	-0.40288100
C	0.25125600	-1.97811000	-1.79772200
Pd	1.08965700	0.20653000	0.02601400
H	-0.75291600	-2.17235100	1.44404800
H	-2.50152500	-3.95970600	-2.03160100
H	-2.48618500	-3.57973100	0.43425900
O	1.26093600	-1.39721800	-2.49038500
C	1.50904900	-1.76818200	-3.83814900
H	2.45930300	-1.29874100	-4.09159100
H	1.59719100	-2.85715400	-3.94335300
H	0.71998500	-1.40215300	-4.50763600
H	-0.74773000	-2.94267800	-3.44884400
C	2.95640700	-0.65257000	0.51561700
C	3.48645300	-0.61220300	1.96505300
C	2.15981100	-2.45211400	1.82041700
C	2.17868600	-1.86204900	0.40345500
C	3.64338000	-2.14536400	2.19208900
H	3.89039300	-2.41975600	3.22417400
H	4.36734300	-2.61252900	1.51642700
C	2.35999700	-0.28451100	2.96661900
H	2.77380400	-0.18770200	3.97565000
H	1.85585700	0.65148400	2.71808300
C	1.43283700	-1.53341400	2.84868200
H	1.35048300	-2.06618800	3.80120400
H	0.42798600	-1.25332200	2.54332800
H	4.37693200	0.00439100	2.07136700
H	2.37385700	-2.51100800	-0.44255900
C	3.84939400	-0.22096000	-0.60168800
O	3.92642600	-0.74830500	-1.69699400
C	5.39374100	1.42354800	-1.27306100
H	5.92070500	2.25470800	-0.80561500
H	6.09972800	0.69049300	-1.67357000

H	4.75712800	1.78635400	-2.08458700
C	-0.49404000	3.06604100	-0.00411900
C	1.06202900	3.20622800	0.17549500
O	1.78275200	2.13625200	0.31640500
O	1.48279100	4.35258800	0.25067200
C	-2.34878100	0.76529200	-0.14410600
C	-2.46612800	0.18095100	1.12231200
C	-3.48211600	0.74417600	-0.96806800
C	-3.64386400	-0.42423900	1.54484900
C	-4.67378400	0.14934800	-0.55972000
C	-4.75223300	-0.43921900	0.70060800
F	-3.44360000	1.29097500	-2.18641000
F	-5.73839200	0.14046400	-1.36689400
F	-5.88526500	-1.01696000	1.09906800
F	-3.71105100	-1.00321800	2.74816100
F	-1.42987200	0.16182700	1.97321400
C	-1.11670300	3.17359200	1.39164600
H	-0.85044800	4.15696500	1.78890900
H	-2.20791300	3.09930900	1.35093600
H	-0.72933700	2.40930600	2.06599100
C	-1.04109200	4.14022500	-0.94571300
H	-0.60817700	4.05177800	-1.94536400
H	-2.13074400	4.06988900	-1.02815600
H	-0.76593300	5.11807000	-0.54429400
S	-0.81927800	1.38389300	-0.81257700
H	1.83985900	-3.49490700	1.85210600
O	4.58922400	0.84436000	-0.23567200

int4'

C	0.10292700	-1.34355200	2.66762600
C	1.21625200	-2.00943400	2.18153500
C	1.14725700	-2.72587300	0.97645700
C	-0.01843000	-2.70540600	0.22825500
C	-1.16492500	-1.98279200	0.64386900
C	-1.10782200	-1.36578400	1.93471400
Pd	-0.99624200	0.28335400	0.00206000
H	-0.06836600	-3.26596500	-0.69568300
H	2.13904100	-1.99449400	2.75416700
H	2.00740600	-3.28402900	0.62078400
O	-2.29831300	-0.98766600	2.47511500
C	-2.30321500	-0.00681900	3.51177700

H	-3.35228800	0.23182900	3.68242500
H	-1.86941000	-0.39802800	4.43900200
H	-1.76788400	0.89361600	3.19044900
H	0.14629000	-0.83691700	3.62366000
C	-2.84985200	-0.48969200	-0.38734900
C	-3.33626100	-0.49458400	-1.86672700
C	-2.64603000	-2.62954700	-1.50164400
C	-2.50524000	-1.98133100	-0.09846500
C	-3.94664600	-1.91921800	-1.95660200
H	-4.24782600	-2.18578500	-2.97574400
H	-4.78744000	-2.06815000	-1.27545300
C	-2.14361600	-0.63185400	-2.83488600
H	-2.50103600	-0.53338200	-3.86560200
H	-1.38782800	0.13815800	-2.67244800
C	-1.63492200	-2.07847200	-2.54981400
H	-1.67963800	-2.70029700	-3.44983000
H	-0.59821700	-2.07741500	-2.21515000
H	-3.99564200	0.34239900	-2.10196700
H	-3.26718800	-2.42012400	0.55726000
C	-3.93625500	0.06735600	0.50365300
O	-4.96088000	-0.53541700	0.76390500
C	-4.79358100	1.95615600	1.61933400
H	-4.42817300	2.94290200	1.90253900
H	-5.66380800	2.04491900	0.96352000
H	-5.08315700	1.37850500	2.50181200
C	0.96630600	2.75478800	-0.84746300
C	-0.55827200	3.01473800	-1.12548700
O	-1.40677200	2.04057700	-0.98872800
O	-0.83794600	4.12315300	-1.56116500
C	2.57521200	0.51642800	0.13129700
C	2.61178200	-0.51815400	-0.81160300
C	3.74442500	0.75918700	0.86399900
C	3.74378900	-1.30560400	-0.99070200
C	4.89159800	-0.01311700	0.69262100
C	4.88809600	-1.05160300	-0.23635400
F	3.78551100	1.74437000	1.76646000
F	5.99068100	0.23504100	1.41068600
F	5.97633900	-1.80299800	-0.40254700
F	3.73380300	-2.31404200	-1.86896500
F	1.54199900	-0.80459800	-1.56517500
C	1.57057100	2.26940000	-2.17140500

H	1.39267800	3.05003600	-2.91641900
H	2.65048100	2.11475700	-2.08634400
H	1.10083500	1.34623200	-2.51444900
C	1.66301500	4.01978700	-0.34395700
H	1.22374200	4.36679600	0.59452100
H	2.73092200	3.83846800	-0.18385800
H	1.53262600	4.80816700	-1.08831600
S	1.10282800	1.44136200	0.51296000
H	-2.68476000	-3.72184100	-1.46350300
O	-3.70502100	1.32729900	0.92491100

int3”

C	1.12010000	-3.43541500	-1.35218300
C	0.65320900	-4.07702800	-0.19967800
C	0.19850000	-3.33412300	0.88716400
C	0.23097700	-1.93395300	0.82436000
C	0.70876800	-1.27540600	-0.30673800
C	1.13284900	-2.03568800	-1.41157300
Pd	0.70526500	0.74672700	-0.46486900
H	-0.10754800	-1.35189000	1.67879000
H	0.64158800	-5.16264300	-0.16367800
H	-0.16986200	-3.83131900	1.77993800
O	1.52545900	-1.32130100	-2.51026100
C	2.34582000	-1.96156800	-3.47666700
H	2.66373800	-1.17764900	-4.16515800
H	3.23045100	-2.40521300	-3.00505900
H	1.79690000	-2.73046800	-4.03662100
H	1.45345600	-4.02547600	-2.19897800
C	2.66642100	0.38265200	0.83867700
C	2.38807200	0.35306400	2.33804600
C	2.24502200	2.51825400	1.67602800
C	2.57674600	1.70313600	0.44312300
C	1.39184200	1.52118400	2.49353900
H	1.26216900	1.83098700	3.53536200
H	0.41050300	1.33548500	2.04870600
C	3.67118100	0.99511500	2.96797300
H	3.62852900	0.91116400	4.05795600
H	4.58361600	0.49346000	2.63469200
C	3.57879200	2.48543600	2.50544600
H	3.49328800	3.16592100	3.35781000
H	4.44281400	2.80370800	1.91540300

H	2.11394100	-0.62015500	2.74043400
H	3.02777000	2.11394100	-0.45371600
C	3.48692400	-0.63878700	0.12765700
O	3.95741000	-0.51524600	-0.98550100
C	4.40572100	-2.80139100	0.31070200
H	4.56562200	-3.52645800	1.10835800
H	3.81027100	-3.24604700	-0.49093400
H	5.35801500	-2.44803100	-0.09236400
C	-1.72574600	2.31957700	-1.89375400
C	-0.81837100	3.25658900	-1.02717300
O	0.35154700	2.81703300	-0.68036100
O	-1.24133000	4.38894800	-0.83527800
C	-2.39179300	-0.09454800	-0.29408200
C	-2.52225100	0.52555600	0.95240200
C	-3.00961400	-1.33674300	-0.47073000
C	-3.24299600	-0.05961200	1.98691200
C	-3.72986300	-1.94270600	0.55662700
C	-3.84905300	-1.30024800	1.78619600
F	-2.88949500	-1.99494500	-1.62663400
F	-4.29995700	-3.13543700	0.36848500
F	-4.53838700	-1.87063200	2.77433100
F	-3.34682500	0.55049600	3.17080300
F	-1.92313000	1.70122800	1.18823300
C	-3.20923000	2.59940300	-1.68422800
H	-3.37730400	3.64932200	-1.93272000
H	-3.83276400	1.96648900	-2.32328100
H	-3.50319700	2.46551900	-0.64212900
C	-1.31108500	2.53536900	-3.36210500
H	-0.26317200	2.26598200	-3.52583300
H	-1.94147400	1.96014800	-4.04684200
H	-1.42394300	3.60070600	-3.58330300
S	-1.32664900	0.49089700	-1.60380100
O	3.67315100	-1.72057100	0.91075000
H	1.82539500	3.50270600	1.48058200

TS2''

C	1.11590400	-2.77845500	-1.91043800
C	0.40879600	-3.58049200	-1.01080800
C	0.04317500	-3.08935500	0.24253800
C	0.39922300	-1.78770800	0.59666100
C	1.09548700	-0.94657700	-0.28588300

C	1.45783000	-1.46945100	-1.55551700
Pd	0.56061500	1.09358400	-0.36969400
H	0.12121800	-1.41277900	1.57521800
H	0.14107200	-4.59256100	-1.29976000
H	-0.50899700	-3.71230000	0.93933300
O	2.10723600	-0.60857100	-2.38343100
C	2.72472700	-1.10874800	-3.56183000
H	3.30784700	-0.28018700	-3.96326600
H	3.39463400	-1.94822000	-3.33674500
H	1.97963000	-1.42682000	-4.30160600
H	1.37243200	-3.16839800	-2.88863300
C	2.55750600	0.10093500	0.73182900
C	2.41964600	-0.19166200	2.23125700
C	2.09574600	2.04397700	2.02577100
C	2.32724100	1.52227300	0.61102000
C	1.37092800	0.84763900	2.68327400
H	1.31192800	0.92872100	3.77333900
H	0.36691000	0.68918200	2.28233600
C	3.70936400	0.42745500	2.86865000
H	3.75987700	0.12268700	3.91811300
H	4.62698500	0.07630900	2.38873600
C	3.48563000	1.96632000	2.72831200
H	3.44650900	2.45574800	3.70670500
H	4.27031600	2.45516000	2.14402500
H	2.26386200	-1.23929700	2.48231100
H	2.92002600	2.10017800	-0.09623200
C	3.72075800	-0.53006600	0.00424500
O	4.43584800	0.03517800	-0.79284600
C	4.97820100	-2.50482400	-0.24187300
H	5.02503000	-3.48235100	0.23726100
H	4.77415200	-2.61520100	-1.31118900
H	5.91955000	-1.96377300	-0.11637900
C	-2.16988500	2.51503800	-1.41439400
C	-1.31306700	3.39182400	-0.43374200
O	-0.07580500	3.06451100	-0.22621000
O	-1.85792300	4.40836700	-0.02118000
C	-2.42343100	-0.24241000	-0.32313300
C	-2.52603500	0.09523100	1.03113800
C	-2.89559300	-1.50186600	-0.70857000
C	-3.08135600	-0.77319700	1.96438900
C	-3.44336600	-2.39082200	0.21330200

C	-3.54163900	-2.02332700	1.55228500
F	-2.78346400	-1.91000400	-1.97717000
F	-3.86035000	-3.59892200	-0.17925000
F	-4.06277600	-2.86956800	2.44268700
F	-3.15782100	-0.42539500	3.25277000
F	-2.05644100	1.27001000	1.47337500
C	-3.65397100	2.55497700	-1.06464500
H	-3.96857300	3.59992400	-1.08781000
H	-4.24804300	1.97558800	-1.77817900
H	-3.83964800	2.18622200	-0.05448400
C	-1.91283300	3.06733300	-2.83019200
H	-0.85992100	2.97108300	-3.11344300
H	-2.53322100	2.56278000	-3.57708400
H	-2.16142100	4.13248400	-2.81896900
S	-1.54651800	0.72891900	-1.53450000
O	3.89958000	-1.80852800	0.40011300
H	1.59609700	3.01126500	2.06916300

int4”

C	0.60644800	-1.56641500	-2.47590000
C	-0.36085300	-2.37053500	-1.89729100
C	-0.36096200	-2.59940200	-0.51088000
C	0.59340900	-1.99501400	0.28930100
C	1.59440800	-1.14429600	-0.25151000
C	1.59950900	-0.96026000	-1.66983900
Pd	0.59288800	0.91030700	-0.32501500
H	0.58370800	-2.16973400	1.35783800
H	-1.12808400	-2.81761100	-2.52167100
H	-1.11956800	-3.23344700	-0.06363800
O	2.69454100	-0.34522800	-2.19589200
C	2.56859300	0.33655000	-3.44273600
H	3.48468900	0.91708200	-3.55454500
H	2.48123100	-0.36480600	-4.28076800
H	1.70331500	1.00963700	-3.42634100
H	0.61525500	-1.40814400	-3.54734900
C	2.73370300	-0.51755600	0.58785800
C	2.70625200	-0.86398500	2.11969400
C	2.29618100	1.36894500	2.07774000
C	2.40624200	0.99420000	0.60303900
C	1.63432400	0.10633800	2.67455800
H	1.61577400	0.10659800	3.76949800

H	0.61761300	-0.05545900	2.31069500
C	3.96886000	-0.26322500	2.78936300
H	3.99374600	-0.58688400	3.83469400
H	4.90635700	-0.57925500	2.32906300
C	3.73043800	1.27687100	2.68017700
H	3.76569600	1.76136700	3.66134000
H	4.47279800	1.75821200	2.03868300
H	2.57639400	-1.93111500	2.31516900
H	3.05677800	1.62036000	-0.00976100
C	4.09519800	-0.85573600	-0.00758900
O	5.02009400	-0.08325400	-0.13179500
C	5.41643400	-2.58313400	-0.90635700
H	5.31510800	-3.65231200	-1.09262600
H	5.59713600	-2.04451200	-1.84070400
H	6.24531900	-2.38716800	-0.22106200
C	-2.06186700	2.72839500	-0.83247400
C	-1.10551500	3.25656300	0.29093200
O	0.11016800	2.79800700	0.34186200
O	-1.53649500	4.17054800	0.98112800
C	-2.62441000	-0.11440300	-0.29282100
C	-2.54030300	-0.09596700	1.10404100
C	-3.40598800	-1.11851200	-0.87507100
C	-3.19823300	-1.03468700	1.89173400
C	-4.06926200	-2.07098400	-0.10465500
C	-3.96795600	-2.02627100	1.28385000
F	-3.50046600	-1.22080900	-2.20726700
F	-4.79638300	-3.02772900	-0.69113000
F	-4.59996800	-2.93288800	2.03027200
F	-3.08781600	-0.99928500	3.22250200
F	-1.79209500	0.82405700	1.72509600
C	-3.52905200	2.86954200	-0.43865700
H	-3.71487400	3.92086300	-0.21210500
H	-4.18987500	2.54420300	-1.24796700
H	-3.75970700	2.30055700	0.46444000
C	-1.73792800	3.54521500	-2.09860300
H	-0.70143600	3.39260200	-2.41581200
H	-2.40980500	3.28923700	-2.92337600
H	-1.86058300	4.60440800	-1.85425500
S	-1.67491400	0.95169300	-1.35953200
O	4.16920500	-2.16700200	-0.32713800
H	1.78319700	2.31599900	2.24573000

int3'''

C	-0.10867800	-3.08036000	2.14398200
C	0.76562700	-3.77832500	1.30501500
C	1.08696900	-3.27378500	0.04777400
C	0.51775500	-2.06251300	-0.37226000
C	-0.35956200	-1.35156200	0.44583400
C	-0.65885600	-1.86388000	1.72071700
Pd	-0.90265000	0.52864500	-0.09935700
H	0.74893700	-1.68137200	-1.36308100
H	1.19612500	-4.71492400	1.64746500
H	1.76938000	-3.80901000	-0.60643700
O	-1.48286600	-1.09173700	2.50150200
C	-1.81701200	-1.55066900	3.80202500
H	-2.47619300	-0.79184000	4.22691800
H	-2.34776000	-2.51115500	3.76901500
H	-0.92693700	-1.65280800	4.43636000
H	-0.33895400	-3.48234500	3.12389300
C	-2.85559300	-0.59569100	-1.12583200
C	-4.19432200	-0.58121800	-0.37507200
C	-3.88059300	1.50484300	-1.20119500
C	-2.66828900	0.67591400	-1.62182700
C	-4.96484700	0.38973600	-1.31714400
H	-5.94354300	0.69386200	-0.92882300
H	-5.08538100	0.00130200	-2.33336100
C	-4.08814600	0.29207200	0.90991300
H	-5.01756100	0.20901600	1.48269400
H	-3.26476000	-0.03335200	1.54591000
C	-3.90011100	1.73364000	0.34044100
H	-4.75137100	2.37465700	0.59055700
H	-2.99408400	2.23275700	0.68124100
H	-4.61408000	-1.57329100	-0.21612900
H	-1.98575000	0.95499900	-2.41696100
C	-2.23351300	-1.81110800	-1.71183500
O	-1.45171600	-1.80912600	-2.64376400
C	-2.14032500	-4.16271600	-1.60737900
H	-1.07107000	-4.20643300	-1.39018100
H	-2.67132700	-4.95152500	-1.07494800
H	-2.29821500	-4.24722800	-2.68556300
C	0.79478600	3.04628200	0.99104200
C	-0.08860400	3.42125300	-0.24570300

O	-1.00827400	2.58366700	-0.60943900
O	0.08375600	4.53999600	-0.71064900
C	2.31122900	0.58354400	0.32912300
C	2.52860600	0.84581800	-1.02678200
C	3.15970500	-0.32843000	0.96444000
C	3.55922400	0.23305000	-1.73045700
C	4.19107700	-0.95951100	0.27352100
C	4.39322900	-0.67297500	-1.07441000
F	2.97006300	-0.65200800	2.24685200
F	4.97989600	-1.84042500	0.89456600
F	5.38075800	-1.26956100	-1.74179600
F	3.74836800	0.49706600	-3.02503200
F	1.71693200	1.67922300	-1.68651200
C	2.18481600	3.66623500	0.91176800
H	2.05125600	4.74667200	0.82671900
H	2.77990000	3.43767800	1.80140500
H	2.72213100	3.33666800	0.02133000
C	0.03122300	3.52433800	2.24145200
H	-0.93667700	3.02164900	2.33601300
H	0.61033100	3.35979300	3.15505600
H	-0.15511000	4.59570300	2.12474300
S	0.89725200	1.17542500	1.24376600
H	-4.01312200	2.41370100	-1.78715300
O	-2.68830000	-2.92782600	-1.11166400

TS2'''

C	0.32311600	-2.75486200	1.55841300
C	1.01500700	-3.31419800	0.48075000
C	0.81834600	-2.83290700	-0.81275300
C	-0.08624400	-1.79000200	-1.02058300
C	-0.77496000	-1.18947900	0.04821400
C	-0.57788300	-1.70295800	1.35119700
Pd	-0.90430100	0.87059300	-0.31650800
H	-0.27789100	-1.44418900	-2.03140600
H	1.71266100	-4.12618800	0.66392100
H	1.35403700	-3.26311700	-1.65301300
O	-1.25627100	-1.09400500	2.36016500
C	-0.86361100	-1.35659000	3.70254700
H	-1.44723500	-0.67340900	4.32096200
H	-1.08873400	-2.38909900	3.99767300
H	0.20615500	-1.15852800	3.84187900

H	0.49827800	-3.13636700	2.55681000
C	-2.74705700	-0.66440400	-0.48501600
C	-3.82268900	-0.38948700	0.58992100
C	-3.91749200	1.38577300	-0.82928800
C	-2.71493200	0.53758100	-1.29356200
C	-4.87468300	0.23871000	-0.37800400
H	-5.77274800	0.59198300	0.14170300
H	-5.17677200	-0.42579200	-1.19418500
C	-3.49663200	0.83638500	1.48821100
H	-4.21687500	0.87302300	2.31224400
H	-2.50049800	0.75604400	1.92162900
C	-3.65108100	2.06318900	0.53518500
H	-4.51620200	2.67553700	0.81190200
H	-2.77507000	2.71197100	0.50696100
H	-4.11765000	-1.28191200	1.13834300
H	-2.51746400	0.45171000	-2.35980500
C	-2.84433200	-1.99413200	-1.19734400
O	-2.72248100	-2.13739900	-2.39638100
C	-3.16209100	-4.30740700	-0.94371000
H	-2.18422400	-4.55293600	-1.36692100
H	-3.41350800	-4.99242800	-0.13442100
H	-3.91421100	-4.34877200	-1.73547200
C	1.19721600	3.20215900	0.54856600
C	0.32683300	3.54042000	-0.71352600
O	-0.74249100	2.83974900	-0.93942900
O	0.66018700	4.54278200	-1.33148500
C	2.29936700	0.43363300	0.35415800
C	2.58368600	0.43762400	-1.01520000
C	2.95794500	-0.51114700	1.14765700
C	3.50418400	-0.44155100	-1.57444800
C	3.86664200	-1.41359800	0.60323000
C	4.14730200	-1.37200200	-0.75957200
F	2.68972700	-0.60525400	2.45824400
F	4.45166300	-2.33304800	1.37864400
F	5.01212700	-2.23874800	-1.29019000
F	3.75032000	-0.42200200	-2.88722600
F	1.93790500	1.28057400	-1.83056300
C	2.66378400	3.56842700	0.34615700
H	2.70482500	4.63074700	0.09831000
H	3.25086800	3.37847800	1.24999800
H	3.10212900	3.02509000	-0.49201000

C	0.57917000	3.99185900	1.71974400
H	-0.45185000	3.67915600	1.91490200
H	1.16708000	3.87889100	2.63550600
H	0.56066700	5.04733800	1.43364300
S	1.00618000	1.40174900	1.10261500
H	-4.28251700	2.06430000	-1.60118700
O	-3.12312300	-2.99946300	-0.34615300

int4'''

C	-0.81674100	-2.19380900	2.10974100
C	0.27626700	-2.58459100	1.31282900
C	0.30041500	-2.30210100	-0.03839000
C	-0.74977900	-1.54252300	-0.60514100
C	-1.84083000	-1.07341500	0.18825300
C	-1.88561700	-1.49468600	1.55862300
Pd	-0.52822900	0.72443700	-0.29084600
H	-0.82373300	-1.47827000	-1.68692200
H	1.09373500	-3.12851800	1.77561900
H	1.11519300	-2.64113000	-0.66893600
O	-3.02160500	-1.20073500	2.23271700
C	-3.10285800	-1.50959200	3.61866600
H	-4.08134700	-1.15490100	3.94344900
H	-3.03032700	-2.59010500	3.79369500
H	-2.31972100	-0.99437600	4.18896100
H	-0.82963100	-2.47772600	3.15440800
C	-2.98259600	-0.37370800	-0.58847200
C	-4.12824500	0.41043200	0.12759300
C	-3.19835700	2.00112800	-1.20961100
C	-2.27694300	0.77518300	-1.35897600
C	-4.57716500	1.29978000	-1.06219200
H	-5.38063800	1.99487300	-0.79556700
H	-4.88436300	0.73540100	-1.94840100
C	-3.58202100	1.48162000	1.11414400
H	-4.39252600	1.81200200	1.77187000
H	-2.79299300	1.08919200	1.75541100
C	-3.07448400	2.63126800	0.19357600
H	-3.72570100	3.51018900	0.25750700
H	-2.05728600	2.95516100	0.41324800
H	-4.87840700	-0.24704600	0.56357300
H	-2.03191200	0.53137900	-2.39446400
C	-3.57501100	-1.44646300	-1.50786600

O	-3.36928000	-1.54859800	-2.69921600
C	-4.87276300	-3.41295700	-1.57013300
H	-4.07292800	-4.00321000	-2.02539800
H	-5.43864600	-4.01521400	-0.85949500
H	-5.52539700	-3.03614400	-2.36198100
C	1.75387300	2.64387700	0.96210000
C	1.10206300	3.19709700	-0.35206600
O	0.01197800	2.63970100	-0.79321300
O	1.60187700	4.21105400	-0.81815200
C	2.73862800	-0.06863500	0.36171800
C	3.03751400	0.12358600	-0.99171500
C	3.42106900	-1.08964100	1.03264400
C	3.97845700	-0.66032400	-1.65347400
C	4.35676900	-1.89309500	0.38607100
C	4.64103800	-1.67279300	-0.96006400
F	3.15570300	-1.35341700	2.31942200
F	4.98024400	-2.87236100	1.04999600
F	5.53998900	-2.43317600	-1.58616800
F	4.24291600	-0.45621700	-2.94597200
F	2.39958800	1.06508700	-1.69482300
C	3.24494300	2.95862800	1.02850700
H	3.36353000	4.03930500	0.93290400
H	3.67876900	2.62106300	1.97471900
H	3.78931900	2.50026000	0.20036700
C	0.98771600	3.29491400	2.13106900
H	-0.07140900	3.01762700	2.11851000
H	1.42004900	3.01879500	3.09748700
H	1.05170300	4.38016000	2.00942900
S	1.44407700	0.79729600	1.22662800
H	-3.09088100	2.71470400	-2.02755900
O	-4.32411100	-2.32375100	-0.80666700

N-Ag-TS3'

C	2.13781400	2.53245900	-2.96939100
C	0.97757300	1.84234400	-3.33990400
C	0.37314600	0.95585800	-2.45775300
C	0.90783600	0.75286800	-1.16600300
C	2.02860800	1.51053800	-0.75430300
C	2.66032000	2.36533600	-1.68368300
Pd	-0.02564700	-0.22957700	0.41385000
H	0.93418800	-0.72351700	-1.12412600

H	0.56725400	1.98901000	-4.33528800
H	-0.47931900	0.36610900	-2.77919000
C	1.56167400	0.55622800	1.56451700
C	0.91837400	1.49839800	2.61473900
C	2.21850600	2.88107200	1.37871700
C	2.46088100	1.49194200	0.69016300
C	0.73714000	2.79024200	1.79119000
H	0.41440600	3.63893800	2.40392300
H	0.05129600	2.68336500	0.94717100
C	2.01444200	1.95317500	3.61964300
H	1.54826000	2.51421400	4.43661000
H	2.54659500	1.11411500	4.07201600
C	2.92947800	2.87247400	2.75138500
H	2.97933000	3.88685600	3.16019600
H	3.95793700	2.50231200	2.67764000
H	0.03507500	1.07072800	3.08759400
H	3.52607500	1.24078100	0.77095000
C	2.19835000	-0.65951900	2.09265000
O	3.13570300	-1.30965600	1.56268100
C	2.06034100	-2.39338300	3.69773400
H	3.13128100	-2.45461000	3.90571700
H	1.47577100	-2.55508100	4.60192500
H	1.79320500	-3.13011200	2.93594500
C	-2.28730400	-2.44948700	0.62386800
C	-1.86423400	-1.91777500	2.03276500
O	-0.91279400	-1.03720300	2.09951100
O	-2.41714800	-2.42700600	3.00048600
C	-3.36288900	-0.00289100	-0.49629900
C	-4.52688800	-0.23755800	-1.24374200
C	-3.35345300	1.12544000	0.33434700
C	-5.63316800	0.60302200	-1.17118600
C	-4.45012500	1.98166100	0.41514300
C	-5.59211600	1.71898200	-0.33738600
F	-2.28961100	1.43741300	1.08136800
F	-4.40992300	3.05323300	1.21124500
F	-6.64373800	2.53370800	-0.26129000
F	-6.72881000	0.34774400	-1.89220100
F	-4.60572500	-1.30166800	-2.05183900
C	-1.33707800	-3.59645100	0.23083500
H	-1.38969100	-4.35372000	1.01889900
H	-1.64006300	-4.05091100	-0.71714600

H	-0.30121000	-3.25855900	0.13779300
C	-3.74288700	-2.90737400	0.61656100
H	-4.41806700	-2.09885600	0.90628300
H	-4.03569300	-3.28593400	-0.36628100
H	-3.84794100	-3.69508000	1.36501900
S	-1.99313400	-1.13294400	-0.71152900
O	0.96819000	-1.86600300	-1.91166800
C	1.87236100	-1.97404600	-2.81063100
O	3.10933400	-1.78592300	-2.61456700
C	1.41454700	-2.32261200	-4.20758400
H	0.96999500	-1.42142600	-4.64422500
H	2.24838000	-2.65121300	-4.82806100
H	0.63571400	-3.08718800	-4.16452500
Ag	3.47952100	-1.41278800	-0.54348300
O	1.70174600	-1.07457800	3.25037900
H	2.50316500	3.71604000	0.73910900
H	2.61709000	3.19229500	-3.68236000
O	3.78731700	2.99429700	-1.22809500
C	4.47977600	3.87033100	-2.10563000
H	3.84956600	4.71456600	-2.41490300
H	5.33337300	4.24766700	-1.54063900
H	4.84176600	3.34496800	-2.99893700

N-Ag-TS22'

C	1.67584800	-2.27138100	1.72261100
C	2.10176800	-1.30007500	0.79851100
C	1.14259200	-0.55325400	0.11055300
C	-0.23550400	-0.76069600	0.31985300
C	-0.65672800	-1.67466900	1.31178700
C	0.31621600	-2.44931700	1.98101400
Pd	-1.79921800	0.44375300	-0.36873800
H	-0.67633500	-0.88305200	-1.06629800
H	1.46910600	0.11688200	-0.67679500
C	-3.00050500	-0.75208500	0.89903800
C	-3.61643300	0.19270800	1.96216400
C	-2.31470600	-1.20443200	3.18095300
C	-2.10466200	-1.73820600	1.71940200
C	-2.45021900	0.31492900	2.96398900
H	-2.73051200	0.85052200	3.87731300
H	-1.55455800	0.78035300	2.54174400
C	-4.64348700	-0.60805400	2.81143800

H	-5.18622300	0.07922300	3.46881300
H	-5.38882400	-1.11768500	2.19714700
C	-3.74316800	-1.58482500	3.63114100
H	-3.85742700	-1.42400000	4.70804400
H	-3.96748900	-2.63885400	3.43535200
H	-4.01460500	1.11190100	1.53611600
H	-2.46935300	-2.77174500	1.66720700
C	-3.94315200	-1.36314500	-0.05005700
O	-3.80089100	-2.45695900	-0.65324200
C	-5.91004900	-1.05657100	-1.32956800
H	-6.32657600	-2.04896500	-1.14077800
H	-6.69585400	-0.30339600	-1.36022500
H	-5.35414900	-1.06821300	-2.27045700
C	-1.98911700	3.10924100	-2.20345800
C	-3.27378900	2.83715600	-1.35523300
O	-3.38644700	1.69946800	-0.73806700
O	-4.15001300	3.68935700	-1.41533900
C	0.31072200	2.94154800	-0.34134300
C	1.70897600	2.98120800	-0.37365500
C	-0.32022000	3.48215200	0.78464800
C	2.45197700	3.52773400	0.66869300
C	0.40438200	4.04584300	1.83064800
C	1.79782700	4.06603000	1.77410800
F	-1.65345100	3.45356300	0.89094600
F	-0.22583000	4.55360900	2.89224300
F	2.49941000	4.59091200	2.77780500
F	3.78960700	3.50608600	0.62248100
F	2.37959000	2.43219200	-1.39643000
C	-2.27563000	2.58083600	-3.62353400
H	-3.17845200	3.08129600	-3.98470300
H	-1.44836700	2.79817500	-4.30557100
H	-2.46124900	1.50209000	-3.62187000
C	-1.62353600	4.58995700	-2.22383300
H	-1.41448900	4.96826400	-1.22135200
H	-0.75912000	4.77672100	-2.86826600
H	-2.48943200	5.13671500	-2.60242200
S	-0.52033800	2.05645700	-1.65115300
O	-0.22220600	-1.22742800	-2.34969400
C	0.44536000	-2.31105600	-2.47519500
O	0.05132400	-3.44682300	-2.07079100
C	1.81458200	-2.21893800	-3.10701600

H	1.81963800	-1.45495500	-3.88664400
H	2.51783700	-1.90587900	-2.32603600
H	2.13353700	-3.18389100	-3.50221600
Ag	-1.91072400	-3.27760200	-1.23416400
O	-5.04634600	-0.65346300	-0.25245900
H	-1.53243000	-1.53941100	3.86172000
H	2.42050500	-2.85747000	2.24674100
O	-0.17545100	-3.35736700	2.87738900
C	0.74045400	-4.18338700	3.58294700
H	1.42248400	-3.58991600	4.20565800
H	0.13327600	-4.82357300	4.22438600
H	1.32858500	-4.80935500	2.89954500
C	5.75437100	-2.03140400	0.07686400
C	6.27259400	-0.73808200	-0.08046100
C	5.42177400	0.36659400	0.06110900
C	4.07735700	0.17905700	0.35317200
C	3.54396000	-1.11133000	0.51195700
C	4.40584500	-2.21312700	0.36945700
H	6.40896900	-2.88723700	-0.04117900
H	5.83101300	1.36446100	-0.05396700
H	3.43525400	1.03901300	0.48309900
H	4.00569500	-3.21846200	0.46275200
C	7.70416200	-0.48071200	-0.39634700
O	8.19044400	0.62453800	-0.54135600
O	8.42322600	-1.62273500	-0.50844700
C	9.81380500	-1.43687100	-0.81539400
H	10.30569400	-0.84977800	-0.03501800
H	10.24056500	-2.43856300	-0.86924800
H	9.93167700	-0.91608100	-1.76960700

N-Ag-TS29'

C	-1.63632500	2.20629300	1.34743900
C	-0.31597700	2.35593400	1.78110900
C	0.59022700	1.32012800	1.56335400
C	0.24587700	0.19604600	0.80183400
C	-1.06953400	0.07888800	0.27882200
C	-2.02254900	1.06298500	0.62711500
Pd	1.64043600	-0.97440800	-0.22450000
H	0.95254700	-0.84331200	1.55980700
H	1.56575000	1.40057700	2.02549900
C	-0.06697800	-1.80008200	-1.15706700

C	0.08739600	-1.56575400	-2.68140500
C	-1.76238100	-0.37700300	-2.14402900
C	-1.34887800	-0.99096500	-0.76134800
C	-0.40093600	-0.10909400	-2.81058300
H	-0.49309700	0.21618800	-3.85217600
H	0.21844300	0.61201600	-2.27153800
C	-1.05384700	-2.32019900	-3.41998600
H	-0.87514400	-2.28154200	-4.49961700
H	-1.10761000	-3.37575500	-3.14417500
C	-2.32928300	-1.51121800	-3.02669200
H	-2.82595900	-1.09408600	-3.90849500
H	-3.07203400	-2.11293800	-2.49177700
H	1.08454100	-1.79695000	-3.05020100
H	-2.14394900	-1.66672100	-0.42973700
C	-0.02316700	-3.19960800	-0.71141800
O	-0.60489800	-3.68921800	0.29086000
C	0.95291500	-5.33341200	-1.02289400
H	1.44717200	-5.30801100	-0.04838300
H	0.01816000	-5.89340800	-0.94131400
H	1.60733400	-5.77654500	-1.77201600
C	4.84777800	-0.63825200	-0.77056400
C	4.09454200	-1.52235400	-1.81854900
O	2.89133300	-1.93192600	-1.54666800
O	4.74527900	-1.86744900	-2.79573400
C	3.22453400	1.82089600	-0.29627800
C	3.12145600	2.91173400	0.57552200
C	2.73141200	1.98907400	-1.59435900
C	2.49830700	4.09792100	0.19668600
C	2.11874500	3.16963500	-1.99770300
C	1.99599900	4.22602500	-1.09507500
F	2.79621000	0.98451500	-2.47820100
F	1.63013900	3.28760200	-3.23546000
F	1.39136600	5.35573300	-1.46790100
F	2.36099600	5.10211600	1.06785800
F	3.53688900	2.80298100	1.84454200
C	5.61038700	-1.60958800	0.15315100
H	6.24967300	-2.23207400	-0.47906000
H	6.23313400	-1.07041500	0.87310100
H	4.92590400	-2.26885600	0.69659400
C	5.79654300	0.35168000	-1.43959100
H	5.26194800	1.04101600	-2.09520600

H	6.36394500	0.92196800	-0.69779800
H	6.48322300	-0.22374900	-2.06371800
S	3.67201600	0.24051300	0.41582900
O	1.45689400	-1.15803200	2.79303100
C	0.68031800	-1.01872900	3.80178400
O	-0.49663500	-1.48280900	3.87148200
C	1.19809100	-0.20705100	4.96516000
H	2.25921000	-0.41117000	5.12193400
H	1.09853800	0.85173600	4.69846000
H	0.62394000	-0.40289800	5.87096500
Ag	-0.93627600	-2.63122200	2.11854400
O	0.70427300	-3.99477600	-1.48745000
H	-2.43181100	0.47691900	-2.04623600
H	-2.38892800	2.94844600	1.58687600
O	0.17975700	3.44019400	2.44648500
C	-0.61711800	4.61514200	2.50812400
H	-1.50408000	4.47358400	3.13913800
H	0.01866300	5.38547700	2.94589000
H	-0.93491700	4.93417500	1.50673900
C	-5.49761100	1.84665100	-0.69611300
C	-6.19707900	0.68314700	-0.34918900
C	-5.52741200	-0.35150700	0.31837300
C	-4.17815600	-0.22749200	0.62593100
C	-3.46247700	0.92900000	0.27224000
C	-4.14605200	1.96558600	-0.38402000
H	-6.01415100	2.64742600	-1.21265000
H	-6.08721500	-1.23928200	0.59310800
H	-3.66970200	-1.02264300	1.16331900
H	-3.60152400	2.86154400	-0.66767100
C	-7.64207300	0.49406200	-0.65486200
O	-8.28199000	-0.50010700	-0.36988800
O	-8.17991000	1.56004700	-1.29214900
C	-9.57435500	1.43549600	-1.61363500
H	-10.16834600	1.30068100	-0.70557600
H	-9.84540500	2.36428000	-2.11579100
H	-9.74286300	0.57832600	-2.27117500
L-Ag-TS35'			
C	3.03951900	-2.58711500	-2.44155200
C	2.07214500	-1.99486700	-3.26392400
C	0.89956700	-1.49550600	-2.71556500

C	0.71178100	-1.52811300	-1.31857500
C	1.73973600	-1.99885300	-0.47267900
C	2.86232400	-2.61729200	-1.05484200
Pd	-0.67614200	-0.41022500	-0.28884000
H	-0.49848200	-2.14866600	-1.18049600
H	2.22918800	-1.97309000	-4.33837300
H	0.09950200	-1.13755800	-3.35646100
O	3.73255800	-3.21879500	-0.18490200
C	4.92645200	-3.78608100	-0.70162000
H	5.46222500	-4.19134700	0.15809100
H	4.71691300	-4.59739700	-1.41049400
H	5.55190200	-3.02864000	-1.19340800
H	3.92021200	-3.02677900	-2.89391900
C	0.14593500	-1.34347500	1.37204400
C	0.35854600	-0.27846700	2.45406900
C	2.49038600	-0.67311500	1.72037200
C	1.58951800	-1.80390400	1.00526400
C	1.51689600	0.52440600	1.85571100
H	1.90699500	1.29566300	2.52970100
H	1.25035500	0.99438400	0.90623900
C	1.04129000	-0.98878500	3.66398100
H	0.96161600	-0.35727900	4.55449800
H	0.56567600	-1.94444300	3.90223000
C	2.52228400	-1.14248600	3.20270200
H	3.16403900	-0.49057700	3.79943300
H	2.90296300	-2.16319500	3.30484100
H	-0.53415200	0.28742100	2.71889500
H	1.79759100	-2.75871800	1.49882900
C	-0.80972800	-2.47205600	1.70909000
O	-0.52975700	-3.65425500	1.50678900
N	-1.98506300	-2.10105900	2.29501300
H	-2.21537700	-1.11923200	2.33471800
C	-2.99268100	-3.09390100	2.64291000
H	-3.80872800	-2.59582200	3.17058700
H	-3.38103100	-3.58843900	1.74727400
H	-2.55395500	-3.85416600	3.29471400
C	3.85331100	-0.34695500	1.06691900
C	3.69005200	0.55295300	-0.17666700
C	4.87415000	0.31710100	2.01646900
H	4.30155300	-1.29317400	0.75200600
C	5.01456800	0.78435400	-0.90975500

H	3.31304600	1.52702100	0.15423100
H	2.94567100	0.14968000	-0.86448600
C	6.21409500	0.57569900	1.30547500
H	4.46903200	1.26813100	2.39257900
H	5.05683600	-0.31607500	2.89070300
C	6.04820000	1.41590800	0.03139200
H	4.84546900	1.42604600	-1.78205600
H	5.39344500	-0.17581400	-1.28997900
H	6.91585600	1.06036900	1.99515500
H	6.65995700	-0.39326700	1.03678800
H	7.01436400	1.53825800	-0.47323800
H	5.70494900	2.42420100	0.30422200
C	-3.33071800	2.88827200	0.78265200
C	-2.98542200	1.42603800	0.46167700
O	-1.81604800	1.04570800	0.78629000
O	-3.86101100	0.72869200	-0.12425400
C	-1.03256000	3.67118900	-0.78114000
C	-0.19465200	4.58780500	-0.13101000
C	-0.40981500	2.66973300	-1.53770600
C	1.19286200	4.52486000	-0.24320600
C	0.97281000	2.59230500	-1.67163200
C	1.77514400	3.53432500	-1.03051500
F	-1.14589100	1.72742900	-2.16058400
F	1.53551600	1.62315400	-2.40113200
F	3.10265000	3.48780900	-1.16438900
F	1.96686300	5.41600700	0.38413900
F	-0.71096300	5.56298800	0.62292800
C	-4.84419500	3.11313100	0.86986400
H	-5.24136200	2.53512200	1.71028600
H	-5.06465400	4.16998700	1.04402500
H	-5.35180000	2.77613600	-0.03519800
C	-2.60858100	3.38857500	2.03380700
H	-1.53121100	3.24092800	1.95801800
H	-2.81737600	4.44865700	2.19301900
H	-2.96193400	2.82479700	2.90508000
S	-2.80029100	3.85937600	-0.75087300
Ag	-3.49096700	-1.33143300	-0.52678700
O	-1.22899600	-3.25498900	-1.62518500
C	-2.16144100	-3.90934200	-1.07070700
O	-3.25761300	-3.42027900	-0.64138100
C	-1.96148200	-5.39651700	-0.88364900

H	-1.36385400	-5.80417700	-1.70061500
H	-1.39935500	-5.51112100	0.04884700
H	-2.91647600	-5.91678100	-0.79721800

L-Ag-TS50'

C	-3.16906000	0.19901500	-2.12890500
C	-3.14991100	-0.46165900	-0.88368600
C	-1.92329100	-0.88196000	-0.37103700
C	-0.72178500	-0.57833500	-1.04031500
C	-0.74096100	0.22002400	-2.20572100
C	-1.98480600	0.50832400	-2.79841500
Pd	1.14950200	-0.58846800	-0.15583700
H	-0.12265700	-1.78360900	-1.14769400
H	-1.88753100	-1.47267700	0.53884900
C	1.77289900	0.07821700	-2.02469900
C	2.75887300	1.23176600	-1.80694300
C	0.87045500	2.32046800	-2.50584300
C	0.55618500	0.75173100	-2.72814100
C	1.82242200	2.32583000	-1.28447000
H	2.31600700	3.29577300	-1.15536600
H	1.34642000	2.05024800	-0.34072800
C	3.14490800	1.77835800	-3.21686800
H	4.04380600	2.39778100	-3.13800600
H	3.36768900	0.97425600	-3.92413700
C	1.90192200	2.62484000	-3.62913000
H	2.16269100	3.68563200	-3.63482000
H	1.51901800	2.37392700	-4.62289600
H	3.61354200	0.98882700	-1.17607700
H	0.60336400	0.55030900	-3.80305800
C	2.30266300	-1.15244000	-2.73584400
O	1.69088000	-1.69077600	-3.65983300
N	3.51844700	-1.60612000	-2.31758600
H	3.93000800	-1.19481300	-1.49303700
C	4.12452400	-2.78560200	-2.92067900
H	4.29883700	-2.61783000	-3.98766200
H	5.07955100	-2.97907200	-2.42797900
H	3.47139100	-3.65568500	-2.80780800
C	-0.34732700	3.26662900	-2.39865600
C	-1.01804900	3.18294400	-1.01015600
C	-0.03372800	4.74892400	-2.69758300
H	-1.07383900	2.95318600	-3.15311500

C	-2.30059600	4.01599700	-0.92783400
H	-0.31513200	3.57329500	-0.26608200
H	-1.22362200	2.14952700	-0.72831100
C	-1.30171100	5.61654500	-2.61009500
H	0.71619200	5.12208600	-1.98475400
H	0.39899800	4.85797600	-3.69730500
C	-2.00902700	5.48637900	-1.25389000
H	-2.73722800	3.92196700	0.07311700
H	-3.04150000	3.61687400	-1.63658400
H	-1.05137900	6.66515700	-2.81174100
H	-1.99481300	5.30354400	-3.40483700
H	-2.93144000	6.07964800	-1.24607600
H	-1.36203600	5.89874100	-0.46643400
C	4.29685400	-0.36040800	2.87041500
C	3.52130700	-1.03753300	1.72880600
O	3.01875300	-0.25665100	0.85975200
O	3.41327000	-2.29611100	1.75881000
C	1.92939000	1.20452000	3.43734200
C	2.19260800	2.57666900	3.55179900
C	0.73828200	0.84040300	2.79577900
C	1.31028100	3.53886100	3.06457300
C	-0.16479400	1.78286300	2.31384800
C	0.12084000	3.13895300	2.45993000
F	0.43332400	-0.46061900	2.61087600
F	-1.29386000	1.40153400	1.70687400
F	-0.74026800	4.05757300	2.01597200
F	1.58771400	4.84041300	3.18895200
F	3.31222500	3.00603400	4.14154500
C	5.27345800	-1.32444600	3.55198500
H	6.03507200	-1.62915900	2.82733200
H	5.77312600	-0.83319800	4.39155300
H	4.76821200	-2.22596600	3.90177200
C	4.99002700	0.92252600	2.41239500
H	4.28506300	1.60974600	1.94475800
H	5.46960200	1.41765000	3.25938400
H	5.75620800	0.67280600	1.66912600
S	2.99101600	-0.00490200	4.19367700
Ag	2.38462000	-3.35249800	0.21376200
O	-0.30243200	-3.13566300	-1.42414400
C	0.49260100	-3.96494000	-1.96416800
O	1.59867200	-4.35242800	-1.46638800

C	0.11105100	-4.53921800	-3.30966800
H	-0.97354100	-4.63057800	-3.38843400
H	0.45555800	-3.81761500	-4.05749200
H	0.59969600	-5.49899600	-3.48380100
O	-1.93789500	1.10382500	-4.02954800
C	-3.15687300	1.50812100	-4.63539700
H	-3.68774700	2.24366200	-4.01597000
H	-2.88106400	1.96890000	-5.58495100
H	-3.81712200	0.65294700	-4.82756200
C	-5.82195100	-2.18352300	1.18629300
C	-6.82383400	-1.20339600	1.22143500
C	-6.61699800	0.01656600	0.56349500
C	-5.42886100	0.25207000	-0.11736200
C	-4.41707000	-0.72425700	-0.16111000
C	-4.63491000	-1.94500500	0.50133000
H	-5.98367900	-3.13096400	1.68735200
H	-7.39755400	0.76869000	0.60784300
H	-5.26389900	1.21130200	-0.59916100
H	-3.87610900	-2.72008300	0.45379000
C	-8.11457600	-1.40002500	1.93488700
O	-9.00775700	-0.57543300	1.98664300
O	-8.19725100	-2.61245200	2.53245500
C	-9.42341500	-2.85930800	3.23727400
H	-10.27756500	-2.80293800	2.55682300
H	-9.32851000	-3.86294400	3.65218500
H	-9.56451500	-2.12452500	4.03475200
H	-4.12740200	0.44258200	-2.57058600

L-Ag-TS55'

C	-2.71671900	0.02469300	2.78116600
C	-1.48761500	0.05584200	3.45795700
C	-0.33219900	-0.31886100	2.77680500
C	-0.39621800	-0.59391400	1.39522800
C	-1.60789400	-0.43540400	0.67822000
C	-2.80247500	-0.24227200	1.41145500
Pd	1.27382100	-0.59733600	0.18438900
H	0.12237600	-1.82606800	1.29790100
H	0.60503600	-0.47307600	3.29848900
H	-3.61834600	0.18047700	3.36467100
C	-0.12227900	-0.92626700	-1.31431400
C	0.22660000	0.00715600	-2.47985500

C	-1.61877900	1.00839300	-1.57128900
C	-1.50418800	-0.41430400	-0.82095400
C	-0.14677100	1.37055800	-1.88598400
H	-0.07068900	2.19444300	-2.60496400
H	0.45234400	1.62026000	-1.00691800
C	-0.87364900	-0.18555600	-3.56993500
H	-0.52993900	0.23761400	-4.51891700
H	-1.09683000	-1.24119400	-3.74959400
C	-2.08924100	0.60592900	-2.99841600
H	-2.26996800	1.49428100	-3.60725700
H	-3.01610400	0.02444700	-2.98005500
H	1.24576500	-0.09339100	-2.85366200
H	-2.27253600	-1.05787400	-1.24951700
C	-0.08855200	-2.41745400	-1.59151900
O	-1.01293900	-3.16555900	-1.26343900
N	1.00546700	-2.87587700	-2.26073600
H	1.77288500	-2.23983300	-2.42040500
C	1.15772900	-4.29191100	-2.56789100
H	0.32021800	-4.63587000	-3.18153200
H	2.08876600	-4.43240400	-3.12062800
H	1.18296700	-4.88617300	-1.64966900
C	-2.44370500	2.09562600	-0.85143900
C	-1.63893500	2.77541400	0.27606500
C	-3.01677500	3.18525900	-1.78253900
H	-3.31182200	1.60643000	-0.40222500
C	-2.47273700	3.78386100	1.07348400
H	-0.80129700	3.31641500	-0.17754000
H	-1.20366200	2.03459700	0.94966900
C	-3.85900500	4.20408300	-0.99628800
H	-2.19565400	3.70506200	-2.29811400
H	-3.64386500	2.73541500	-2.55897500
C	-3.06636600	4.85240600	0.14661400
H	-1.84671800	4.24735700	1.84496200
H	-3.28212300	3.25696900	1.59817900
H	-4.24827500	4.97159800	-1.67616900
H	-4.73281400	3.68466100	-0.57690800
H	-3.70314000	5.54609000	0.70888300
H	-2.24517100	5.44905000	-0.27630700
C	5.29991000	0.21182300	-1.33780900
C	4.15059500	-0.69106000	-0.86201300
O	2.97618300	-0.26641300	-1.10088600

O	4.45275500	-1.75390300	-0.24866700
C	4.11624800	2.33582000	0.23085100
C	3.93196300	3.51838500	-0.49955200
C	3.10772700	1.99189000	1.14049700
C	2.81118800	4.32735400	-0.32177100
C	1.98792800	2.79143100	1.34569200
C	1.84608900	3.97046800	0.61716600
F	3.18592200	0.84534400	1.84674900
F	1.04439100	2.43340500	2.22522200
F	0.78493900	4.75630800	0.81246800
F	2.66435900	5.45014900	-1.03152200
F	4.83927700	3.90881000	-1.39961200
C	6.61370100	-0.56207600	-1.49006500
H	6.49552400	-1.31035100	-2.28013700
H	7.42524100	0.11351100	-1.77466100
H	6.87843000	-1.08752700	-0.57132600
C	4.93844700	0.97490300	-2.61217400
H	4.01318400	1.53773100	-2.48950200
H	5.74405900	1.65961800	-2.88544800
H	4.78936200	0.26121700	-3.43093100
S	5.61950300	1.39424600	0.10348400
Ag	2.94214700	-3.11988500	0.37969200
O	0.11829200	-3.12676600	1.82219200
C	0.36009700	-4.24348100	1.27376000
O	1.46388700	-4.57742700	0.73080100
C	-0.74934000	-5.27097800	1.24298800
H	-1.38113700	-5.17439000	2.12743300
H	-1.35105200	-5.04139100	0.35758100
H	-0.35013400	-6.28236000	1.15397600
O	-1.54687400	0.38960300	4.77761800
C	-0.32553500	0.43028900	5.50352300
H	-0.58147800	0.77720800	6.50569000
H	0.13684500	-0.56322700	5.57289400
H	0.38894200	1.12821800	5.04682500
C	-6.43217000	0.43159400	0.50239900
C	-6.71834600	-0.66193900	-0.32621700
C	-5.72379000	-1.61851000	-0.57249500
C	-4.45915800	-1.47993200	-0.01215300
C	-4.15438500	-0.37367300	0.80108300
C	-5.16511000	0.56749000	1.06096400
H	-7.19968500	1.17151500	0.69817800

H	-5.96571900	-2.46868200	-1.20137300
H	-3.70012600	-2.23590500	-0.19165800
H	-4.94173100	1.42732700	1.68527600
C	-8.04907600	-0.85898800	-0.96245300
O	-8.33596900	-1.79129600	-1.68909800
O	-8.92568000	0.12402600	-0.64592600
C	-10.22907900	-0.01437700	-1.23185700
H	-10.70028500	-0.94652400	-0.90813100
H	-10.80170600	0.84598300	-0.88488300
H	-10.16294700	-0.01852200	-2.32334600