

Supporting Information

Computational Exploration of Palladium-Catalyzed Synthesis of Dibenzosilepin Derivatives

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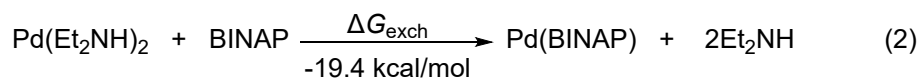
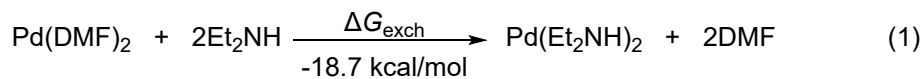
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Table of Contents

Ligand exchange energy.	S2
Gibbs free energy profiles for the reaction of 1,5-palladium migration and alkyne insertion without the diphosphine ligand.	S2
Transition state of intramolecular alkyne insertions.	S3
The other possible conformations of intramolecular alkyne insertions.	S4
Gibbs free energy profiles for the reaction of 1,4-palladium migration, C–H activation and reductive elimination without the diphosphine ligand.	S5
Gibbs free energy profiles for the formal 1,4-palladium migration without the diphosphine ligand.	S6
Gibbs free energy profiles for the reaction of 1,5-palladium migration with the (<i>R</i>)-BINAP ligand.	S7
Gibbs free energy profiles for the reaction of 1,4-palladium migration and C–H activation with the (<i>R</i>)-BINAP ligand.	S7
Visual analysis of non-covalent interactions.	S8
The intramolecular alkyne insertion TSs with the (<i>R</i>)-BINAP ligand.	S8
Tables of energies.	S9
Cartesian coordinates of the structures.	S11



Scheme S1 Calculated ligand exchange energy ΔG_{exch} .

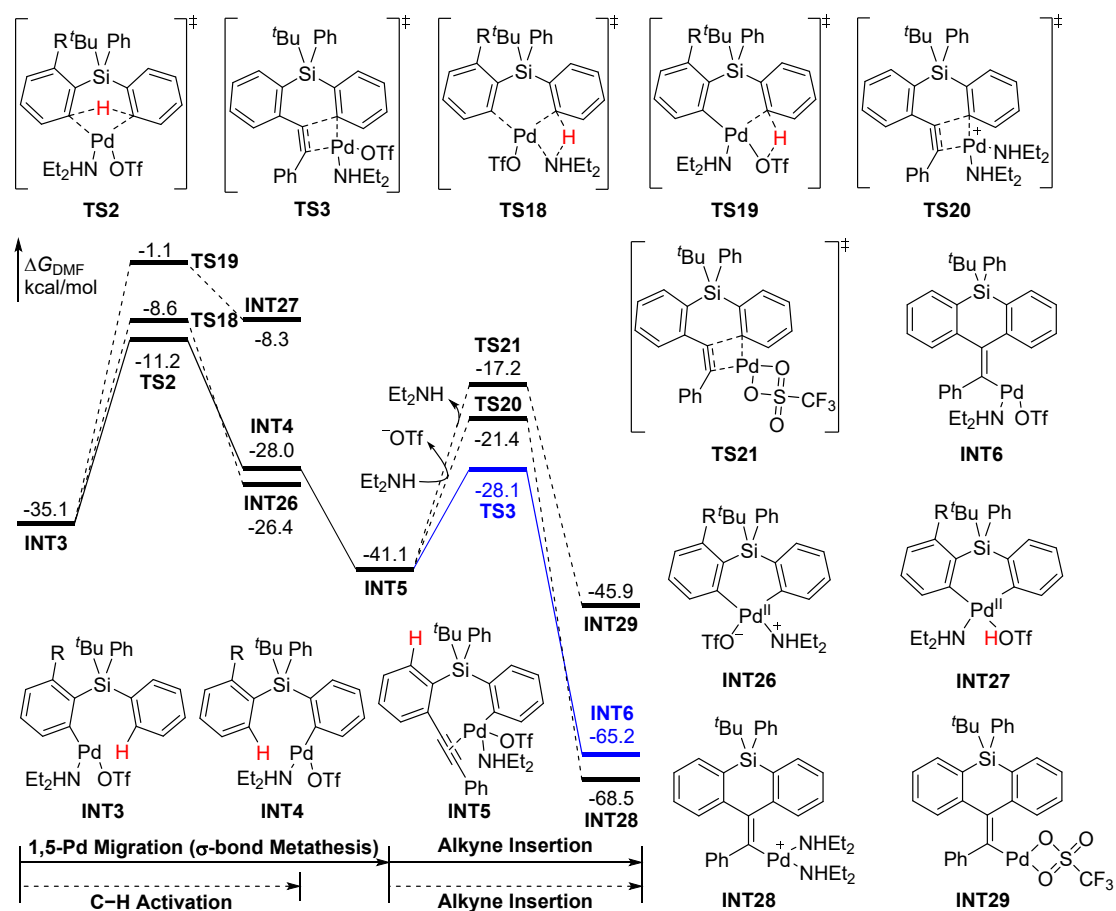


Fig. S1 Gibbs free energy profiles for the reaction of 1,5-palladium migration and alkyne insertion without the diphosphine ligand.

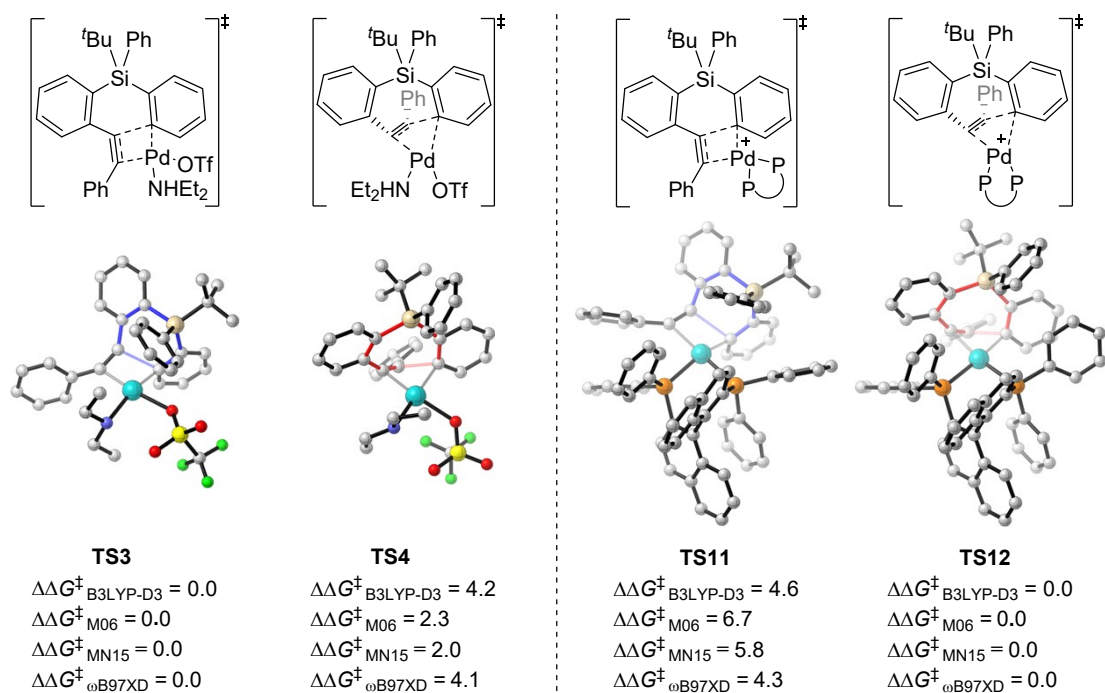


Fig. S2 Transition states of intramolecular alkyne insertions. Geometry optimization was performed with B3LYP-D3. The LANL2DZ basis set with ECP was used for Pd, and the 6-31G(d) basis set was used for other atoms. The single-point energies from B3LYP-D3, M06, MN15 and ω B97XD calculations. The SDD-6-311++G(d,p) basis set by using the SMD solvation model (Solvent = DMF). Gibbs free energies are shown in kcal/mol. Hydrogen atoms omitted for clarity.

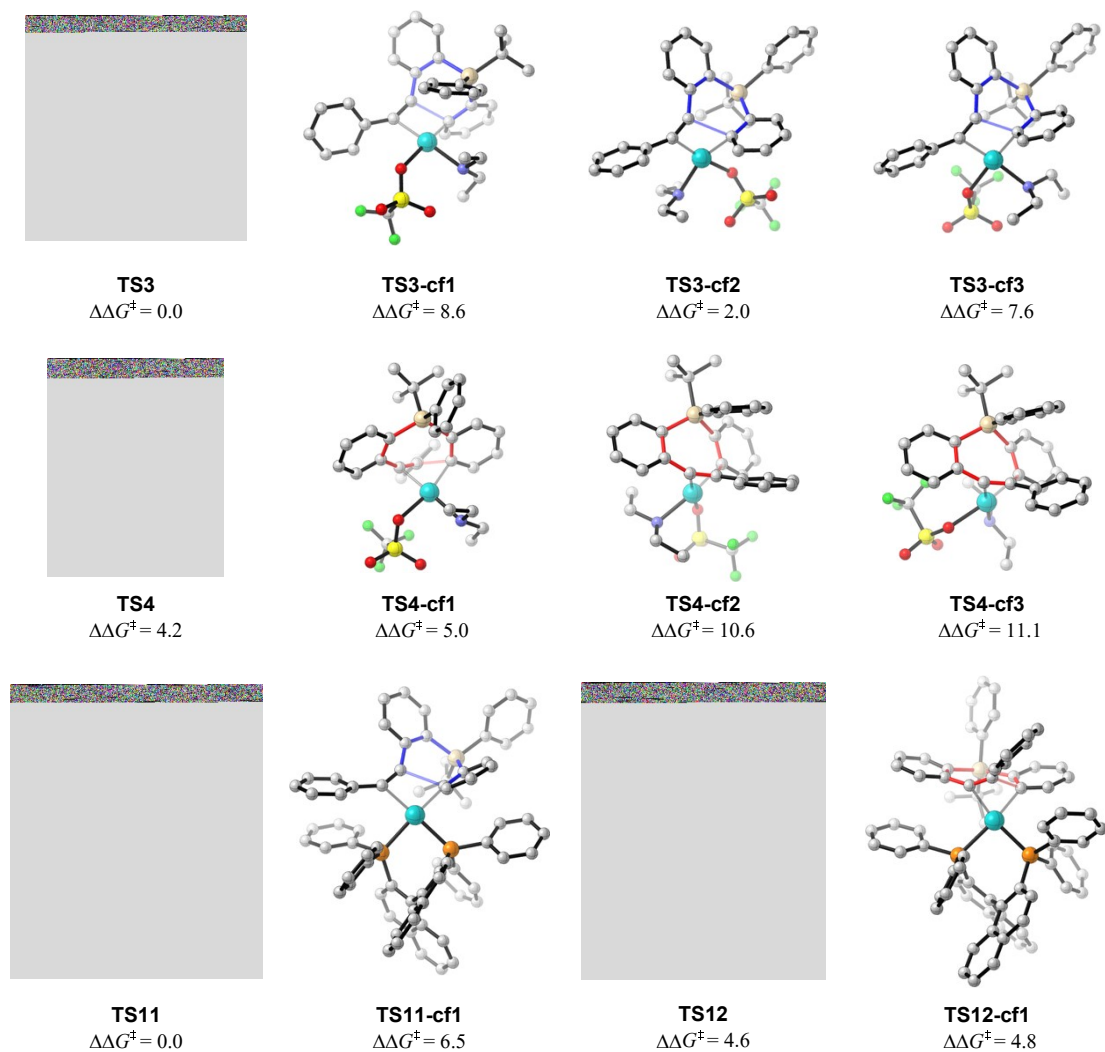


Fig. S3 The other possible conformations of intramolecular alkyne insertion TSs. Hydrogen atoms omitted for clarity. Gibbs free energies are shown in kcal/mol.

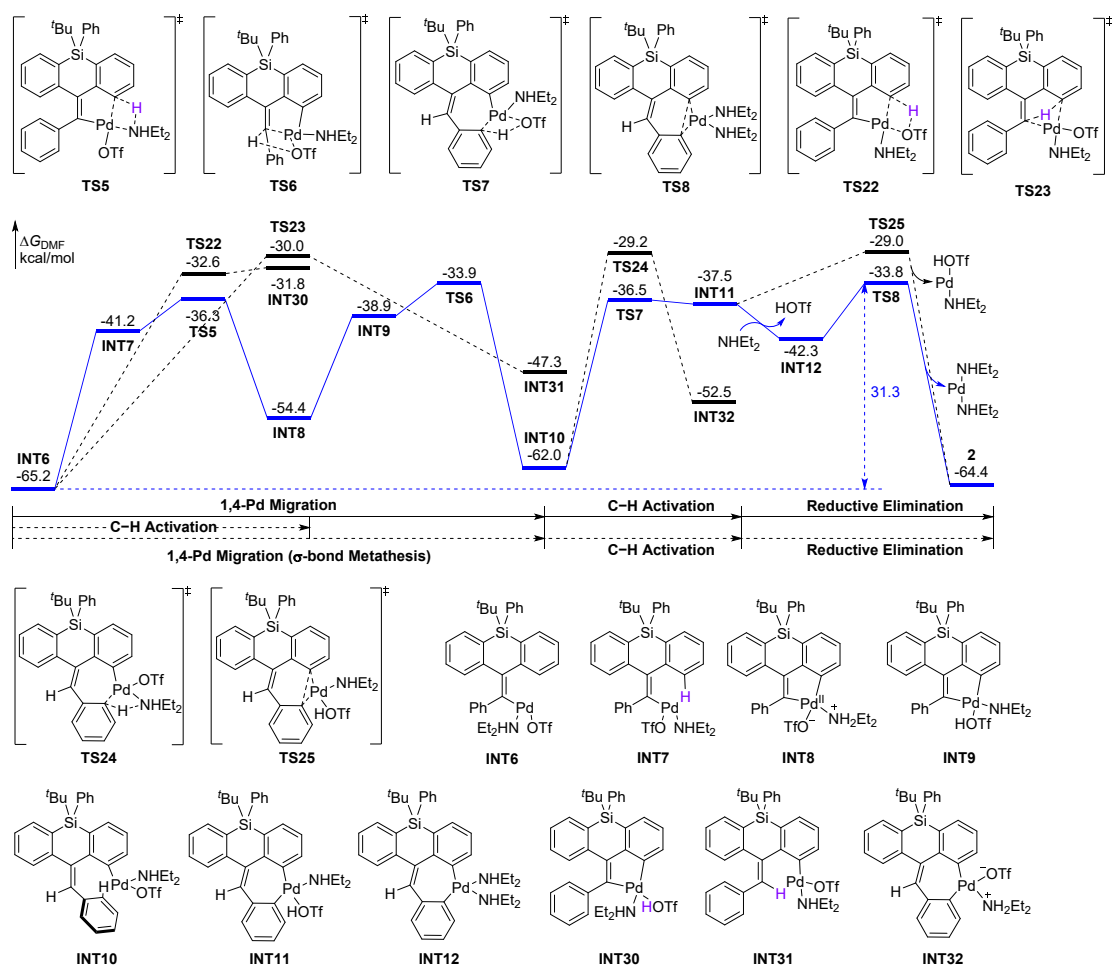


Fig. S4 Gibbs free energy profiles for the reaction of 1,4-palladium migration, C-H activation and reductive elimination without the diphosphine ligand.

The position of triflate in **INT6** can be exchanged with diethylamine to form the alkenylpalladium intermediate **INT7** to bring the diethylamine close to the reacting C–H bond. The diethylamine-assisted concerted metalation/deprotonation (CMD) process occurs via **TS5** to generate alkenyl(aryl)palladium(II) species **INT8**, which requires a barrier of 28.9 kcal/mol. Then the intramolecular proton exchange generates the arylpalladium intermediate **INT9**, which further shifts the proton via **TS6** to the alkenyl moiety to form the *Z*-alkene arylpalladium intermediate **INT10**. This concerted protodepalladation process is concomitant with the *E*→*Z* alkene isomerization. In addition, the triflic acid can dissociate from **INT9** to form **INT33**, which undergoes an outer-sphere protonation by triflic acid to give intermediate **INT34**. The subsequent depalladation generates intermediate **INT35**, which is then subjected to a *E*→*Z* isomerization via **TS27** through the rotation of the alkene C–C bond to form intermediate **INT10**. Therefore, in the formal 1,4-palladium migration process from **INT6** to **INT10**, the largest energy span for both the concerted mechanism via **TS6** and the stepwise mechanism via **TS26/TS27** is 31.3 kcal/mol.

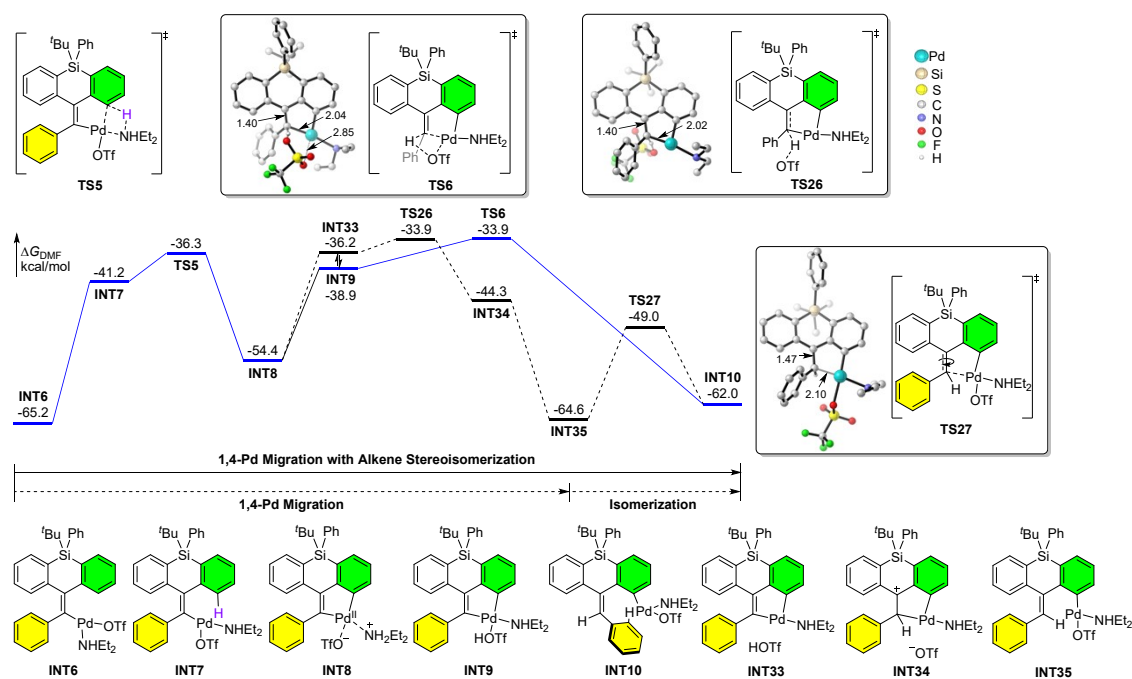


Fig. S5 Gibbs free energy profiles for the formal 1,4-palladium migration without the diphosphine ligand.

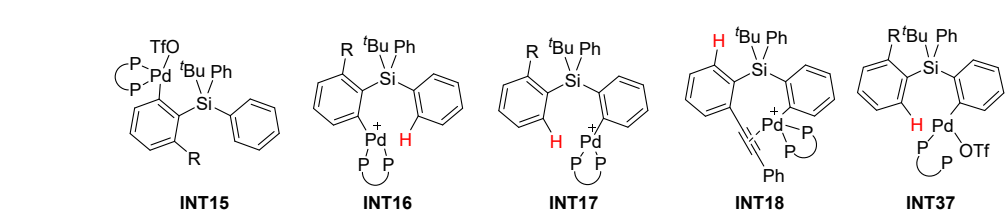
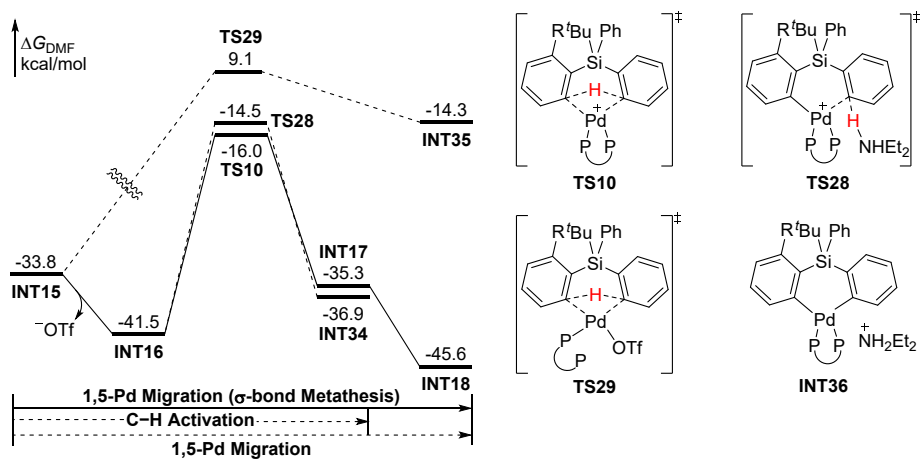


Fig. S6 Gibbs free energy profiles for the reaction of 1,5-palladium migration with the (*R*)-BINAP ligand.

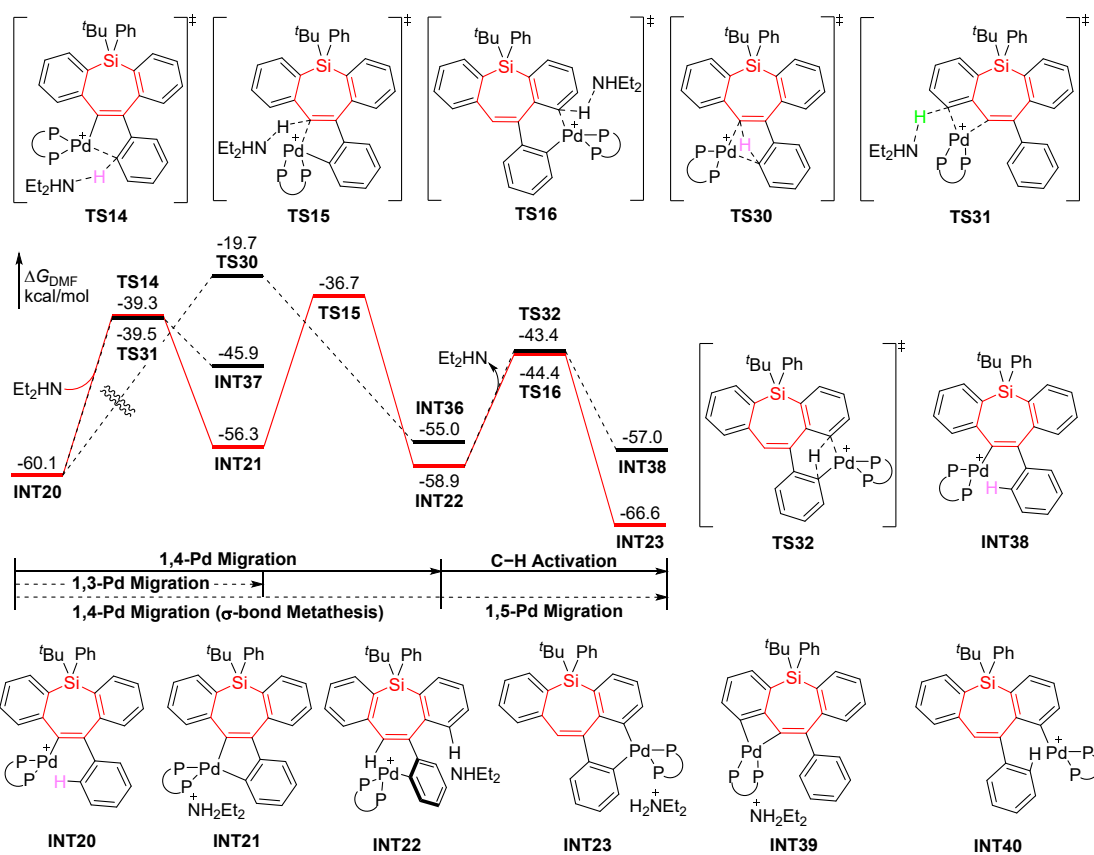


Fig. S7 Gibbs free energy profiles for the reaction of 1,4-palladium migration and C-H activation with the (*R*)-BINAP ligand.

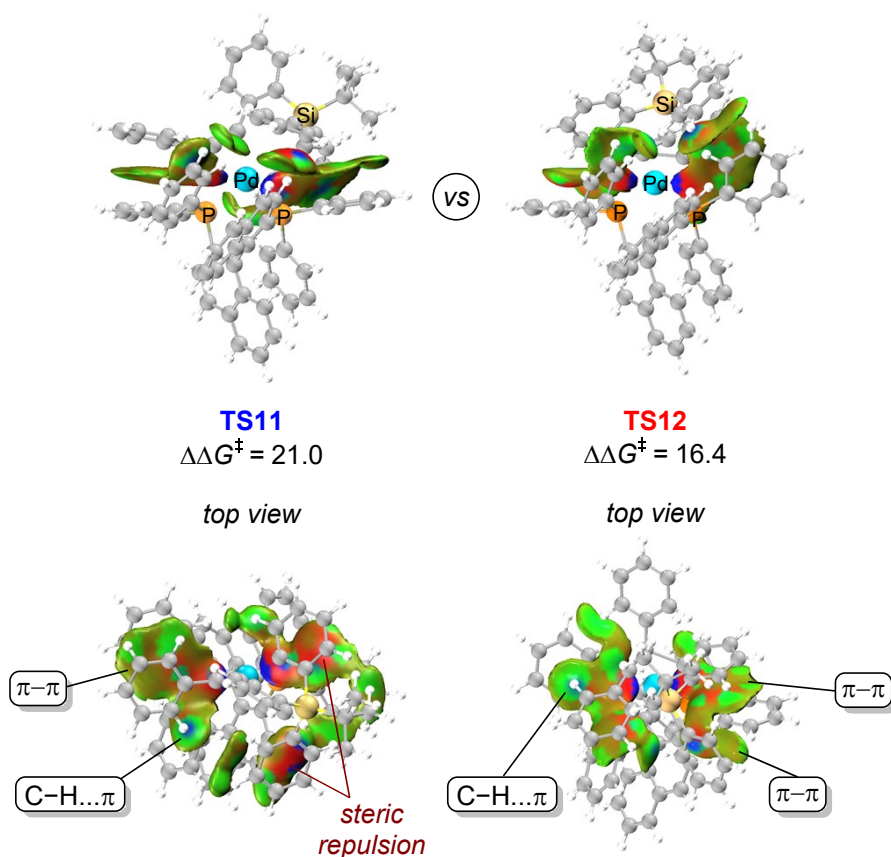


Fig. S8 Ligand steric effects on divergent alkyne insertion TSs. Visual analysis of non-covalent interactions. For IGM analysis, blue, attraction; green, weak interaction; red, steric effect. Gibbs free energies are shown in kcal/mol.

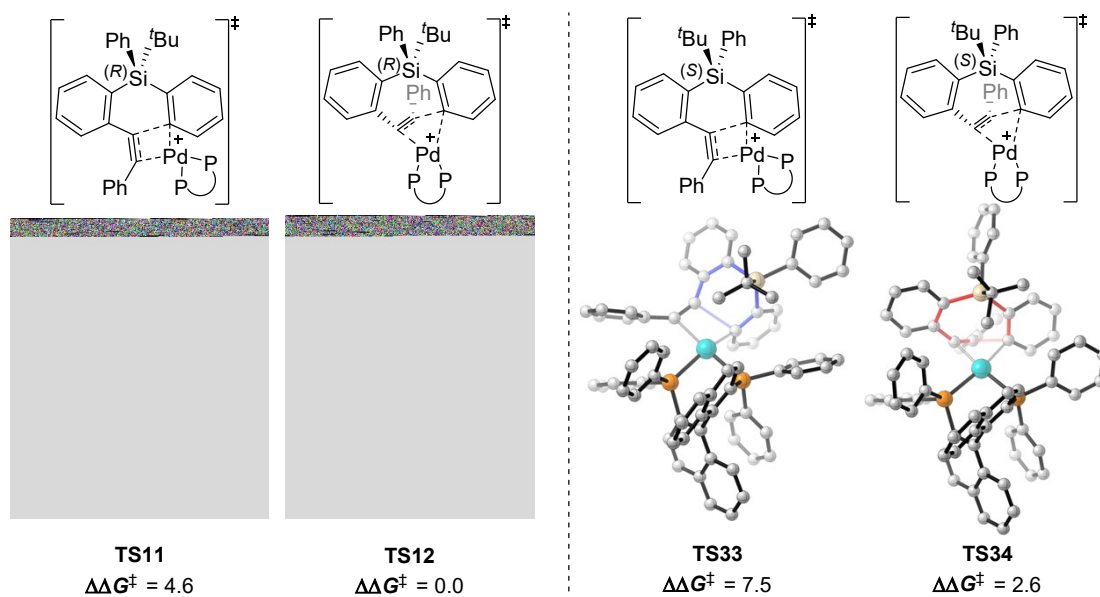


Fig. S9 The intramolecular alkyne insertion TSs with the (*R*)-BINAP ligand. Hydrogen atoms omitted for clarity. Gibbs free energies are shown in kcal/mol.

Table S1. Electronic Energies, Enthalpies, and Free Energies (in Hartree) of the Structures Calculated at the SMD_(DMF)-B3LYP-D3/6-311++G(d,p)-[SDD for Pd]/B3LYP-D3/6-31G(d)[LANL2DZ for Pd] Level of Theory

Structures	ZPE	TCE	TCH	TCG	E _{sol}	G _{sol} (E _{sol} +TCG)	Imaginary Frequency
Et₂NH	0.150542	0.157344	0.158288	0.120568	-213.879098	-213.758530	—
DMF	0.103060	0.109129	0.110073	0.073953	-248.607783	-248.533830	—
Pd(Et₂NH)₂	0.305330	0.321921	0.322865	0.258380	-555.729050	-555.470670	—
Pd(DMF)₂	0.208114	0.223802	0.224746	0.161026	-625.152476	-624.991450	—
Et₂NH₂⁺	0.165872	0.172836	0.173780	0.135592	-214.354354	-214.218762	—
Pd(BINAP)	0.624462	0.663420	0.664364	0.550407	-2507.258725	-2506.708318	—
OTf	0.027217	0.034402	0.035346	-0.005344	-961.809171	-961.814515	—
HOTf	0.038558	0.046423	0.047368	0.005380	-962.233006	-962.227626	—
1	0.508168	0.544746	0.545690	0.437008	-2410.950207	-2410.513199	—
INT1	0.813595	0.868360	0.869305	0.720159	-2966.706451	-2965.986292	—
TS1	0.812067	0.866703	0.867647	0.718986	-2966.690053	-2965.971067	180.10 <i>i</i>
INT2	0.817430	0.870991	0.871935	0.728456	-2966.749858	-2966.021402	—
INT3	0.663272	0.709342	0.710286	0.581341	-2752.862628	-2752.281287	—
TS2	0.656510	0.702525	0.703470	0.575531	-2752.818661	-2752.243130	1374.31 <i>i</i>
INT4	0.662591	0.708784	0.709729	0.581003	-2752.850967	-2752.269964	—
INT5	0.662159	0.708297	0.709241	0.579765	-2752.870576	-2752.290811	—
TS3	0.661779	0.707151	0.708095	0.582239	-2752.852401	-2752.270162	170.48 <i>i</i>
INT6	0.664464	0.709735	0.710679	0.584431	-2752.913739	-2752.329308	—
TS4	0.661467	0.706729	0.707673	0.581246	-2752.844714	-2752.263468	255.09 <i>i</i>
INT13	0.663944	0.709142	0.710086	0.584491	-2752.892308	-2752.307817	—
INT7	0.661409	0.707735	0.708679	0.577913	-2752.868868	-2752.290955	—
TS5	0.657815	0.703053	0.703997	0.576705	-2752.859894	-2752.283189	1176.58 <i>i</i>
INT8	0.665756	0.710773	0.711717	0.585395	-2752.897442	-2752.312047	—
INT9	0.661548	0.707500	0.708444	0.578060	-2752.865393	-2752.287333	—
TS6	0.656189	0.701778	0.702722	0.572737	-2752.852157	-2752.279420	1415.75 <i>i</i>
INT10	0.664255	0.709427	0.710371	0.582616	-2752.906724	-2752.324108	—
TS7	0.657051	0.701994	0.702939	0.575348	-2752.858822	-2752.283474	1111.52 <i>i</i>
INT11	0.661577	0.707119	0.708063	0.578726	-2752.863790	-2752.285064	—
INT12	0.775920	0.819800	0.820744	0.698768	-2004.522380	-2003.823612	—
TS8	0.773577	0.817493	0.818437	0.695263	-2004.505421	-2003.810158	277.69 <i>i</i>
2	0.470445	0.496408	0.497352	0.414700	-1448.802973	-1448.388273	—
INT14	1.134164	1.211045	1.211990	1.017685	-4918.258640	-4917.240955	—
TS9	1.132251	1.208933	1.209877	1.016993	-4918.227115	-4917.210122	159.08 <i>i</i>
INT15	1.136583	1.212792	1.213736	1.022982	-4918.298357	-4917.275375	—
INT16	1.107140	1.174771	1.175715	1.003560	-3956.448295	-3955.444735	—
TS10	1.101170	1.168406	1.169351	0.998907	-3956.435182	-3955.436275	1273.08 <i>i</i>
INT17	1.107257	1.174777	1.175721	1.004685	-3956.471729	-3955.467044	—
INT18	1.107624	1.174922	1.175866	1.005698	-3956.485442	-3955.479744	—

TS12	1.106474	1.172987	1.173931	1.006210	-3956.459789	-3955.453579	318.74i
INT19	1.109359	1.175929	1.176873	1.008809	-3956.504317	-3955.495508	—
TS11	1.106654	1.173342	1.174286	1.007417	-3956.453601	-3955.446184	75.49
INT25	1.109125	1.175763	1.176707	1.007836	-3956.525475	-3955.517639	—
TS13	1.107881	1.174044	1.174988	1.006081	-3956.476679	-3955.470598	25.22i
INT20	1.109413	1.175905	1.176849	1.008204	-3956.510939	-3955.502735	—
TS14	1.258688	1.332442	1.333386	1.150204	-4170.378341	-4169.228137	1415.55i
INT21	1.265003	1.339183	1.340127	1.154974	-4170.410194	-4169.255220	—
TS15	1.258256	1.331901	1.332845	1.149861	-4170.373803	-4169.223942	1311.14i
INT22	1.261937	1.336911	1.337855	1.149556	-4170.408843	-4169.259287	—
TS16	1.257876	1.331946	1.332890	1.147408	-4170.383556	-4169.236148	1425.78i
INT23	1.263942	1.338569	1.339513	1.151878	-4170.423382	-4169.271504	—
INT24	1.096353	1.162379	1.163323	0.996099	-3956.043265	-3955.047166	291.81i
TS17	1.094299	1.160182	1.161126	0.993436	-3956.025092	-3955.031656	—
3	0.470116	0.496131	0.497075	0.414767	-1448.784762	-1448.369995	—
TS18	0.655693	0.701854	0.702798	0.572097	-2752.811219	-2752.239122	984.83i
INT26	0.662780	0.709326	0.710270	0.579320	-2752.846756	-2752.267436	—
TS19	0.653981	0.700466	0.701410	0.570068	-2752.797138	-2752.227070	1421.95i
INT27	0.658994	0.705974	0.706918	0.574386	-2752.813014	-2752.238628	—
TS20	0.788022	0.832135	0.833079	0.713346	-2004.916765	-2004.203419	215.83i
INT28	0.790111	0.834204	0.835148	0.714644	-2004.993127	-2004.278483	—
TS21	0.506220	0.544214	0.545158	0.434449	-2538.928608	-2538.494159	325.32i
INT29	0.509095	0.546945	0.547890	0.436937	-2538.976910	-2538.539973	—
TS22	0.657994	0.702871	0.703815	0.578412	-2752.855635	-2752.277223	795.30i
INT30	0.661591	0.707098	0.708042	0.580792	-2752.856729	-2752.275937	—
TS23	0.658790	0.703715	0.704659	0.579883	-2752.852966	-2752.273083	1321.40i
INT31	0.663419	0.708498	0.709442	0.583850	-2752.884643	-2752.300793	—
TS24	0.657470	0.702611	0.703556	0.576341	-2752.848266	-2752.271925	897.76i
INT32	0.664619	0.710215	0.711159	0.582258	-2752.891334	-2752.309076	—
TS25	0.660598	0.705733	0.706677	0.579739	-2752.851277	-2752.271538	259.39i
INT33	0.661296	0.707424	0.708368	0.576881	-2752.859867	-2752.282986	—
TS26	0.656713	0.702183	0.703127	0.573954	-2752.85337	-2752.279416	1355.68i
INT34	0.661401	0.707460	0.708404	0.575263	-2752.87112	-2752.295857	—
INT35	0.664186	0.709469	0.710413	0.582948	-2752.911178	-2752.328230	—
TS27	0.662683	0.707177	0.708121	0.582328	-2752.885739	-2752.303411	8.1i
TS28	1.255316	1.330419	1.331363	1.143653	-4170.332209	-4169.188556	1176.49i
INT36	1.262340	1.337797	1.338741	1.150267	-4170.374461	-4169.224194	—
TS29	1.127985	1.204371	1.205316	1.014879	-4918.221923	-4917.207044	1431.67i
INT37	1.134152	1.210828	1.211772	1.019754	-4918.264033	-4917.244279	—
TS30	1.103860	1.170146	1.171090	1.002860	-3956.441262	-3955.438402	1501.31i
INT38	1.108542	1.174988	1.175933	1.006347	-3956.500960	-3955.494613	—
TS31	1.258284	1.332350	1.333294	1.148148	-4170.376501	-4169.228353	943.96i
INT39	1.264353	1.338733	1.339677	1.153940	-4170.392451	-4169.238511	—
TS32	1.103582	1.169650	1.170595	1.003111	-3956.479304	-3955.476193	1391.57i

INT40	1.110096	1.176322	1.177266	1.010449	-3956.508243	-3955.497794	—
TS3-cf1	0.662887	0.707775	0.708719	0.585196	-2752.841675	-2752.256479	172.04 <i>i</i>
TS3-cf2	0.661145	0.706728	0.707673	0.579653	-2752.846549	-2752.266896	145.99 <i>i</i>
TS3-cf3	0.661810	0.707094	0.708038	0.582482	-2752.840519	-2752.258037	205.71 <i>i</i>
TS4-cf1	0.661110	0.706484	0.707428	0.581453	-2752.843721	-2752.262268	373.00 <i>i</i>
TS4-cf2	0.661405	0.706858	0.707802	0.581313	-2752.834510	-2752.253197	193.21 <i>i</i>
TS4-cf3	0.661123	0.706472	0.707417	0.581546	-2752.834073	-2752.252527	330.00 <i>i</i>
TS11-cf1	1.106392	1.172973	1.173918	1.006039	-3956.451984	-3955.445945	101.53 <i>i</i>
TS12-cf1	1.105995	1.172930	1.173875	1.003363	-3956.446641	-3955.443278	244.43 <i>i</i>
TS33	1.106575	1.173084	1.174028	1.007008	-3956.448595	-3955.441587	112.47 <i>i</i>
TS34	1.106108	1.173026	1.173970	1.003413	-3956.452800	-3955.449387	312.11 <i>i</i>

ZPVE = zero-point vibrational energy; **TCE** = thermal correction to energy; **TCH** = thermal correction to enthalpy; **TCG** = thermal correction to Gibbs free energy.

Cartesian coordinates of the structures

Et₂NH

N	0.00001700	-0.27541000	-0.07360900
H	0.00007900	-0.96824300	0.67566700
C	1.22176600	0.51995600	0.02202300
C	2.46090200	-0.37193300	-0.03206600
H	1.25338500	1.14737800	0.93593100
H	1.23229900	1.21701700	-0.82721200
H	3.37733600	0.22782300	-0.00225200
H	2.48710400	-1.06143300	0.82196700
H	2.46152500	-0.97068600	-0.94885100
C	-1.22180500	0.51992900	0.02222400
C	-2.46088400	-0.37194300	-0.03214800
H	-1.23234300	1.21713200	-0.82687600
H	-1.25347700	1.14707800	0.93628800
H	-3.37730200	0.22783700	-0.00207200
H	-2.46160000	-0.97035000	-0.94915800
H	-2.48700000	-1.06173400	0.82163300

DMF

C	-0.82436100	-0.69305200	0.02980800
O	-1.92281200	-0.15956000	-0.00014100
N	0.35778100	-0.01700700	0.04989400
H	-0.68783200	-1.79387300	0.04977400
C	0.30484700	1.44090200	-0.00988800
H	-0.71692000	1.78719800	0.58501700
H	1.32323400	1.83662700	0.55013500
H	0.26302300	1.82742800	-1.18465900

C	1.64393000	-0.68792600	-0.04979000
H	2.15089800	-0.44480000	-0.99969300
H	2.31016700	-0.40551900	0.78081800
H	1.48896200	-1.77108400	-0.02030100

Pd (Et₂NH)₂

N	-2.17069300	0.04204200	0.17550600
H	-2.31190700	0.46355900	1.09649800
C	-2.86637400	0.90424300	-0.81240900
C	-2.40831900	2.35657100	-0.73492000
H	-3.95769200	0.84813100	-0.65479700
H	-2.65709100	0.49149500	-1.80421500
H	-2.94993400	2.96230200	-1.47066300
H	-2.60388900	2.77939300	0.25886400
H	-1.33273100	2.42402700	-0.92734200
C	-2.77057100	-1.31504400	0.21896400
C	-2.21015300	-2.15712200	1.36000000
H	-2.56135300	-1.79078000	-0.74426800
H	-3.86752800	-1.23634700	0.31682500
H	-2.67900500	-3.14795200	1.36305000
H	-1.12600400	-2.26550700	1.25148700
H	-2.40894000	-1.68719300	2.33164500
Pd	0.00000100	0.04907200	-0.00000900
N	2.17072400	0.04216500	-0.17555300
H	2.31191100	0.46378400	-1.09650000
C	2.86611100	0.90447100	0.81249300
C	2.40790500	2.35674300	0.73490500
H	3.95747000	0.84849700	0.65508200
H	2.65669600	0.49168600	1.80425000
H	2.94934100	2.96253000	1.47073500
H	2.60359900	2.77958300	-0.25884700
H	1.33227600	2.42409200	0.92714200
C	2.77091100	-1.31475000	-0.21903100
C	2.21046800	-2.15700400	-1.35992500
H	2.56197500	-1.79049800	0.74426000
H	3.86783400	-1.23580500	-0.31708000
H	2.67955000	-3.14772500	-1.36304100
H	1.12636500	-2.26562400	-1.25118500
H	2.40893700	-1.68705600	-2.33162700

Pd (DMF)₂

C	2.99438700	-0.95096200	-0.22436100
O	1.82458900	-1.10212600	-0.58406800
N	3.53640600	0.08756600	0.45359500

H	3.73093900	-1.73626300	-0.45928300
C	2.77281900	1.25219300	0.88275000
H	1.72550900	1.14640900	0.56178800
H	2.81210500	1.34105200	1.97583700
H	3.19871400	2.16035400	0.43817700
C	4.95023400	0.08836100	0.79037300
H	5.45357100	0.95169900	0.33649500
H	5.08714000	0.14289700	1.87807900
H	5.42725800	-0.82527300	0.42424600
Pd	0.00007300	-0.00070100	-0.53676300
C	-2.99413400	0.95080400	-0.22603200
O	-1.82442300	1.10066100	-0.58652800
N	-3.53638300	-0.08607600	0.45427800
H	-3.73039600	1.73605500	-0.46203400
C	-2.77340900	-1.25068300	0.88457500
H	-1.72567300	-1.14495700	0.56506200
H	-2.81433000	-1.33937800	1.97760000
H	-3.19858000	-2.15896700	0.43951400
C	-4.95034800	-0.08608700	0.79045800
H	-5.45399200	-0.94932000	0.33668200
H	-5.08764700	-0.14020900	1.87812300
H	-5.42677700	0.82768900	0.42391000
Et₂NH₂⁺			
H	-0.00015700	-0.88560100	-0.81694300
N	-0.00002700	-0.26157400	-0.00014500
C	1.28530000	0.55098700	-0.00011200
C	-1.28531000	0.55106900	0.00011800
H	0.00006100	-0.88589600	0.81642600
H	1.24097800	1.18732800	0.88734500
H	1.24118000	1.18707000	-0.88777900
H	-1.24114000	1.18751000	-0.88727600
H	-1.24115900	1.18703200	0.88786200
C	-2.50515100	-0.35873100	0.00000900
H	-2.54009700	-0.99390500	0.89209800
H	-3.40710000	0.26005800	0.00036600
H	-2.54046000	-0.99337100	-0.89245200
C	2.50518400	-0.35870700	0.00012100
H	2.54058200	-0.99363600	-0.89211000
H	3.40701600	0.26029600	0.00025000
H	2.54034200	-0.99357100	0.89241300
Pd (BINAP)			
P	0.59886400	-1.62665800	-0.12980200

P	0.59896900	1.62667400	0.12976200
C	-1.50637300	5.35347000	1.99524800
C	-0.86465700	5.46815000	0.76681000
C	-0.17775300	4.38138300	0.22440000
C	-0.12264200	3.15590300	0.89774700
C	-0.79651300	3.04974700	2.12591700
C	-1.46839100	4.13681700	2.67522400
H	0.30738700	4.50273300	-0.73784900
H	-0.81282300	2.09867400	2.64969500
C	-1.50719200	-5.35320600	-1.99498500
C	-0.86548200	-5.46790700	-0.76654400
C	-0.17833000	-4.38124000	-0.22424800
C	-0.12294700	-3.15584000	-0.89771800
C	-0.79681900	-3.04965700	-2.12588800
C	-1.46894900	-4.13663000	-2.67508200
H	0.30678600	-4.50259900	0.73801200
H	-0.81295700	-2.09862800	-2.64974900
C	2.82272700	-3.34663200	3.57483200
C	3.16703100	-3.77034400	2.29153100
C	2.49643600	-3.25868300	1.18609600
C	1.45909300	-2.33141000	1.34632800
C	1.10754800	-1.93092500	2.63559400
C	1.79012700	-2.42858900	3.74449600
H	2.78873300	-3.57920100	0.18877300
H	0.31045900	-1.20441800	2.76504500
C	2.82301700	3.34649300	-3.57485900
C	3.16734200	3.77017700	-2.29155500
C	2.49668600	3.25857600	-1.18613200
C	1.45926300	2.33139600	-1.34636600
C	1.10768400	1.93095500	-2.63564200
C	1.79033000	2.42854700	-3.74453300
H	2.78900600	3.57904500	-0.18879800
H	0.31053200	1.20452200	-2.76510800
H	6.75320400	-2.29711600	1.67860600
C	3.00609500	0.25491700	0.70675000
C	2.07139100	1.17254700	1.17216700
C	2.16291200	1.63955200	2.50965900
H	1.45204500	2.37272500	2.87201900
C	3.13608000	1.19337100	3.36079900
H	3.18427500	1.56566400	4.38110900
C	4.10089300	0.25380600	2.92391900
C	4.04526000	-0.21425900	1.58281700
H	5.00325000	-1.54229400	0.15435800
C	5.03252600	-1.15092100	1.16495800

C	6.01286300	-1.58059900	2.02286400
H	6.83557600	-1.46722200	4.02797900
C	6.05823100	-1.11333500	3.35679500
H	5.13603300	0.14922000	4.81933800
C	5.11772500	-0.21816700	3.79627600
H	6.83572400	1.46676600	-4.02798100
C	3.13608700	-1.19364000	-3.36079600
H	3.18430200	-1.56599500	-4.38108300
C	2.16287400	-1.63973000	-2.50966300
H	1.45198200	-2.37287900	-2.87201600
C	2.07132800	-1.17265600	-1.17219500
C	3.00609300	-0.25507300	-0.70679100
C	4.04527500	0.21403500	-1.58286300
C	4.10092700	-0.25409200	-2.92394000
H	5.13614300	-0.14964600	-4.81932700
C	5.11780700	0.21779700	-3.79628500
C	6.05832900	1.11295300	-3.35681400
H	6.75326900	2.29682900	-1.67867800
C	6.01292600	1.58030100	-2.02291400
H	5.00323400	1.54212800	-0.15444000
C	5.03254500	1.15070200	-1.16501900
H	-2.03894000	6.20084600	2.41760000
H	-2.03996600	-6.20050500	-2.41722900
H	3.35999700	-3.73090600	4.43741300
H	3.36033100	3.73072600	-4.43743100
H	-0.89534900	6.40645800	0.21993300
H	-1.97373700	4.02775300	3.63083500
H	-0.89637600	-6.40616000	-0.21958400
H	-1.97429200	-4.02754200	-3.63069100
H	1.51804600	2.09088800	-4.74085800
H	3.97435300	4.48373700	-2.15113000
H	1.51785700	-2.09091100	4.74081700
H	3.97397600	-4.48398000	2.15111500
Pd	-0.96158300	0.00006000	-0.00001700

OTf⁻

O	-10.99025166	9.85821716	4.52273628
S	-11.03590666	9.04464316	3.29247028
O	-9.88044866	8.13324516	3.09347628
O	-12.34731266	8.44893216	2.93847428
C	-10.76090266	10.28469116	1.93122428
F	-10.86683166	9.68401216	0.71673028
F	-11.64476166	11.29021916	1.96489628
F	-9.52032066	10.81388216	2.00435228

HOTf

O	-1.27473100	-0.71859200	-1.27052900
S	-0.85366500	-0.14825100	-0.00049600
O	-1.27775100	-0.71541900	1.27060900
C	1.01062100	-0.00099700	0.00000400
F	1.41085800	0.64486100	1.08993300
F	1.49800900	-1.24003200	0.00005700
F	1.41086800	0.64477200	-1.08997400
O	-1.09984000	1.47124700	-0.00160300
H	-2.06413200	1.63369400	0.04996200

1

C	1.76777200	-2.62640400	-1.32347900
C	1.44032500	-1.45743800	-0.64185400
C	0.13383800	-1.02167300	-0.37595600
C	-0.89001400	-1.93890700	-0.76662600
C	-0.57514700	-3.14794300	-1.42317500
C	0.74020400	-3.47927800	-1.71638800
Si	-0.22723900	0.70334600	0.41787600
C	-1.72958300	1.46874600	-0.45241900
C	-2.45842300	2.50532600	0.15915700
C	-2.06764500	1.14154400	-1.77893700
C	-3.09382200	1.80193300	-2.45615500
C	-3.80967200	2.82024600	-1.82305600
C	-3.48550100	3.17403500	-0.51235000
H	2.80408000	-2.86540500	-1.52233200
H	-1.38615300	-3.81368400	-1.69993400
H	0.97154900	-4.40198100	-2.23977200
H	-2.22402400	2.81018800	1.17367300
H	-1.53017600	0.34899300	-2.29226600
H	-3.33724800	1.51783900	-3.47662600
H	-4.61103200	3.33391500	-2.34752900
H	-4.03107100	3.96896300	-0.01003100
O	3.64461600	-2.55689100	0.95547500
S	3.72142600	-1.12357000	0.72151000
O	3.90760200	-0.17053300	1.80095100
O	2.49707500	-0.60411100	-0.23365500
C	5.07920500	-0.79152400	-0.51794800
F	5.07672000	0.49274300	-0.85210700
F	4.88197900	-1.54355100	-1.60535400
F	6.24337400	-1.11653400	0.04247400
C	1.17869900	1.90669400	-0.00185400
C	2.23378500	2.22091500	0.87259000

C	1.20531700	2.49170800	-1.28210800
C	3.27769600	3.06067500	0.48420000
H	2.27607700	1.77827900	1.85978000
C	2.24857800	3.33015300	-1.67959400
H	0.39911400	2.29583500	-1.98410900
C	3.29099000	3.61606000	-0.79662600
H	4.08521500	3.27021500	1.18078500
H	2.24421800	3.76162000	-2.67756400
H	4.10565000	4.26748000	-1.10292500
C	-0.48400300	0.43593700	2.31407800
C	0.62071400	-0.50360300	2.85300000
C	-0.43971900	1.75814100	3.11423300
C	-1.85199600	-0.23742100	2.56575500
H	0.63031100	-1.46623200	2.32815300
H	1.62228000	-0.07156700	2.77632100
H	0.43890400	-0.71443800	3.91643800
H	-1.28585600	2.41254300	2.88076200
H	-0.49884700	1.53505300	4.18920400
H	0.47627400	2.33078000	2.94579600
H	-2.00597700	-0.36275300	3.64729600
H	-2.68607900	0.35670500	2.17618000
H	-1.91282300	-1.22807400	2.10631200
C	-2.27038200	-1.70921000	-0.50212600
C	-3.46298300	-1.59067900	-0.30192800
C	-4.84208300	-1.34611600	-0.05294800
C	-5.77113200	-2.40415100	-0.00832400
C	-5.29076500	-0.02484100	0.14843100
C	-7.11732700	-2.14365300	0.23568300
H	-5.42514600	-3.42162700	-0.16363900
C	-6.63918100	0.22352000	0.38999900
H	-4.57650000	0.78877700	0.10502100
C	-7.55568400	-0.83118700	0.43551700
H	-7.82679100	-2.96596800	0.27027800
H	-6.97578300	1.24564600	0.54130200
H	-8.60699500	-0.63210700	0.62498800

INT1

C	1.85332800	0.25503000	-1.86398400
C	1.11240400	0.60547500	-0.68025800
C	-0.29083300	0.30963600	-0.56633100
C	-0.90390300	-0.27392300	-1.69749500
C	-0.18128300	-0.56382100	-2.89343400
C	1.16459900	-0.30907300	-2.97326600
Si	-1.37851200	0.51357300	1.00095200

C	-2.69876000	1.81115400	0.60584800
C	-2.52771200	2.66709000	-0.49891200
C	-3.84928300	1.99888100	1.39593700
C	-4.78898200	2.98761800	1.09566200
C	-4.59763000	3.82187000	-0.00728100
C	-3.46124500	3.65918400	-0.80340100
H	2.80331600	0.74775300	-2.04588500
H	-0.72492900	-0.97236900	-3.73911800
H	1.71078100	-0.49171600	-3.89504500
H	-1.65828700	2.55382800	-1.14081400
H	-4.02898100	1.36455500	2.25838400
H	-5.67078500	3.10204700	1.72122300
H	-5.32657800	4.59284500	-0.24394600
H	-3.29939800	4.30436900	-1.66296000
O	1.06621400	3.13094600	-2.02241400
S	1.47969400	3.23242000	-0.62969800
O	0.86690100	4.17993100	0.28701000
O	1.58621200	1.76046200	0.07901700
C	3.31415100	3.59584100	-0.59917100
F	3.76192000	3.54629000	0.65626600
F	3.97915000	2.69571900	-1.33649900
F	3.52029200	4.81199100	-1.10268100
C	-2.08574200	-1.23194400	1.26654400
C	-1.20019100	-2.32477800	1.21853700
C	-3.44065700	-1.50831800	1.51207500
C	-1.64196000	-3.63355000	1.41735700
H	-0.15034400	-2.15135100	0.99153400
C	-3.89269200	-2.81560200	1.70510600
H	-4.16877000	-0.70348800	1.50836000
C	-2.99379200	-3.88347000	1.66371100
H	-0.93299500	-4.45743300	1.36888900
H	-4.95138800	-2.99886500	1.87029700
H	-3.34538800	-4.90156000	1.81193400
C	-0.55131000	0.97947400	2.69242900
C	0.64172100	0.05243000	2.97725200
C	-1.60953600	0.75595600	3.80170100
C	-0.09014800	2.44610700	2.77962300
H	1.40118000	0.12050900	2.19248900
H	0.32636800	-0.99408800	3.05302600
H	1.11185500	0.32667600	3.93455500
H	-2.43149900	1.47593600	3.72942700
H	-1.13875400	0.90698900	4.78398900
H	-2.03215500	-0.25432700	3.78823500
H	0.17066700	2.68662100	3.82127300

H	-0.87084000	3.14557400	2.46215400
H	0.79044800	2.63373300	2.16875300
C	-2.30299100	-0.54372200	-1.70526400
C	-3.50438200	-0.72471200	-1.69587400
C	-4.91308100	-0.84933600	-1.53197400
C	-5.67598500	0.29343400	-1.21623600
C	-5.55179900	-2.10086000	-1.61936600
C	-7.04566100	0.17770200	-0.99189400
H	-5.18091100	1.25530400	-1.13983100
C	-6.92302000	-2.20474000	-1.39578800
H	-4.95905100	-2.98195100	-1.84454000
C	-7.67385400	-1.06810900	-1.08101600
H	-7.62291000	1.06409300	-0.74236200
H	-7.40699000	-3.17568200	-1.46184400
H	-8.74270900	-1.15388300	-0.90387500
N	3.06114100	-3.22892000	-1.09865100
H	2.93598700	-3.86831900	-0.31505800
C	4.48740400	-3.26665100	-1.48361600
C	4.87628600	-2.14170400	-2.44082900
H	5.07564900	-3.17388100	-0.56172900
H	4.74653600	-4.24205800	-1.93112400
H	4.65958800	-1.16807000	-1.98979500
H	4.32663100	-2.20789100	-3.38527100
H	5.94603200	-2.19782200	-2.67140900
C	2.14934200	-3.67960300	-2.17345000
C	0.72581000	-3.85916200	-1.65677900
H	2.15309200	-2.91980600	-2.95960600
H	2.51690400	-4.62166500	-2.61724100
H	0.07605000	-4.22936000	-2.45670000
H	0.31828600	-2.90987200	-1.29845500
H	0.68768200	-4.58436700	-0.83328900
Pd	2.28813200	-1.09994900	-0.24816600
N	3.64603800	-1.55237700	1.76586000
H	4.35358900	-2.09686500	1.26992900
C	3.14193400	-2.38553100	2.87467200
C	2.48783200	-3.66977500	2.37649400
H	3.95463000	-2.62927300	3.58141100
H	2.41092300	-1.79011600	3.42583800
H	2.10002200	-4.25318900	3.21814800
H	3.21065600	-4.30394100	1.84460300
H	1.65521500	-3.44350300	1.70277600
C	4.30510700	-0.32156700	2.25622300
C	4.98263400	0.44777800	1.12774500
H	3.53217200	0.29968900	2.71813200

H	5.04108100	-0.56467000	3.04251000
H	5.45133600	1.35848200	1.51501200
H	4.25019300	0.73195500	0.36717900
H	5.76291200	-0.15660100	0.64638800
TS1			
C	1.60603000	0.49750600	-2.21471500
C	1.00128800	0.41329700	-0.94571100
C	-0.37738100	0.29995000	-0.70086400
C	-1.14588800	0.00382500	-1.87749100
C	-0.55144100	-0.02743800	-3.15299700
C	0.80854800	0.23142700	-3.32044800
Si	-1.35048500	0.46964900	0.95453100
C	-2.61351400	1.84565400	0.64893000
C	-2.34535600	2.83211300	-0.31935600
C	-3.78205300	1.99543100	1.41918400
C	-4.65425100	3.06850200	1.22137100
C	-4.37353600	4.02677600	0.24605900
C	-3.21238400	3.90669400	-0.52179400
H	2.64744500	0.76601500	-2.31297500
H	-1.18410600	-0.21460100	-4.01429200
H	1.24469800	0.24912700	-4.31545500
H	-1.44758500	2.76422600	-0.92863600
H	-4.02782500	1.26870500	2.18754600
H	-5.55315100	3.15154200	1.82717800
H	-5.04923200	4.86388800	0.08999200
H	-2.97731300	4.65237400	-1.27669600
O	1.81381400	3.35599100	-1.72282200
S	2.20789500	3.13098300	-0.33112600
O	2.01170800	4.18784100	0.65956800
O	1.74741000	1.76238000	0.22246000
C	4.05268100	2.85880100	-0.37086400
F	4.52395500	2.66292700	0.86872300
F	4.35524500	1.76331700	-1.10461800
F	4.66925300	3.91109900	-0.91002700
C	-2.13024300	-1.24785600	1.18549600
C	-1.28424900	-2.37073800	1.24025700
C	-3.51074100	-1.47447700	1.31278400
C	-1.78782500	-3.65905800	1.42725500
H	-0.21118100	-2.23881600	1.10832200
C	-4.02479500	-2.75996200	1.49418300
H	-4.20657200	-0.64732500	1.22831000
C	-3.16421200	-3.85731500	1.55747600
H	-1.10989000	-4.50814600	1.45843500

H	-5.09995300	-2.90140300	1.56848400
H	-3.56231200	-4.85937900	1.69639000
C	-0.47183500	0.92353500	2.62764000
C	0.83563500	0.15530900	2.87447900
C	-1.45905100	0.53274100	3.75815300
C	-0.20987800	2.44062600	2.73522000
H	1.59856600	0.40661700	2.12640900
H	0.67350300	-0.92832800	2.87927500
H	1.25128800	0.42541700	3.85755800
H	-2.40987000	1.07070500	3.67920900
H	-1.01957500	0.80453000	4.72849700
H	-1.67491400	-0.54076800	3.77537000
H	0.23413600	2.66500000	3.71639700
H	-1.13925000	3.01398800	2.65637700
H	0.47807300	2.80387700	1.97314900
C	-2.55385700	-0.20388200	-1.80226000
C	-3.75682300	-0.35484100	-1.73347200
C	-5.16126900	-0.45784500	-1.52088100
C	-5.90202500	0.69789100	-1.20150600
C	-5.81352800	-1.70471400	-1.56766900
C	-7.26607900	0.59991600	-0.93657400
H	-5.39365100	1.65468400	-1.14979700
C	-7.17870300	-1.79048300	-1.30289000
H	-5.23625200	-2.59507200	-1.79601300
C	-7.90851800	-0.64061800	-0.98700600
H	-7.82815300	1.49548300	-0.68561500
H	-7.67417800	-2.75706100	-1.33928200
H	-8.97266100	-0.71197400	-0.77854300
N	3.00130300	-2.88104500	-1.65347100
H	2.83868800	-3.72404200	-1.10783700
C	4.44307800	-2.75951800	-1.91386700
C	4.85346600	-1.33653100	-2.28737500
H	4.97245000	-3.05189000	-0.99649500
H	4.77211600	-3.46188100	-2.70152900
H	4.60905500	-0.64174600	-1.47912900
H	4.34000900	-0.99513900	-3.19228600
H	5.93158800	-1.28732100	-2.47776800
C	2.17086400	-2.97334700	-2.86088600
C	0.71774800	-3.26645500	-2.49874000
H	2.22706300	-2.01756200	-3.38812100
H	2.55425500	-3.74804200	-3.55092100
H	0.09966400	-3.32234200	-3.40028400
H	0.31049900	-2.48053500	-1.85560100
H	0.62599700	-4.22457000	-1.97020400

Pd	1.96768300	-0.91682500	0.12792600
N	3.16896900	-2.33406500	1.60431900
H	3.82144600	-2.77484200	0.95490400
C	2.42001000	-3.40686300	2.29441000
C	1.85722300	-4.43400400	1.31802900
H	3.06518000	-3.91361200	3.03134700
H	1.60579900	-2.93371800	2.85254200
H	1.27755100	-5.18986300	1.85743200
H	2.66378300	-4.95925100	0.78862500
H	1.20403700	-3.96157200	0.57843400
C	3.96936800	-1.52196600	2.55065400
C	4.77436400	-0.44855700	1.82664800
H	3.27026800	-1.05862000	3.25363100
H	4.63861300	-2.17191500	3.13843600
H	5.39098000	0.11083800	2.53788400
H	4.11933100	0.26662400	1.31995200
H	5.44195000	-0.89034200	1.07591900

INT2

C	1.20984900	0.76720500	-2.32453800
C	0.73742000	0.32819600	-1.07892200
C	-0.63514700	0.36736200	-0.74873100
C	-1.51888900	0.55987100	-1.86940100
C	-1.03732000	0.90167400	-3.14586100
C	0.32535400	1.07579400	-3.35413100
Si	-1.46061200	0.45364900	1.01208000
C	-2.83736300	1.75958700	0.88012800
C	-2.67658900	2.91706300	0.09524600
C	-3.99453200	1.67372900	1.67504700
C	-4.95446100	2.68907300	1.67996000
C	-4.77728800	3.82311700	0.88543300
C	-3.63214300	3.93375800	0.09187500
H	2.27396500	0.86708700	-2.49339300
H	-1.74977800	1.04342500	-3.95249300
H	0.70059700	1.41064200	-4.31769900
H	-1.79644700	3.02402300	-0.53310100
H	-4.15400700	0.80310200	2.30513200
H	-5.84062700	2.59083400	2.30224000
H	-5.52127600	4.61590200	0.88725800
H	-3.48105200	4.81394200	-0.52794700
O	2.50602200	2.91629000	-0.62418000
S	3.48369500	2.32529100	0.29257800
O	4.07103700	3.14065500	1.35556700
O	3.09211300	0.94530900	0.83060200

C	4.91376000	1.90840800	-0.82847700
F	5.93541900	1.37007200	-0.14132500
F	4.53127000	1.00658400	-1.77137600
F	5.35054300	2.99940700	-1.45766100
C	-2.25663000	-1.20197400	1.51739300
C	-1.58052500	-2.15275500	2.30534200
C	-3.53887900	-1.55864600	1.05534300
C	-2.13582200	-3.40143000	2.59395900
H	-0.60031300	-1.92536400	2.70156500
C	-4.10307800	-2.80334800	1.33865200
H	-4.11124900	-0.85529800	0.46642900
C	-3.39930900	-3.73568800	2.10371800
H	-1.58139400	-4.10989200	3.20533600
H	-5.09372600	-3.03874900	0.95726200
H	-3.83433000	-4.70741600	2.32376300
C	-0.33164900	1.16074500	2.41729900
C	0.81363000	0.23250600	2.86835700
C	-1.20574300	1.44245400	3.66310200
C	0.25002400	2.49920700	1.90962400
H	1.30245800	-0.26433200	2.02704500
H	0.45976400	-0.53783500	3.56201400
H	1.58980900	0.81055300	3.38602200
H	-1.98046100	2.18923300	3.46728600
H	-0.56870800	1.82900500	4.47152400
H	-1.69631900	0.53333500	4.03451400
H	0.95099800	2.91178500	2.64791600
H	-0.53961400	3.24160600	1.75326700
H	0.79211800	2.38987100	0.97034500
C	-2.92894900	0.35389000	-1.77506700
C	-4.12416100	0.13453800	-1.79867400
C	-5.52579400	-0.08709800	-1.66164000
C	-6.35051600	0.93115700	-1.14259600
C	-6.09541900	-1.33343100	-1.98828800
C	-7.71232400	0.70123600	-0.96092300
H	-5.90621700	1.88335700	-0.87405600
C	-7.45886200	-1.55271300	-1.80253900
H	-5.45720100	-2.11990500	-2.37985500
C	-8.27103000	-0.53726400	-1.28947600
H	-8.33935500	1.49123000	-0.55628300
H	-7.88868800	-2.51783200	-2.05728200
H	-9.33369800	-0.71169800	-1.14406300
N	1.62346300	-2.54365200	-1.25787300
H	1.54618400	-3.22723400	-0.50295100
C	2.78680800	-2.96753000	-2.09575400

C	3.12242600	-1.99142300	-3.21691700
H	3.65396500	-3.07832000	-1.44144700
H	2.56642500	-3.96050500	-2.51610100
H	3.47281500	-1.03860300	-2.81520700
H	2.25672400	-1.79282200	-3.85531600
H	3.91683100	-2.41659300	-3.83981300
C	0.34134000	-2.63179300	-2.02999100
C	-0.81662500	-3.02046100	-1.12707300
H	0.16212400	-1.66950700	-2.50702200
H	0.46780200	-3.37925100	-2.82565300
H	-1.76135900	-2.96803800	-1.67611000
H	-0.89756700	-2.34053600	-0.28104600
H	-0.70172700	-4.04159400	-0.74075900
Pd	2.15590000	-0.70877500	-0.10896700
N	3.73630500	-2.03958600	1.05552300
H	3.81092700	-2.94870000	0.59458400
C	3.24559100	-2.30720000	2.43014900
C	2.00548300	-3.19470300	2.41266600
H	4.03764600	-2.79238100	3.02186900
H	3.03578600	-1.34222400	2.89775300
H	1.64046100	-3.36398600	3.43073100
H	2.23000700	-4.17773900	1.97535700
H	1.19402300	-2.73868600	1.83947000
C	5.10138200	-1.44939500	1.06119800
C	5.78958700	-1.62417500	-0.28730000
H	4.99664500	-0.39285200	1.30999400
H	5.70525400	-1.92721900	1.84808000
H	6.77502700	-1.15083800	-0.26788800
H	5.21461900	-1.15538100	-1.08794000
H	5.93171300	-2.68690600	-0.52655600

INT3

C	-0.27034800	-2.65558100	-1.75256900
C	-0.08231400	-1.53322000	-0.93558900
C	1.21951000	-1.10368400	-0.58623600
C	2.32011000	-1.90436500	-1.01485400
C	2.10823500	-3.05498800	-1.80146100
C	0.82363600	-3.41234200	-2.18318100
Si	1.39819600	0.51291800	0.40212500
H	-1.26127600	-2.94188900	-2.08251000
H	2.96554400	-3.64205700	-2.11557300
H	0.66449300	-4.28050300	-2.81802000
C	-0.17406500	1.48274800	-0.08443400
C	-0.73035800	2.51215400	0.71770000

C	-0.68805600	1.35680900	-1.41207100
C	-1.73786900	3.33595900	0.24525400
H	-0.36732300	2.66556400	1.72551900
C	-1.71772700	2.20280200	-1.88382600
H	-0.18234100	0.72117800	-2.13297300
C	-2.23989200	3.18211900	-1.05826800
H	-2.15936600	4.09757300	0.89423400
H	-2.08255700	2.08060300	-2.89943900
H	-3.03839800	3.82626300	-1.40857300
C	3.66676300	-1.58299900	-0.68079600
C	4.83084700	-1.34591600	-0.42323800
C	6.16984200	-0.98784500	-0.10152100
C	7.20053300	-1.94834100	-0.11368000
C	6.47606300	0.34734100	0.23159800
C	8.50540000	-1.57932800	0.20385500
H	6.96486800	-2.97660900	-0.37099000
C	7.78434800	0.70485200	0.54610900
H	5.68478200	1.08741900	0.23225800
C	8.80190900	-0.25370100	0.53468900
H	9.29359100	-2.32726300	0.19337500
H	8.01021700	1.73733600	0.79899900
H	9.82139200	0.03023900	0.78121600
Pd	-1.66645700	-0.52311500	-0.22932700
O	-5.32460400	-0.37910000	1.43000300
S	-4.66521900	0.87536000	1.01484400
O	-3.17459200	0.73046000	0.82635600
O	-5.02774600	2.11134100	1.71027500
C	-5.27216300	1.11694600	-0.73789200
F	-5.07410100	2.37427100	-1.15878900
F	-6.57681600	0.84060600	-0.82668700
F	-4.61109800	0.28933100	-1.58341400
C	2.80727000	1.58736200	-0.26119000
C	3.43054600	2.58261600	0.51297700
C	3.18574300	1.48680400	-1.61337000
C	4.39126300	3.43780200	-0.03399600
H	3.17382700	2.70033500	1.56065300
C	4.14978000	2.33079900	-2.16456100
H	2.73386900	0.72437800	-2.24278000
C	4.75640100	3.31094600	-1.37514700
H	4.85641700	4.19704300	0.58962700
H	4.43192800	2.22036800	-3.20827100
H	5.50842000	3.96895700	-1.80233200
C	1.56180800	0.11010200	2.28695400
C	1.31002100	1.29754000	3.24434800

C	0.54423100	-0.99117600	2.65343900
C	2.98994800	-0.43058600	2.53227900
H	1.90370500	2.18644000	3.00940200
H	0.25532900	1.58797400	3.26244000
H	1.57268200	0.99764800	4.26868700
H	0.67158700	-1.88980000	2.03973900
H	0.66910000	-1.28144000	3.70653200
H	-0.48498800	-0.63441800	2.52986600
H	3.10275200	-0.70377900	3.59116500
H	3.20042100	-1.32236400	1.93499100
H	3.76120700	0.31036700	2.29515000
N	-2.66144500	-2.40014800	0.26784400
H	-2.00796900	-3.12520000	-0.03368300
C	-2.79190600	-2.49848800	1.75766500
C	-3.30383200	-3.85030500	2.26151500
H	-3.45096500	-1.68742300	2.07061500
H	-1.79700000	-2.31127600	2.16498200
H	-3.20400400	-3.88337700	3.35175300
H	-4.35895800	-4.01233700	2.02479400
H	-2.71925600	-4.68258000	1.84772400
C	-3.96286300	-2.61034900	-0.43876300
C	-3.84401400	-2.60677000	-1.95759800
H	-4.63354200	-1.82557000	-0.09308600
H	-4.38607300	-3.56879400	-0.11479700
H	-4.84821200	-2.63643500	-2.39255000
H	-3.34949500	-1.70090200	-2.32002500
H	-3.29760800	-3.48174800	-2.32914500

TS2

C	-0.38197800	-1.90539200	-2.59179700
C	-0.16504700	-0.94248400	-1.59618100
C	1.09939500	-0.74747900	-0.99552800
C	2.12267000	-1.67822900	-1.34114200
C	1.87550600	-2.69067600	-2.29193400
C	0.64476800	-2.78536600	-2.93385900
Si	1.42586900	0.78750900	0.11341900
H	-1.34635100	-1.97291100	-3.08115000
H	2.67631500	-3.38217700	-2.53544500
H	0.48428800	-3.54475600	-3.69441000
C	0.02533900	1.98142400	-0.34117200
C	0.17277300	3.37364400	-0.19661200
C	-1.17262800	1.51743300	-0.90393900
C	-0.83874900	4.24636800	-0.59744300
H	1.09149900	3.77960700	0.21881000

C	-2.17617900	2.38217300	-1.35575900
H	-0.82129700	0.33626600	-1.67610700
C	-2.01051500	3.75491300	-1.18291600
H	-0.70780200	5.31757500	-0.46841000
H	-3.08454200	1.99149700	-1.79900200
H	-2.79285300	4.43814400	-1.50150200
C	3.41987200	-1.61190800	-0.75783900
C	4.54115100	-1.55702900	-0.29226600
C	5.83971100	-1.39727600	0.26873300
C	6.66537300	-2.51023200	0.51969100
C	6.30908400	-0.10404100	0.57659500
C	7.93152700	-2.33080900	1.07155200
H	6.30284200	-3.50574700	0.28191600
C	7.57701700	0.06269300	1.12681300
H	5.67599800	0.75196000	0.37450300
C	8.39074400	-1.04622900	1.37701500
H	8.56168600	-3.19464900	1.26446900
H	7.93136400	1.06318100	1.35961800
H	9.37916000	-0.91067100	1.80746200
Pd	-1.83040600	-0.42062000	-0.40120100
O	-5.07733100	-0.97633300	1.65193300
S	-4.53594300	0.39170600	1.53972200
O	-3.06152500	0.43233000	1.18443400
O	-4.88814200	1.36257800	2.57426000
C	-5.32381400	1.03739200	-0.02151100
F	-5.01955300	2.32636800	-0.22614300
F	-6.65173600	0.91119900	0.02917700
F	-4.87843100	0.33379600	-1.09758300
C	3.00773700	1.66330000	-0.44546900
C	3.66831000	2.59194400	0.38114800
C	3.51005300	1.48693800	-1.74802300
C	4.78448300	3.30447300	-0.06589600
H	3.31815000	2.76707100	1.39362500
C	4.62948200	2.18726600	-2.19853500
H	3.02951600	0.78124500	-2.42017200
C	5.27254500	3.09824700	-1.35719600
H	5.27379300	4.01353100	0.59700900
H	5.00194600	2.01976100	-3.20569800
H	6.14542900	3.64343800	-1.70623800
C	1.41679800	0.39316000	2.00391400
C	1.01791900	1.65572000	2.80295300
C	0.36958700	-0.69852000	2.29908000
C	2.79653700	-0.11302100	2.47799100
H	1.72145100	2.48566700	2.67044000

H	0.02140000	2.01373600	2.52393900
H	0.99911400	1.41868100	3.87583600
H	0.58819300	-1.62236800	1.75045400
H	0.37364600	-0.93854600	3.37196600
H	-0.64625300	-0.37346400	2.04578000
H	2.76648400	-0.29806200	3.56117900
H	3.07430200	-1.05074100	1.98738900
H	3.60053600	0.60467800	2.28755400
N	-2.49701900	-2.51838500	-0.06497700
H	-1.80550500	-3.06944700	-0.57847600
C	-2.40377300	-2.89594900	1.37726100
C	-2.60347300	-4.38603800	1.66661300
H	-3.13849100	-2.28803600	1.90752200
H	-1.41174800	-2.59191800	1.71543200
H	-2.37831600	-4.58182200	2.72068700
H	-3.63089400	-4.71484200	1.48564300
H	-1.92886500	-5.00604300	1.06101000
C	-3.83977500	-2.80432500	-0.65003400
C	-3.90609100	-2.52658200	-2.14718000
H	-4.55430300	-2.18600500	-0.10635300
H	-4.10253800	-3.85451100	-0.46993900
H	-4.92155200	-2.72136700	-2.50793200
H	-3.66629500	-1.48228000	-2.37111300
H	-3.22346600	-3.17478300	-2.71049100

INT4

C	-0.40199700	-0.58935500	-3.43221000
C	-0.09660400	0.29686400	-2.37269800
C	0.84877400	-0.03519900	-1.35291900
C	1.52191600	-1.29432700	-1.49848200
C	1.18070200	-2.17115800	-2.54061400
C	0.21460800	-1.82910200	-3.49766400
Si	1.31192100	1.29100300	-0.02255000
H	-1.11340400	-0.28079200	-4.19162000
H	1.71222500	-3.11474000	-2.62126300
H	-0.01586600	-2.52138100	-4.30240100
C	-0.12028200	2.49488000	-0.21137100
C	-0.02273300	3.89743300	-0.16935200
C	-1.39677300	1.92757800	-0.33379500
C	-1.16603400	4.69499200	-0.23289500
H	0.95469800	4.36819600	-0.09644200
C	-2.55016600	2.70759700	-0.39003100
H	-0.44400200	1.32052200	-2.46490900
C	-2.42580100	4.10105100	-0.33799500

H	-1.07587300	5.77762900	-0.20006100
H	-3.53242500	2.25670800	-0.46287300
H	-3.32000200	4.71839500	-0.37753600
C	2.65032200	-1.61138200	-0.69007200
C	3.70550400	-1.82690400	-0.12535800
C	4.95920900	-1.98590400	0.53119900
C	5.36214100	-3.23493400	1.04060400
C	5.81226600	-0.87089000	0.67098800
C	6.59212900	-3.36284300	1.68135900
H	4.70304200	-4.09102800	0.93362100
C	7.03956900	-1.01192000	1.31272500
H	5.50078100	0.08936100	0.27106400
C	7.43226600	-2.25427400	1.81980200
H	6.89532100	-4.32860600	2.07582100
H	7.69138400	-0.14923300	1.41832300
H	8.39007400	-2.35843300	2.32195300
Pd	-1.58958200	-0.06005300	-0.54928900
O	-4.06655400	-1.96723500	1.59479100
S	-3.93006300	-0.52707800	1.87396900
O	-2.64060100	0.08598000	1.34170200
O	-4.24226400	-0.04381400	3.21694500
C	-5.20455600	0.25113100	0.75923500
F	-5.31015300	1.56701900	0.98416600
F	-6.39944300	-0.31600500	0.93689000
F	-4.84786100	0.08209200	-0.54083900
C	2.95189700	2.07514500	-0.53563900
C	3.46873100	3.17559000	0.17686500
C	3.71417900	1.58132000	-1.60893800
C	4.69337500	3.75268200	-0.16174900
H	2.91498100	3.58619400	1.01838000
C	4.94433100	2.14966600	-1.94968600
H	3.35318200	0.73461900	-2.18588600
C	5.43797800	3.23620300	-1.22505800
H	5.06826200	4.60025500	0.40612900
H	5.51601200	1.74300800	-2.78003900
H	6.39474600	3.67964600	-1.48815300
C	1.37173900	0.69792600	1.83712300
C	0.58260600	1.72371600	2.68760600
C	0.72243000	-0.68467900	2.04861300
C	2.82180800	0.63937800	2.36325000
H	0.96730900	2.74548500	2.57626500
H	-0.48082500	1.73489000	2.43057300
H	0.66795000	1.45334600	3.74921400
H	1.24132600	-1.47032300	1.49108300

H	0.77389900	-0.95013800	3.11427600
H	-0.33625500	-0.68756100	1.77545400
H	2.81326600	0.30998000	3.41166300
H	3.43680300	-0.06716600	1.80280200
H	3.32090400	1.61259900	2.33077400
N	-1.86527200	-2.29607700	-0.92955900
H	-1.22340400	-2.46977500	-1.70343200
C	-1.38588100	-3.10837200	0.22321700
C	-1.25105300	-4.60729600	-0.05964900
H	-2.06863900	-2.92085700	1.05325900
H	-0.40797900	-2.70571200	0.49709500
H	-0.77890000	-5.09956900	0.79772700
H	-2.21819900	-5.09170300	-0.22417900
H	-0.61922800	-4.78979000	-0.93952200
C	-3.23058200	-2.65610300	-1.39908400
C	-3.61196000	-1.89509100	-2.66570400
H	-3.91823200	-2.42984600	-0.58434100
H	-3.29048900	-3.73496800	-1.59625600
H	-4.62489300	-2.17471500	-2.97414900
H	-3.59715500	-0.81306400	-2.50146500
H	-2.93050500	-2.12513300	-3.49376700

INT5

C	1.38295900	-0.27829400	-1.60137800
C	1.86641700	-0.74722900	-2.84968500
C	-0.00672200	-0.26992800	-1.42612100
C	1.01522700	-1.11238700	-3.88801500
H	2.93802900	-0.84524500	-3.00181100
C	-0.87216600	-0.62915400	-2.46782400
C	-0.36556800	-1.03546900	-3.70228600
H	1.42691500	-1.46335600	-4.83048400
H	-1.94509200	-0.62683100	-2.31558700
H	-1.04895400	-1.31957700	-4.49871300
C	2.37124600	0.75791000	1.35237600
C	1.27626100	1.56894100	1.74699700
C	3.33867000	0.48213600	2.33216500
C	1.21194000	2.13294700	3.03522800
C	3.25940300	1.01125200	3.62311300
C	2.20643800	1.85968300	3.96933600
H	0.37113100	2.76990500	3.29343600
H	4.02818300	0.77149800	4.35251600
H	2.15120600	2.29441800	4.96321300
C	0.17101000	1.78092600	0.86231900
C	-0.75798500	2.15044000	0.12120300

H	4.18374200	-0.15089600	2.07838900
Pd	-0.94343600	-0.03486600	0.33327500
O	-2.38921900	-4.39726500	0.28915200
S	-2.57771800	-2.96072600	0.46243400
O	-3.29565800	-2.49202200	1.67104400
O	-1.31655500	-2.16364800	0.17298600
C	-3.69635700	-2.42738700	-0.92620400
F	-4.91267400	-2.95639900	-0.77992400
F	-3.81935700	-1.07632900	-0.91974500
F	-3.20108300	-2.79142400	-2.11415800
Si	2.77628600	0.29492700	-0.45189000
C	-1.65348900	3.00087200	-0.61263900
C	-2.19258900	4.13246000	0.02892000
C	-2.00522900	2.72288400	-1.94524000
C	-3.06843800	4.97040000	-0.65634200
H	-1.92149800	4.33998400	1.05960800
C	-2.87987200	3.56988400	-2.62124600
H	-1.58794400	1.84921000	-2.43255500
C	-3.41583900	4.69098100	-1.98110900
H	-3.48221500	5.84085600	-0.15518100
H	-3.14658900	3.35120800	-3.65125600
H	-4.10295600	5.34394300	-2.51173000
C	3.97296800	-1.16635200	-0.35933200
C	5.37449600	-1.05551800	-0.31571400
C	3.41705900	-2.45859600	-0.26819000
C	6.18909100	-2.18373000	-0.18907000
H	5.84733000	-0.08039500	-0.38358900
C	4.22547200	-3.58811700	-0.13534700
H	2.33754800	-2.58595300	-0.31171700
C	5.61534700	-3.45287100	-0.09696100
H	7.27001800	-2.07031400	-0.16385700
H	3.76995600	-4.57247200	-0.06682200
H	6.24726800	-4.33172700	0.00187800
C	3.55919700	1.91024600	-1.19535100
C	4.55428400	2.55768000	-0.20571900
H	4.97162000	3.47406700	-0.64715500
H	4.07182200	2.83479000	0.73739400
H	5.39864900	1.90331600	0.03779500
C	4.28969800	1.62040800	-2.52498000
H	3.59471400	1.29362000	-3.30476200
H	4.77578900	2.53768100	-2.88753800
H	5.06570000	0.85387500	-2.42125800
C	2.43292700	2.93103900	-1.47566600
H	1.66867500	2.52541500	-2.14792400

H	1.93314500	3.25307100	-0.55580400
H	2.85472400	3.82947800	-1.94900900
N	-2.13242000	0.04128500	2.28010700
H	-2.69655500	-0.80617300	2.14211300
C	-1.34969900	-0.17234000	3.52042400
C	-0.38694400	-1.35034400	3.40548300
H	-2.04481100	-0.33579500	4.35911700
H	-0.79880100	0.74764100	3.73393400
H	0.09544700	-1.53090700	4.37223800
H	-0.91932300	-2.25710800	3.10463100
H	0.39764400	-1.15382200	2.66770500
C	-3.05247000	1.19227400	2.39691600
C	-4.10511900	1.19250600	1.29174600
H	-2.45204100	2.10948900	2.35838000
H	-3.54814900	1.17152600	3.38047900
H	-4.78632500	2.04004600	1.42174000
H	-3.64653300	1.27691700	0.30298100
H	-4.69124000	0.26801100	1.31349100

TS3

C	-1.52958900	0.94301300	-1.55937200
C	-1.82475100	1.75580700	-2.66972600
C	-0.44651400	0.06322500	-1.71210800
C	-1.10953100	1.66592100	-3.86624700
H	-2.63471700	2.47271800	-2.61087100
C	0.21795200	-0.11381800	-2.92807500
C	-0.10246300	0.71291100	-4.00805200
H	-1.36310900	2.32067000	-4.69546800
H	0.99802200	-0.86265700	-3.03049500
H	0.43371400	0.60899800	-4.94767200
C	-3.21250700	-1.10924600	-0.32605800
C	-2.23196300	-2.09509700	-0.59747700
C	-4.54701200	-1.54328400	-0.26317000
C	-2.60039600	-3.43798100	-0.81896500
C	-4.91443700	-2.87307500	-0.47608600
C	-3.93487900	-3.82437100	-0.76217300
H	-1.82661000	-4.17206600	-1.02555100
H	-5.96065900	-3.16147200	-0.42196900
H	-4.20519500	-4.86195700	-0.93804400
H	-5.33058200	-0.82812600	-0.04368600
Pd	0.87068500	-0.44030700	-0.20910500
O	1.24220400	1.76433800	-0.15269500
S	2.18288800	2.69191800	0.57689300
O	3.27249100	1.97599100	1.28731500

O	1.51202200	3.77345200	1.30528100
C	3.02854600	3.52500000	-0.85592800
F	3.60906300	2.60680200	-1.65112700
F	3.97214700	4.36449800	-0.41624600
F	2.13869200	4.20974500	-1.58297200
Si	-2.70514300	0.71127300	-0.09131100
C	-0.79769200	-1.86276900	-0.59382400
C	0.34720500	-2.40680600	-0.45532700
C	1.11268000	-3.62493400	-0.29618000
C	0.77982600	-4.52762800	0.73071900
C	2.17390300	-3.93055800	-1.16472000
C	1.49976700	-5.71181800	0.88140000
H	-0.03920100	-4.28657300	1.40177600
C	2.88550500	-5.11925100	-1.01143300
H	2.43376800	-3.22800000	-1.95083000
C	2.55326200	-6.01035100	0.01277500
H	1.23862300	-6.40145100	1.67922200
H	3.70270500	-5.34817500	-1.68961000
H	3.11321000	-6.93328300	0.13372300
N	2.67454000	-0.79837000	1.04976300
H	2.89492400	0.18111000	1.27624200
C	3.86070700	-1.33930700	0.34149000
C	4.13069500	-0.62046500	-0.97511400
H	4.73596800	-1.24474300	1.00207500
H	3.69505300	-2.40727200	0.17498500
H	5.05059000	-1.00529600	-1.42974800
H	4.24321200	0.45462400	-0.81858500
H	3.30862900	-0.77214300	-1.68489800
C	2.43395700	-1.51496700	2.32521300
C	1.37221400	-0.82050900	3.16585500
H	2.13635200	-2.54048700	2.08279900
H	3.38060400	-1.57418000	2.88463300
H	1.24321800	-1.34138100	4.12078500
H	0.40480300	-0.80111300	2.65628200
H	1.65408600	0.21535200	3.37791700
C	-4.20037600	1.93629000	-0.11929000
C	-5.05665700	1.74137400	1.15658300
C	-3.64427000	3.38116300	-0.06685900
C	-5.11311300	1.78278400	-1.35650000
H	-5.51663000	0.74917300	1.21847300
H	-4.46697100	1.88698400	2.06709500
H	-5.87320300	2.47746000	1.16562600
H	-3.01928900	3.63481700	-0.92869600
H	-4.47858200	4.09681300	-0.04445100

H	-3.04501900	3.54860000	0.83451100
H	-5.92982000	2.51733200	-1.30695800
H	-4.58314700	1.94939700	-2.29858900
H	-5.57047400	0.79035600	-1.41843300
C	-1.91094100	0.87885200	1.60451200
C	-1.05600600	1.95413800	1.90349300
C	-2.30282100	0.03089500	2.65826400
C	-0.60878900	2.18071000	3.20640600
H	-0.71307200	2.61471700	1.11702400
C	-1.87105300	0.26248800	3.96591500
H	-2.95942400	-0.81324200	2.45761800
C	-1.02566900	1.34096300	4.24163700
H	0.07275200	3.00528400	3.39092000
H	-2.18909300	-0.40019800	4.76723400
H	-0.68453100	1.51817400	5.25859700

INT6

C	1.11521800	-1.73146400	-1.33889900
C	0.36252100	-2.77520700	-1.86663200
C	0.82384600	-0.40865500	-1.79143700
C	-0.66346900	-2.55752600	-2.80741100
H	0.54842000	-3.79405000	-1.54592200
C	-0.16844600	-0.19556000	-2.78645300
C	-0.92121500	-1.28334700	-3.27574900
H	-1.24186500	-3.40123200	-3.17213800
H	-0.23401700	0.77198700	-3.27646000
H	-1.69030600	-1.10953200	-4.02194600
C	3.65410600	-0.43150000	-0.62460000
C	3.04912700	0.73730300	-1.15736200
C	5.05499700	-0.45472100	-0.53219300
C	3.83285600	1.83169200	-1.54838500
C	5.83472700	0.63350000	-0.93022700
C	5.22057200	1.78181000	-1.43272600
H	3.34694500	2.71693300	-1.94754500
H	6.91715800	0.58390700	-0.84649500
H	5.82036800	2.63325400	-1.74324900
H	5.55814800	-1.33357800	-0.14392500
Pd	-1.01335800	0.79598600	-0.76687300
O	-2.67441000	-0.68899400	-0.72320600
S	-3.26956100	-1.24379800	0.55173800
O	-3.46772500	-0.19549000	1.58451900
O	-2.69641800	-2.51802600	0.99919400
C	-4.98884500	-1.63978400	-0.03644900
F	-5.60233200	-0.51429200	-0.44620300

F	-5.70546700	-2.17750000	0.95576400
F	-4.94723300	-2.49968200	-1.06060400
Si	2.47980900	-1.79816400	-0.03200600
C	1.57280800	0.78242600	-1.27357100
C	0.73801300	1.75097500	-0.84407400
C	1.04997300	3.04822600	-0.24686100
C	1.80090500	3.12523800	0.94050900
C	0.57281100	4.23555300	-0.82921700
C	2.05613000	4.36079400	1.53208300
H	2.16283900	2.20847300	1.39566600
C	0.83745100	5.47095200	-0.23842600
H	-0.00743200	4.17604500	-1.74624500
C	1.57444900	5.53622100	0.94750300
H	2.63015100	4.40712700	2.45366500
H	0.46515900	6.38169800	-0.69983400
H	1.77286300	6.49763000	1.41317800
N	-2.20969600	2.13424600	0.44146700
H	-2.84845800	1.41463500	0.80918300
C	-2.99466200	3.08839000	-0.38359100
C	-3.76578700	2.40757800	-1.51088000
H	-3.69637200	3.61783300	0.27853400
H	-2.29431600	3.83292700	-0.77616000
H	-4.41269300	3.13970100	-2.00685300
H	-4.38872200	1.59217300	-1.13166700
H	-3.08602200	1.98518300	-2.25843700
C	-1.61352900	2.80409300	1.62761900
C	-0.92319800	1.81318800	2.55002700
H	-0.92202600	3.57031600	1.27414800
H	-2.42522700	3.31742300	2.16492500
H	-0.50663200	2.33728700	3.41643000
H	-0.10374400	1.29820200	2.04184000
H	-1.62466000	1.05260600	2.90037100
C	3.30169100	-3.51915500	0.19966700
C	4.34390200	-3.45136400	1.34085600
C	2.24094700	-4.55997800	0.62854000
C	3.97733700	-3.97674300	-1.10874800
H	5.17948400	-2.77980000	1.12204900
H	3.88849500	-3.12067500	2.28128200
H	4.77019600	-4.45033100	1.51127100
H	1.50513800	-4.76528400	-0.15430400
H	2.73464300	-5.51475400	0.85964100
H	1.69571700	-4.24285000	1.52435400
H	4.44292800	-4.96375700	-0.97409400
H	3.25356500	-4.06212300	-1.92855900

H	4.76096300	-3.28147100	-1.43142500
C	1.67046000	-1.29218600	1.59119000
C	0.35278200	-1.70411700	1.86640600
C	2.37230000	-0.59745700	2.59280700
C	-0.23489900	-1.46086100	3.10884700
H	-0.23890100	-2.21308700	1.11101300
C	1.78594800	-0.34667000	3.83630300
H	3.38686900	-0.25229900	2.40096700
C	0.48616900	-0.78914100	4.09873700
H	-1.25902400	-1.77909200	3.27844600
H	2.34290200	0.19088200	4.60006500
H	0.03120500	-0.59398900	5.06652800

TS4

C	1.22072200	0.50217700	-1.48499000
C	1.60511400	0.50963700	-2.84423400
C	-0.15239100	0.71501900	-1.23250000
C	0.70260400	0.79397000	-3.86909100
H	2.63762700	0.29721100	-3.10830900
C	-1.06706100	1.02160800	-2.24883900
C	-0.63547500	1.06554500	-3.57182000
H	1.04556800	0.80415600	-4.90012200
H	-2.11159700	1.18006700	-2.01058200
H	-1.34623700	1.27940500	-4.36518900
C	2.35907500	-0.09027400	1.56822500
C	1.20141300	0.35883500	2.25539800
C	3.36265700	-0.70210000	2.33562400
C	1.08869900	0.24117800	3.64749300
C	3.24553800	-0.84091600	3.72256200
C	2.11575100	-0.35292600	4.38062500
H	0.19902400	0.61671000	4.14338700
H	4.03959900	-1.32248700	4.28644400
H	2.02807500	-0.44135000	5.45984700
C	0.13310200	0.85998700	1.42578800
C	-0.32862400	1.70336800	0.57358600
H	4.25311700	-1.08157400	1.84205500
Pd	-0.93732500	-0.44571700	0.26900200
O	-4.21169200	-2.65452500	-2.17412200
S	-3.61530500	-1.99486200	-1.01519200
O	-3.84707400	-2.59828500	0.32127200
O	-2.17498300	-1.58271900	-1.22294200
C	-4.48242400	-0.34854300	-0.89819000
F	-5.78455700	-0.51313000	-0.65517100
F	-3.95523600	0.39663400	0.10079300

F	-4.34113400	0.34662900	-2.04064400
Si	2.69376300	0.29447500	-0.27168500
C	-0.81865900	3.05914900	0.41025200
C	-1.51754500	3.63667600	1.48855000
C	-0.58649600	3.82482200	-0.74582600
C	-1.96733100	4.95212200	1.41162700
H	-1.70713500	3.03578000	2.37268200
C	-1.03447800	5.14193000	-0.81235600
H	-0.04972500	3.38704800	-1.57893600
C	-1.72716700	5.70833200	0.26117700
H	-2.51017400	5.38497000	2.24710500
H	-0.84292300	5.72772800	-1.70685100
H	-2.08196700	6.73332700	0.19990200
C	3.67525900	-1.18590300	-0.92218600
C	4.75864100	-1.09721300	-1.81421200
C	3.25022300	-2.47481400	-0.54476100
C	5.38887600	-2.24150900	-2.30959300
H	5.12529700	-0.12632900	-2.13297300
C	3.87124300	-3.62202500	-1.03848200
H	2.42362500	-2.58498500	0.15163200
C	4.94493300	-3.50744000	-1.92454800
H	6.22576700	-2.14286700	-2.99621800
H	3.51694400	-4.60319900	-0.73294400
H	5.43213100	-4.39849000	-2.31152400
C	3.71232200	1.94517000	-0.25274900
C	5.07229600	1.69931400	0.43780000
H	5.64867900	2.63502900	0.46729400
H	4.94624300	1.36197800	1.47245800
H	5.67931500	0.95317700	-0.08635700
C	3.95605300	2.51964000	-1.66460500
H	3.01756600	2.74411500	-2.18180400
H	4.52494400	3.45711100	-1.58652100
H	4.53452700	1.84613400	-2.30629900
C	2.93740800	3.00795600	0.55847800
H	1.98251900	3.26598900	0.09018000
H	2.73290200	2.67963400	1.58338100
H	3.53020200	3.93185900	0.62031200
N	-1.40787100	-2.06126800	1.74263100
H	-2.23327700	-2.45651600	1.27327500
C	-0.34228800	-3.09030900	1.77900300
C	-0.15228600	-3.75694200	0.41815100
H	-0.59716400	-3.85405000	2.53077300
H	0.58208400	-2.60310900	2.11336700
H	0.62851600	-4.52294900	0.48269500

H	-1.07948300	-4.23514700	0.08556200
H	0.13486200	-3.03370900	-0.35158300
C	-1.84006300	-1.66102800	3.10002900
C	-2.92408600	-0.58809400	3.06131400
H	-0.95700200	-1.30875900	3.64080000
H	-2.21006200	-2.55046600	3.63378500
H	-3.30513100	-0.40087800	4.07153500
H	-2.53205300	0.35140100	2.65773600
H	-3.75597800	-0.90434100	2.42550900

INT13

C	0.46160100	-0.12324000	-1.44778100
C	-0.40289500	-0.55022800	-2.49541700
C	0.60662000	1.30544000	-1.27055600
C	-1.01535000	0.35386800	-3.34692000
H	-0.59878400	-1.60935600	-2.62129200
C	-0.02387800	2.20896500	-2.14786900
C	-0.81148100	1.73434500	-3.18503800
H	-1.67368900	-0.00500700	-4.13199400
H	0.10002200	3.27512000	-1.98369400
H	-1.30760000	2.43388300	-3.85144700
C	2.11727400	-1.15869000	1.21646600
C	1.79648400	0.07242900	1.85730300
C	2.78770200	-2.13265800	1.96755700
C	2.14596500	0.29833400	3.19196500
C	3.14037000	-1.90441500	3.30323600
C	2.82476800	-0.68931400	3.91127300
H	1.90095400	1.24560000	3.66317900
H	3.65666200	-2.67707600	3.86629500
H	3.10160100	-0.50851100	4.94637000
C	1.04869200	0.94755200	0.95236000
C	1.47092300	1.68518300	-0.10243500
H	3.02250400	-3.09475000	1.51950500
Pd	-0.76758700	0.29078500	0.45435300
O	-5.16863600	-0.58940300	-0.74617600
S	-4.06460000	0.14389600	-0.13263100
O	-4.23964000	0.60746100	1.26961500
O	-2.70774700	-0.47708400	-0.37174300
C	-3.93775200	1.73854000	-1.08469800
F	-5.04152600	2.47465200	-0.92464000
F	-2.88189400	2.45922500	-0.64329700
F	-3.76323400	1.50321900	-2.39342400
Si	1.61955100	-1.46078900	-0.61581600
C	2.66546700	2.52892300	-0.21843800

C	3.36227500	2.94870400	0.93117700
C	3.14656200	2.94120100	-1.47621600
C	4.51520000	3.72042400	0.82439900
H	2.98614200	2.66950700	1.90958500
C	4.29626600	3.72257900	-1.57961600
H	2.62780500	2.62930900	-2.37737200
C	4.98897600	4.11232100	-0.43162500
H	5.04076900	4.02806900	1.72448200
H	4.65332000	4.02364400	-2.56080100
H	5.88396800	4.72279200	-0.51274200
C	0.62570600	-3.06971900	-0.62660100
C	0.44780000	-3.85178900	-1.78437800
C	-0.02445400	-3.49588200	0.54567400
C	-0.34927500	-4.99768900	-1.77530300
H	0.93416900	-3.56852500	-2.71393800
C	-0.82644400	-4.63820500	0.56202700
H	0.09586000	-2.92712600	1.46243500
C	-0.99290300	-5.39195100	-0.60045800
H	-0.46962700	-5.57998400	-2.68512500
H	-1.32510700	-4.93418400	1.48116800
H	-1.61959800	-6.27963200	-0.59224800
C	3.23462100	-1.60807000	-1.67568600
C	3.85974400	-3.00901800	-1.49062000
H	4.77852300	-3.08576700	-2.08975700
H	4.14187100	-3.19286600	-0.44736900
H	3.18951600	-3.81586100	-1.80245700
C	2.93528600	-1.37564200	-3.17216400
H	2.52763100	-0.37495600	-3.35453800
H	3.86160500	-1.46923600	-3.75677800
H	2.22110100	-2.10015900	-3.58034300
C	4.26733600	-0.55595000	-1.21792400
H	3.91348700	0.46645300	-1.37124400
H	4.52170200	-0.66354800	-0.15791500
H	5.19506100	-0.67009100	-1.79726500
N	-1.64941600	0.46865700	2.42761700
H	-2.63987000	0.53654700	2.14603000
C	-1.49297800	-0.75913000	3.25216400
C	-2.35601000	-1.90048500	2.71838400
H	-1.78665400	-0.52883200	4.28747700
H	-0.43032500	-1.02381600	3.27007100
H	-2.17853300	-2.80663300	3.30800000
H	-3.41825800	-1.64430200	2.78345100
H	-2.13619100	-2.11636800	1.67009800
C	-1.31406000	1.70827900	3.16748800

C	-1.58445100	2.96143800	2.34115900
H	-0.26219200	1.65055400	3.46102600
H	-1.91044600	1.73052400	4.09221800
H	-1.46667600	3.85269100	2.96724800
H	-0.88760000	3.03417500	1.50081500
H	-2.60253600	2.94938100	1.94017500

INT7

C	-2.10565700	-1.90077400	-0.47824800
C	-1.94171200	-3.05298700	-1.24653100
C	-1.02987600	-1.51933700	0.36807300
C	-0.74546400	-3.79840600	-1.23863100
H	-2.74336100	-3.38609000	-1.89806500
C	0.17017900	-2.28374200	0.41761400
C	0.30336000	-3.41670600	-0.42097400
H	-0.65581500	-4.67495900	-1.87386200
H	1.22744700	-3.98630100	-0.39519500
C	-3.55879900	-0.08491300	1.30629400
C	-2.28385100	0.13316000	1.89292800
C	-4.69423200	0.22632500	2.06842800
C	-2.17689500	0.68049600	3.17823200
C	-4.58481000	0.75814600	3.35574800
C	-3.32354800	0.99694700	3.90494500
H	-1.19177300	0.84739200	3.60427100
H	-5.48122700	0.98942100	3.92499600
H	-3.23207100	1.41766700	4.90276600
H	-5.68557000	0.05717300	1.65971400
Pd	1.24465700	-0.40936600	-0.36693000
O	2.31366900	1.31884400	-1.31086000
S	3.34534400	0.46935500	-2.02800700
O	3.84337000	0.97709800	-3.29869800
O	2.89555500	-0.96357300	-1.96793300
C	4.78859400	0.53368500	-0.84539800
F	5.34554700	1.74459600	-0.85835300
F	5.70710300	-0.38036900	-1.17211000
F	4.36474000	0.27596700	0.41439600
Si	-3.51482600	-0.63558700	-0.50417700
C	-1.07184800	-0.24336300	1.12790700
C	0.03570200	0.49591600	0.90757400
C	0.34330000	1.89219300	1.18756400
C	1.61383700	2.27743900	1.65782900
C	-0.62186100	2.88597200	0.93019400
C	1.89828700	3.61832800	1.89897700
H	2.37538300	1.52010900	1.81007400

C	-0.32937700	4.22515000	1.16838600
H	-1.58722500	2.59576000	0.53262600
C	0.92725700	4.59484200	1.65802000
H	2.88064000	3.90448400	2.26419700
H	-1.08016300	4.98297300	0.96176100
H	1.15365300	5.64202700	1.84005100
C	-2.84962600	0.85487800	-1.46231100
C	-1.65984900	0.78223900	-2.20959500
C	-3.46886900	2.11385600	-1.33929200
C	-1.09245400	1.91952600	-2.78779800
H	-1.14662400	-0.16997800	-2.31829200
C	-2.92222900	3.25069700	-1.93870500
H	-4.37215400	2.21800000	-0.74191300
C	-1.72597500	3.15657900	-2.65458300
H	-0.14777400	1.84100100	-3.31819100
H	-3.41718000	4.21243200	-1.82823200
H	-1.28300000	4.04484200	-3.09664500
C	-5.16595300	-1.27421400	-1.23359000
C	-4.95821600	-1.67140000	-2.71363900
H	-5.92003700	-1.96420600	-3.15836200
H	-4.55950000	-0.83798400	-3.30373000
H	-4.27885500	-2.52058200	-2.83536400
C	-6.23836100	-0.16077800	-1.21098100
H	-7.17442200	-0.54121800	-1.64434400
H	-6.47007800	0.19125100	-0.20097100
H	-5.93058800	0.70603500	-1.80621200
C	-5.66118300	-2.49265600	-0.42744700
H	-6.60134600	-2.87445700	-0.85075700
H	-4.93440000	-3.31391500	-0.44239000
H	-5.84946900	-2.23836800	0.62230900
H	0.89561200	-2.13737700	1.22471500
N	2.92005800	-2.01886600	2.20986500
H	3.51360600	-1.21386300	2.01840300
C	2.51275300	-2.01018000	3.61458300
C	1.82077100	-0.69869000	3.98106400
H	3.36427200	-2.19139800	4.29856300
H	1.81689500	-2.84773500	3.76231200
H	1.49673200	-0.70911300	5.02751300
H	2.49750900	0.15492600	3.85080100
H	0.94728700	-0.53070300	3.34341600
C	3.62087700	-3.23998600	1.80673200
C	4.18389000	-3.11988300	0.39200800
H	2.89835100	-4.06746600	1.85593900
H	4.43547300	-3.50060100	2.50969300

H	4.65008000	-4.06194100	0.08306800
H	3.40459800	-2.86036000	-0.33029600
H	4.94630400	-2.33625900	0.33423700

TS5

C	-2.11786000	-1.80231700	-0.41999500
C	-2.01322300	-2.98985500	-1.15809200
C	-0.91772900	-1.14531300	-0.05948100
C	-0.77984500	-3.48601200	-1.60402600
H	-2.91210000	-3.53431500	-1.43045700
C	0.35276600	-1.63870400	-0.49301600
C	0.38787000	-2.78574000	-1.31807500
H	-0.74457400	-4.39766000	-2.19470400
H	1.34328000	-3.13468100	-1.70132400
C	-3.23994900	0.08800300	1.51008600
C	-1.89995800	0.54831200	1.62456800
C	-4.14410700	0.38281200	2.54195800
C	-1.53517300	1.31311400	2.74792000
C	-3.76613900	1.13201600	3.65650900
C	-2.45740200	1.60875300	3.74809100
H	-0.51802700	1.67585700	2.84013300
H	-4.48665900	1.34568800	4.44153600
H	-2.14845700	2.20223100	4.60474200
H	-5.16678300	0.02476100	2.48152100
Pd	1.65885000	-0.04403100	-0.74570800
O	3.44048600	1.42316400	-1.11939300
S	4.39022100	0.29584500	-1.42207400
O	5.49434700	0.56025300	-2.33365000
O	3.58664700	-0.95985300	-1.65562800
C	5.18594800	-0.03076500	0.23782000
F	6.01805700	0.95628300	0.56443800
F	5.85632900	-1.18923100	0.22277600
F	4.23786500	-0.11595200	1.21083300
Si	-3.65719900	-0.75842700	-0.11584900
C	-0.86987000	0.15630400	0.62448900
C	0.23616500	0.88408000	0.28566400
C	0.44443400	2.31805200	0.47545500
C	1.65142600	2.82533900	0.99630300
C	-0.57186400	3.22311200	0.10036700
C	1.82269900	4.19707600	1.16797700
H	2.45013200	2.13754000	1.25429200
C	-0.38826600	4.59229800	0.26312500
H	-1.49478500	2.83536100	-0.32046100
C	0.80578500	5.08327300	0.80268400

H	2.75576100	4.57591800	1.57567000
H	-1.17648000	5.27952200	-0.03280000
H	0.94659600	6.15353100	0.92823400
C	-3.59220100	0.60923000	-1.42285100
C	-2.99189700	0.40437500	-2.67763200
C	-4.09700700	1.89149100	-1.13639800
C	-2.90010100	1.43781000	-3.61277300
H	-2.56803800	-0.56746700	-2.92048500
C	-4.01035700	2.92817900	-2.06796800
H	-4.54208500	2.08956900	-0.16353600
C	-3.40885400	2.70245100	-3.30880200
H	-2.42259200	1.25917700	-4.57273300
H	-4.40267200	3.91223800	-1.82331100
H	-3.33029200	3.50997100	-4.03197600
C	-5.34099800	-1.67075700	-0.19636200
C	-5.52922200	-2.29336900	-1.59931200
H	-6.53621200	-2.72709100	-1.68129600
H	-5.42554200	-1.54430400	-2.39309200
H	-4.81763300	-3.09915900	-1.80384100
C	-6.49493100	-0.66174900	0.00816000
H	-7.46081600	-1.17673000	-0.09565800
H	-6.48394100	-0.19376100	0.99709000
H	-6.46482200	0.13952400	-0.73917000
C	-5.40784400	-2.77598500	0.87655500
H	-6.37061900	-3.30470700	0.82387600
H	-4.61394300	-3.52079600	0.73994600
H	-5.30831100	-2.36928300	1.88984700
H	1.24390400	-1.78681200	0.51157100
N	1.94010700	-2.29809800	1.64180500
H	2.77005800	-1.71267300	1.73795600
C	1.03782600	-2.12554100	2.80119900
C	1.23332700	-0.75085200	3.43269700
H	1.22175300	-2.91995600	3.53731200
H	0.00957200	-2.24356800	2.43692000
H	0.46945200	-0.56704500	4.19330200
H	2.22002300	-0.67229700	3.90487500
H	1.14711400	0.02972000	2.67260100
C	2.32726500	-3.68276700	1.30887500
C	3.52197100	-3.69556900	0.35876000
H	1.45253000	-4.15877000	0.84825600
H	2.55731800	-4.23730600	2.22977900
H	3.75616400	-4.72319500	0.06353600
H	3.33238300	-3.10542700	-0.54152100
H	4.41053200	-3.27012300	0.83845200

INT8

C	-2.04889700	-1.25134700	-0.57540000
C	-2.07827900	-2.50027200	-1.23662000
C	-0.83752300	-0.52850700	-0.57403100
C	-0.95777400	-3.02178600	-1.87431000
H	-3.00533700	-3.06469100	-1.27715600
C	0.30636200	-1.07440400	-1.21475400
C	0.24653900	-2.29790000	-1.86901900
H	-1.01409800	-3.98157700	-2.38236800
H	1.12756400	-2.69581500	-2.36708300
C	-2.95565900	1.16408100	0.87579300
C	-1.59541700	1.57411600	0.77910400
C	-3.85385600	1.96989700	1.60488200
C	-1.19009600	2.69416500	1.54262200
C	-3.44718400	3.11127400	2.28904400
C	-2.09244500	3.45029900	2.27967000
H	-0.14880700	2.98623200	1.55173700
H	-4.16782000	3.71182600	2.83751000
H	-1.73544800	4.30939000	2.84197900
H	-4.90453200	1.69507100	1.63600500
Pd	1.96473700	-0.00349200	-1.10979400
O	4.25531000	0.77068300	-1.01394200
S	4.79251000	-0.62532300	-1.08737400
O	6.06059500	-0.84518200	-1.77012900
O	3.66569400	-1.57236300	-1.41665000
C	5.14208400	-1.02003100	0.71084700
F	6.30421700	-0.50820100	1.10171200
F	5.14438900	-2.34376400	0.92822800
F	4.16637500	-0.48855400	1.51031200
Si	-3.55806100	-0.49635700	0.23319200
C	-0.59892400	0.83670800	-0.04345500
C	0.64052100	1.31227200	-0.40517900
C	1.13127200	2.69475300	-0.42599300
C	2.38107500	3.05125300	0.11861800
C	0.37416900	3.69403000	-1.07523200
C	2.83860600	4.36692700	0.04803700
H	3.00244800	2.28998400	0.57899800
C	0.83911100	5.00255400	-1.15092700
H	-0.58342100	3.42284800	-1.50929100
C	2.07130500	5.34724100	-0.58361900
H	3.80437100	4.62133400	0.47621500
H	0.24201000	5.75745100	-1.65587700
H	2.43417400	6.36958400	-0.64586100

C	-4.98260600	-0.27304600	-0.99041700
C	-5.57765900	-1.36890500	-1.64699800
C	-5.47095600	1.00956200	-1.30315300
C	-6.61899300	-1.19528400	-2.55927000
H	-5.22177100	-2.37775600	-1.45903100
C	-6.51440700	1.19001800	-2.21406000
H	-5.02583300	1.88378100	-0.83693600
C	-7.09418400	0.08723600	-2.84236500
H	-7.05688500	-2.06005700	-3.05145300
H	-6.87020300	2.19312300	-2.43559600
H	-7.90549800	0.22514000	-3.55243200
C	-4.10340700	-1.58992700	1.74351000
C	-4.45594700	-3.02717000	1.30513100
H	-4.71867300	-3.63109300	2.18631900
H	-5.32034500	-3.04996400	0.63287800
H	-3.61682000	-3.52655300	0.80918300
C	-5.33372500	-0.99187900	2.45690200
H	-5.67736800	-1.67312500	3.24917000
H	-5.10510200	-0.03385300	2.93377300
H	-6.17157900	-0.84001500	1.76567700
C	-2.92760400	-1.66158200	2.73989100
H	-3.20801900	-2.25423200	3.62313100
H	-2.05246400	-2.14281600	2.28514900
H	-2.62877800	-0.66537600	3.08814500
H	1.58439100	-1.03341600	0.81015500
N	1.52062100	-1.54847800	1.73438300
H	2.48903400	-1.58741700	2.06567000
C	0.69155800	-0.73116400	2.68395500
C	1.38106500	0.58434000	3.01363000
H	0.52730500	-1.34350300	3.57585000
H	-0.26715400	-0.56758700	2.19223000
H	0.73487300	1.17140200	3.67206300
H	2.34002500	0.42436800	3.51932400
H	1.55258200	1.16612700	2.10554800
C	1.02027200	-2.94087000	1.46334800
C	2.07254400	-3.73974200	0.70578700
H	0.09895600	-2.82994500	0.88841800
H	0.78387800	-3.38995500	2.43299000
H	1.66456200	-4.72331800	0.45541500
H	2.36218600	-3.23744900	-0.21994100
H	2.97478700	-3.88590500	1.31032300
INT9			
C	2.11056600	-1.20339800	-0.70951100

C	2.28043100	-2.54852100	-1.09596500
C	0.81018300	-0.66842700	-0.67288000
C	1.19704400	-3.33329300	-1.47352300
H	3.27954700	-2.97881100	-1.10073100
C	-0.28728400	-1.45367700	-1.11915500
C	-0.09108700	-2.77071500	-1.51305600
H	1.34151900	-4.37361900	-1.75511800
H	-0.92490100	-3.38013000	-1.84701600
C	2.77203300	1.43523400	0.40987300
C	1.36630200	1.63859900	0.41743600
C	3.59830300	2.32274700	1.12083100
C	0.85324200	2.71214900	1.17641400
C	3.07698200	3.40081800	1.83124000
C	1.69218600	3.58545700	1.85952200
H	-0.21711100	2.85471000	1.24884900
H	3.73575600	4.07485300	2.37246500
H	1.26040800	4.40294600	2.43153900
H	4.67319900	2.15252200	1.12978500
Si	3.53402900	-0.00971700	-0.50693000
C	0.43985100	0.71168100	-0.28398300
C	-0.86154800	0.97804000	-0.58927200
C	-1.59180300	2.24090900	-0.68918800
C	-1.10191400	3.27517800	-1.51804800
C	-1.83304300	4.44310300	-1.70472800
H	-0.13901800	3.14092300	-2.00191100
C	-3.57659000	3.59304100	-0.26148600
C	-3.07570300	4.60704500	-1.07935600
H	-1.43739100	5.23019700	-2.34139800
H	-4.53684800	3.71510100	0.23293700
H	-3.64535200	5.52007500	-1.22962400
Pd	-2.04687600	-0.47490600	-1.26430300
H	-1.48414400	-1.30689800	0.73410300
C	4.91160500	-0.80970800	0.50674700
C	4.56356000	-1.79004300	1.45700200
C	6.27127600	-0.46282000	0.40243400
C	5.52689600	-2.39434500	2.26628000
H	3.52351300	-2.08942500	1.56118200
C	7.24048400	-1.06338900	1.20906300
H	6.58885000	0.28439500	-0.31818900
C	6.86997200	-2.03171200	2.14388500
H	5.22951300	-3.14863600	2.99049600
H	8.28402600	-0.77633700	1.10571600
H	7.62285700	-2.50150800	2.77169900
C	4.09688900	0.56400600	-2.26034300

C	4.83845300	-0.57891800	-2.98142900
C	2.82816500	0.93189500	-3.06377700
C	4.99616900	1.81628600	-2.19072300
H	5.75684200	-0.86737600	-2.45686600
H	4.20796300	-1.47247000	-3.06910300
H	5.11790500	-0.27197000	-4.00016400
H	2.24973100	1.72195300	-2.56840100
H	3.10952800	1.30175800	-4.06060000
H	2.16495900	0.07105300	-3.19999200
H	5.23412200	2.16445900	-3.20669500
H	4.50159600	2.64061400	-1.66426500
H	5.95077800	1.62502100	-1.68822100
S	-2.91712900	-1.14725200	2.36052100
C	-2.20963700	0.28334900	3.32994800
F	-1.54576400	1.09333400	2.50148600
F	-1.38650900	-0.16951000	4.26927300
F	-3.21708200	0.95311000	3.89244000
O	-3.82489100	-0.56347000	1.37021000
O	-1.58299300	-1.68399000	1.66800300
O	-3.37318100	-2.14078200	3.31415600
C	-2.84700500	2.41867700	-0.06686900
H	-3.23373900	1.64131000	0.58351700
N	-3.76802600	-1.76705500	-2.09267000
H	-3.67729400	-1.62342400	-3.10014300
C	-3.74519400	-3.23865300	-1.87230400
C	-3.59247600	-3.63305300	-0.40707300
H	-2.90646600	-3.63322100	-2.45418800
H	-4.66428600	-3.68244800	-2.28722400
H	-3.64472500	-4.72315400	-0.31351500
H	-2.62995700	-3.30400000	-0.00967700
H	-4.38300800	-3.20575000	0.21662800
C	-5.06133800	-1.15129000	-1.68442100
C	-5.18307800	0.28532600	-2.18589400
H	-5.11160300	-1.17267800	-0.59417400
H	-5.89558900	-1.75488000	-2.07563200
H	-6.15802000	0.69644200	-1.90419400
H	-4.41865700	0.94089600	-1.75166300
H	-5.09897200	0.33871900	-3.27878600

TS6

C	2.33969700	-1.33142500	0.00739600
C	2.58874300	-2.70740300	0.12811400
C	1.01142000	-0.89808100	-0.21407400
C	1.56104400	-3.63740400	-0.01887600

H	3.60030700	-3.05449100	0.32530200
C	-0.02582700	-1.85130000	-0.42761200
C	0.26498800	-3.20924600	-0.34006400
H	1.76542500	-4.69981000	0.09339800
H	-0.50900400	-3.95089400	-0.50530600
C	2.86091500	1.55729900	-0.00852300
C	1.44704300	1.66414000	-0.09859900
C	3.61440900	2.70380700	0.28804300
C	0.84908900	2.91592900	0.16968000
C	3.01028700	3.94012000	0.50728200
C	1.61710600	4.03683300	0.45890600
H	-0.22961600	3.00599800	0.17601100
H	3.61495900	4.81291300	0.73903000
H	1.12546300	4.98408900	0.66256000
H	4.69584700	2.62060500	0.37294600
Si	3.72035700	-0.09329200	-0.22485600
C	0.58074700	0.49308700	-0.36451900
C	-0.78178500	0.59415200	-0.67628300
C	-1.39720100	1.65476000	-1.49732800
C	-0.74080700	2.10277200	-2.66524700
C	-1.33541500	3.03561600	-3.50757100
H	0.24068800	1.70084200	-2.89993700
C	-3.27150400	3.10595600	-2.06593800
C	-2.60619200	3.54349500	-3.21221500
H	-0.81075700	3.36610300	-4.40041400
H	-4.25729400	3.49515400	-1.82489500
H	-3.07096000	4.27091300	-3.87224900
Pd	-1.82751500	-1.13963000	-0.89538200
H	-1.31237100	0.54581800	0.62994800
C	5.04772500	-0.34525900	1.08932800
C	4.66797200	-0.88386800	2.33460600
C	6.39918800	0.00751700	0.91807000
C	5.59499700	-1.05988400	3.36302000
H	3.63366100	-1.17479000	2.50069600
C	7.33140400	-0.16685400	1.94307000
H	6.73950200	0.42166600	-0.02603900
C	6.93063600	-0.70126800	3.16901800
H	5.27493400	-1.47783300	4.31401200
H	8.36975000	0.11262800	1.78329800
H	7.65500600	-0.83869800	3.96768300
C	4.36788200	-0.24487900	-2.03560700
C	5.19473500	-1.53583400	-2.19841800
C	3.14182700	-0.30501500	-2.97506000
C	5.21832600	0.97876700	-2.43833800

H	6.08314000	-1.53781200	-1.55636400
H	4.60192700	-2.42575900	-1.95445100
H	5.53415900	-1.64216000	-3.23909800
H	2.51097900	0.58752700	-2.87492300
H	3.47411900	-0.35711300	-4.02182000
H	2.51452000	-1.18090200	-2.77840800
H	5.51323800	0.89752300	-3.49466400
H	4.66235100	1.91582400	-2.32049100
H	6.14221500	1.06294500	-1.85558700
S	-3.15225300	0.12094900	2.06219400
C	-4.00374100	1.61580100	2.77840500
F	-3.99355800	2.61722900	1.88627300
F	-3.38624000	2.01634500	3.89032400
F	-5.27186200	1.30347300	3.06338700
O	-3.89149800	-0.15431500	0.80972600
O	-1.75667200	0.71853300	1.77882600
O	-3.14842300	-0.89574800	3.10899600
C	-2.67849100	2.17063900	-1.21659400
H	-3.20670400	1.84299600	-0.33115900
N	-3.25686900	-2.85564700	-1.31655800
H	-2.96602800	-3.21883600	-2.22513800
C	-3.28686900	-4.00300600	-0.36498300
C	-3.25754400	-3.56919300	1.09643600
H	-2.41701100	-4.62891700	-0.58696500
H	-4.17923000	-4.61570000	-0.56782100
H	-3.35022700	-4.44766500	1.74472300
H	-2.31955600	-3.06049500	1.33432600
H	-4.06954700	-2.88019400	1.33888500
C	-4.60536000	-2.24862800	-1.50092000
C	-4.58173800	-1.10876800	-2.51616300
H	-4.93026200	-1.87087400	-0.53019600
H	-5.31485100	-3.02727100	-1.82160800
H	-5.59960900	-0.74192700	-2.68573700
H	-3.98901500	-0.25536000	-2.16288600
H	-4.17389500	-1.43403200	-3.48117500

INT10

C	2.40282100	0.72476400	-0.74400100
C	2.63850100	1.10923700	-2.07280200
C	1.07450900	0.69859600	-0.24758700
C	1.58763000	1.48860800	-2.90474200
H	3.65560100	1.10894200	-2.45813300
C	0.00783500	0.96863500	-1.13308400
C	0.27345100	1.40533200	-2.43307800

H	1.77958500	1.81610700	-3.92373200
H	-0.54730600	1.66034700	-3.09916000
C	2.94183000	-0.89091700	1.64517600
C	1.57603900	-0.63971000	1.91271300
C	3.58912500	-1.92015400	2.34737600
C	0.89316900	-1.43859900	2.84630500
C	2.91122200	-2.69498500	3.28920600
C	1.55696700	-2.45439700	3.53201900
H	-0.17113400	-1.28635100	3.00361800
H	3.42966900	-3.49074500	3.81749700
H	1.01033900	-3.06864200	4.24250500
H	4.63641300	-2.12940000	2.14071900
Si	3.81633300	0.17268500	0.36998400
C	0.83970600	0.45066600	1.21077700
C	-0.01868800	1.23128700	1.90227600
C	-0.84061700	2.29090400	1.27031500
C	-0.28253500	3.48389000	0.78767900
C	-1.07344800	4.41271900	0.11403200
H	0.77946900	3.66273400	0.92059300
C	-3.01043400	2.99429400	0.36940600
C	-2.43086600	4.16306000	-0.12060700
H	-0.62217200	5.32960400	-0.25591100
H	-4.06420100	2.78128800	0.22112500
H	-3.03155300	4.88052800	-0.67189300
Pd	-1.90011300	0.57894000	-0.69068200
H	-0.16824100	1.05497400	2.96547300
C	4.98398000	-0.92062300	-0.63429800
C	4.54721400	-2.22084000	-0.95987900
C	6.23739800	-0.51654900	-1.12737600
C	5.32473400	-3.07677400	-1.74005000
H	3.58674000	-2.57204200	-0.58957300
C	7.02189800	-1.36875800	-1.90875800
H	6.61888500	0.47422300	-0.90220300
C	6.56705000	-2.65145400	-2.21718100
H	4.96387200	-4.07532700	-1.97339900
H	7.98814300	-1.03026300	-2.27420300
H	7.17650600	-3.31629100	-2.82381100
C	4.66832800	1.67399400	1.21390700
C	5.10989100	2.72646700	0.17510100
C	3.64584600	2.33631600	2.16389200
C	5.87812200	1.19672700	2.04391400
H	5.87101600	2.34888400	-0.51627800
H	4.26227700	3.07681800	-0.42583600
H	5.54129400	3.60037400	0.68458800

H	3.30381200	1.64764300	2.94394200
H	4.10231800	3.20539100	2.65922500
H	2.76081800	2.68912800	1.62276500
H	6.33656700	2.04633700	2.57056400
H	5.57761200	0.46364800	2.80292700
H	6.65370800	0.73435100	1.42363400
S	-4.21198000	-1.14217800	0.53894500
C	-6.04908700	-1.14771800	0.82477100
F	-6.41404800	-0.03041000	1.46694700
F	-6.38962900	-2.20686400	1.56588700
F	-6.69768500	-1.20645600	-0.34477600
O	-4.06099300	0.10443700	-0.31430500
O	-3.59305800	-1.02288000	1.86902200
O	-3.93039100	-2.37595100	-0.23160400
C	-2.22911500	2.06273300	1.09095500
H	-2.70959300	1.24026800	1.61716300
N	-1.82325200	-1.16874100	-1.97266900
H	-2.64791800	-1.64947400	-1.58972100
C	-2.07439700	-0.89383900	-3.40913300
C	-3.27520100	0.02144600	-3.62585600
H	-2.23405400	-1.85482100	-3.92016900
H	-1.16238700	-0.45382500	-3.82317400
H	-3.49914500	0.09459500	-4.69559500
H	-4.15972500	-0.35946300	-3.10578400
H	-3.07818900	1.02942600	-3.24348500
C	-0.65695900	-2.07348600	-1.77216700
C	-0.57785800	-2.58581000	-0.33962100
H	0.24343600	-1.51664000	-2.04470400
H	-0.75460300	-2.91790700	-2.47051600
H	0.30706000	-3.21939100	-0.21887900
H	-0.49512200	-1.75766300	0.36796200
H	-1.46940500	-3.16179100	-0.07601200

TS7

C	2.34307100	0.05408500	-1.08996500
C	2.58151900	-0.49860100	-2.35672300
C	1.00982900	0.17113100	-0.61757100
C	1.52530800	-0.92000800	-3.16267000
H	3.60417600	-0.60169100	-2.71291700
C	-0.04227800	-0.35418000	-1.39109300
C	0.21809000	-0.85356100	-2.67355500
H	1.71455000	-1.31661900	-4.15755200
H	-0.60020700	-1.21102900	-3.29335300
C	3.00923100	0.46236700	1.72876100

C	1.61000700	0.62843400	1.85680300
C	3.77302800	0.23270200	2.88376400
C	1.02089200	0.55508200	3.13124300
C	3.18104700	0.16741900	4.14586900
C	1.79892500	0.32943900	4.26574100
H	-0.05738200	0.65143600	3.22464300
H	3.79002500	-0.01610100	5.02721200
H	1.32287400	0.26721900	5.24088900
H	4.84769200	0.09116200	2.79155500
Si	3.76275400	0.59267700	0.01437000
C	0.74642600	0.89313300	0.66894300
C	-0.17858600	1.87839300	0.75093200
C	-1.10761400	2.30158700	-0.31503700
C	-1.04997800	3.62496200	-0.77890000
C	-1.90308300	4.05714300	-1.79279100
H	-0.31438600	4.30704100	-0.35902800
C	-2.94650600	1.88383200	-1.84814500
C	-2.85481300	3.18489500	-2.33438400
H	-1.83303300	5.07908100	-2.15697500
H	-3.71857800	1.22432800	-2.23573700
H	-3.52642200	3.52820900	-3.11707900
Pd	-1.83634000	-0.67405100	-0.62224700
H	-0.19979900	2.47886000	1.65962100
C	5.16618100	-0.66603500	-0.11776100
C	4.93153500	-1.95148900	0.41166500
C	6.41065200	-0.43690700	-0.73006700
C	5.89155300	-2.96000300	0.33208600
H	3.98360200	-2.16340200	0.90161700
C	7.37812100	-1.44199800	-0.81293100
H	6.64098300	0.53691300	-1.14966900
C	7.12062100	-2.70652200	-0.28244900
H	5.68357100	-3.94157500	0.75071100
H	8.33239500	-1.23520900	-1.29089900
H	7.87227200	-3.48924400	-0.34530400
C	4.27696000	2.40409800	-0.36800100
C	4.66277600	2.56754900	-1.85359600
C	3.06496800	3.32082000	-0.08530600
C	5.44559100	2.83123500	0.54374900
H	5.54485400	1.98081000	-2.13194800
H	3.84184000	2.26610600	-2.51485400
H	4.89344300	3.62119600	-2.06853700
H	2.74275600	3.26119000	0.96004500
H	3.33369700	4.36676800	-0.29407200
H	2.20498600	3.06550000	-0.71465700

H	5.70964600	3.88237800	0.35667100
H	5.17712900	2.74310700	1.60386900
H	6.34693400	2.23055000	0.37844300
S	-4.44694200	-0.27508500	1.31886600
C	-6.04036800	0.27560800	0.52815100
F	-5.77139300	0.80785500	-0.67046700
F	-6.64005400	1.18658200	1.29171800
F	-6.84241300	-0.77895300	0.37198900
O	-3.88268900	-1.23649100	0.32747200
O	-3.62243400	1.02941600	1.31369300
O	-4.75698200	-0.75735700	2.65476800
C	-2.08910900	1.40799900	-0.82714000
H	-2.90474700	1.09463300	0.35519200
N	-1.46540300	-2.84970900	-0.37743500
H	-2.30146700	-3.09487800	0.15880500
C	-1.47460400	-3.64194900	-1.62946900
C	-2.73612300	-3.39364300	-2.45010200
H	-1.38229400	-4.71222400	-1.38740900
H	-0.58240000	-3.35683900	-2.19464800
H	-2.73712000	-4.02911800	-3.34212000
H	-3.63806000	-3.61920000	-1.86890400
H	-2.79745200	-2.34677600	-2.76710400
C	-0.27401100	-3.14295100	0.46073900
C	-0.40027200	-2.53278800	1.85189400
H	0.59509200	-2.73142300	-0.06145400
H	-0.13767900	-4.23319900	0.53379500
H	0.49341800	-2.75290300	2.44434700
H	-0.50314800	-1.44637400	1.79159300
H	-1.27211000	-2.93206300	2.38484600

INT11

C	2.41183000	-0.09809500	-1.09363400
C	2.71165800	-0.79391100	-2.27298800
C	1.06151100	0.00943500	-0.66346400
C	1.70062400	-1.37571900	-3.03561800
H	3.74742400	-0.88518600	-2.59290900
C	0.05174500	-0.64621800	-1.39702000
C	0.37834100	-1.30141400	-2.59336500
H	1.93740500	-1.89584200	-3.96112300
H	-0.40392400	-1.77390900	-3.18153000
C	3.01816900	0.65593100	1.65701400
C	1.60858800	0.74293600	1.75429000
C	3.77998500	0.59317500	2.83395400
C	1.01211100	0.75716600	3.02840000

C	3.17850600	0.61500700	4.09294400
C	1.78763000	0.69717000	4.18543900
H	-0.07015300	0.79535700	3.10862600
H	3.78665500	0.56086200	4.99215700
H	1.30280900	0.70258700	5.15844200
H	4.86259800	0.51411200	2.76236000
Si	3.77966800	0.65828400	-0.05728200
C	0.74142200	0.84048500	0.54074800
C	-0.24721000	1.77022900	0.55141600
C	-1.23363000	2.08402600	-0.49802600
C	-1.50538100	3.44495300	-0.75714700
C	-2.43140800	3.82121100	-1.72378900
H	-0.96475900	4.20590700	-0.19799800
C	-2.88852700	1.48891200	-2.16965500
C	-3.12412000	2.83778800	-2.43841900
H	-2.61756400	4.87419900	-1.91807900
H	-3.45084200	0.73620500	-2.71702400
H	-3.85409900	3.12312100	-3.19229000
Pd	-1.78446700	-0.86852800	-0.68416900
H	-0.28142500	2.43487700	1.41395900
C	5.27714900	-0.49644400	-0.05105600
C	5.15448200	-1.71622500	0.64512700
C	6.49088300	-0.25374500	-0.71795100
C	6.19180300	-2.64825100	0.67386500
H	4.23352800	-1.93626700	1.18033800
C	7.53507000	-1.18218600	-0.69349400
H	6.63621700	0.67130200	-1.26618800
C	7.38800100	-2.38245100	0.00259400
H	6.06894000	-3.57987500	1.22071400
H	8.46270600	-0.96584400	-1.21755700
H	8.19942200	-3.10552800	0.02357300
C	4.16912100	2.45212300	-0.62831900
C	4.53175500	2.48794000	-2.12831800
C	2.90347900	3.31505300	-0.42276100
C	5.31469200	3.04370600	0.21861700
H	5.44751600	1.93300100	-2.35940000
H	3.72666600	2.06925400	-2.74347600
H	4.69230800	3.52683900	-2.45174200
H	2.59573400	3.34465100	0.62825800
H	3.10305500	4.34834800	-0.74264600
H	2.05509300	2.94329800	-1.00773400
H	5.50720500	4.08560900	-0.07665800
H	5.06091200	3.04618000	1.28611500
H	6.25231800	2.48906600	0.10168900

S	-4.50413800	-0.16971000	1.23265800
C	-6.02153800	0.53456500	0.40191700
F	-5.66510300	1.07849400	-0.76044900
F	-6.57007400	1.45726100	1.18527000
F	-6.88421100	-0.45813300	0.19205100
O	-3.95234000	-1.14266300	0.27146400
O	-3.58418800	1.12564500	1.30762600
O	-4.86224800	-0.57556100	2.57622700
C	-1.95915700	1.07908300	-1.19216700
H	-2.99613900	1.20112700	0.49117300
N	-1.49430500	-2.98196900	0.04527200
H	-2.41293200	-3.21705600	0.42833400
C	-1.16653400	-3.96836100	-1.00816300
C	-2.25999500	-4.03706200	-2.06930800
H	-1.01063500	-4.96216500	-0.55868000
H	-0.21800000	-3.65614900	-1.45572400
H	-1.99677600	-4.76998400	-2.83930900
H	-3.22010300	-4.33759700	-1.63134500
H	-2.39891900	-3.06159600	-2.54812000
C	-0.51392200	-3.00014500	1.16000700
C	-0.98354100	-2.14698000	2.33412500
H	0.43066900	-2.61362100	0.76357400
H	-0.34076100	-4.03735500	1.48871900
H	-0.24269600	-2.17054500	3.13930500
H	-1.10983200	-1.10554800	2.02327800
H	-1.93997900	-2.50646500	2.73406500

INT12

C	-1.72248000	0.16744100	-1.11905800
C	-1.82618700	0.87966900	-2.32359400
C	-0.44290200	-0.06810200	-0.54621400
C	-0.68840200	1.36076700	-2.96670200
H	-2.80780900	1.06769200	-2.75300700
C	0.71188600	0.46381400	-1.16998700
C	0.56460700	1.15201800	-2.38597400
H	-0.77382600	1.90108300	-3.90748600
H	1.44716600	1.53887700	-2.89033900
C	-2.71524000	-0.47722700	1.54135100
C	-1.33886300	-0.67358100	1.80629300
C	-3.60299100	-0.30351200	2.61378700
C	-0.90270400	-0.68387600	3.14447100
C	-3.15978100	-0.32614500	3.93661000
C	-1.80126400	-0.51734800	4.19729900
H	0.15548200	-0.80489400	3.35729900

H	-3.86253800	-0.18694600	4.75411300
H	-1.43644800	-0.52297900	5.22169800
H	-4.65886600	-0.13998000	2.40745900
Si	-3.26055500	-0.45855800	-0.25128300
C	-0.34690800	-0.88858000	0.70660700
C	0.54066800	-1.90474200	0.86967900
C	1.58041600	-2.38091500	-0.05538700
C	1.71006600	-3.77445500	-0.22681800
C	2.44560500	-1.50651700	-0.75241300
C	2.62570500	-4.30821400	-1.12956900
H	1.06030800	-4.43859900	0.34091000
C	3.33999400	-2.06313600	-1.68180700
C	3.43474400	-3.44507400	-1.87341100
H	2.70040600	-5.38474900	-1.26056400
H	3.98648900	-1.40929000	-2.26369400
H	4.14351000	-3.84605600	-2.59513100
Pd	2.50678600	0.44183000	-0.27201200
H	0.40372100	-2.52630100	1.75474800
C	-4.64075400	0.82058400	-0.45784200
C	-4.29932900	2.17399300	-0.25917600
C	-5.98374400	0.53252300	-0.75667300
C	-5.25093700	3.18923400	-0.35240200
H	-3.26754700	2.43637600	-0.03595800
C	-6.94360600	1.54403600	-0.85305400
H	-6.29732400	-0.49307900	-0.92168600
C	-6.57963200	2.87552300	-0.65056500
H	-4.95748100	4.22438200	-0.19534700
H	-7.97447100	1.29005700	-1.08749300
H	-7.32444800	3.66387600	-0.72564000
C	-3.72579500	-2.22433700	-0.85163300
C	-4.16707900	-2.17913700	-2.32950800
C	-2.47173300	-3.12107200	-0.74078800
C	-4.83564000	-2.83929900	0.02653700
H	-5.06762400	-1.57378300	-2.48181500
H	-3.37635000	-1.76517800	-2.96714200
H	-4.38604300	-3.19453700	-2.69151600
H	-2.12434700	-3.20749100	0.29439400
H	-2.70655600	-4.13379700	-1.10043000
H	-1.63650200	-2.73895900	-1.33747200
H	-5.04681500	-3.86910700	-0.29752000
H	-4.53380900	-2.87908100	1.08011300
H	-5.77841100	-2.28385000	-0.02584500
N	4.48161600	0.19769400	0.91447000
H	4.69750400	1.11897900	1.30082500

C	4.26164000	-0.73088400	2.05259200
C	3.20581200	-0.21724500	3.02359300
H	5.21207500	-0.90415800	2.58356700
H	3.94014200	-1.68433000	1.62283600
H	3.08032300	-0.92537600	3.84987500
H	3.49056300	0.75117900	3.45493100
H	2.24513400	-0.10514300	2.51452700
C	5.64594200	-0.23851600	0.10834400
C	5.94458900	0.71121500	-1.04442600
H	5.40416900	-1.23203900	-0.27956200
H	6.53311500	-0.34218700	0.75455600
H	6.83305700	0.37477100	-1.58967300
H	5.10182400	0.74593800	-1.74051900
H	6.13746500	1.73091700	-0.68796300
N	2.31512100	2.70968600	0.14241400
H	1.49282500	2.88311500	-0.43920100
C	1.96187400	3.05351500	1.53876600
C	0.62753400	2.44691900	1.95763200
H	1.92941200	4.14926200	1.65952900
H	2.76909000	2.68647000	2.18375100
H	0.39632600	2.71582900	2.99356900
H	-0.18893100	2.81025600	1.32237100
H	0.64012500	1.35979900	1.87649700
C	3.42559800	3.53660500	-0.37449600
C	3.55065900	3.43890800	-1.89158200
H	4.34910100	3.19492800	0.10849300
H	3.28561800	4.59048600	-0.08191200
H	4.40687700	4.02526900	-2.24146900
H	3.68425000	2.40044700	-2.20578800
H	2.65030600	3.82675900	-2.38243000

TS8

C	-1.65487700	0.02370900	-1.14787600
C	-1.70832500	0.62830000	-2.40881900
C	-0.39255400	-0.31470900	-0.58054100
C	-0.54103000	0.88068800	-3.14102600
H	-2.67338800	0.89332400	-2.83532400
C	0.79842200	0.02551500	-1.28677300
C	0.69297900	0.56680000	-2.58729200
H	-0.60123000	1.32456800	-4.13256100
H	1.60199900	0.75934800	-3.15232600
C	-2.67300100	-0.61086900	1.51802900
C	-1.31108300	-0.90565400	1.77091000
C	-3.55336400	-0.44019100	2.59747500

C	-0.88506700	-1.00449400	3.11122500
C	-3.12147200	-0.56099500	3.91789900
C	-1.77696500	-0.84355400	4.16918200
H	0.16482800	-1.18194300	3.32415800
H	-3.81890700	-0.42352100	4.74014900
H	-1.41613300	-0.92133200	5.19201600
H	-4.59581200	-0.19952500	2.39771200
Si	-3.22795300	-0.46631100	-0.26222500
C	-0.30909500	-1.08695400	0.68027600
C	0.65123300	-2.05185200	0.84810100
C	1.71270700	-2.37340600	-0.08248500
C	2.18254800	-3.70371500	-0.17477800
C	2.26143400	-1.37878800	-0.94012800
C	3.10267800	-4.07273000	-1.14566100
H	1.78432800	-4.45057400	0.51006100
C	3.14237900	-1.79192000	-1.96622200
C	3.56616000	-3.11297700	-2.06287200
H	3.44258500	-5.10277200	-1.21359000
H	3.51796600	-1.05531400	-2.67305200
H	4.26924400	-3.40188300	-2.84125200
Pd	2.45884000	0.50954300	-0.21887500
H	0.54525700	-2.72033600	1.70071000
C	-4.50245900	0.92211600	-0.42912100
C	-4.04018800	2.25279000	-0.46876000
C	-5.89442900	0.72216700	-0.46062000
C	-4.92322300	3.33106600	-0.53571300
H	-2.97004400	2.44544900	-0.45754700
C	-6.78522600	1.79646900	-0.52791500
H	-6.30001300	-0.28427400	-0.43583500
C	-6.30135500	3.10496400	-0.56553900
H	-4.53715000	4.34710100	-0.56754300
H	-7.85612800	1.61021800	-0.55291000
H	-6.99245700	3.94240400	-0.61942700
C	-3.84348700	-2.17096700	-0.91208000
C	-4.41050500	-2.01972000	-2.33811200
C	-2.62975500	-3.12759200	-0.95498800
C	-4.90558700	-2.78629700	0.02288100
H	-5.28905900	-1.36494300	-2.36850800
H	-3.66058500	-1.60488300	-3.02301200
H	-4.71219100	-3.00050500	-2.73450000
H	-2.18448000	-3.26649200	0.03668900
H	-2.94650100	-4.11581600	-1.31973200
H	-1.84186700	-2.76086500	-1.62151700
H	-5.18465500	-3.78914500	-0.33277700

H	-4.52752200	-2.89016500	1.04663400
H	-5.82686800	-2.19481200	0.06817600
N	4.43712100	0.30402500	1.01846500
H	4.66531100	1.19758200	1.45859400
C	4.21980000	-0.69232100	2.09252700
C	3.14807600	-0.24300800	3.07868900
H	5.16546100	-0.89244000	2.62445800
H	3.90967200	-1.62310700	1.60607200
H	3.02474000	-0.99045000	3.87013400
H	3.41469300	0.70872000	3.55686500
H	2.19015500	-0.11875000	2.56666800
C	5.57200100	-0.08303100	0.15246600
C	5.88719900	0.98714400	-0.88585800
H	5.28738500	-1.01478300	-0.34779500
H	6.46651400	-0.29253000	0.76352500
H	6.75321000	0.69008400	-1.48726200
H	5.03248200	1.13339100	-1.55265200
H	6.12287200	1.94938100	-0.41245400
N	2.05387700	2.77106300	0.24981600
H	1.21370400	2.89271800	-0.31766900
C	1.69683300	3.04721900	1.65682300
C	0.41389100	2.32856400	2.06060800
H	1.58678700	4.13332100	1.81990400
H	2.53450500	2.71354000	2.28151700
H	0.17874800	2.52140500	3.11239100
H	-0.43687900	2.66918100	1.45747300
H	0.50163500	1.25060200	1.91714700
C	3.09495900	3.67906800	-0.26804200
C	3.19520200	3.60690900	-1.78897300
H	4.04764200	3.38668400	0.19048600
H	2.89458800	4.71913100	0.04221800
H	4.00659500	4.24749400	-2.15061300
H	3.38160000	2.57982400	-2.11569100
H	2.26237500	3.94297500	-2.25816600

2

C	-1.60413000	3.97782900	-0.46598300
C	-1.94849100	2.68209300	-0.08860200
C	-0.98905500	1.66034900	0.00515400
C	0.36868900	1.94691900	-0.28160900
C	0.68815200	3.25184300	-0.71490600
C	-0.27509700	4.25333900	-0.79267900
C	1.46265300	0.93009600	-0.18297200
C	1.24582700	-0.51088400	-0.32571800

C	-0.05765300	-1.09075400	-0.25249500
C	-0.22991800	-2.44762500	-0.50772200
H	-1.22817700	-2.87833500	-0.46461900
C	0.86371100	-3.27288400	-0.80597700
C	2.37443800	-1.37302000	-0.52173500
H	-2.36203300	4.75394000	-0.53073300
H	-2.99054400	2.44870200	0.11874800
H	1.69932700	3.48468200	-1.03085000
H	0.01194900	5.24611600	-1.12973300
H	0.71513500	-4.32798500	-1.01974900
C	3.73031700	-0.85168900	-0.41255300
C	2.75141700	1.36939200	-0.00710300
C	3.89728600	0.52369000	-0.09352700
H	2.93838100	2.41973400	0.19249300
C	5.19776600	1.05419400	0.08505300
C	6.31516000	0.25654800	-0.05987500
H	7.30922300	0.67302200	0.07713900
C	4.89408600	-1.64159000	-0.56401400
C	6.15740200	-1.10276200	-0.39261200
H	7.03230200	-1.73582500	-0.51310900
H	5.30168800	2.10841200	0.33136300
H	4.81179800	-2.69354900	-0.81343200
Si	-1.47868100	-0.08840700	0.43506100
C	-3.09310000	-0.51739300	-0.44625300
C	-4.10865600	-1.32517100	0.09611900
C	-3.28040300	-0.03276200	-1.75667300
C	-5.25880100	-1.63766000	-0.63317900
H	-4.01276000	-1.71894800	1.10275200
C	-4.42577900	-0.34114700	-2.49078600
H	-2.52135900	0.60245600	-2.20697600
C	-5.41996300	-1.14621400	-1.92920200
H	-6.02816100	-2.26312800	-0.18735700
H	-4.54405400	0.04775400	-3.49903600
H	-6.31443100	-1.38720800	-2.49792700
C	-1.53754700	-0.30932100	2.34647600
C	-1.63066900	-1.79400500	2.75545800
C	-0.22624900	0.26693900	2.92809700
C	-2.72888400	0.48121800	2.92650600
H	-2.55766900	-2.27136000	2.41941100
H	-0.79362500	-2.37504200	2.35163300
H	-1.60012600	-1.88409100	3.85113100
H	-0.10719400	1.33049900	2.69347500
H	-0.22657300	0.16426900	4.02293200
H	0.65561600	-0.26048800	2.54654800

H	-2.73566300	0.40840100	4.02388900
H	-2.66585200	1.54598500	2.66927600
H	-3.69316000	0.10752700	2.56419200
C	2.13910500	-2.74320900	-0.78313600
H	2.97781800	-3.40600000	-0.96364500

INT14

C	-0.68972000	-1.49659500	-2.29566000
C	-1.60949300	-1.68829200	-1.22978600
C	-2.68734900	-0.85765400	-0.93093100
C	-2.93071800	0.20930100	-1.87493900
C	-2.07259800	0.40577900	-2.96444600
C	-0.94236200	-0.39726600	-3.15773400
Si	-3.76160000	-1.08024400	0.64779900
C	-3.96089600	0.60771700	1.48985700
C	-3.07038900	1.66586900	1.23692400
C	-4.90259000	0.78966100	2.52028800
C	-4.97179700	1.98283900	3.24468100
C	-4.08840200	3.02538200	2.95907300
C	-3.13271100	2.86148900	1.95439100
H	-0.00209300	-2.27689100	-2.58802800
H	-2.27828700	1.21811800	-3.65470700
H	-0.33919300	-0.27869800	-4.05265300
H	-2.31868500	1.56747300	0.46099900
H	-5.58333200	-0.01307900	2.78458600
H	-5.71340900	2.09416200	4.03202300
H	-4.14267000	3.95806100	3.51484800
H	-2.44440200	3.66559900	1.71688100
O	-0.74331900	-4.88775600	0.67607600
S	-0.69599300	-4.19569800	-0.59515600
O	0.53085600	-4.05898100	-1.36602900
O	-1.43059500	-2.77682900	-0.32692200
C	-1.93408600	-5.02920900	-1.73677200
F	-2.37291400	-4.15731200	-2.65090500
F	-2.96169400	-5.49372900	-1.03109600
F	-1.31861300	-6.04050500	-2.34646300
C	-2.83033100	-2.05893000	1.98200200
C	-3.15574100	-3.35410100	2.41598600
C	-1.74905000	-1.41669000	2.61806300
C	-2.45379200	-3.97553700	3.45120600
H	-3.96203000	-3.90433500	1.94376900
C	-1.03425000	-2.03501400	3.64284800
H	-1.45468100	-0.41532400	2.31538400
C	-1.39477900	-3.31516900	4.07226300

H	-2.73150300	-4.97869000	3.76415400
H	-0.19033600	-1.52387000	4.09585400
H	-0.84663600	-3.79555500	4.87932300
C	-5.42284500	-1.92033400	0.12835100
C	-6.32782800	-2.25302300	1.33716800
C	-6.22901400	-1.00939900	-0.82218600
C	-5.08814700	-3.22294300	-0.63311400
H	-7.16908700	-2.87863700	1.00511900
H	-5.81002900	-2.79228300	2.13569200
H	-6.76159300	-1.34652000	1.77179900
H	-5.69737400	-0.81750200	-1.75843000
H	-7.18178600	-1.49757100	-1.07546200
H	-6.45899900	-0.03912200	-0.36931900
H	-6.01484100	-3.69433400	-0.99145700
H	-4.45822000	-3.02943900	-1.50827300
H	-4.56968400	-3.95726700	-0.01169800
C	-3.96219500	1.17016300	-1.71246600
C	-4.76573500	2.07773400	-1.60819700
C	-5.66254700	3.14839600	-1.34987400
C	-6.19254200	3.31896400	-0.05332200
C	-6.00281900	4.07500900	-2.35679300
C	-7.03847700	4.39014100	0.21936000
H	-5.92040200	2.61627100	0.72567600
C	-6.84901000	5.14402900	-2.07093600
H	-5.59726500	3.94446000	-3.35595800
C	-7.37023700	5.30626100	-0.78381500
H	-7.43557500	4.51343100	1.22352900
H	-7.10382900	5.85221100	-2.85500500
H	-8.02967900	6.14164400	-0.56444600
P	1.14513300	2.23580400	-0.52443700
P	2.60272300	-1.12746200	-0.74058000
C	3.68720100	-3.45724800	-4.62737000
C	3.67982200	-4.13621100	-3.40923600
C	3.40514900	-3.45680600	-2.21926100
C	3.12553000	-2.08362100	-2.23230400
C	3.11542700	-1.41242300	-3.47045200
C	3.40548400	-2.08747800	-4.65406200
H	3.38674300	-4.00605300	-1.28551500
H	2.87805400	-0.35204700	-3.50069300
C	-2.05746600	5.60878000	-0.26801400
C	-0.95561400	5.66318400	0.59312000
C	0.00510600	4.65256400	0.56662300
C	-0.11288000	3.57870700	-0.33372200
C	-1.22798400	3.53046500	-1.18162900

C	-2.19721700	4.53659300	-1.14847300
H	0.83541900	4.68809300	1.26520900
H	-1.34446600	2.68600700	-1.85267700
C	4.74305900	4.48986200	-2.42654600
C	4.26340400	4.91097700	-1.18355200
C	3.18904600	4.25312000	-0.58883200
C	2.58093600	3.16019200	-1.22487100
C	3.06711400	2.74915400	-2.47312800
C	4.14221400	3.40867000	-3.07180500
H	2.84775700	4.57538700	0.38835400
H	2.60165200	1.89946200	-2.96488500
C	3.13060100	-4.11698800	2.76767800
C	4.24404700	-3.74116200	2.00994800
C	4.09596600	-2.83919000	0.95851800
C	2.83214000	-2.30705500	0.65077100
C	1.72784100	-2.67357800	1.42713500
C	1.87583500	-3.58283600	2.47664900
H	4.96223100	-2.54415400	0.37196800
H	0.75144800	-2.24503100	1.22036900
H	5.90993100	4.57976800	2.74334500
C	3.91934300	0.99500600	0.57894400
C	4.01307400	0.04481000	-0.43998700
C	5.16287100	0.02912400	-1.27731800
H	5.23914400	-0.71617500	-2.06058300
C	6.17185900	0.94772400	-1.12466700
H	7.03441000	0.92803100	-1.78693600
C	6.11062000	1.92974700	-0.10619400
C	4.98359500	1.93668400	0.77696700
H	4.10782200	2.92986700	2.49347300
C	4.94974400	2.91507700	1.81078400
C	5.95941600	3.84152200	1.94729400
H	7.84955700	4.58147300	1.17419500
C	7.06154800	3.84215900	1.05884100
H	7.97606100	2.88830700	-0.63021000
C	7.13276400	2.90191000	0.05635200
H	3.20367000	-1.28051800	6.31742700
C	0.65098500	1.24095000	3.41276000
H	-0.16846900	1.30348100	4.12497400
C	0.52809800	1.82163600	2.17560000
H	-0.39593700	2.32804500	1.92713600
C	1.57579400	1.75510800	1.21171300
C	2.75140300	1.06684000	1.52478600
C	2.89322400	0.44963700	2.81366700
C	1.82833500	0.53684800	3.76834500

H	1.15265000	-0.00997300	5.74832800
C	1.96948600	-0.09123100	5.03466700
C	3.10946800	-0.79481200	5.35001600
H	5.05702200	-1.45228700	4.65610400
C	4.16316700	-0.88643500	4.40944300
H	4.87225100	-0.36067100	2.46673300
C	4.06237400	-0.27405200	3.18101200
H	3.90278300	-3.98912100	-5.55022500
H	-2.81448200	6.38756600	-0.23539300
H	5.58706300	4.99884700	-2.88433200
H	3.24384000	-4.82363600	3.58576800
H	3.88434100	-5.20323400	-3.37876700
H	3.40354300	-1.54763500	-5.59771000
H	-0.85146300	6.48758600	1.29398300
H	-3.06979300	4.46613800	-1.78992300
H	1.00392700	-3.87173000	3.05164800
H	5.22531400	-4.14902600	2.23947100
H	4.51400800	3.07053000	-4.03542100
H	4.74074900	5.73804300	-0.66616900
Pd	0.64904100	0.09341800	-1.37747200

TS9

C	0.24542800	1.50695600	-2.56982900
C	0.86656700	1.79455300	-1.33633500
C	2.19818300	1.49970000	-0.99006300
C	2.85723400	0.66065100	-1.93408200
C	2.21241600	0.23061400	-3.12353700
C	0.93217600	0.65431800	-3.44397000
Si	2.95217200	2.14806400	0.65035200
C	3.83822500	0.72487300	1.55007700
C	3.57700000	-0.61794300	1.22957200
C	4.68638400	0.96527200	2.64819500
C	5.26449100	-0.08312600	3.36978200
C	5.00273600	-1.40757900	3.01370300
C	4.15161300	-1.67389800	1.93973000
H	-0.68009500	1.98884500	-2.85557700
H	2.76481700	-0.40776900	-3.80548400
H	0.47597400	0.36413000	-4.38617500
H	2.92015900	-0.84908800	0.40067400
H	4.89129900	1.98118900	2.96805000
H	5.91708900	0.13790600	4.21093800
H	5.45813200	-2.22488600	3.56709400
H	3.94061000	-2.69717300	1.64391700
O	-0.35247700	5.59232400	0.28592100

S	-0.67336300	4.37279600	-0.45721200
O	-1.61231800	3.39575800	0.14354900
O	0.56779600	3.69722900	-1.05600400
C	-1.55836200	4.96962100	-1.98547700
F	-1.78166100	3.94726100	-2.82845700
F	-0.82679500	5.89036600	-2.61815500
F	-2.73607500	5.50383800	-1.64290600
C	1.51605900	2.55481900	1.81351500
C	1.16470000	3.83984900	2.24870300
C	0.76819800	1.46713300	2.31846100
C	0.11929700	4.03823300	3.15518300
H	1.67450700	4.71087100	1.85588600
C	-0.27694700	1.65888300	3.22461800
H	1.03865300	0.44985200	2.05215800
C	-0.59773200	2.95063800	3.64992200
H	-0.14288400	5.04935300	3.45261600
H	-0.83666200	0.80344800	3.58948300
H	-1.41105300	3.10503600	4.35484700
C	4.13478000	3.62579700	0.26649500
C	4.62934800	4.33707100	1.54822100
C	5.37326700	3.10039800	-0.49450200
C	3.42289400	4.66415100	-0.63027500
H	5.18204000	5.24515300	1.26779100
H	3.81702400	4.64076500	2.21502300
H	5.32159800	3.71343900	2.12234100
H	5.10692900	2.66965600	-1.46438000
H	6.06911700	3.93123000	-0.68133300
H	5.91366700	2.33296500	0.07151700
H	4.12903300	5.46960900	-0.88005600
H	3.07311800	4.22040400	-1.56717600
H	2.55082700	5.11722800	-0.15157600
C	4.17394100	0.16767100	-1.71943100
C	5.26266300	-0.34461200	-1.54829900
C	6.49946800	-0.96016900	-1.21548200
C	7.02684600	-0.80586800	0.08322400
C	7.18915100	-1.75926800	-2.14935800
C	8.21518300	-1.44180600	0.43161100
H	6.48910700	-0.20266600	0.80582600
C	8.37746000	-2.39040900	-1.78895500
H	6.78304900	-1.87563700	-3.14996900
C	8.89376600	-2.23454300	-0.49887300
H	8.60945100	-1.32175800	1.43701000
H	8.90264000	-3.00451400	-2.51554800
H	9.82037500	-2.72937200	-0.22077400

P	0.42704000	-2.15551400	-0.55940600
P	-2.96799900	0.26913300	-0.12704100
C	-4.55427300	2.80169700	-3.70671900
C	-4.82471800	3.19313300	-2.39602500
C	-4.39408200	2.41258900	-1.32126200
C	-3.68204100	1.22583500	-1.54397300
C	-3.39865800	0.84893400	-2.86856400
C	-3.83875100	1.62421000	-3.94004000
H	-4.60186800	2.73911000	-0.30855100
H	-2.85142000	-0.06693400	-3.06329700
C	4.06108600	-5.04577800	-0.10226800
C	2.91629500	-5.28553000	0.66330600
C	1.80728200	-4.44458800	0.55169000
C	1.82615800	-3.34986600	-0.32872900
C	2.97859000	-3.12770700	-1.09899800
C	4.08936900	-3.96520100	-0.98613400
H	0.92960200	-4.63043700	1.16399500
H	3.02124700	-2.27340000	-1.76696100
C	-1.96720400	-4.19904600	-3.98394800
C	-1.32227800	-5.00745000	-3.04430300
C	-0.61135900	-4.43136300	-1.99219800
C	-0.54442000	-3.03580200	-1.86001900
C	-1.17140300	-2.23476300	-2.82453500
C	-1.88823100	-2.80972700	-3.87460500
H	-0.11480300	-5.07020000	-1.27009200
H	-1.08686900	-1.15603300	-2.74220500
C	-5.67691800	1.60160200	3.39757900
C	-6.17170700	0.68560300	2.46399800
C	-5.37176200	0.27106300	1.40072400
C	-4.06557200	0.76612200	1.26341800
C	-3.58271000	1.70037500	2.18772800
C	-4.38658700	2.11273800	3.25278400
H	-5.75869400	-0.44824000	0.68443300
H	-2.59009600	2.11594400	2.06420900
H	-2.41167700	-7.09611500	0.78835800
C	-2.82968600	-2.51883000	0.20862100
C	-3.47088200	-1.47913000	-0.46176400
C	-4.49633300	-1.77756900	-1.40332000
H	-5.00752500	-0.96616800	-1.90848100
C	-4.83536600	-3.07399200	-1.70013700
H	-5.60827300	-3.28278500	-2.43602800
C	-4.18539000	-4.15785000	-1.05960000
C	-3.19275900	-3.87766900	-0.06691800
H	-1.83654000	-4.77377100	1.36464300

C	-2.57607900	-4.97423600	0.59750500
C	-2.89865900	-6.27299600	0.27249600
H	-4.10315700	-7.57456700	-0.98037500
C	-3.86092700	-6.54541800	-0.72950900
H	-5.24005200	-5.70510900	-2.14066100
C	-4.49337900	-5.50721400	-1.37533500
H	-3.70498100	-1.52670200	6.26130900
C	-0.05078300	-1.89869300	3.46367100
H	0.64479900	-1.74072500	4.28436300
C	0.42245800	-2.07402400	2.19052700
H	1.49337300	-2.05270200	2.03050600
C	-0.45038200	-2.26645100	1.07402500
C	-1.82570600	-2.27240000	1.29536000
C	-2.34326500	-2.11084900	2.63039800
C	-1.44431300	-1.89946400	3.72423100
H	-1.26008400	-1.51771300	5.84353100
C	-1.96054800	-1.68940700	5.02959400
C	-3.31790400	-1.69792800	5.26062800
H	-5.28127500	-1.94446500	4.37222800
C	-4.21058400	-1.93750600	4.19043600
H	-4.43524600	-2.32295200	2.10626300
C	-3.73639500	-2.14724200	2.91447300
H	-4.88910200	3.41210300	-4.54092800
H	4.92923100	-5.69170800	-0.00225900
H	-2.52492300	-4.65136100	-4.79978500
H	-6.29967500	1.91948800	4.22973700
H	-5.36332000	4.11636300	-2.20234600
H	-3.62059600	1.30910700	-4.95742900
H	2.88779700	-6.12524100	1.35315400
H	4.98388400	-3.75324500	-1.56498000
H	-4.00016300	2.83601000	3.96593900
H	-7.17993700	0.29246700	2.56677700
H	-2.38130300	-2.17390300	-4.60586000
H	-1.38256400	-6.08916200	-3.12343800
Pd	-0.65464600	1.06643600	-0.26606000

INT15

C	-1.03782600	-2.20744900	-2.31660400
C	-1.26736100	-1.51604800	-1.11660100
C	-2.57412400	-1.22619500	-0.67837100
C	-3.62385500	-1.46455500	-1.62675900
C	-3.37910900	-2.11868400	-2.84799500
C	-2.09384900	-2.54199300	-3.16420300
Si	-3.04526000	-0.82359600	1.13763600

C	-3.85135700	0.88569300	1.30643400
C	-3.99722200	1.77145500	0.22506400
C	-4.31990500	1.31844500	2.56387900
C	-4.90378700	2.57570200	2.73523600
C	-5.03340800	3.43850500	1.64355500
C	-4.57809200	3.03182400	0.38863600
H	-0.02928400	-2.49574500	-2.59559100
H	-4.20645000	-2.28620800	-3.53085900
H	-1.90412500	-3.08932100	-4.08394000
H	-3.67108600	1.47088100	-0.76307300
H	-4.22613100	0.66581100	3.42827000
H	-5.25902600	2.87882500	3.71718500
H	-5.49226100	4.41593000	1.76998200
H	-4.68152600	3.68663700	-0.47121600
O	1.26500300	-4.99866100	1.49415000
S	0.68331400	-4.39976300	0.28338400
O	1.24468900	-3.01825500	0.01718300
O	-0.76582100	-4.51855000	0.07154500
C	1.43997200	-5.34130200	-1.13801000
F	1.23780600	-4.68016300	-2.29995600
F	0.88838800	-6.55380500	-1.24520900
F	2.76108500	-5.48177900	-0.96500700
C	-1.50670800	-0.82671400	2.23271500
C	-0.74255700	-2.00703200	2.32003100
C	-1.17064900	0.22358500	3.10013800
C	0.31827100	-2.12700800	3.21547000
H	-1.00237400	-2.85425500	1.69824500
C	-0.09345500	0.12254800	3.98411000
H	-1.75787000	1.13339100	3.09375500
C	0.65462900	-1.05283300	4.04271000
H	0.87864000	-3.05493400	3.24657700
H	0.16239500	0.96518200	4.62215300
H	1.49991400	-1.13120100	4.71915000
C	-4.21985800	-2.22036200	1.86750300
C	-3.83957200	-2.49834100	3.34330900
C	-5.71263200	-1.82375700	1.85887100
C	-4.04865100	-3.53238600	1.06829800
H	-4.55195400	-3.22008400	3.76773600
H	-2.83830200	-2.92232800	3.44828100
H	-3.87918400	-1.59527800	3.96558300
H	-6.09577900	-1.67030200	0.85030700
H	-6.30439700	-2.62872700	2.31859800
H	-5.90290800	-0.91084300	2.43389500
H	-4.61573800	-4.33742200	1.55829500

H	-4.43103200	-3.43603400	0.04724100
H	-3.00554800	-3.85812500	0.99632700
C	-4.93822800	-0.96066000	-1.41196700
C	-6.02814800	-0.43149500	-1.30217600
C	-7.27268900	0.21670000	-1.06809500
C	-7.46656300	0.95664100	0.11777200
C	-8.31973800	0.14060900	-2.00813200
C	-8.67912900	1.60078400	0.34729400
H	-6.66288200	1.01894300	0.84183500
C	-9.52831200	0.78954700	-1.76751600
H	-8.17226200	-0.43079000	-2.91977300
C	-9.71275500	1.52150500	-0.59071300
H	-8.81568200	2.16874900	1.26366700
H	-10.32952100	0.72293600	-2.49877300
H	-10.65744900	2.02587300	-0.40586400
P	0.30442500	1.22794800	-1.15378600
P	2.97662000	-0.53503800	0.22277500
C	5.49948900	-3.67144100	-2.12633400
C	6.02269200	-3.07258000	-0.97754100
C	5.26431100	-2.14503100	-0.26431900
C	3.97429700	-1.79098500	-0.69710500
C	3.45430500	-2.41570500	-1.83706000
C	4.21066400	-3.34709200	-2.54824300
H	5.67589500	-1.69581100	0.63433800
H	2.43261900	-2.22597900	-2.13782800
C	-3.37888300	3.05363900	-3.32117700
C	-2.62777500	3.84892900	-2.45317200
C	-1.54964900	3.30441400	-1.75577700
C	-1.20751500	1.95234400	-1.92031700
C	-1.93942800	1.17163300	-2.82693400
C	-3.02604500	1.71675900	-3.51101400
H	-0.98949500	3.93584200	-1.07462100
H	-1.67339300	0.13752300	-2.99766200
C	3.12362200	2.18359200	-4.71517500
C	2.52727100	3.22559200	-3.99864500
C	1.69715100	2.94452800	-2.91661700
C	1.47548400	1.61671000	-2.52202900
C	2.05929800	0.57846600	-3.25481300
C	2.88232500	0.86011200	-4.34685000
H	1.23830700	3.76089700	-2.36898800
H	1.87279300	-0.44874700	-2.96800300
C	4.29364600	-1.55058100	4.55169700
C	4.36779700	-0.22842900	4.11120700
C	3.97606600	0.09931500	2.81137200

C	3.49128700	-0.88884500	1.94975800
C	3.39630300	-2.21728200	2.40171500
C	3.80805700	-2.54185300	3.69254800
H	4.05888800	1.12301900	2.47348700
H	2.99238800	-2.99001200	1.75663100
H	3.19180500	6.87133200	-0.98803600
C	3.18407000	2.32824700	-0.02275000
C	3.77744400	1.08495000	-0.25455300
C	4.98099000	1.03121700	-1.01831300
H	5.45094400	0.07581400	-1.20495000
C	5.55782700	2.15637500	-1.54613900
H	6.47276000	2.07632900	-2.12806900
C	4.95904000	3.42619500	-1.37405200
C	3.76208700	3.51790000	-0.59753900
H	2.23411500	4.89958500	0.09430600
C	3.14885900	4.79895500	-0.47702200
C	3.68644600	5.90928100	-1.08958000
H	5.29370600	6.69420700	-2.32205400
C	4.87734100	5.80974800	-1.84799300
H	6.41116900	4.49424400	-2.56649100
C	5.49968800	4.59014800	-1.98155800
H	2.44952100	4.90432900	5.58982800
C	-0.34087400	3.26640700	2.30485700
H	-1.22769500	3.53355200	2.87378500
C	-0.47432000	2.62319300	1.10253500
H	-1.46901300	2.37359800	0.75323900
C	0.66399500	2.26825100	0.32352700
C	1.94693300	2.54063000	0.80021400
C	2.09927500	3.18480700	2.07928000
C	0.93933900	3.54247100	2.84001400
H	0.19886200	4.41415900	4.67412600
C	1.09310400	4.16217600	4.10943000
C	2.34247100	4.43571500	4.61566300
H	4.47958200	4.34672800	4.24884000
C	3.49343300	4.11406100	3.85676600
H	4.26823200	3.29604200	2.04917700
C	3.37484300	3.51601700	2.62222900
H	6.08564000	-4.40400800	-2.67444100
H	-4.23090800	3.47434400	-3.84781100
H	3.77168200	2.40548400	-5.55863500
H	4.60845100	-1.80872300	5.55942100
H	7.01804200	-3.33451600	-0.62910900
H	3.77148500	-3.84587800	-3.40686300
H	-2.88554700	4.89442200	-2.30744400

H	-3.60041500	1.08486500	-4.18156800
H	3.73254100	-3.57221700	4.02850000
H	4.73623500	0.55280900	4.77081800
H	3.33742800	0.04298300	-4.89952400
H	2.71740100	4.25903400	-4.27325700
Pd	0.54425400	-0.92253300	-0.34393300

INT16

C	1.17966000	-2.08154000	-2.40494000
C	1.44004000	-1.00011000	-1.56253000
C	2.71109000	-0.79133000	-0.99107000
C	3.58995000	-1.91987000	-0.99882000
C	3.27262000	-3.07056000	-1.74769000
C	2.11546000	-3.11313000	-2.51343000
Si	3.36514000	0.90124000	-0.35365000
H	0.22584000	-2.17588000	-2.91256000
H	3.96034000	-3.90990000	-1.73574000
H	1.90126000	-3.97691000	-3.13601000
C	2.30726000	2.19420000	-1.30687000
C	2.72814000	3.52225000	-1.50757000
C	1.13533000	1.81451000	-1.99782000
C	2.01601000	4.39193000	-2.33928000
H	3.65163000	3.87444000	-1.05775000
C	0.37275000	2.70024000	-2.77540000
H	1.06062000	0.74503000	-2.30750000
C	0.82119000	3.99889000	-2.95628000
H	2.39795000	5.39516000	-2.50893000
H	-0.51836000	2.33716000	-3.28009000
H	0.27248000	4.69460000	-3.58358000
C	4.79011000	-1.91186000	-0.23294000
C	5.81739000	-1.90433000	0.41822000
C	7.04611000	-1.79383000	1.13099000
C	7.54527000	-2.86429000	1.89763000
C	7.77873000	-0.59057000	1.06065000
C	8.75100000	-2.73011000	2.58194000
H	6.98229000	-3.79136000	1.94871000
C	8.98246000	-0.46895000	1.74947000
H	7.39945000	0.22932000	0.46089000
C	9.47157000	-1.53421000	2.51111000
H	9.13049000	-3.56001000	3.17124000
H	9.54256000	0.45994000	1.68817000
H	10.41188000	-1.43447000	3.04582000
P	-1.74378000	1.68214000	0.25569000
P	-1.45097000	-1.72424000	-0.32551000

C	1.20956000	-5.46753000	0.34809000
C	0.12790000	-5.55308000	-0.52928000
C	-0.70358000	-4.45052000	-0.73677000
C	-0.45872000	-3.24766000	-0.05965000
C	0.63489000	-3.16902000	0.81706000
C	1.46151000	-4.27050000	1.02296000
H	-1.52322000	-4.53079000	-1.44117000
H	0.85432000	-2.23904000	1.32540000
C	-1.54135000	6.30524000	-0.03656000
C	-2.78521000	5.67322000	-0.11014000
C	-2.86826000	4.28157000	-0.07114000
C	-1.70176000	3.50392000	0.02787000
C	-0.45866000	4.14661000	0.09799000
C	-0.38010000	5.53874000	0.07018000
H	-3.84230000	3.80533000	-0.12301000
H	0.45222000	3.56409000	0.16190000
C	-2.01417000	1.40765000	4.87665000
C	-2.87391000	2.26307000	4.18225000
C	-2.80820000	2.34703000	2.79351000
C	-1.88888000	1.56092000	2.08197000
C	-1.02614000	0.71175000	2.78565000
C	-1.08667000	0.63519000	4.17656000
H	-3.47461000	3.02214000	2.26691000
H	-0.31752000	0.09853000	2.24410000
C	-4.14171000	-2.58637000	-3.99973000
C	-4.33562000	-3.29371000	-2.81055000
C	-3.53288000	-3.03209000	-1.70185000
C	-2.51804000	-2.06282000	-1.77585000
C	-2.33604000	-1.35187000	-2.97015000
C	-3.14245000	-1.61515000	-4.07751000
H	-3.71079000	-3.56249000	-0.77099000
H	-1.57432000	-0.57903000	-3.02572000
H	-6.97113000	1.31670000	3.67240000
C	-3.66719000	-0.71961000	1.14710000
C	-2.60212000	-1.62594000	1.12140000
C	-2.30806000	-2.39739000	2.28031000
H	-1.50299000	-3.12147000	2.25494000
C	-3.02893000	-2.23801000	3.43883000
H	-2.78634000	-2.83409000	4.31479000
C	-4.08286000	-1.29535000	3.51915000
C	-4.42291000	-0.54074000	2.35051000
H	-5.75452000	0.97975000	1.56365000
C	-5.48655000	0.40080000	2.44023000
C	-6.16514000	0.59024000	3.62276000

H	-6.36282000	0.00947000	5.70497000
C	-5.81986000	-0.15207000	4.77830000
H	-4.53077000	-1.65288000	5.60505000
C	-4.80175000	-1.07658000	4.72428000
H	-8.31905000	-1.54011000	-2.90506000
C	-4.70162000	1.29781000	-2.52999000
H	-4.92891000	1.76159000	-3.48651000
C	-3.63140000	1.73196000	-1.79083000
H	-3.01853000	2.54554000	-2.16515000
C	-3.31577000	1.13601000	-0.53416000
C	-4.05986000	0.05316000	-0.07605000
C	-5.21470000	-0.38220000	-0.81429000
C	-5.53320000	0.24968000	-2.05922000
H	-6.88444000	0.29554000	-3.74615000
C	-6.65913000	-0.19240000	-2.80131000
C	-7.45525000	-1.21353000	-2.33343000
H	-7.77878000	-2.64317000	-0.73592000
C	-7.14740000	-1.83895000	-1.10279000
H	-5.82900000	-1.93633000	0.57051000
C	-6.05312000	-1.44054000	-0.36643000
H	1.85870000	-6.32523000	0.49875000
H	-1.47978000	7.38941000	-0.06328000
H	-2.06832000	1.34609000	5.95965000
H	-4.77575000	-2.78526000	-4.85858000
H	-0.06966000	-6.47863000	-1.06252000
H	2.31105000	-4.18566000	1.69414000
H	-3.69360000	6.26325000	-0.19233000
H	0.59221000	6.01997000	0.12010000
H	-2.99686000	-1.05263000	-4.99515000
H	-5.12651000	-4.03370000	-2.73853000
H	-0.41477000	-0.03274000	4.70783000
H	-3.60045000	2.86206000	4.72286000
Pd	-0.09943000	0.22212000	-0.78460000
C	5.11540000	1.28123000	-0.97170000
C	5.69883000	0.56570000	-2.03331000
C	5.84568000	2.36804000	-0.44891000
C	6.96318000	0.89369000	-2.52510000
H	5.16878000	-0.27151000	-2.47704000
C	7.11004000	2.70495000	-0.93912000
H	5.43345000	2.96789000	0.35762000
C	7.67734000	1.95998000	-1.97472000
H	7.39259000	0.31186000	-3.33601000
H	7.65075000	3.54363000	-0.50865000
H	8.66434000	2.21119000	-2.35295000

C	3.18727000	1.01731000	1.58700000
C	2.47678000	-0.26302000	2.07161000
C	4.54419000	1.09475000	2.32070000
C	2.32461000	2.23283000	1.98161000
H	1.51716000	-0.39506000	1.56406000
H	3.08051000	-1.15732000	1.88454000
H	2.28052000	-0.20030000	3.15132000
H	5.05443000	2.04856000	2.16463000
H	4.37399000	0.99637000	3.40191000
H	5.22705000	0.29636000	2.01803000
H	2.23401000	2.29539000	3.07476000
H	2.75230000	3.17975000	1.62995000
H	1.30815000	2.15500000	1.58097000

TS10

C	1.19809300	-2.01098500	-2.52111700
C	1.51912300	-0.88487200	-1.75504500
C	2.73828300	-0.76352800	-1.05978900
C	3.56441900	-1.92409300	-1.00963900
C	3.21073100	-3.07902400	-1.73689800
C	2.06225500	-3.10629400	-2.52014300
Si	3.35857600	0.91450600	-0.36454400
H	0.26975800	-2.05528900	-3.07982800
H	3.86084700	-3.94665200	-1.68693700
H	1.81451600	-3.99498100	-3.09248900
C	2.26598600	2.18368100	-1.27914400
C	2.72302300	3.48050400	-1.58160000
C	1.03811100	1.79101000	-1.84318400
C	1.99387400	4.32702400	-2.41885100
H	3.67713900	3.82317000	-1.19182700
C	0.31831000	2.61868800	-2.71817600
H	1.14202500	0.46457000	-2.15804000
C	0.79951300	3.89368800	-3.00430600
H	2.37183600	5.32198300	-2.63783100
H	-0.60713600	2.26810800	-3.16747400
H	0.24845900	4.54836200	-3.67337900
C	4.75941100	-1.93271000	-0.23612500
C	5.79486900	-1.91297400	0.40133100
C	7.02582400	-1.79922900	1.10896100
C	7.52605500	-2.86955600	1.87518900
C	7.75697100	-0.59507600	1.03709500
C	8.73143300	-2.73406900	2.55935200
H	6.96348000	-3.79680800	1.92678500
C	8.96096500	-0.47260900	1.72538100

H	7.37635500	0.22456100	0.43782800
C	9.45061300	-1.53732200	2.48755700
H	9.11179100	-3.56315000	3.14914900
H	9.52049300	0.45653400	1.66381800
H	10.39079300	-1.43643600	3.02225400
P	-1.75847500	1.67391300	0.22709600
P	-1.48188300	-1.73203700	-0.34235800
C	1.19015700	-5.47171900	0.32510900
C	0.11047100	-5.55868200	-0.55512500
C	-0.72264700	-4.45756900	-0.76336500
C	-0.48156600	-3.25303800	-0.08687800
C	0.61178900	-3.17282500	0.78989400
C	1.43907800	-4.27398100	0.99944000
H	-1.54456500	-4.54046100	-1.46499100
H	0.82629100	-2.24354900	1.30194200
C	-1.56439900	6.29894200	-0.05988900
C	-2.80642000	5.66350800	-0.13298600
C	-2.88533700	4.27124600	-0.09803200
C	-1.71619300	3.49658100	0.00027300
C	-0.47499800	4.14330900	0.07491800
C	-0.40104300	5.53551100	0.04655400
H	-3.85821000	3.79298200	-0.15203100
H	0.43790900	3.56508600	0.14092500
C	-2.03579700	1.40341100	4.84836500
C	-2.89321100	2.25756800	4.14961000
C	-2.82309500	2.33892600	2.76086800
C	-1.90145100	1.55049800	2.05350100
C	-1.04250200	0.70162800	2.76115500
C	-1.10725700	0.62875600	4.15219400
H	-3.48779100	3.01340400	2.23159600
H	-0.33357000	0.08604500	2.22287100
C	-4.16360500	-2.58984800	-4.02571400
C	-4.36102900	-3.30014500	-2.83892000
C	-3.55989000	-3.04268200	-1.72823700
C	-2.54417900	-2.07486400	-1.79571800
C	-2.35958800	-1.35986800	-2.98797900
C	-3.16338900	-1.61910800	-4.09840000
H	-3.74031600	-3.57499000	-0.79883100
H	-1.60202900	-0.58252700	-3.03965500
H	-6.99434100	1.31424900	3.64905300
C	-3.69187500	-0.72905600	1.12618900
C	-2.63579700	-1.64495900	1.10032100
C	-2.33974400	-2.41132400	2.26075500
H	-1.53692800	-3.13828800	2.23490700

C	-3.05461000	-2.24281900	3.42151400
H	-2.81119600	-2.83460700	4.30020500
C	-4.10666800	-1.29814000	3.49921900
C	-4.44587000	-0.54437200	2.32966600
H	-5.77624400	0.97649800	1.54147900
C	-5.50838000	0.39820300	2.41861600
C	-6.18803000	0.58800100	3.60056600
H	-6.38804700	0.00793600	5.68278100
C	-5.84399800	-0.15373300	4.75677700
H	-4.55540900	-1.65404600	5.58497800
C	-4.82573700	-1.07790500	4.70384300
H	-8.33977100	-1.54298500	-2.92860200
C	-4.72202600	1.29441800	-2.55240700
H	-4.94991400	1.76001200	-3.50787100
C	-3.64891200	1.72459300	-1.81514500
H	-3.03474700	2.53686200	-2.18979500
C	-3.33130500	1.12570000	-0.56002100
C	-4.07906200	0.04562400	-0.09855500
C	-5.23555400	-0.38570400	-0.83701000
C	-5.55419000	0.24679200	-2.08167700
H	-6.90540700	0.29325100	-3.76871200
C	-6.68030300	-0.19487200	-2.82393400
C	-7.47630500	-1.21627800	-2.35653100
H	-7.80011300	-2.64637800	-0.75938500
C	-7.16879600	-1.84193500	-1.12585900
H	-5.85039400	-1.93966000	0.54741900
C	-6.07478100	-1.44360300	-0.38924200
H	1.83839000	-6.32952100	0.47949900
H	-1.50579200	7.38328300	-0.08635200
H	-2.09294500	1.34404200	5.93130900
H	-4.79607000	-2.78548900	-4.88650400
H	-0.08573400	-6.48533000	-1.08711600
H	2.28596900	-4.18848400	1.67408500
H	-3.71673600	6.25075200	-0.21362200
H	0.57009700	6.01894900	0.09668200
H	-3.01630600	-1.05305400	-5.01369800
H	-5.15329600	-4.03910400	-2.77078500
H	-0.43767800	-0.03893000	4.68664400
H	-3.62153700	2.85773800	4.68641200
Pd	-0.13357500	0.24382200	-0.81123200
C	5.10152300	1.28948400	-0.98920100
C	5.67854600	0.56806800	-2.05062000
C	5.83576300	2.37348100	-0.46935100
C	6.94221000	0.89086900	-2.54682600

H	5.14394800	-0.26763300	-2.49164200
C	7.09914400	2.70525300	-0.96386500
H	5.42586300	2.97612300	0.33642000
C	7.66028300	1.95648700	-2.00005300
H	7.36797500	0.30693400	-3.35814000
H	7.64391800	3.54330300	-0.53744800
H	8.64658300	2.20470200	-2.38204700
C	3.17146500	1.00415300	1.57032900
C	2.45570300	-0.27497000	2.04712700
C	4.52556700	1.08427800	2.30682000
C	2.30736100	2.22163300	1.96082600
H	1.49974000	-0.40313500	1.53133500
H	3.05919000	-1.17034300	1.86358600
H	2.25051100	-0.21510300	3.12533600
H	5.03550300	2.03770500	2.14647200
H	4.35417700	0.99087400	3.38828900
H	5.20954400	0.28508100	2.00866400
H	2.21384600	2.28379900	3.05374500
H	2.73736000	3.16765400	1.61005300
H	1.29337100	2.14429300	1.55518600

INT17

C	1.32102400	-1.78095200	-2.92994000
C	1.73532700	-0.59850500	-2.29056200
C	2.75801200	-0.58350700	-1.30776200
C	3.39565500	-1.82818500	-1.03724400
C	2.97045500	-3.00559300	-1.68454000
C	1.93430000	-2.98780900	-2.61472200
Si	3.32417300	1.05357600	-0.47268600
H	0.53960900	-1.73955300	-3.68194500
H	3.47445700	-3.93749500	-1.45147000
H	1.62348300	-3.90895300	-3.09559300
C	2.18731600	2.36040700	-1.25615800
C	2.75725800	3.50240700	-1.85900000
C	0.80490800	2.15605600	-1.43603900
C	2.00074400	4.38405400	-2.63205700
H	3.82180400	3.68711000	-1.74963200
C	0.05842500	3.00207400	-2.26221300
H	1.37899200	0.34248400	-2.70585500
C	0.65303900	4.11620600	-2.86138000
H	2.47165600	5.25592000	-3.07767800
H	-0.99471200	2.81404800	-2.44174700
H	0.05805800	4.77053200	-3.49334100
C	4.53425800	-1.89766300	-0.18446800

C	5.57374800	-1.93119600	0.44611300
C	6.80963300	-1.87721600	1.15124200
C	7.25320700	-2.96578000	1.92684100
C	7.60554300	-0.71508000	1.06544700
C	8.46612100	-2.88973400	2.60661500
H	6.64095500	-3.86038500	1.98884500
C	8.81633500	-0.65204800	1.74949300
H	7.26882500	0.11915500	0.45951600
C	9.24923600	-1.73467300	2.52089000
H	8.80252600	-3.73230600	3.20393400
H	9.42523900	0.24465100	1.67760400
H	10.19502600	-1.68000700	3.05239600
P	-1.73285800	1.67907800	0.36067600
P	-1.37311600	-1.71466700	-0.43822700
C	1.25355600	-5.49197600	0.22876400
C	0.26074000	-5.51935400	-0.75227800
C	-0.54402400	-4.39996000	-0.97542400
C	-0.36233300	-3.23509400	-0.21584000
C	0.64718800	-3.21369800	0.75951800
C	1.44514500	-4.33409400	0.98603200
H	-1.30207800	-4.43794600	-1.74933800
H	0.81110900	-2.32111500	1.35025600
C	-1.86430500	6.31282200	0.58117700
C	-3.04670300	5.59643700	0.39017600
C	-3.01374100	4.20622700	0.26987900
C	-1.79005700	3.51724300	0.33133200
C	-0.60755100	4.24542200	0.53403700
C	-0.64694600	5.63280400	0.65714800
H	-3.94437400	3.66672400	0.12878300
H	0.34668000	3.73749000	0.57385300
C	-1.98408200	0.93030900	4.92968600
C	-2.84525100	1.84456800	4.31798700
C	-2.77371700	2.06558000	2.94474600
C	-1.84585600	1.35546700	2.16424300
C	-0.98423600	0.44472100	2.78449800
C	-1.05084000	0.23393700	4.16094600
H	-3.44180500	2.78643500	2.48684300
H	-0.26967500	-0.10738800	2.19089000
C	-3.95729400	-2.38223600	-4.22903800
C	-4.15978100	-3.18492700	-3.10341900
C	-3.38608200	-2.99404200	-1.96012100
C	-2.39205700	-2.00252200	-1.93389100
C	-2.20062800	-1.19678800	-3.06622600
C	-2.97862500	-1.38704800	-4.20854000

H	-3.57070800	-3.59881100	-1.07685900
H	-1.46007800	-0.40203000	-3.04602800
H	-6.97297400	1.04032200	3.63768800
C	-3.62707400	-0.84573900	1.04922300
C	-2.57231700	-1.75858500	0.97811300
C	-2.31898900	-2.61755900	2.08252000
H	-1.52460800	-3.35094600	2.02371100
C	-3.06251500	-2.53226800	3.23465000
H	-2.84787800	-3.19491000	4.06922500
C	-4.10498800	-1.58296200	3.36184000
C	-4.41048400	-0.74286000	2.24352000
H	-5.71459400	0.84023500	1.53655500
C	-5.46855100	0.19953700	2.37608400
C	-6.17128600	0.31207000	3.55458800
H	-6.42060000	-0.41210300	5.58576100
C	-5.85818300	-0.51304900	4.66214100
H	-4.60249900	-2.08370400	5.40647400
C	-4.84793100	-1.44236600	4.56392200
H	-8.17463500	-1.47985000	-3.13302000
C	-4.65022500	1.42453800	-2.48393100
H	-4.88438300	1.96382200	-3.39809000
C	-3.60122200	1.82705800	-1.69909600
H	-3.02611700	2.69758000	-1.99208100
C	-3.27240100	1.13488500	-0.49451400
C	-3.99748400	0.00421700	-0.12747000
C	-5.13099700	-0.40059300	-0.91562500
C	-5.45194800	0.31507400	-2.11323100
H	-6.78176800	0.45258300	-3.81222800
C	-6.55500600	-0.09934900	-2.90375000
C	-7.32806700	-1.17389800	-2.52534600
H	-7.63337900	-2.72726600	-1.04401400
C	-7.01969400	-1.88131100	-1.34002800
H	-5.72049100	-2.06926900	0.34050200
C	-5.94674500	-1.51056600	-0.55955300
H	1.87637900	-6.36539700	0.39953700
H	-1.89164600	7.39489800	0.67122100
H	-2.04164800	0.76336900	6.00125000
H	-4.56914400	-2.52585300	-5.11469900
H	0.10834200	-6.41467000	-1.34852600
H	2.22375000	-4.29431700	1.74229000
H	-3.99906200	6.11587900	0.33537900
H	0.27862200	6.18146700	0.80384000
H	-2.82802900	-0.75006200	-5.07544300
H	-4.93484500	-3.94509700	-3.10815700

H	-0.37759300	-0.47971600	4.62672000
H	-3.57810000	2.38455000	4.90948500
Pd	-0.10774200	0.43190900	-0.76577400
C	5.09684500	1.41670700	-1.01363400
C	5.74657200	0.62444100	-1.97762300
C	5.81305500	2.50679000	-0.48083000
C	7.05873500	0.89023300	-2.37340100
H	5.23025100	-0.22219400	-2.41986800
C	7.12518600	2.77971700	-0.87232800
H	5.34487500	3.16219000	0.24953600
C	7.75454800	1.96499800	-1.81652100
H	7.53895800	0.25457700	-3.11222700
H	7.65427200	3.62513800	-0.44079500
H	8.77768300	2.16983500	-2.11935300
C	3.13285500	1.00915800	1.47188700
C	2.42067300	-0.28639700	1.90242500
C	4.48317900	1.07849600	2.21485300
C	2.26430900	2.20277700	1.92322200
H	1.49489400	-0.42750100	1.33585000
H	3.04604900	-1.16920900	1.74624500
H	2.15845600	-0.23875000	2.96905400
H	4.98878700	2.03771400	2.07477900
H	4.30866800	0.96031900	3.29366300
H	5.17093400	0.29045800	1.90277400
H	2.19642300	2.22433000	3.01969800
H	2.67269600	3.16608500	1.59482800
H	1.24477500	2.12131800	1.53715100

INT18

C	2.20487000	2.53570700	1.03110800
C	2.08977400	1.45453700	1.60738400
C	2.21974100	0.28933300	2.43506400
C	2.08075800	0.84076900	-1.38676900
C	2.84353300	-0.87568100	1.91587900
C	3.26545500	0.10529100	-1.19400200
C	2.84430600	1.61981100	-3.56187600
H	2.67651100	2.21733900	-4.45411900
C	3.97940600	0.82067700	-3.44278500
H	4.70726000	0.76867500	-4.24760000
C	4.17462300	0.07957100	-2.27918400
H	5.05542800	-0.55070900	-2.22445900
C	1.89322100	1.61160100	-2.54105100
H	0.98624600	2.19362400	-2.67314900
C	1.81544400	-0.78680100	4.56834900

H	1.42781100	-0.74944000	5.58200800
C	2.40284400	-1.95305300	4.07701300
H	2.47356100	-2.83556300	4.70622900
C	2.91213600	-1.98582900	2.77652700
H	3.38037200	-2.90082100	2.42710800
C	1.72179000	0.33366800	3.74972300
H	1.26632700	1.24693800	4.11325500
Si	3.85147900	-0.94074900	0.29481200
C	5.63692600	-0.41371300	0.87109600
C	3.74754000	-2.73917900	-0.30110900
C	4.77502200	-3.35327500	-1.04010600
C	2.55573800	-3.47176300	-0.12643900
C	4.62112500	-4.63148900	-1.58363800
H	5.71574200	-2.83465300	-1.19856500
C	2.39078300	-4.74611400	-0.67067600
H	1.73183900	-3.03906000	0.43605600
C	3.42570600	-5.33089000	-1.40403000
H	5.43545100	-5.08107400	-2.14545800
H	1.45591900	-5.28080000	-0.52107300
H	3.30401100	-6.32375400	-1.82796200
Pd	0.55307200	0.78048800	-0.02941300
P	-1.33754100	0.67579300	1.60156400
P	-0.78297900	-0.20757100	-1.71031600
C	1.62751000	-2.18421000	-5.15688600
C	0.57372200	-1.32505900	-5.47165600
C	-0.17604600	-0.72014700	-4.46044500
C	0.12418300	-0.97575600	-3.11471500
C	1.20305300	-1.81966600	-2.81094600
C	1.94363600	-2.43028200	-3.81894700
H	-0.97284200	-0.03946200	-4.73324000
H	1.48729200	-1.98782300	-1.78189300
C	-0.91054800	3.97995300	4.84164500
C	-0.70232500	4.25824700	3.48837000
C	-0.82605500	3.24439100	2.53886000
C	-1.19719700	1.94471000	2.92371800
C	-1.40466300	1.67493400	4.28426200
C	-1.25470100	2.68606400	5.23589900
H	-0.63839500	3.46120700	1.49052400
H	-1.66221600	0.67379200	4.60976700
C	-1.81377500	-3.43153200	3.68210400
C	-0.70442300	-3.16456300	2.87861100
C	-0.56863000	-1.91843800	2.26887100
C	-1.54145300	-0.92876000	2.45410300
C	-2.66034300	-1.20593700	3.25683600

C	-2.78935100	-2.44902000	3.87332600
H	0.29449700	-1.71188100	1.64760500
H	-3.44225800	-0.46129400	3.37604600
C	-3.54988900	2.95702400	-3.65297800
C	-3.70876300	1.60612800	-3.96951300
C	-2.89080600	0.64800900	-3.37399200
C	-1.89471300	1.03496400	-2.46217400
C	-1.74590000	2.39283700	-2.14484000
C	-2.57103200	3.34858400	-2.73755600
H	-3.04375500	-0.40290600	-3.59916600
H	-0.99522000	2.69773100	-1.42026600
H	-6.43892100	-3.06825900	2.29527400
C	-2.98802100	-1.29172200	-0.24735300
C	-1.83837000	-1.55250700	-0.99759500
C	-1.35769200	-2.88916000	-1.10739200
H	-0.47877700	-3.10168900	-1.70112600
C	-1.99854300	-3.92906700	-0.48372800
H	-1.61179500	-4.94055900	-0.58056500
C	-3.17543600	-3.71163800	0.27302200
C	-3.69029700	-2.38012100	0.37855600
H	-5.29138300	-1.18591900	1.22939600
C	-4.88441600	-2.18464400	1.12913900
C	-5.52678300	-3.24300700	1.73187000
H	-5.52221400	-5.37991200	2.11401300
C	-5.00708800	-4.55503700	1.63040100
H	-3.44333900	-5.78388400	0.82846000
C	-3.85222700	-4.78064100	0.91688900
H	-7.90019900	1.49192100	-2.85611300
C	-4.69588000	2.64823100	0.25437100
H	-5.13551400	3.63344400	0.38795900
C	-3.57634200	2.29352600	0.96530200
H	-3.15084900	3.00464600	1.66218300
C	-2.97572600	1.01453500	0.80339900
C	-3.54991700	0.08863300	-0.06929200
C	-4.73708400	0.43512500	-0.79848600
C	-5.29887700	1.74382800	-0.65281100
H	-6.85267500	3.10425200	-1.29449900
C	-6.44244100	2.10472300	-1.41368600
C	-7.02394900	1.20803600	-2.28059300
H	-6.94746600	-0.79949200	-3.09863500
C	-6.48185700	-0.09245600	-2.41791700
H	-4.96293700	-1.46551700	-1.82281000
C	-5.36946200	-0.46864900	-1.69871800
H	2.20706500	-2.64848800	-5.94974500

H	-0.80263100	4.76653400	5.58265100
H	-1.92533300	-4.40399900	4.15266400
H	-4.19531900	3.70067300	-4.11101500
H	0.33222700	-1.11610400	-6.50999100
H	2.77191200	-3.07827200	-3.54819700
H	-0.43931400	5.26538100	3.17690500
H	-1.41181200	2.46033700	6.28678400
H	-2.45281300	4.39661400	-2.47811900
H	-4.48637400	1.29405600	-4.65926600
H	-3.66391900	-2.66039600	4.48080300
H	0.05766800	-3.92246900	2.72235100
C	2.50445300	3.75991100	0.36805000
C	1.89119900	4.96422000	0.76658600
C	3.45731000	3.77548700	-0.67339400
C	2.21215700	6.15648400	0.12455700
H	1.18894300	4.95364400	1.59112900
C	3.76976400	4.97430400	-1.30669700
H	3.93355200	2.85079200	-0.97650900
C	3.14677500	6.16336100	-0.91569000
H	1.73999400	7.08257500	0.43909700
H	4.50222900	4.98011900	-2.10829400
H	3.39521800	7.09563600	-1.41459700
C	6.67380500	-0.20343900	-0.25396400
H	6.40293500	0.62498500	-0.91506200
H	7.64486900	0.04445000	0.19610200
H	6.83092800	-1.09628400	-0.86948400
C	6.18090800	-1.49954300	1.82836400
H	7.17345800	-1.20526400	2.19605300
H	5.53983500	-1.63669900	2.70510000
H	6.28693600	-2.47057900	1.33103800
C	5.53032800	0.92394800	1.64219600
H	5.12333100	1.72737900	1.01633100
H	4.90406600	0.84102700	2.53580600
H	6.52946200	1.23973200	1.97225200

TS12

C	2.47224700	2.04878800	0.03081500
C	2.09238300	1.47854800	1.10838500
C	2.32987700	0.63472000	2.24828400
C	2.16392200	0.74501800	-1.48506400
C	2.94688900	-0.61884400	1.97742200
C	3.13437800	-0.26734600	-1.30288900
C	2.53759200	0.78360400	-3.88287900
H	2.30681700	1.18589800	-4.86515000

C	3.46188700	-0.25463800	-3.73938400
H	3.95745000	-0.66990400	-4.61181600
C	3.74250700	-0.76808100	-2.47379300
H	4.45105600	-1.58743900	-2.40013700
C	1.89046800	1.28090700	-2.75664500
H	1.15892800	2.07603100	-2.86137400
C	2.08810900	0.07553900	4.58979500
H	1.77093700	0.34655500	5.59247000
C	2.64673300	-1.17944100	4.34181000
H	2.75711400	-1.89687900	5.14978500
C	3.07967500	-1.51026600	3.05401300
H	3.52463600	-2.48696900	2.88553800
C	1.92543900	0.98314800	3.54639800
H	1.48936800	1.95762200	3.72542700
Si	3.78499400	-1.06292200	0.32210500
C	5.64732600	-0.58588700	0.56515500
C	3.48356100	-2.91831700	0.08035600
C	4.39613900	-3.77760000	-0.55797600
C	2.23845600	-3.46335700	0.45358900
C	4.07863000	-5.11299700	-0.82199200
H	5.37435100	-3.41081900	-0.85410000
C	1.90978500	-4.79285000	0.18707400
H	1.50218800	-2.83813700	0.95100600
C	2.83148200	-5.62333400	-0.45506600
H	4.80623900	-5.75422300	-1.31216300
H	0.93590100	-5.17673000	0.48052100
H	2.58283300	-6.66028600	-0.66299600
Pd	0.50955100	0.70223900	-0.15000900
P	-1.25912300	0.91835800	1.51234900
P	-0.99816000	-0.38517100	-1.70819400
C	1.23720600	-3.08306100	-4.75891200
C	0.28054800	-2.18027600	-5.22918900
C	-0.41029700	-1.35304700	-4.34196200
C	-0.14220700	-1.41620200	-2.96582100
C	0.85099200	-2.29683500	-2.51074100
C	1.52273000	-3.13990800	-3.39388300
H	-1.14628200	-0.65831700	-4.72935300
H	1.11165000	-2.32616500	-1.46071300
C	-0.29154100	4.57015600	4.21714600
C	-0.02348300	4.59656700	2.84592700
C	-0.33088900	3.49087800	2.05263100
C	-0.93302400	2.35174500	2.61586300
C	-1.20544100	2.33777700	3.99128100
C	-0.88223200	3.43966800	4.78571400

H	-0.09766300	3.50955800	0.99195500
H	-1.64546700	1.46076300	4.45227900
C	-1.84235300	-2.76248300	4.25035900
C	-0.70481100	-2.63636000	3.45074300
C	-0.54813200	-1.51586000	2.63644000
C	-1.52639500	-0.51298500	2.61326400
C	-2.66568800	-0.64324700	3.42273000
C	-2.81898700	-1.76291900	4.23881300
H	0.33913900	-1.41164800	2.02317200
H	-3.44509100	0.11236400	3.39080200
C	-3.65996900	2.57382700	-4.07101400
C	-3.89394300	1.20103600	-4.18116000
C	-3.10418600	0.29815000	-3.47163600
C	-2.06521100	0.76197500	-2.64873200
C	-1.83863000	2.14196400	-2.54138400
C	-2.63293300	3.04350200	-3.24986300
H	-3.30951500	-0.76615500	-3.53850500
H	-1.05706000	2.50785600	-1.88081900
H	-6.60464200	-2.17875500	2.92120800
C	-3.18031700	-1.09247500	-0.01552900
C	-2.11265600	-1.55400000	-0.78889500
C	-1.75951100	-2.93287700	-0.73776200
H	-0.95048100	-3.30743300	-1.35042300
C	-2.43304600	-3.81202600	0.07251800
H	-2.13895600	-4.85850700	0.09950100
C	-3.52990800	-3.38564300	0.86012300
C	-3.93105700	-2.01346400	0.79336400
H	-5.38668500	-0.57745700	1.52349900
C	-5.06068100	-1.60996800	1.56069500
C	-5.74239500	-2.50975800	2.34927000
H	-5.87178900	-4.55840200	3.05627700
C	-5.32807700	-3.86075900	2.42591400
H	-3.91822600	-5.32295000	1.73865600
C	-4.24222000	-4.28623300	1.69541200
H	-7.94084800	1.83190200	-2.75082100
C	-4.43592300	3.04363000	-0.00626600
H	-4.75512900	4.08279300	-0.00332900
C	-3.32688600	2.66426700	0.70844700
H	-2.78675500	3.41171900	1.27633600
C	-2.88312200	1.31188100	0.71631800
C	-3.59495100	0.34866200	-0.00108700
C	-4.77668600	0.72463000	-0.72393500
C	-5.18708800	2.09600600	-0.74349300
H	-6.62844900	3.51959500	-1.50049900

C	-6.33357300	2.47339400	-1.49172000
C	-7.06225300	1.53460100	-2.18568300
H	-7.24978400	-0.56307900	-2.70466900
C	-6.66885800	0.17510800	-2.15908800
H	-5.26205000	-1.26242200	-1.44880200
C	-5.55526100	-0.21915500	-1.45175900
H	1.76299200	-3.73070400	-5.45492100
H	-0.04104300	5.42540900	4.83797100
H	-1.97223700	-3.63842600	4.87934600
H	-4.28431200	3.27533200	-4.61648500
H	0.06431800	-2.12059400	-6.29223100
H	2.27768800	-3.81856500	-3.00754800
H	0.43012500	5.47489600	2.39502200
H	-1.09150900	3.41242500	5.85128100
H	-2.45698500	4.11081500	-3.15118700
H	-4.70629800	0.83412400	-4.80065700
H	-3.71273100	-1.86709100	4.84595900
H	0.06223900	-3.40552100	3.45695600
C	3.13903600	3.25095800	-0.43999200
C	2.94833200	4.43225700	0.30429300
C	4.01836400	3.26326200	-1.53727800
C	3.61426900	5.60206800	-0.05152700
H	2.28323400	4.40965100	1.16110100
C	4.68732700	4.43575100	-1.87987900
H	4.19135600	2.35492000	-2.10107900
C	4.48279700	5.60800100	-1.14633700
H	3.45876700	6.50807300	0.52718200
H	5.37438500	4.43340300	-2.72094600
H	5.00239100	6.52053600	-1.42371400
C	6.49408900	-0.67916000	-0.72184900
H	6.12719300	-0.00858900	-1.50537100
H	7.52896200	-0.38677700	-0.49728400
H	6.53411300	-1.69276700	-1.13622200
C	6.26640500	-1.50966600	1.63816500
H	7.31777500	-1.23546000	1.80080700
H	5.75512200	-1.41670200	2.60220500
H	6.24192200	-2.56470900	1.34241800
C	5.71747900	0.87608500	1.06552000
H	5.31891800	1.58221300	0.32878300
H	5.17167000	1.02049600	2.00394000
H	6.76477200	1.15325800	1.24864000
INT19			
C	2.93169300	1.19881800	-1.25045600

C	2.23447400	1.31145700	-0.10061500
C	2.67183500	1.51678100	1.27540500
C	2.55448500	-0.09749100	-1.90928700
C	3.19320300	0.30955000	1.82484900
C	2.65942400	-1.24695400	-1.04538200
C	1.95133900	-1.50771900	-3.79082400
H	1.67440500	-1.61538100	-4.83571200
C	2.06136500	-2.64221600	-2.97393600
H	1.86408800	-3.62860500	-3.38168700
C	2.40031000	-2.50946600	-1.63324600
H	2.47228900	-3.40389400	-1.02574900
C	2.19647100	-0.24538000	-3.26421700
H	2.12741200	0.64107200	-3.88831600
C	2.91198000	2.63324400	3.40565000
H	2.81616500	3.52899700	4.01273300
C	3.38215300	1.44852200	3.97544300
H	3.64421000	1.41720600	5.02923000
C	3.52491000	0.30086900	3.18748700
H	3.88505500	-0.61348800	3.65135100
C	2.54729000	2.66935600	2.05924700
H	2.16198500	3.58185000	1.62124100
Si	3.44670400	-1.25266700	0.74379200
C	5.34249300	-1.56808600	0.55651300
C	2.56505000	-2.65153100	1.67658200
C	2.96450300	-4.00010500	1.62741100
C	1.42329500	-2.34989200	2.44438600
C	2.26195200	-4.99536400	2.31242800
H	3.83912700	-4.28978600	1.05338800
C	0.71086600	-3.33711300	3.12741500
H	1.07213800	-1.32790800	2.50615400
C	1.12998000	-4.66776100	3.06260700
H	2.60177500	-6.02658800	2.26241300
H	-0.17106500	-3.06298400	3.69978300
H	0.58423400	-5.44225700	3.59435200
Pd	0.59518200	0.07771000	-0.39570100
P	-0.85797100	1.73367400	0.47583800
P	-1.26219600	-1.45339500	-0.99128500
C	-0.10736700	-5.88152900	-1.90022600
C	-0.84329300	-5.14988000	-2.83278500
C	-1.22094300	-3.83318300	-2.56013800
C	-0.86358400	-3.22224200	-1.34683700
C	-0.09260200	-3.95821800	-0.43082800
C	0.26578500	-5.27940400	-0.69699700
H	-1.78525900	-3.28879800	-3.30657200

H	0.26151000	-3.49828300	0.48271400
C	0.93980900	5.97757700	-0.11022800
C	1.10302500	4.99462300	-1.09021700
C	0.54739600	3.72846100	-0.90684200
C	-0.18276900	3.43119200	0.25660500
C	-0.35419900	4.42770400	1.22835200
C	0.20595900	5.69345100	1.04347900
H	0.69181900	2.96581800	-1.66368000
H	-0.90212200	4.21616000	2.13972100
C	-1.66383900	1.41846500	5.02200500
C	-0.50992700	0.86034900	4.46743800
C	-0.28027400	0.95338000	3.09573800
C	-1.20624200	1.59820700	2.26472600
C	-2.35107800	2.17851300	2.83062500
C	-2.57844700	2.08455100	4.20316500
H	0.63025100	0.54751100	2.67603700
H	-3.07375000	2.68294500	2.19800300
C	-3.50921800	-0.12759900	-4.81870200
C	-4.07333900	-1.10544700	-3.99493500
C	-3.41841400	-1.49866500	-2.83008800
C	-2.18748400	-0.92050000	-2.47854600
C	-1.62672000	0.05704200	-3.31179900
C	-2.28700300	0.45312100	-4.47617000
H	-3.86783300	-2.24792000	-2.18529700
H	-0.67777800	0.51187800	-3.04303000
H	-6.47727300	1.49228500	3.51559300
C	-3.29703500	-0.36866500	0.69028100
C	-2.45583600	-1.45471200	0.43409800
C	-2.37350000	-2.51137900	1.38438100
H	-1.74756200	-3.36998300	1.18585800
C	-3.08213300	-2.47338000	2.55886500
H	-2.99383400	-3.28958300	3.27181100
C	-3.95694500	-1.39832100	2.84835500
C	-4.09739700	-0.34866900	1.88544200
H	-5.17631400	1.48363400	1.44282000
C	-5.03497700	0.68709600	2.16345800
C	-5.76491700	0.69314100	3.33081800
H	-6.17281600	-0.30993000	5.21311200
C	-5.59548100	-0.33066100	4.29343900
H	-4.58049900	-2.15660900	4.77519300
C	-4.70949400	-1.35518600	4.05222400
H	-7.81169900	0.94100600	-3.36881700
C	-3.81703800	2.87833100	-2.12262200
H	-3.95259200	3.69051900	-2.83213900

C	-2.69576000	2.83734800	-1.33378000
H	-1.96273500	3.62805900	-1.42633600
C	-2.48602900	1.78101800	-0.40144400
C	-3.44556300	0.77339400	-0.27173100
C	-4.63762000	0.82187700	-1.07243200
C	-4.81203200	1.87657600	-2.02447100
H	-6.08095300	2.70214300	-3.56836900
C	-5.96833600	1.89581700	-2.84829100
C	-6.92893500	0.91699400	-2.73653000
H	-7.52958400	-0.89319300	-1.70340700
C	-6.76776100	-0.12382900	-1.79078300
H	-5.54345400	-0.98183000	-0.27193300
C	-5.65379900	-0.17207900	-0.98305800
H	0.17940100	-6.90774000	-2.11159800
H	1.38265800	6.96006300	-0.24590900
H	-1.84907000	1.33948000	6.08936800
H	-4.02560300	0.18377600	-5.72209200
H	-1.13060700	-5.60130600	-3.77832200
H	0.85304400	-5.82346400	0.03533200
H	1.67716200	5.20383900	-1.98770700
H	0.07311100	6.45477900	1.80672800
H	-1.84917700	1.21841300	-5.11089800
H	-5.03227400	-1.54637600	-4.24836300
H	-3.48082800	2.51384500	4.62677600
H	0.21782500	0.35687600	5.09698300
C	4.03929700	2.03890500	-1.72377600
C	4.26134600	3.30725200	-1.15190100
C	4.88825000	1.61582900	-2.76462300
C	5.31524800	4.10701600	-1.58412100
H	3.59368800	3.66443800	-0.37645800
C	5.93686500	2.42385000	-3.20088300
H	4.73981900	0.64144800	-3.21999100
C	6.15810900	3.67025500	-2.61077700
H	5.47453200	5.07924300	-1.12582600
H	6.58543500	2.07640600	-4.00012700
H	6.97539700	4.29898800	-2.95192900
C	5.64230500	-2.60931100	-0.54357300
H	5.27249200	-2.28678200	-1.52313200
H	6.72813300	-2.75148100	-0.63078200
H	5.20679100	-3.59278400	-0.33342400
C	5.92985800	-2.05524700	1.90050500
H	7.00619100	-2.24287500	1.78432000
H	5.82056000	-1.30053400	2.68691300
H	5.46896700	-2.98273900	2.25541700

C	6.04346200	-0.24668200	0.17181200
H	5.72826500	0.11710900	-0.80954100
H	5.85431700	0.55008400	0.89950700
H	7.12999400	-0.40467800	0.12636200

TS11

C	3.29534800	-1.12697600	-1.33850800
C	3.93052200	-1.87379900	-2.35458700
C	2.19715800	-0.34787000	-1.73157200
C	3.51516500	-1.83723700	-3.68424400
H	4.77204300	-2.50569900	-2.10601800
C	1.82086200	-0.23696900	-3.07597000
C	2.46555000	-0.99688800	-4.05419600
H	4.02721400	-2.43943700	-4.42937600
H	1.01394500	0.42617300	-3.37337500
H	2.14768500	-0.92683600	-5.09099200
C	4.80448400	0.89782000	0.07305900
C	3.98272400	1.88352500	-0.52643300
C	6.12585300	1.27468800	0.36448400
C	4.51197500	3.13584600	-0.90386300
C	6.64491800	2.52444200	0.02266800
C	5.84008500	3.45114500	-0.63861100
H	3.86116300	3.86718400	-1.37268200
H	7.67591200	2.76610500	0.26457600
H	6.23458800	4.41976300	-0.93145900
H	6.77871700	0.57907000	0.87623200
Pd	0.62034200	0.52077700	-0.61972700
Si	4.16569300	-0.87572900	0.33346100
C	2.53488600	1.82669700	-0.63468800
C	1.49692300	2.53316300	-0.53951600
C	1.01201000	3.88258900	-0.32753200
C	1.04413300	4.79903300	-1.39355700
C	0.61252000	4.32079300	0.94530900
C	0.67989700	6.12670600	-1.18500400
H	1.34203500	4.45804200	-2.37939300
C	0.24893100	5.65093500	1.14528300
H	0.59775100	3.62356100	1.77284800
C	0.27950900	6.55703300	0.08282400
H	0.70291800	6.82482400	-2.01650000
H	-0.05355000	5.97900000	2.13565100
H	-0.00555900	7.59307400	0.24113900
C	3.08260000	-0.83369200	1.89917500
C	2.78888600	-1.99560300	2.64042600
C	2.74981600	0.40067000	2.49341700

C	2.24457300	-1.93052100	3.92556600
H	2.99083000	-2.97404000	2.22210000
C	2.17633500	0.47287300	3.76544300
H	2.96840200	1.32760100	1.97439100
C	1.94028000	-0.69255500	4.49600600
H	2.05447900	-2.84802900	4.47634200
H	1.94730100	1.44422800	4.19670800
H	1.52903700	-0.63725600	5.50044100
C	5.61682800	-2.14271600	0.61771700
C	5.11559100	-3.60218200	0.47259800
H	5.95500800	-4.29168800	0.63873300
H	4.34336900	-3.86383600	1.20021200
H	4.70430000	-3.81860200	-0.51653100
C	6.16889900	-1.97715500	2.05686600
H	5.41505300	-2.19761600	2.81778600
H	7.00691200	-2.67099100	2.20928800
H	6.54450700	-0.96731900	2.25511500
C	6.80223200	-1.96201000	-0.36633000
H	7.57152700	-2.71269000	-0.13897000
H	6.52075500	-2.09864600	-1.41327900
H	7.27661700	-0.98196300	-0.29246400
P	-0.37783200	-1.65512400	-0.38046400
P	-1.64537400	1.50550700	-0.27669500
C	-2.13546500	5.10670000	-3.15978600
C	-2.55622900	5.24074100	-1.83658600
C	-2.40086100	4.18592700	-0.93412700
C	-1.80947200	2.98798900	-1.34925700
C	-1.35710200	2.87212000	-2.67494100
C	-1.52939100	3.91880600	-3.57796700
H	-2.72100500	4.31198600	0.09355900
H	-0.87275200	1.95594400	-3.00274100
C	2.05362600	-5.60902500	-0.12091700
C	1.27784900	-5.23668100	0.97722600
C	0.55359800	-4.04185200	0.95935900
C	0.60935900	-3.19607900	-0.15855500
C	1.37134300	-3.59388500	-1.27121600
C	2.08901700	-4.78704200	-1.24957500
H	-0.06257900	-3.79301400	1.81399100
H	1.38843600	-2.98399100	-2.16718200
C	-2.91653900	-3.09213900	-3.98520000
C	-2.77481700	-3.90341200	-2.85619100
C	-2.02173600	-3.46450200	-1.77041700
C	-1.41592600	-2.19716300	-1.79578000
C	-1.55497300	-1.39443200	-2.93344300

C	-2.30255500	-1.83965200	-4.02387600
H	-1.90650900	-4.10540700	-0.90181200
H	-1.09095300	-0.41580100	-2.95937100
C	-2.54155100	2.61354100	4.12391300
C	-3.53420700	2.78678000	3.15526300
C	-3.27497600	2.46684400	1.82385600
C	-2.01053100	1.98535900	1.44727600
C	-1.02644500	1.79418300	2.42723000
C	-1.29117100	2.11259400	3.75864000
H	-4.06288400	2.56427700	1.08251800
H	-0.06457100	1.36872000	2.15723400
H	-5.97336600	-4.57225200	-0.13537800
C	-3.44418600	-0.69585300	-0.15044200
C	-3.11665300	0.49224600	-0.80703300
C	-3.85816200	0.87402300	-1.95963200
H	-3.64308800	1.81009200	-2.45735800
C	-4.85101700	0.06895600	-2.46399000
H	-5.40097200	0.37831900	-3.34915700
C	-5.16556300	-1.17132500	-1.85873200
C	-4.46775300	-1.54999100	-0.66785000
H	-4.26824700	-3.09365300	0.84256500
C	-4.79045600	-2.79544200	-0.05983400
C	-5.74306000	-3.62279100	-0.61009700
H	-7.17472600	-3.91174600	-2.21596300
C	-6.42608900	-3.24806500	-1.79316500
H	-6.66480400	-1.74874500	-3.30760600
C	-6.14398100	-2.04596800	-2.40106100
H	-5.29764600	-0.39661700	5.78196500
C	-1.37344600	-1.37430700	3.56294900
H	-0.81911800	-1.44673300	4.49408200
C	-0.72082800	-1.54757600	2.37031700
H	0.34479900	-1.72533600	2.37459400
C	-1.41441000	-1.46179600	1.13128800
C	-2.74698400	-1.06038000	1.11916700
C	-3.45052800	-0.87722500	2.36018800
C	-2.75586000	-1.06576000	3.59822200
H	-2.90284800	-1.03208400	5.75440100
C	-3.44643100	-0.88538400	4.82452300
C	-4.77585900	-0.52852600	4.83854200
H	-6.51086600	-0.03775700	3.63435100
C	-5.46377900	-0.32638800	3.61914500
H	-5.36087300	-0.32287500	1.48989800
C	-4.81850800	-0.48837400	2.41283100
H	-2.26580700	5.92732000	-3.85931500

H	2.61553900	-6.53836100	-0.10332600
H	-3.50349500	-3.43708800	-4.83138900
H	-2.75131800	2.85045300	5.16280400
H	-3.00462200	6.17038200	-1.49870200
H	-1.18406900	3.81142900	-4.60246300
H	1.22151400	-5.88061100	1.85042200
H	2.67530600	-5.07125900	-2.11846500
H	-0.52635100	1.94315000	4.51088500
H	-4.51672300	3.15032300	3.44054100
H	-2.41043400	-1.20395200	-4.89799300
H	-3.25600000	-4.87587100	-2.81873200

INT25

C	3.57545200	-1.59248600	-1.22716800
C	3.51447100	-2.81068300	-1.90882200
C	2.77904100	-0.51518400	-1.71395700
C	2.63553500	-3.01254000	-2.98455600
H	4.14334200	-3.63798200	-1.59657100
C	1.89796400	-0.72195800	-2.79776000
C	1.80461000	-1.98105500	-3.40777700
H	2.60157200	-3.97835800	-3.48030500
H	1.37508300	0.12906500	-3.22517000
H	1.11791300	-2.13109800	-4.23536800
C	5.32221500	0.51419000	-0.33381900
C	4.40118400	1.33840200	-1.03019400
C	6.64129100	0.96815200	-0.18383200
C	4.82905300	2.55736800	-1.57219600
C	7.05570500	2.19286900	-0.71000100
C	6.14708000	2.98365000	-1.41205600
H	4.13500300	3.16936400	-2.13330000
H	8.08332400	2.52049500	-0.58054000
H	6.46228800	3.92956000	-1.84354900
H	7.36676200	0.36086500	0.34668000
Pd	0.44454100	0.11838300	-0.61474400
Si	4.65298200	-1.14095900	0.26708100
C	2.98230200	0.87828800	-1.18324000
C	1.90047700	1.58035600	-0.78759200
C	1.87474700	2.96298900	-0.29651700
C	1.93802800	4.05208400	-1.18439700
C	1.80026100	3.23049000	1.08120700
C	1.93379800	5.36147000	-0.71033500
H	1.96711800	3.86420700	-2.25185400
C	1.79033900	4.54048400	1.55524100
H	1.77563800	2.40252800	1.77638900

C	1.85575400	5.61254100	0.66167200
H	1.97949900	6.18608700	-1.41570100
H	1.73522400	4.72277900	2.62501700
H	1.84790200	6.63409800	1.03107900
C	3.50472800	-0.81805100	1.73962200
C	2.61709800	-1.80470800	2.20940900
C	3.54709500	0.40395500	2.43450700
C	1.81843600	-1.58812100	3.33359600
H	2.54362500	-2.75967600	1.70079700
C	2.74068500	0.63128100	3.55375400
H	4.21126300	1.19372700	2.09316800
C	1.87468600	-0.36594800	4.00800900
H	1.17037000	-2.38289400	3.69273400
H	2.79575800	1.58438700	4.07393800
H	1.25823600	-0.19851600	4.88751200
C	5.97184400	-2.45036200	0.73099900
C	5.30366000	-3.79321700	1.10911100
H	6.07839300	-4.53245400	1.35526200
H	4.65936000	-3.69292900	1.98891200
H	4.70062900	-4.21691700	0.29910600
C	6.75748100	-1.96898500	1.97406000
H	6.09317100	-1.79058900	2.82752100
H	7.48396900	-2.73704500	2.27338400
H	7.31967600	-1.04781900	1.79306900
C	6.94332500	-2.67477300	-0.44825600
H	7.70952500	-3.41146900	-0.16962400
H	6.43028000	-3.05583700	-1.33890700
H	7.46036400	-1.75396700	-0.73838900
P	-1.04743500	-1.80260800	-0.11668900
P	-1.33993000	1.62159800	-0.43227500
C	-0.81225400	5.22694800	-3.30048900
C	-1.23078800	5.45943300	-1.99106900
C	-1.37520900	4.39773800	-1.09450900
C	-1.09720100	3.08992700	-1.50527900
C	-0.64381400	2.86561800	-2.81739500
C	-0.51360200	3.92423600	-3.71274500
H	-1.67036400	4.60414400	-0.07317500
H	-0.39149700	1.85746800	-3.13521200
C	0.74875300	-5.91396800	1.05013100
C	-0.51521500	-5.56976200	1.53918900
C	-1.07272500	-4.32742900	1.23709300
C	-0.36017900	-3.40748900	0.44886000
C	0.90227300	-3.76129600	-0.03629900
C	1.45491700	-5.00865000	0.25692400

H	-2.05206600	-4.07283600	1.63020900
H	1.45609800	-3.05559200	-0.63889700
C	-3.56908900	-3.12983900	-3.77789900
C	-3.78831000	-3.73402900	-2.53689600
C	-3.04700200	-3.33935000	-1.42569600
C	-2.08454500	-2.32479400	-1.54127800
C	-1.86428000	-1.72938800	-2.79082300
C	-2.60359300	-2.13025600	-3.90438700
H	-3.22765900	-3.81509800	-0.46748900
H	-1.12264400	-0.94220800	-2.88490600
C	-2.04852200	3.02911000	3.91400200
C	-2.90591000	3.45894200	2.89807800
C	-2.70362200	3.03438200	1.58631400
C	-1.62538000	2.18777400	1.27824500
C	-0.78531400	1.73915300	2.30636300
C	-0.99496400	2.16315800	3.61690800
H	-3.40035500	3.33732200	0.81043500
H	0.01636900	1.04072300	2.08973900
H	-7.22335100	-2.99799000	-0.19295500
C	-3.66950600	-0.02778900	-0.29699300
C	-2.95771800	0.92687600	-1.02963500
C	-3.42873200	1.30443900	-2.31981900
H	-2.91095800	2.06728800	-2.88455200
C	-4.54440600	0.72397600	-2.86926900
H	-4.88096900	1.02761400	-3.85721700
C	-5.27017800	-0.27059500	-2.17128100
C	-4.84053900	-0.63695400	-0.85629900
H	-5.26707300	-1.92944600	0.83437900
C	-5.57915000	-1.63599900	-0.16107100
C	-6.67436600	-2.23668500	-0.73963700
H	-7.95642900	-2.35777800	-2.48711200
C	-7.09140300	-1.87380600	-2.04315400
H	-6.71354700	-0.62211500	-3.74298700
C	-6.40206800	-0.90938800	-2.74213300
H	-5.91954600	1.39373000	5.33383400
C	-2.38052800	-1.06628400	3.68554600
H	-2.02811800	-1.29254600	4.68880800
C	-1.70385900	-1.55030800	2.59499400
H	-0.81650500	-2.15007700	2.74441400
C	-2.14142300	-1.26597400	1.27000100
C	-3.24317200	-0.43925900	1.07596900
C	-3.98305000	0.05305000	2.20445400
C	-3.54068600	-0.26731800	3.52791900
H	-3.90600800	-0.01490800	5.64395600

C	-4.25678000	0.23461000	4.64578700
C	-5.37502300	1.01859200	4.47221300
H	-6.70033600	1.95572000	3.03439000
C	-5.81747600	1.33681500	3.16663000
H	-5.48609800	1.13138200	1.06946800
C	-5.13747400	0.87237500	2.06233500
H	-0.70545700	6.05533900	-3.99476400
H	1.17766000	-6.88323100	1.28743800
H	-4.15032100	-3.43850500	-4.64193200
H	-2.21557600	3.35392000	4.93672700
H	-1.43795300	6.47146300	-1.65601900
H	-0.17003200	3.73585300	-4.72594000
H	-1.06981200	-6.27141100	2.15575300
H	2.43748100	-5.26499400	-0.12874000
H	-0.33993600	1.80143000	4.40374900
H	-3.74697700	4.10472900	3.13024700
H	-2.43115600	-1.65534700	-4.86623600
H	-4.54369200	-4.50695200	-2.43278800

TS13

C	-2.36465700	-1.95646600	0.08356800
C	-1.96810600	-0.99943400	1.01922000
C	-2.55179300	-0.05618900	1.90850700
C	-2.89635200	-1.65912200	-1.26815500
C	-3.48310900	0.87708800	1.37433700
C	-3.44530600	-0.39426600	-1.59719000
C	-3.32990900	-2.46929500	-3.52130300
H	-3.30479600	-3.27883900	-4.24446300
C	-3.77403500	-1.19838000	-3.89437300
H	-4.10044000	-1.00484600	-4.91230100
C	-3.81518700	-0.18035600	-2.94156900
H	-4.18406400	0.79748800	-3.24052900
C	-2.85636500	-2.68283600	-2.23198500
H	-2.43710900	-3.64647300	-1.96019000
C	-2.53476600	1.06760400	4.05719800
H	-2.19908100	1.12489900	5.08778200
C	-3.38245100	2.04683300	3.52548000
H	-3.69930900	2.88332400	4.14187400
C	-3.82218600	1.95908100	2.20363000
H	-4.45223900	2.75260500	1.81388200
C	-2.08009200	0.04870800	3.23693400
H	-1.38597500	-0.69477800	3.60427900
Si	-4.16403100	0.89338700	-0.40697800
C	-6.06345000	0.54035700	-0.30000400

C	-3.70149900	2.59719200	-1.07053100
C	-4.51078300	3.73613800	-0.90374800
C	-2.43108100	2.77640200	-1.65310900
C	-4.07031200	5.00315400	-1.29329600
H	-5.50115100	3.64253700	-0.46783300
C	-1.98293400	4.04135300	-2.03616700
H	-1.77616100	1.92132700	-1.80765000
C	-2.80150500	5.15857500	-1.85557100
H	-4.71660200	5.86613400	-1.15792000
H	-0.98946700	4.15503300	-2.45668600
H	-2.45344300	6.14410700	-2.15265700
Pd	-0.16969300	-1.18235400	0.28897000
P	1.26143100	0.18990600	1.74568900
P	1.52981700	-1.29500700	-1.52344400
C	0.46045200	-2.82479100	-5.78479200
C	1.68991800	-3.17244100	-5.22284800
C	2.02732600	-2.73539000	-3.94154600
C	1.13049400	-1.95068900	-3.19755700
C	-0.12446900	-1.64848700	-3.75203000
C	-0.44507900	-2.06353200	-5.04496100
H	2.98941100	-3.01266900	-3.52782300
H	-0.85211500	-1.08170500	-3.17965000
C	0.86309600	-1.82765100	5.91663400
C	1.07877600	-2.58018400	4.75812700
C	1.22095600	-1.93965000	3.52829600
C	1.16035100	-0.53724300	3.43563300
C	0.95679900	0.20874400	4.60478500
C	0.80573500	-0.43529900	5.83574800
H	1.38336100	-2.53144100	2.63082900
H	0.88521100	1.28932600	4.55762400
C	0.14454000	4.67075300	2.09054400
C	-0.61410600	3.81421900	1.29168300
C	-0.27254300	2.46437700	1.20059300
C	0.82733100	1.96071400	1.90652200
C	1.60339800	2.83574500	2.68585100
C	1.25475200	4.18148400	2.78519600
H	-0.85376800	1.80759400	0.56398800
H	2.48735500	2.46711100	3.19950800
C	5.36226700	-3.60384800	-0.33417300
C	5.43501000	-2.63739700	-1.34064800
C	4.29525800	-1.92295500	-1.70577600
C	3.07182400	-2.16267600	-1.06146900
C	3.00646300	-3.13874800	-0.05667500
C	4.14697900	-3.85685100	0.30526500

H	4.36157800	-1.16299200	-2.47748400
H	2.05879700	-3.33766500	0.43877200
H	3.83408700	5.54165400	0.52366200
C	2.63544500	1.28449200	-0.87044600
C	1.90495100	0.51247100	-1.78028700
C	1.21064900	1.16508200	-2.84052900
H	0.68378700	0.57659400	-3.57964900
C	1.21664300	2.53035200	-2.97465800
H	0.69713900	2.99380200	-3.80987100
C	1.89978500	3.34982500	-2.04384800
C	2.63019000	2.71938500	-0.98627600
H	3.89036400	3.10120600	0.73693800
C	3.33301300	3.55505000	-0.07334700
C	3.29885900	4.92596800	-0.19342200
H	2.55930500	6.62503100	-1.32459900
C	2.57191000	5.54230300	-1.23947700
H	1.33683000	5.22484500	-2.96380600
C	1.88994100	4.76592600	-2.14775600
H	8.78242700	0.43142800	-0.86866500
C	5.33283600	-0.36069800	2.08780500
H	6.01921100	-0.76797700	2.82583800
C	3.98719000	-0.31427400	2.35142100
H	3.62083400	-0.68111800	3.30245600
C	3.07116400	0.20759700	1.39517300
C	3.53683800	0.69092000	0.17467500
C	4.94521500	0.66806200	-0.10619200
C	5.84892100	0.11593100	0.85779100
H	7.90594400	-0.38285900	1.30036900
C	7.23497000	0.04216500	0.55822200
C	7.72089500	0.49389100	-0.64741900
H	7.22200600	1.41010400	-2.54956300
C	6.83377000	1.04882200	-1.60155000
H	4.82076600	1.56281600	-2.08093100
C	5.48511200	1.13819800	-1.33737000
H	0.20558900	-3.15366200	-6.78825700
H	0.74121400	-2.32443100	6.87468800
H	-0.11775500	5.72263100	2.16086700
H	6.25228800	-4.15673800	-0.04761600
H	2.39486900	-3.77979700	-5.78349700
H	-1.41058800	-1.80016300	-5.46352200
H	1.12984900	-3.66407700	4.81218600
H	0.64116300	0.15541500	6.73266400
H	4.08723500	-4.60970900	1.08616500
H	6.38097000	-2.42454000	-1.82899700

H	1.85893900	4.85179000	3.39007000
H	-1.46256400	4.18917100	0.72865100
C	-2.70271700	-3.24598600	0.77859400
C	-1.85274300	-3.79335500	1.75843200
C	-3.93715700	-3.87713200	0.53045700
C	-2.22434300	-4.93520300	2.46766200
H	-0.89008200	-3.32887100	1.94811100
C	-4.29626400	-5.02527300	1.23117100
H	-4.61084000	-3.46500300	-0.21170100
C	-3.44534500	-5.55754200	2.20573700
H	-1.55169300	-5.34405400	3.21651500
H	-5.24822100	-5.50397200	1.01981100
H	-3.73151600	-6.45292200	2.74965100
C	-6.76670600	0.92369200	-1.62017900
H	-6.38691900	0.34686500	-2.46948900
H	-7.84200300	0.71252400	-1.54114100
H	-6.65574800	1.98788300	-1.85678600
C	-6.74846200	1.29030500	0.86377500
H	-7.81808100	1.04081900	0.87760700
H	-6.33513800	1.00889500	1.83745000
H	-6.67784700	2.37989900	0.76910800
C	-6.24246700	-0.97698600	-0.06061300
H	-5.87092500	-1.56479100	-0.90675900
H	-5.72377400	-1.31814700	0.84480900
H	-7.30797400	-1.21325400	0.06441200

INT20

C	2.22944700	-1.08345700	-0.24705200
C	1.94835500	0.26770400	-0.23476900
C	2.71720400	1.47389500	-0.08573500
C	3.20203100	-1.68692900	0.72266500
C	4.14026600	1.52558000	-0.26051100
C	4.57840400	-1.37002200	0.69469300
C	3.56695000	-3.25599600	2.54663500
H	3.15794600	-3.95100400	3.27434400
C	4.93788500	-3.00852200	2.48497700
H	5.62167200	-3.52430300	3.15325200
C	5.42486000	-2.06285500	1.58328300
H	6.48720900	-1.83805700	1.58668700
C	2.70696000	-2.59513700	1.67272000
H	1.63964300	-2.77207700	1.73768200
C	2.64300300	3.91544400	0.12791800
H	2.06588700	4.82170800	0.28545100
C	4.01832700	3.97455700	-0.10175200

H	4.53006600	4.93245700	-0.13436800
C	4.74439600	2.79193100	-0.26889300
H	5.82166000	2.86302500	-0.38665100
C	2.01050400	2.68197100	0.13538200
H	0.94410200	2.63383100	0.29990900
Si	5.33019900	0.03574800	-0.32987700
C	5.73913900	-0.42216500	-2.14966900
C	6.85259600	0.59535600	0.65285900
C	8.18794800	0.42799100	0.24711000
C	6.63125200	1.17175500	1.92148600
C	9.25340200	0.82238700	1.06193100
H	8.41767000	-0.01543800	-0.71538500
C	7.68798700	1.56737200	2.73975900
H	5.61316700	1.31697300	2.27621500
C	9.00644400	1.39404300	2.30969200
H	10.27480600	0.68158300	0.71874300
H	7.48517600	2.01008600	3.71140900
H	9.83348900	1.70145600	2.94383200
Pd	-0.03372500	-0.18271100	-0.03815800
P	-1.40031300	1.56550700	-0.73802000
P	-1.84031300	-1.41096700	0.96815500
C	0.30411400	-3.78204700	4.32874700
C	-0.43701300	-4.47507800	3.37012300
C	-1.13301000	-3.78097600	2.37650700
C	-1.08196100	-2.38038100	2.32867700
C	-0.30510900	-1.69130200	3.28023100
C	0.36802600	-2.38600100	4.28248100
H	-1.70888400	-4.33163500	1.64041700
H	-0.21756600	-0.60904300	3.22620500
C	0.80282400	4.05030500	-3.98635500
C	0.68091700	2.66225100	-4.10140800
C	-0.01558900	1.94226400	-3.13433000
C	-0.62037100	2.59608400	-2.04625500
C	-0.49200200	3.98826100	-1.93901100
C	0.21653600	4.70716700	-2.90518000
H	-0.08527300	0.86347500	-3.21657200
H	-0.92486100	4.51798600	-1.09843000
C	-2.63467600	4.47521800	2.64181000
C	-1.68445700	3.48146800	2.88556000
C	-1.30765300	2.60949100	1.86431000
C	-1.88253900	2.72461500	0.59049400
C	-2.84176300	3.72313200	0.35363000
C	-3.21003900	4.59694700	1.37465400
H	-0.58049300	1.82502500	2.05548700

H	-3.31495400	3.80246000	-0.62077300
C	-4.13201200	-4.28884500	-1.82051800
C	-4.54228000	-4.15017200	-0.49107500
C	-3.84927000	-3.29970300	0.36792600
C	-2.73206200	-2.58870800	-0.09920400
C	-2.31890700	-2.73769600	-1.42955700
C	-3.02021600	-3.58546200	-2.28661800
H	-4.18515700	-3.17295600	1.39363600
H	-1.46493700	-2.18079800	-1.79920300
H	-7.15297100	3.78725400	0.67173800
C	-3.93802300	0.45326300	0.90012300
C	-3.13827700	-0.34114300	1.72414000
C	-3.22708200	-0.21059000	3.13666100
H	-2.63103600	-0.85132600	3.77505700
C	-4.06172200	0.71732900	3.70994400
H	-4.11264200	0.80855300	4.79201000
C	-4.87336900	1.55854400	2.91030200
C	-4.83698000	1.40587500	1.48649700
H	-5.68145300	2.12919700	-0.37737400
C	-5.68805600	2.23405800	0.70123600
C	-6.51124900	3.16692700	1.29098500
H	-7.18152300	4.06867300	3.14876400
C	-6.52889700	3.32701600	2.69745200
H	-5.73794100	2.64358100	4.56947500
C	-5.72632800	2.53651600	3.48781000
H	-8.03780900	-2.32913000	-2.83234300
C	-4.12510100	0.04357300	-3.40668300
H	-4.19418000	-0.04282900	-4.48811300
C	-3.08044600	0.72931300	-2.83922900
H	-2.34337700	1.18850600	-3.48536100
C	-2.96727200	0.86484900	-1.42676500
C	-3.94693600	0.30939000	-0.59648400
C	-5.05528700	-0.39504500	-1.18123500
C	-5.13368500	-0.54254100	-2.60372300
H	-6.26238400	-1.35551000	-4.25943600
C	-6.22089900	-1.25261500	-3.17813500
C	-7.20654100	-1.79251000	-2.38438700
H	-7.91810000	-2.07448100	-0.35534200
C	-7.13861500	-1.64550400	-0.97847300
H	-6.05135000	-0.87763300	0.68610700
C	-6.09209700	-0.97012300	-0.39245000
H	0.83642800	-4.32565900	5.10400300
H	1.35622300	4.61272300	-4.73259900
H	-2.93413300	5.14865400	3.43937300

H	-4.68405800	-4.94072300	-2.49137000
H	-0.48160700	-5.56012400	3.39600500
H	0.96011500	-1.84133300	5.01184200
H	1.13744100	2.14013600	-4.93751500
H	0.31210100	5.78451600	-2.80475200
H	-2.69778300	-3.68847400	-3.31832900
H	-5.41265700	-4.69007300	-0.13021200
H	-3.96371100	5.35533800	1.18781700
H	-1.24330800	3.37749200	3.87250200
C	1.57518300	-1.97895500	-1.26727300
C	1.23477400	-1.43391100	-2.52871200
C	1.37543300	-3.36268900	-1.08211900
C	0.68147600	-2.22114400	-3.53603500
H	1.47512100	-0.39763100	-2.72686700
C	0.83124700	-4.14768900	-2.09646500
H	1.65118300	-3.83151000	-0.14694500
C	0.47335100	-3.58570900	-3.32480700
H	0.44622300	-1.77244000	-4.49746100
H	0.68577200	-5.21001100	-1.92333200
H	0.05840300	-4.20795700	-4.11222100
C	6.59732300	-1.70501700	-2.20553100
H	6.08143300	-2.55149200	-1.73674800
H	6.79662500	-1.97620700	-3.25178300
H	7.56615000	-1.59431500	-1.70890000
C	6.47027100	0.75550200	-2.83195500
H	6.68935500	0.50110000	-3.87845700
H	5.85068500	1.66076200	-2.83787300
H	7.41938300	1.00730200	-2.34978600
C	4.43418100	-0.68755000	-2.92300500
H	3.90279600	-1.56084400	-2.53562100
H	3.75509400	0.17287300	-2.88583100
H	4.65771900	-0.88651600	-3.98079800

TS14

C	1.90653500	0.39204600	0.01685400
C	2.45277200	-0.75481500	-0.73177800
C	3.98362200	1.84595700	0.54946100
C	3.61297900	-1.50558000	-0.36987700
C	5.12007900	1.01138500	0.41255800
C	1.71110900	-1.19706800	-1.84854100
H	0.86914100	-0.59618200	-2.16421300
C	1.99158000	-2.37335500	-2.52949200
H	1.37138100	-2.67101400	-3.37059600
C	3.84742000	-2.72047300	-1.04620700

C	3.04492800	-3.17536400	-2.09063200
H	4.71313200	-3.31546300	-0.77009000
H	3.25943900	-4.12561800	-2.57151200
C	6.37440500	1.61139200	0.18662100
C	6.54014700	2.99158200	0.09267400
C	5.42663600	3.81592600	0.24443200
H	5.52619000	4.89714500	0.19443800
H	7.52499300	3.41512200	-0.08240200
H	7.24885500	0.97629400	0.08261700
C	2.56461100	1.38525700	0.68959800
C	1.65921100	2.31628100	1.40861600
C	1.95545800	2.87084400	2.66260300
C	-0.37265600	3.64384400	1.32068500
H	2.86829900	2.58552900	3.17695000
H	-1.26914300	3.97286700	0.80838200
C	-0.05932800	4.21479000	2.55200500
C	1.09409300	3.80628400	3.23368800
H	1.33220600	4.23587700	4.20326200
H	-0.71029000	4.96936900	2.98521600
Si	5.07202700	-0.85588700	0.65696900
C	5.06734500	-1.22622300	2.53998600
C	6.31760700	-0.61597000	3.21243700
C	3.82616800	-0.56088700	3.17243900
C	5.02319700	-2.74862500	2.78675100
H	7.25333400	-1.04766700	2.84491100
H	6.37017200	0.46776600	3.05504800
H	6.27903600	-0.79142700	4.29705000
H	2.89920700	-0.85004400	2.67376700
H	3.74760100	-0.83932700	4.23374600
H	3.89800700	0.53036800	3.12443400
H	4.89650600	-2.95666700	3.85952800
H	4.19260400	-3.22093400	2.25577900
H	5.94321000	-3.24822000	2.46836700
C	6.60555500	-1.54134500	-0.23018700
C	6.73708200	-1.24436900	-1.60377600
C	7.62123000	-2.31393500	0.35745600
C	7.82562700	-1.69176800	-2.34992600
H	5.97082000	-0.65218900	-2.09963900
C	8.71544700	-2.77022600	-0.38434500
H	7.57406800	-2.57281500	1.40913100
C	8.82125700	-2.46004500	-1.73949500
H	7.89840900	-1.44435900	-3.40583700
H	9.48368500	-3.36686500	0.10034500
H	9.67152400	-2.81261300	-2.31702300

C	4.17680400	3.24893800	0.47671700
H	3.33351300	3.91584700	0.62743300
C	0.46176000	2.67405300	0.72068100
Pd	-0.22416600	0.72355300	0.02641000
P	-0.98950600	-1.54034400	0.08581600
P	-2.54426600	1.48170200	-0.22782000
C	-2.54710100	5.32537000	-2.85132700
C	-3.23294400	5.33646600	-1.63607600
C	-3.25985400	4.19607600	-0.82869000
C	-2.58129100	3.03352800	-1.22071300
C	-1.87338100	3.04053300	-2.43409000
C	-1.87096000	4.16920900	-3.25265300
H	-3.80251200	4.22055700	0.11012000
H	-1.33913500	2.14887800	-2.74700300
C	1.85519100	-4.53139800	2.20378700
C	1.60094300	-3.26559600	2.73790500
C	0.81380000	-2.35658700	2.03607800
C	0.20916900	-2.72378900	0.82171700
C	0.51272400	-3.97439400	0.26844100
C	1.33807300	-4.86791200	0.95430700
H	0.66227900	-1.35617900	2.43281600
H	0.12491800	-4.25589200	-0.70194100
C	-2.45584600	-3.47538300	-3.87071000
C	-1.94295200	-2.17594600	-3.87245000
C	-1.50266700	-1.59793300	-2.68363200
C	-1.56685700	-2.30909600	-1.47752300
C	-2.11427900	-3.60213500	-1.48041100
C	-2.54511100	-4.18444400	-2.67202800
H	-1.13900100	-0.57560100	-2.68414100
H	-2.22447700	-4.14743000	-0.54812700
C	-4.68841400	2.26755600	3.79549700
C	-5.39565700	2.41278500	2.59944400
C	-4.75740800	2.19215900	1.38021000
C	-3.39858800	1.83994600	1.34813300
C	-2.69400800	1.69619100	2.55271700
C	-3.33927500	1.90849000	3.77033400
H	-5.32167800	2.26613600	0.45463500
H	-1.64875600	1.40733600	2.53566100
H	-6.27047000	-4.89538300	-1.23055200
C	-4.07239400	-0.86143300	-0.60334100
C	-3.69691200	0.36376500	-1.15428500
C	-4.10744200	0.69180700	-2.47651200
H	-3.85202900	1.65425000	-2.90015700
C	-4.83909700	-0.19024900	-3.23324600

H	-5.14283100	0.08124600	-4.24120600
C	-5.21520100	-1.45468500	-2.71938300
C	-4.84650700	-1.78944600	-1.37736100
H	-4.98207300	-3.32729500	0.14745300
C	-5.25173100	-3.05470800	-0.86604100
C	-5.97173000	-3.93528800	-1.64159600
H	-6.89025900	-4.30881000	-3.57289800
C	-6.32357700	-3.60340500	-2.97205200
H	-6.21999700	-2.11884300	-4.51597300
C	-5.95147500	-2.38716100	-3.49736400
H	-7.70717800	-0.96160200	4.41745600
C	-3.28127900	-1.89331600	3.51351900
H	-3.09231000	-2.16753100	4.54841700
C	-2.26762500	-1.96866000	2.59164600
H	-1.30130600	-2.32242800	2.92085700
C	-2.47138500	-1.62139600	1.22581900
C	-3.74580600	-1.22058200	0.81446200
C	-4.82469700	-1.15638200	1.76529800
C	-4.58117600	-1.48055700	3.13723000
H	-5.43057200	-1.64546600	5.11877400
C	-5.63864800	-1.39695600	4.08121800
C	-6.90199100	-1.01724500	3.69061600
H	-8.15070800	-0.39903000	2.02889200
C	-7.15272400	-0.70008700	2.33466300
H	-6.35591300	-0.50215400	0.37010500
C	-6.14385400	-0.76230300	1.39980500
H	-2.53956300	6.20911800	-3.48264500
H	2.47892900	-5.23545700	2.74682900
H	-2.80293200	-3.92563600	-4.79587800
H	-5.19233100	2.42372500	4.74482700
H	-3.75760900	6.23172600	-1.31507100
H	-1.33850500	4.14922100	-4.19995400
H	2.04224900	-2.97447400	3.68545300
H	1.56766400	-5.83148300	0.50863700
H	-2.78898500	1.78404500	4.69835800
H	-6.44964400	2.67286700	2.61691600
H	-2.97416900	-5.18149500	-2.65811200
H	-1.90000700	-1.60658700	-4.79639500
H	0.84078400	2.87263700	-0.62628200
N	1.61334900	3.26165700	-1.63169600
C	1.47108300	2.40972600	-2.83910300
C	1.44977500	4.72515200	-1.79433200
H	2.53432400	3.08314300	-1.22608400
H	0.95045100	2.98666200	-3.60925100

H	0.82535500	1.56941000	-2.55825300
H	1.43844700	5.14311300	-0.78090400
H	0.45782100	4.89546700	-2.22054600
C	2.54549200	5.37454200	-2.63668400
H	2.53803600	5.00009000	-3.66589100
H	2.39964400	6.45917400	-2.67358200
H	3.53514500	5.17811600	-2.20798200
C	2.81103400	1.87857900	-3.34274600
H	3.31059200	1.29976500	-2.55887000
H	2.65596500	1.21081100	-4.19640000
H	3.47408400	2.69190500	-3.65471200

INT21

C	1.93257700	0.46927100	0.01977000
C	2.42894400	-0.69379500	-0.74063500
C	4.09757600	1.84552600	0.26799400
C	3.54339200	-1.50527300	-0.36475100
C	5.17830800	0.93082100	0.22437700
C	1.67916200	-1.08978600	-1.86860800
H	0.85901000	-0.45380100	-2.17845500
C	1.91812700	-2.26985100	-2.56111600
H	1.29767900	-2.53104200	-3.41402600
C	3.72328600	-2.72763700	-1.04288200
C	2.92270200	-3.12659000	-2.11216500
H	4.54414800	-3.37463000	-0.74895900
H	3.09686100	-4.08225100	-2.59859600
C	6.45291100	1.40898200	-0.13931800
C	6.69071900	2.74192800	-0.46637500
C	5.63195000	3.64660400	-0.41443900
H	5.78873100	4.69830000	-0.64137400
H	7.68937300	3.07014600	-0.74016600
H	7.28580800	0.71378400	-0.16654900
C	2.66715700	1.49324100	0.56264600
C	1.86805900	2.48403100	1.32202700
C	2.41058200	3.37364400	2.26235500
C	-0.30506000	3.48250200	1.67256300
H	3.46945900	3.32430200	2.49882200
H	-1.36708500	3.55358700	1.47815100
C	0.25178500	4.40108000	2.57443400
C	1.60659900	4.32852500	2.88912600
H	2.04245200	5.01357700	3.61113600
H	-0.38082100	5.15648300	3.03389800
Si	5.00076300	-0.89118800	0.68950500
C	4.89132100	-1.06164400	2.60036800

C	6.07924000	-0.32968300	3.26568900
C	3.59213100	-0.40331700	3.11325400
C	4.89726500	-2.55275300	3.00246300
H	7.05228400	-0.73406900	2.96996900
H	6.07915200	0.73875800	3.02064300
H	6.00518900	-0.41929800	4.35881200
H	2.70427100	-0.80042500	2.61841000
H	3.48975200	-0.57677800	4.19479300
H	3.59585700	0.67993600	2.95631800
H	4.69577100	-2.65449200	4.07903100
H	4.13228200	-3.12035000	2.46603000
H	5.85836700	-3.03633200	2.80807300
C	6.53872300	-1.74659100	-0.03633800
C	6.71117500	-1.69987800	-1.43716000
C	7.55727300	-2.36593700	0.70822100
C	7.83141900	-2.24788500	-2.05941700
H	5.95151400	-1.22708600	-2.05516200
C	8.68367400	-2.92077400	0.09275400
H	7.48978900	-2.42251300	1.78823400
C	8.82402100	-2.86495100	-1.29308700
H	7.93109700	-2.19485900	-3.14052800
H	9.45010400	-3.39464900	0.70030300
H	9.69877900	-3.29512800	-1.77325300
C	4.36715600	3.20147900	-0.04208000
H	3.57689600	3.93834900	0.05357000
C	0.47346500	2.50082900	1.05108100
Pd	-0.19573700	0.74616500	0.17448100
P	-1.00903400	-1.58509100	0.01852800
P	-2.52198100	1.50436800	-0.06552000
C	-2.41517000	5.50556600	-2.45315000
C	-3.02296900	5.48131300	-1.19764200
C	-3.08498400	4.29351500	-0.46282700
C	-2.51481700	3.11629700	-0.96445500
C	-1.87485500	3.15976700	-2.21582500
C	-1.84594700	4.33500200	-2.96589900
H	-3.57908100	4.29017600	0.50279700
H	-1.43257400	2.25323600	-2.62031700
C	1.84737900	-4.62183000	2.05862500
C	1.56541300	-3.37945100	2.63248200
C	0.76673900	-2.46317200	1.95386000
C	0.17829900	-2.79867600	0.72258200
C	0.49860200	-4.02965000	0.13666100
C	1.33605700	-4.93003100	0.79901400
H	0.58698400	-1.48288500	2.38705800

H	0.11515300	-4.28882400	-0.84202900
C	-2.50567400	-3.33373100	-4.01393600
C	-1.98818700	-2.03745400	-3.95184300
C	-1.53430800	-1.52635000	-2.73798700
C	-1.58916100	-2.29955600	-1.56981300
C	-2.13771000	-3.58960400	-1.63724700
C	-2.58283500	-4.10610900	-2.85414400
H	-1.16919300	-0.50562400	-2.68502400
H	-2.23778200	-4.18396500	-0.73412800
C	-4.83490000	2.04985500	3.90282500
C	-5.47427800	2.32701700	2.69203700
C	-4.78316500	2.18701400	1.48969000
C	-3.43872300	1.78325300	1.49260600
C	-2.80051600	1.51131700	2.71207200
C	-3.49912300	1.64271000	3.91117900
H	-5.29447000	2.36730000	0.54794300
H	-1.76418500	1.18961500	2.71805200
H	-6.32161800	-4.74415100	-1.52927000
C	-4.06169000	-0.79674000	-0.62868600
C	-3.66691500	0.45899800	-1.09210700
C	-4.07749000	0.88176700	-2.38780500
H	-3.82485000	1.87201500	-2.74191600
C	-4.81801400	0.06332600	-3.20517300
H	-5.12239600	0.41160400	-4.18914500
C	-5.20914600	-1.22964600	-2.78249300
C	-4.84517000	-1.65991600	-1.46714100
H	-5.00391900	-3.29671200	-0.05159300
C	-5.27093900	-2.95050500	-1.04290800
C	-6.00727700	-3.76344100	-1.87475700
H	-6.93478100	-3.98901900	-3.82464200
C	-6.35487900	-3.33610600	-3.17871800
H	-6.22618300	-1.75212300	-4.61867700
C	-5.96154200	-2.09398900	-3.62126300
H	-7.76123700	-1.21531100	4.32885200
C	-3.34136900	-2.15615300	3.40177800
H	-3.17105000	-2.51911100	4.41240800
C	-2.31846900	-2.18068800	2.48671100
H	-1.36428800	-2.58250000	2.79622400
C	-2.49737300	-1.72099900	1.15076100
C	-3.75749500	-1.25824100	0.76363500
C	-4.84649900	-1.24306200	1.70494500
C	-4.62773300	-1.68528700	3.04767400
H	-5.50701000	-1.99880900	4.99806000
C	-5.69632300	-1.66023400	3.98257100

C	-6.94710100	-1.22493800	3.60990800
H	-8.16096600	-0.44463800	1.99110200
C	-7.17312600	-0.79022700	2.28251600
H	-6.34537400	-0.44333600	0.35149200
C	-6.15271000	-0.79328200	1.35824000
H	-2.38911500	6.42475000	-3.03114500
H	2.48070800	-5.33231500	2.58208000
H	-2.86540000	-3.73245400	-4.95775900
H	-5.38108700	2.14198100	4.83696300
H	-3.46518900	6.38573200	-0.78993200
H	-1.38336000	4.33935100	-3.94988400
H	1.98754400	-3.11196200	3.59562200
H	1.57996700	-5.87773000	0.32737300
H	-3.00206400	1.41763400	4.85015400
H	-6.51739600	2.62850400	2.68263100
H	-3.01314800	-5.10222800	-2.89016600
H	-1.95433500	-1.41979200	-4.84478700
H	0.71699300	2.75582400	-1.10915300
N	1.46570200	3.12109500	-1.74027100
C	1.38872700	2.46599500	-3.09649600
C	1.44180500	4.62411400	-1.67857700
H	2.31480600	2.77403900	-1.27643100
H	0.92622700	3.18046600	-3.78083600
H	0.71732700	1.61316900	-2.98233400
H	1.49808700	4.86528000	-0.61340300
H	0.45854400	4.93095600	-2.03879400
C	2.56780600	5.27046100	-2.47362600
H	2.46693600	5.08817500	-3.54810300
H	2.53372300	6.35288400	-2.31744800
H	3.54886500	4.91046700	-2.14985400
C	2.75943100	1.99618000	-3.56877000
H	3.16498500	1.24850400	-2.87917800
H	2.66267700	1.52658800	-4.55229000
H	3.47044200	2.82283600	-3.65113500

TS15

C	-1.92506400	0.59029800	0.49894800
C	-2.47572100	-0.76807500	0.75793700
C	-4.08783300	1.98785500	0.61223800
C	-3.62417500	-1.35492900	0.14567700
C	-5.18856500	1.18492400	0.23931600
C	-1.72442100	-1.56850100	1.64415100
H	-0.85471800	-1.12802200	2.11138200
C	-2.03032600	-2.89382800	1.92076900

H	-1.40712000	-3.45768700	2.60977900
C	-3.87931900	-2.71887600	0.39883500
C	-3.10961500	-3.48922500	1.26857000
H	-4.73368400	-3.18890200	-0.07825700
H	-3.35311900	-4.53503500	1.43431700
C	-6.46627100	1.57159700	0.68762900
C	-6.66290700	2.68551900	1.50191700
C	-5.56649400	3.45652700	1.89141800
H	-5.69881600	4.32209400	2.53463400
H	-7.66408900	2.94845700	1.83157400
H	-7.32796600	0.97708700	0.40231000
C	-2.68085800	1.74225900	0.20814900
C	-1.96765800	2.84476900	-0.43031800
C	-2.62852300	3.98980700	-0.93209600
C	0.02920400	3.52852100	-1.60524300
H	-3.68627300	4.12915600	-0.74056900
H	1.06011600	3.38865700	-1.90664400
C	-0.63047900	4.66862400	-2.08209500
C	-1.95990900	4.90599200	-1.73685800
H	-2.48259900	5.77892900	-2.11638400
H	-0.09658000	5.36625400	-2.72242900
Si	-4.98617200	-0.40218200	-0.77293900
C	-4.62511500	-0.07138800	-2.62943600
C	-5.65795400	0.91120500	-3.22284500
C	-3.22256200	0.55048400	-2.80214000
C	-4.65565900	-1.41636000	-3.38823400
H	-6.68560400	0.53780400	-3.17157500
H	-5.63279200	1.87747400	-2.70472500
H	-5.43017200	1.09796000	-4.28187900
H	-2.44169900	-0.03604300	-2.31045400
H	-2.97453200	0.60582900	-3.87260100
H	-3.17762700	1.57060800	-2.41172300
H	-4.37582100	-1.25885700	-4.44006700
H	-3.94149900	-2.12822400	-2.96344900
H	-5.64150100	-1.88919000	-3.38048700
C	-6.60750500	-1.35231400	-0.48861000
C	-6.90653800	-1.76676300	0.82762700
C	-7.58406200	-1.59602300	-1.47008600
C	-8.10677800	-2.40134500	1.14345200
H	-6.18508100	-1.59218100	1.62235700
C	-8.79037800	-2.23237900	-1.16255200
H	-7.41919200	-1.28736900	-2.49595200
C	-9.05478000	-2.63915400	0.14459700
H	-8.30358500	-2.70964900	2.16696200

H	-9.52179000	-2.40733300	-1.94702200
H	-9.99164600	-3.13408900	0.38546500
C	-4.29771600	3.11770000	1.43499000
H	-3.44732000	3.73198100	1.71899400
C	-0.60386800	2.62161700	-0.75138800
Pd	0.18646300	0.83615600	-0.16397500
P	1.05049700	-1.53463600	-0.27659200
P	2.45613900	1.66960200	-0.26038300
C	2.81764600	6.06129500	1.27435500
C	3.77776900	5.56025900	0.39482000
C	3.68060700	4.25318600	-0.08773500
C	2.61678300	3.42663400	0.30190200
C	1.64495700	3.95005700	1.17097400
C	1.74759800	5.25091200	1.66014100
H	4.43029000	3.89561300	-0.78276100
H	0.78643600	3.34537200	1.43504200
C	-1.76997800	-3.52516100	-3.38533500
C	-1.15379400	-2.29548300	-3.63442000
C	-0.35018900	-1.70923400	-2.66061600
C	-0.11907900	-2.35899200	-1.43321500
C	-0.76858900	-3.57205600	-1.18063700
C	-1.59356500	-4.14705300	-2.15036700
H	0.12231600	-0.75160200	-2.86353800
H	-0.65237900	-4.06776400	-0.22620000
C	1.91300400	-4.39138800	3.28520300
C	1.68575200	-3.03132200	3.50332100
C	1.41189700	-2.19109900	2.42511900
C	1.35237100	-2.69528700	1.12021900
C	1.63692300	-4.05295700	0.90445600
C	1.89868900	-4.89798000	1.98326600
H	1.27862100	-1.12747600	2.58796100
H	1.65973400	-4.45067800	-0.10556600
C	4.63215200	1.48303200	-4.34580300
C	5.38170100	1.68877200	-3.18523300
C	4.74823900	1.73964300	-1.94501500
C	3.35502600	1.59020600	-1.85310100
C	2.61110000	1.37256600	-3.02245900
C	3.24764500	1.32215000	-4.26308200
H	5.34405500	1.85296900	-1.04509300
H	1.53486900	1.23818600	-2.95696900
H	5.64980400	-4.43743400	2.61911900
C	3.86792100	-0.57765200	0.77742100
C	3.42611100	0.72696100	1.00142600
C	3.55203400	1.29925200	2.30130900

H	3.23869300	2.32296400	2.46700700
C	4.08432300	0.58473500	3.34554500
H	4.18551600	1.04586000	4.32533300
C	4.51991100	-0.75218000	3.16592000
C	4.41730600	-1.34040200	1.86404500
H	4.75451000	-3.15645000	0.72806900
C	4.84377400	-2.68808600	1.70066200
C	5.34159200	-3.40617700	2.76387700
H	5.85182200	-3.39463800	4.87385300
C	5.45072400	-2.81667900	4.04628700
H	5.12633700	-1.05173200	5.22084000
C	5.04758300	-1.51533200	4.24059600
H	8.44783200	-1.46500900	-3.31569800
C	3.93317200	-2.39456700	-3.13897700
H	3.95779200	-2.86035200	-4.12098600
C	2.74951100	-2.31252000	-2.44887700
H	1.85616400	-2.72689100	-2.89620500
C	2.68114100	-1.69308200	-1.16972100
C	3.84867500	-1.20460600	-0.58465000
C	5.10042800	-1.30499000	-1.28190400
C	5.13334600	-1.88222700	-2.59106400
H	6.36140100	-2.36408700	-4.30429600
C	6.35759000	-1.92669200	-3.30917500
C	7.51576900	-1.42703100	-2.75934100
H	8.41130600	-0.48187600	-1.02423400
C	7.49353100	-0.86794300	-1.45876000
H	6.32377800	-0.37327400	0.25248300
C	6.32075200	-0.81047100	-0.73909900
H	2.89530200	7.07869700	1.64668300
H	-2.40125200	-3.98089000	-4.14251500
H	2.12588700	-5.04916300	4.12285800
H	5.12848100	1.43610100	-5.31078900
H	4.60609600	6.18692100	0.07683200
H	0.98210700	5.63813700	2.32724600
H	-1.31413100	-1.78499400	-4.57932400
H	-2.09499800	-5.08611800	-1.93462600
H	2.66273300	1.14910800	-5.16188200
H	6.46175500	1.78185500	-3.24032800
H	2.10507900	-5.94956800	1.80525000
H	1.74431900	-2.62135500	4.50726900
H	-1.45738700	0.99235100	1.70104200
N	-1.23007500	1.37947400	3.07661300
C	-2.06055000	0.67833200	4.09521800
C	0.21820500	1.36336800	3.40119000

H	-1.54791500	2.34928500	3.00323600
H	-1.81829400	1.07654300	5.09020600
H	-1.75347900	-0.37073300	4.07728600
H	0.76876000	1.41256100	2.45731300
H	0.43683700	0.38619500	3.84053000
C	0.65587400	2.48176600	4.34381700
H	0.12017700	2.44392900	5.29815300
H	1.72624100	2.39114800	4.55377600
H	0.49159100	3.46683700	3.89220400
C	-3.55556000	0.78944100	3.83113900
H	-3.82504500	0.34682600	2.86971800
H	-4.09833700	0.25694400	4.61873900
H	-3.89450000	1.82979900	3.83397100

INT22

C	-2.23407100	0.19161400	-0.93517100
C	-2.87883900	-1.14306000	-0.90211200
C	-3.50753200	1.53350400	0.81684100
C	-4.28354300	-1.35310600	-0.92156400
C	-4.84421900	1.07081400	0.74362800
C	-2.02868100	-2.25369800	-1.00636000
H	-0.96400600	-2.09045200	-0.99467500
C	-2.51125800	-3.55134500	-1.12216100
H	-1.81257300	-4.38080900	-1.18380900
C	-4.74998900	-2.67201100	-1.07680800
C	-3.88820900	-3.76419000	-1.17450700
H	-5.81995600	-2.85172000	-1.11465000
H	-4.28985200	-4.76674800	-1.29251100
C	-5.69125600	1.35037600	1.83460000
C	-5.25142900	2.04188500	2.96259600
C	-3.93427400	2.49845600	3.02090600
H	-3.57605400	3.04493000	3.88920400
H	-5.93599900	2.23073000	3.78476100
H	-6.72157700	1.01167200	1.80365000
C	-2.49600100	1.34954100	-0.25740600
C	-1.74328500	2.57950000	-0.63218100
C	-2.44557200	3.78841200	-0.80585000
C	0.29157600	3.70631300	-1.30884100
H	-3.50984900	3.81767400	-0.59101500
H	1.36085100	3.71558800	-1.48759700
C	-0.42374900	4.88657100	-1.52054900
C	-1.79461700	4.93168100	-1.25628100
H	-2.35235800	5.85215500	-1.40218500
H	0.09463100	5.77106300	-1.88135700

Si	-5.52875900	0.05091900	-0.70767000
C	-5.76938700	1.03671000	-2.35068900
C	-6.47795100	2.38307700	-2.08471600
C	-4.42733400	1.34083500	-3.05427900
C	-6.59966400	0.16347000	-3.32223600
H	-7.46407200	2.26869200	-1.62386400
H	-5.88153500	3.02255700	-1.42225300
H	-6.62085100	2.92661300	-3.02921900
H	-3.84473700	0.43079400	-3.23634200
H	-4.62865900	1.80637900	-4.02960700
H	-3.80447900	2.03745400	-2.48765500
H	-6.73217200	0.69313300	-4.27607100
H	-6.08716800	-0.78171900	-3.54186500
H	-7.59427200	-0.08243300	-2.94206300
C	-7.15911000	-0.67653600	-0.05871700
C	-7.11401700	-1.69323600	0.91868700
C	-8.43052600	-0.17771900	-0.39850000
C	-8.27301000	-2.19668400	1.50958600
H	-6.15766000	-2.10447600	1.22575300
C	-9.59627500	-0.67569800	0.18908900
H	-8.53016300	0.61595900	-1.13026800
C	-9.52180700	-1.68986100	1.14388100
H	-8.20021300	-2.98348300	2.25592400
H	-10.56129500	-0.26866800	-0.10073200
H	-10.42717800	-2.07947900	1.60121800
C	-3.08281400	2.26231100	1.94729600
H	-2.07027900	2.65038100	1.96993000
C	-0.35614200	2.54510900	-0.86853300
Pd	0.50236000	0.71240000	-0.61700800
P	1.63410400	-1.44938600	-1.02480400
P	2.34586500	1.66519000	0.38648700
C	1.05773600	5.27402000	3.00775800
C	2.20754100	5.37772600	2.22594700
C	2.62744900	4.30310900	1.43700000
C	1.88978100	3.11268800	1.42286600
C	0.71933000	3.02479200	2.19504300
C	0.31349400	4.09046900	2.99195800
H	3.51294900	4.41420400	0.82288800
H	0.11576900	2.12559300	2.15584400
C	-0.30483800	-2.81459400	-5.01915000
C	-0.11354600	-1.45891500	-4.73968000
C	0.49854300	-1.07466300	-3.54743000
C	0.93117800	-2.04046200	-2.62096000
C	0.74330900	-3.39808900	-2.91443100

C	0.12733900	-3.77983800	-4.10775100
H	0.63929300	-0.01580200	-3.33663700
H	1.05671000	-4.15781600	-2.20609700
C	1.43194600	-5.05169800	1.86279400
C	0.52550800	-3.99672200	1.98060600
C	0.59319500	-2.90608600	1.11156500
C	1.57706100	-2.87458400	0.11298600
C	2.48712500	-3.93803700	-0.00555900
C	2.41163400	-5.02270400	0.86618900
H	-0.13312900	-2.10480000	1.22521000
H	3.26179300	-3.90914600	-0.76674400
C	5.64569600	3.06937700	-2.53126900
C	5.87772000	3.08223700	-1.15414300
C	4.88653600	2.65137800	-0.27468500
C	3.64511200	2.21690300	-0.76965700
C	3.42187000	2.19748400	-2.15363600
C	4.41996300	2.62299400	-3.02947300
H	5.08927200	2.62524300	0.79177500
H	2.47432300	1.83669900	-2.54220500
H	6.07627500	-4.58106500	2.11629800
C	3.85719200	-0.65387600	1.05092600
C	3.10336400	0.42626100	1.52467100
C	2.79627600	0.52252700	2.91120000
H	2.24272300	1.37485800	3.28294300
C	3.19563400	-0.44858300	3.79436900
H	2.94770300	-0.35687700	4.84860300
C	3.93765900	-1.57158500	3.35490400
C	4.29393400	-1.66622800	1.96991400
H	5.36596100	-2.86665200	0.51428700
C	5.08095400	-2.77847600	1.55560400
C	5.47739600	-3.74078700	2.45541600
H	5.42610100	-4.41910300	4.51698000
C	5.10817200	-3.64989000	3.81933100
H	4.07133100	-2.50091800	5.30332300
C	4.35428700	-2.58587200	4.25742500
H	9.33017400	0.50518500	-1.66693700
C	5.18077000	-0.95480800	-3.05459600
H	5.51864100	-1.02955100	-4.08508800
C	3.88625200	-1.27883100	-2.72991600
H	3.20945300	-1.61200100	-3.50764900
C	3.42248900	-1.17738400	-1.38996500
C	4.29244000	-0.76572600	-0.38149700
C	5.65568300	-0.45039700	-0.69977700
C	6.09475700	-0.52539400	-2.06153200

H	7.74648500	-0.22592800	-3.42493600
C	7.43041600	-0.16803200	-2.38656200
C	8.30960500	0.23795400	-1.40887100
H	8.58432100	0.61546900	0.70930100
C	7.88478100	0.30093500	-0.05994600
H	6.28493800	0.02767500	1.32266500
C	6.59413500	-0.03195600	0.28573800
H	0.73562300	6.11243000	3.61823800
H	-0.79157100	-3.11618500	-5.94196600
H	1.37898500	-5.89517000	2.54544900
H	6.42420500	3.39495400	-3.21466700
H	2.78258700	6.29905500	2.22113800
H	-0.58959800	4.00150300	3.58886800
H	-0.44699900	-0.70208300	-5.44388800
H	-0.02068100	-4.83454500	-4.32118300
H	4.24189900	2.59610900	-4.10032700
H	6.83901800	3.40149600	-0.76460600
H	3.12377000	-5.83775900	0.77596400
H	-0.24144100	-4.01428200	2.74928100
H	-1.53216900	0.28999100	-1.77626500
N	-1.61110700	-0.98482000	2.58967900
C	-2.51477300	-1.77944500	3.42333400
C	-0.43428400	-0.45001300	3.26875500
H	-2.13533300	-0.22324100	2.16349500
H	-2.89553000	-1.22546600	4.29935300
H	-1.94117400	-2.62934600	3.81899100
H	0.18853500	0.01901000	2.49713200
H	0.15779700	-1.29687500	3.63948700
C	-0.68564900	0.54572100	4.41139100
H	-1.20188300	0.07310600	5.25303800
H	0.25989500	0.95440400	4.78815700
H	-1.30721600	1.38185300	4.07031900
C	-3.69513500	-2.27698900	2.59389500
H	-3.35117600	-2.84260300	1.72233400
H	-4.35610500	-2.91125400	3.19503800
H	-4.28305900	-1.42636100	2.23238300

TS16

P	1.94158500	0.09333100	1.79335800
P	1.88986800	0.46019600	-1.66131400
C	3.13122500	3.97090200	-4.42073000
C	2.06691800	3.14502400	-4.78306200
C	1.72670800	2.04418900	-3.99442100
C	2.45272000	1.75489700	-2.83111800

C	3.51085700	2.60503300	-2.46092800
C	3.85438900	3.69684000	-3.25644700
H	0.88612600	1.42191000	-4.28088400
H	4.07062700	2.41361400	-1.55009800
C	1.52372000	0.32275000	6.41101300
C	1.69353500	1.47181500	5.63266700
C	1.78211300	1.36621100	4.24621400
C	1.70056900	0.11268300	3.61655400
C	1.55532800	-1.03608300	4.40494400
C	1.46011200	-0.92761900	5.79506900
H	1.91985300	2.26273700	3.64473800
H	1.51348300	-2.01686700	3.94258400
C	6.53582900	0.68666600	1.80781300
C	5.70113000	1.62241200	1.19427000
C	4.32098700	1.41319900	1.16840300
C	3.76828000	0.26814500	1.75628400
C	4.61007300	-0.65318300	2.39590700
C	5.98828300	-0.45039900	2.40925300
H	3.66583400	2.13567700	0.68781700
H	4.19093100	-1.53598300	2.86854200
C	-0.70130600	-2.61687500	-3.94375600
C	0.49846500	-2.16124300	-4.49881900
C	1.25602000	-1.20398400	-3.82840200
C	0.80238700	-0.67232500	-2.60792600
C	-0.40083600	-1.13102900	-2.05991700
C	-1.14440300	-2.10794400	-2.72470900
H	2.20101500	-0.87182000	-4.24931000
H	-0.74339700	-0.75197400	-1.10397400
H	5.54314400	-5.08843400	1.74907400
C	3.27088900	-1.73952000	-0.50712900
C	3.36040600	-0.63786800	-1.36160900
C	4.59942000	-0.35041200	-2.00043400
H	4.66265600	0.45889300	-2.71565000
C	5.72659600	-1.08771700	-1.73732500
H	6.66261100	-0.84482300	-2.23390300
C	5.69469800	-2.16005200	-0.81387400
C	4.44472000	-2.50974000	-0.21130100
H	3.48743300	-3.87381800	1.17914600
C	4.42492900	-3.59199700	0.71360100
C	5.57925900	-4.27102000	1.03454400
H	7.71601400	-4.46245100	0.69993600
C	6.81421100	-3.91615000	0.43914100
H	7.80739300	-2.60558600	-0.93727000
C	6.86612500	-2.88508500	-0.47094000

H	-0.50776900	-6.44072400	-2.01542900
C	-0.48216700	-3.10452400	1.16988000
H	-1.43477900	-3.43341800	1.57487100
C	0.13739500	-2.00131900	1.69528200
H	-0.34818700	-1.45247700	2.49350300
C	1.39665500	-1.55370000	1.19189000
C	1.97708300	-2.19383700	0.10150600
C	1.32950400	-3.34401700	-0.47224900
C	0.09295400	-3.80998900	0.08132500
H	-1.48633400	-5.27925300	-0.05760400
C	-0.55004700	-4.93747400	-0.49167400
C	-0.00666900	-5.58064100	-1.58069900
H	1.62578000	-5.61795300	-3.00668200
C	1.20654200	-5.11563500	-2.13975100
H	2.78062300	-3.67870800	-2.04907100
C	1.85839900	-4.02847900	-1.60080500
H	3.39472100	4.82504700	-5.03775700
H	1.44980800	0.40279400	7.49163700
H	7.61057100	0.84367900	1.82210900
H	-1.28728500	-3.37294100	-4.45802400
H	1.49322500	3.35709800	-5.68063100
H	4.68264300	4.33637600	-2.96420700
H	1.75795600	2.44731900	6.10658900
H	1.34187400	-1.82532600	6.39535000
H	-2.07150200	-2.46503900	-2.28999300
H	0.85095800	-2.56184000	-5.44511800
H	6.63492500	-1.18313700	2.88246700
H	6.12286400	2.51195600	0.73417400
C	-2.35519300	1.54193400	-0.97076900
C	-3.76717300	-0.16290600	-2.41681800
C	-2.27181600	1.09689900	0.44626400
C	-4.48132400	-1.00349000	-1.52973400
C	-3.20030600	0.19946900	1.04710100
C	-5.02295600	-2.21136300	1.17956900
C	-6.00350900	-2.44388500	2.15920700
C	-4.13244100	-3.26752100	0.89431100
C	-6.09276400	-3.66915100	2.82716600
H	-6.71551300	-1.66609800	2.41457100
C	-4.21466500	-4.49220400	1.55658000
H	-3.36812900	-3.13321800	0.13212700
C	-5.19727300	-4.69622200	2.52940400
H	-6.86406400	-3.81947700	3.57772400
H	-3.51962600	-5.29197400	1.31175800
H	-5.26646900	-5.64957800	3.04595400

C	-6.21148700	0.67020000	0.42752700
C	-7.52023000	-0.00940700	-0.02990800
C	-6.35420000	1.19038000	1.87422800
C	-5.94515900	1.88392700	-0.49205600
H	-7.44457900	-0.36987200	-1.06288200
H	-7.79346400	-0.86263100	0.59972900
H	-8.35147900	0.70858500	0.00841000
H	-5.44422400	1.70142200	2.21045500
H	-7.18108400	1.91210000	1.93238600
H	-6.56854100	0.39492900	2.59575900
H	-6.77383900	2.60122200	-0.40797800
H	-5.02293100	2.40995800	-0.22129400
H	-5.86513200	1.59135000	-1.54438200
C	-2.09539100	0.48565800	3.22917200
H	-2.04471900	0.25910900	4.29093200
C	-1.22956600	1.66566100	1.26677800
C	-1.19385100	1.36163600	2.64044000
H	-0.44315300	1.84007700	3.25877200
C	-3.06376100	-0.10079100	2.41823600
H	-3.75887800	-0.80040500	2.87318200
H	-1.01540700	3.03147000	1.20731800
C	-3.76806600	-0.47437200	-3.79625900
H	-3.22531400	0.17197500	-4.48107400
C	-5.12480800	-2.13901600	-2.05596300
C	-5.08837600	-2.44952200	-3.41549000
H	-5.59996300	-3.33302100	-3.78696700
C	-4.40938500	-1.60172400	-4.29281700
H	-4.37989200	-1.81770900	-5.35712800
H	-5.67447100	-2.79471800	-1.38705700
Pd	0.70488800	1.44529100	0.18146700
C	-1.55238200	2.76286100	-1.30758300
C	-0.17239000	2.79637900	-1.06979800
C	-2.18167700	3.88606100	-1.87284400
C	0.56272900	3.93421500	-1.41950800
C	-1.44797700	5.02755400	-2.20557700
H	-3.25647800	3.86433500	-2.03369900
C	-0.06824100	5.04868900	-1.98637700
H	1.63537500	3.96753700	-1.25719100
H	-1.95029100	5.88948000	-2.63591100
H	0.51868900	5.92337500	-2.25486800
Si	-4.74782500	-0.56899600	0.27223900
C	-2.98708100	1.02273500	-2.06527500
H	-2.77560500	1.60270000	-2.96074900
N	-0.96863200	4.35076500	1.42406600

C	-2.09828400	4.74075500	2.29694000
C	0.38485200	4.62104600	1.95343100
H	-1.07027500	4.77312300	0.49876800
H	-1.99539900	5.79102700	2.59818000
H	-2.02521800	4.12464100	3.20039800
H	1.06140200	3.90897100	1.46047500
H	0.37284300	4.37172300	3.02003900
C	0.85617100	6.05403900	1.72022400
H	0.19948300	6.78100300	2.20984900
H	1.86669800	6.19120700	2.11936600
H	0.88025700	6.27566000	0.64749500
C	-3.43099600	4.49851400	1.59482100
H	-3.55328500	3.44015200	1.34952000
H	-4.25799200	4.79928400	2.24495100
H	-3.49996100	5.07441100	0.66522800

INT23

P	0.94116000	-1.26526800	1.14001700
P	2.69519200	1.37249600	-0.28582600
C	3.90561900	5.59516900	1.22802100
C	4.11924900	5.27189100	-0.11243300
C	3.81030800	3.99466300	-0.59022900
C	3.27544900	3.02835500	0.27024000
C	3.05936100	3.36395100	1.61970200
C	3.37972400	4.63347500	2.09765700
H	3.96501500	3.76372600	-1.63862200
H	2.62862900	2.62712800	2.29333600
C	-2.14067400	-4.52351600	2.36741000
C	-2.17299800	-3.25061300	2.93951600
C	-1.27675000	-2.26882400	2.51592500
C	-0.33398400	-2.54444400	1.51578500
C	-0.30469100	-3.83115000	0.95033300
C	-1.20639400	-4.80946400	1.37007100
H	-1.31423900	-1.28696100	2.96816500
H	0.41886200	-4.07555600	0.17991000
C	4.02279700	-2.17850800	4.48332300
C	3.60564400	-0.86988200	4.23580400
C	2.68924900	-0.61289400	3.21545600
C	2.18714900	-1.65922600	2.43108500
C	2.59660800	-2.97465600	2.69961100
C	3.51477900	-3.22990700	3.71539500
H	2.36707300	0.40459800	3.01178300
H	2.20315600	-3.79808600	2.11247100
C	3.00001300	1.15582700	-4.89826100

C	4.16164500	1.30269800	-4.13517700
C	4.07793300	1.38905700	-2.74688600
C	2.82709700	1.34316800	-2.10980000
C	1.66523600	1.19393600	-2.88058100
C	1.75537500	1.10083700	-4.26946800
H	4.98603600	1.46485700	-2.15469100
H	0.69856400	1.12815800	-2.39601900
H	5.67012000	-5.37502800	0.72621500
C	3.95436400	-1.13794100	-0.00595000
C	4.03529800	0.22549600	0.28319100
C	5.08840400	0.70715800	1.10745900
H	5.17206100	1.76803700	1.31077200
C	6.00468200	-0.15467600	1.66054600
H	6.79903900	0.22972400	2.29547900
C	5.92899600	-1.54893800	1.42440400
C	4.90333300	-2.04752800	0.55835500
H	4.07057100	-3.83773100	-0.33698700
C	4.84063700	-3.44895600	0.32010000
C	5.73539100	-4.30769100	0.91758200
H	7.43997600	-4.50168700	2.24784200
C	6.74186900	-3.81204100	1.78214400
H	7.60720200	-2.07074600	2.68574100
C	6.83618100	-2.46090700	2.02622100
H	4.20576000	-2.92533500	-5.96433500
C	0.90115500	-2.38646000	-2.78944400
H	0.12443800	-2.65066400	-3.50057200
C	0.56215700	-2.08431800	-1.49557100
H	-0.48361000	-2.09775500	-1.20646200
C	1.56434500	-1.76128700	-0.53111300
C	2.89403500	-1.65428100	-0.92976800
C	3.26681600	-1.98416800	-2.27914000
C	2.25389100	-2.36958100	-3.21439700
H	1.83660200	-2.99247700	-5.24185000
C	2.61897100	-2.70312000	-4.54455600
C	3.93529700	-2.66335700	-4.94546100
H	5.97678400	-2.24202700	-4.34853500
C	4.93960400	-2.27697200	-4.02734500
H	5.39584000	-1.63791100	-2.04424100
C	4.61471000	-1.93913400	-2.73209200
H	4.14857400	6.58809200	1.59556400
H	-2.83628800	-5.29026600	2.69648400
H	4.74065900	-2.38092800	5.27300000
H	3.06871200	1.07220100	-5.97903200
H	4.52563300	6.01452000	-0.79320100

H	3.22022100	4.87386000	3.14570800
H	-2.90448700	-3.01311800	3.70647600
H	-1.17277700	-5.79778000	0.92035400
H	0.85120000	0.97291600	-4.85819000
H	5.13310800	1.32847900	-4.62004100
H	3.84128400	-4.24843900	3.90213000
H	3.99728700	-0.04927500	4.83040800
C	-2.14583200	1.05186300	-1.11019000
C	-3.03651700	-0.93584100	-2.49009100
C	-2.50496500	0.72952700	0.30301500
C	-4.15068000	-1.43679900	-1.76845900
C	-3.79858700	0.32361900	0.71495100
C	-6.00364600	-1.72325200	0.60728400
C	-7.39643100	-1.81558000	0.77022400
C	-5.20993000	-2.68043600	1.27357100
C	-7.97378100	-2.80904700	1.56691000
H	-8.05539200	-1.11297500	0.27205200
C	-5.77873700	-3.67355300	2.06888300
H	-4.12874800	-2.65249400	1.16916000
C	-7.16641300	-3.73991400	2.22027100
H	-9.05435800	-2.85437500	1.67333800
H	-5.13968700	-4.39712600	2.56777100
H	-7.61394400	-4.51306200	2.83906300
C	-6.24176700	0.86418500	-1.23700500
C	-7.20810000	0.18957800	-2.23520600
C	-7.03440700	1.60215600	-0.13511100
C	-5.41142100	1.91243000	-2.00656000
H	-6.66091900	-0.31365800	-3.04084600
H	-7.85516100	-0.55612800	-1.76258100
H	-7.86035800	0.94430800	-2.69706000
H	-6.36518400	2.09690900	0.57927100
H	-7.66833400	2.37951900	-0.58506400
H	-7.68853400	0.93888300	0.43792300
H	-6.07832900	2.67303200	-2.43790900
H	-4.69906600	2.42639600	-1.35253300
H	-4.84534700	1.46189400	-2.82857600
C	-3.16451000	0.79078200	3.03545000
H	-3.43513300	0.85786600	4.08682600
C	-1.49621400	0.97596300	1.26845400
C	-1.84393400	1.02653900	2.62523200
H	-1.07590500	1.21560500	3.37428900
C	-4.10393500	0.38320500	2.09179800
H	-5.09462300	0.09031500	2.42773400
H	-1.85531800	3.03656700	1.66322000

C	-2.51510500	-1.68941300	-3.56217800
H	-1.68720300	-1.27771100	-4.13458200
C	-4.65011100	-2.70402000	-2.12517200
C	-4.09814700	-3.45696900	-3.16131700
H	-4.51401800	-4.42968900	-3.40859500
C	-3.02625800	-2.94019600	-3.89138700
H	-2.59920300	-3.50310600	-4.71717900
H	-5.49792200	-3.11081800	-1.58191500
Pd	0.43397600	1.05212000	0.58391900
C	-1.45436400	2.38009300	-1.23660100
C	-0.30289400	2.67415500	-0.47069000
C	-2.00096500	3.35133100	-2.09417900
C	0.24287900	3.96448700	-0.57645400
C	-1.44709800	4.63106500	-2.17800300
H	-2.88036500	3.10626500	-2.68176900
C	-0.32548900	4.94202200	-1.40768100
H	1.12134900	4.23053300	-0.00100000
H	-1.89040100	5.37406700	-2.83515700
H	0.12061700	5.93265100	-1.45966400
Si	-5.07986900	-0.45084400	-0.45000900
C	-2.38580300	0.35713600	-2.24598400
H	-1.96503600	0.80175200	-3.14809300
N	-1.79273100	4.07300100	1.73299600
C	-3.14210400	4.62120300	2.08705000
C	-0.64979700	4.38115900	2.66049200
H	-1.51677600	4.36898900	0.78495400
H	-3.05982700	5.70996600	2.12034800
H	-3.37484600	4.25458500	3.09064600
H	0.16126100	3.72119700	2.34067700
H	-0.96817900	4.08177800	3.66272000
C	-0.22684200	5.84148300	2.59249400
H	-1.00502400	6.52081800	2.95322100
H	0.65959200	5.98539600	3.21679900
H	0.04223400	6.11792900	1.56762400
C	-4.16892100	4.15263300	1.06400700
H	-4.24811500	3.06161000	1.06820500
H	-5.15023300	4.56931100	1.30765500
H	-3.89777300	4.47629900	0.05308300

INT24

C	-2.37670500	-1.92879100	1.12632200
C	-3.12510500	-1.08715400	2.06698300
C	-2.43840600	-0.73429400	-1.16812600
C	-4.28271300	-0.33405900	1.74204500

C	-3.74861100	-0.20850700	-1.29590400
H	-1.93543600	-2.80196600	1.60641000
C	-2.66826800	-1.09897900	3.40243300
H	-1.77857800	-1.67407700	3.64733400
C	-3.30527000	-0.36948600	4.39964800
H	-2.92700100	-0.39813300	5.41887700
C	-4.90669000	0.39707700	2.77172400
C	-4.43350700	0.39095200	4.08364600
H	-5.79271700	0.98241900	2.54314300
H	-4.94810400	0.96157600	4.85237400
C	-1.43294500	-0.34602300	-2.08926600
C	-4.05445400	0.54775900	-2.44755200
C	-3.10143900	0.79286700	-3.43170200
C	-1.77917400	0.38697200	-3.22474900
H	-1.01141400	0.67682500	-3.93784300
H	-3.37058600	1.34878300	-4.32700400
H	-5.05546400	0.95368600	-2.56829700
C	-2.07344400	-1.80199300	-0.18896200
C	-1.27519500	-2.89616100	-0.82895200
C	-0.16069000	-2.56478300	-1.62302500
C	-1.66092500	-4.23726100	-0.68428600
C	0.49283000	-3.58067500	-2.32678800
H	-2.51781700	-4.48422100	-0.06273700
H	1.33441100	-3.34429400	-2.96994200
C	0.08885000	-4.91593300	-2.20041500
C	-0.97512700	-5.24799500	-1.36204100
H	-1.28929900	-6.28318500	-1.25370800
H	0.61249400	-5.69169500	-2.75520400
Si	-5.07985000	-0.36176300	0.02623300
C	-6.16512800	-1.93282300	-0.20602700
C	-6.76264300	-1.95970000	-1.63003800
C	-5.29117100	-3.19511800	-0.03964000
C	-7.28529500	-1.97381300	0.85462500
H	-7.43194700	-1.11647500	-1.82975000
H	-5.97432800	-1.94151800	-2.39165400
H	-7.34562200	-2.88097600	-1.77552700
H	-4.83710800	-3.25027100	0.95562500
H	-5.91052400	-4.09435100	-0.17528400
H	-4.48407100	-3.23318200	-0.77857900
H	-7.88650400	-2.88725000	0.73577500
H	-6.87104000	-1.98016100	1.87016900
H	-7.96781900	-1.12011700	0.78332900
C	-6.07712600	1.25625300	-0.08732100
C	-5.37662600	2.44845400	0.19147300

C	-7.42565800	1.38165100	-0.45901900
C	-5.98570300	3.69943400	0.09957400
H	-4.33259800	2.39650300	0.49205300
C	-8.04648800	2.63180400	-0.55411100
H	-8.01469000	0.49856100	-0.68219700
C	-7.32848100	3.79468800	-0.27722300
H	-5.41333800	4.59715600	0.32089900
H	-9.09206300	2.69328100	-0.84576400
H	-7.80933200	4.76675500	-0.35162100
P	2.59944700	-1.34804400	-0.46002400
P	0.96990100	1.72183800	-0.96664400
C	-2.07908500	5.13126400	-1.90403100
C	-0.70931000	5.38470300	-1.99100700
C	0.21277600	4.37805400	-1.70153800
C	-0.21929700	3.09916800	-1.31003200
C	-1.60230900	2.85508000	-1.23418100
C	-2.52172000	3.86338500	-1.52650900
H	1.27005000	4.59643600	-1.79342800
H	-1.97155200	1.87371100	-0.96484300
C	4.65491300	-4.00454400	-3.66580400
C	4.27050800	-4.57953000	-2.45465500
C	3.69987300	-3.79513600	-1.44897200
C	3.50850200	-2.42139500	-1.64506800
C	3.88488000	-1.85286000	-2.87497900
C	4.46244400	-2.63508000	-3.87294400
H	3.38101200	-4.26339900	-0.52493300
H	3.72740100	-0.79217800	-3.04761500
C	2.09816600	-3.77161300	3.46192500
C	3.36761400	-3.63540900	2.89219500
C	3.52557100	-2.91859300	1.70745700
C	2.41113400	-2.34878700	1.06935700
C	1.14539200	-2.47885500	1.65183400
C	0.99231000	-3.18761900	2.84447600
H	4.51627600	-2.79743300	1.27711200
H	0.28747000	-2.01318000	1.18349800
C	4.91403200	3.32782900	-2.79754800
C	4.48768900	3.84295400	-1.57089300
C	3.30582400	3.38148900	-0.99122900
C	2.54850600	2.38494400	-1.62203200
C	2.97911700	1.87928600	-2.85782600
C	4.15433500	2.35095800	-3.44489100
H	2.98464800	3.78176600	-0.03524700
H	2.38922200	1.11098600	-3.35211100
H	3.54904800	-1.06274900	5.47318500

C	2.12021500	1.00100500	1.57560200
C	1.05074600	1.57793400	0.88459100
C	-0.18863900	1.77409600	1.56177100
H	-1.01262300	2.24566100	1.04298900
C	-0.37636000	1.37232400	2.85823700
H	-1.33876900	1.51912000	3.33901500
C	0.66465200	0.72950500	3.57172700
C	1.93354200	0.55763500	2.93208500
H	3.92980400	-0.24861700	3.19491600
C	2.96733100	-0.08978300	3.66581000
C	2.74993100	-0.55083700	4.94443000
H	1.33578400	-0.74804400	6.58069600
C	1.49261900	-0.37850000	5.57089000
H	-0.50028700	0.39163900	5.35786600
C	0.47337400	0.25266000	4.89549300
H	7.17025800	4.48349000	2.51247200
C	6.15611600	0.72197600	0.03975700
H	7.17475000	0.65566900	-0.33518600
C	5.21116800	-0.18561800	-0.36800300
H	5.49460500	-0.96866500	-1.06096100
C	3.87000200	-0.11799600	0.10247900
C	3.50307400	0.88168500	1.00087800
C	4.48334400	1.83483000	1.44436800
C	5.82317300	1.75784800	0.94666500
H	7.79174900	2.65213200	0.96299900
C	6.77915500	2.72669400	1.35255900
C	6.43274500	3.74441500	2.21170600
H	4.83732600	4.63114600	3.38558600
C	5.10865300	3.82707600	2.70701200
H	3.15257500	2.97485800	2.72367400
C	4.16260100	2.89626900	2.33854000
H	-2.79667800	5.91288400	-2.13985500
H	5.09416100	-4.61806800	-4.44767500
H	1.97606800	-4.32210800	4.39090700
H	5.83687200	3.68580200	-3.24603300
H	-0.35171800	6.36637000	-2.29094200
H	-3.58248800	3.64110500	-1.47917800
H	4.40359900	-5.64537400	-2.29006700
H	4.75230600	-2.17877400	-4.81570400
H	4.47888700	1.95083700	-4.40179000
H	5.08081200	4.59199500	-1.05410500
H	0.00593700	-3.27929000	3.29023300
H	4.23432800	-4.07772600	3.37634000
Pd	0.49215900	-0.62325100	-1.47126400

TS17

C	-2.38198900	-1.99047900	1.24536700
C	-3.13107700	-1.11103200	2.14567600
C	-2.44505700	-0.93725000	-1.12965900
C	-4.22044500	-0.27936200	1.77183800
C	-3.70156200	-0.32003300	-1.28069500
H	-1.91218200	-2.82291800	1.76806600
C	-2.72719400	-1.13735100	3.49861800
H	-1.89301000	-1.77267700	3.78521100
C	-3.34083300	-0.34639200	4.46270100
H	-3.00425300	-0.39140000	5.49554300
C	-4.81343200	0.52142900	2.76653500
C	-4.38778600	0.50106900	4.09484300
H	-5.64082500	1.17167900	2.49696800
H	-4.87886800	1.12664700	4.83553100
C	-1.46064200	-0.82275900	-2.15571600
C	-3.99575400	0.29848900	-2.51738900
C	-3.08500300	0.28028900	-3.57265200
C	-1.80834500	-0.26150900	-3.38896100
H	-1.07552200	-0.21101300	-4.18934600
H	-3.35193600	0.72538300	-4.52846000
H	-4.96036100	0.77947800	-2.65651600
C	-2.07902400	-1.91942300	-0.07500600
C	-1.22199100	-2.96239700	-0.70191800
C	-0.39376800	-2.49541700	-1.74736400
C	-1.29920700	-4.32665700	-0.42064400
C	0.27409700	-3.42114900	-2.55916300
H	-1.95200100	-4.67895100	0.37455300
H	0.90853000	-3.08233300	-3.37327700
C	0.17778700	-4.79021100	-2.28018100
C	-0.58630900	-5.24351000	-1.20258400
H	-0.66001700	-6.30712900	-0.99223200
H	0.71937100	-5.49980400	-2.90127900
Si	-5.01935500	-0.30336500	0.05959300
C	-6.18800100	-1.82229800	-0.10862000
C	-6.83361000	-1.84252900	-1.51122400
C	-5.36600200	-3.12037600	0.05619500
C	-7.27468300	-1.79457600	0.98686600
H	-7.46329100	-0.96726500	-1.70294100
H	-6.07248500	-1.87993500	-2.29931900
H	-7.46919400	-2.73356200	-1.61967300
H	-4.90124400	-3.18611400	1.04568800
H	-6.02567100	-3.99288200	-0.06119700

H	-4.57013200	-3.20154500	-0.69225300
H	-7.91712700	-2.68358100	0.90491200
H	-6.83031800	-1.79825600	1.98941400
H	-7.92354400	-0.91472500	0.91820800
C	-5.90944400	1.36444500	-0.12321000
C	-5.10881000	2.51793700	0.00446800
C	-7.27556600	1.55834700	-0.38722400
C	-5.64077400	3.80004200	-0.12936400
H	-4.04546400	2.41350700	0.20686700
C	-7.81890900	2.84001400	-0.52134400
H	-7.93745500	0.70541700	-0.49340700
C	-7.00312600	3.96451200	-0.39406300
H	-4.99032900	4.66591700	-0.03370800
H	-8.88008700	2.95695700	-0.72687600
H	-7.42421800	4.96109500	-0.50009100
P	2.57905600	-1.34544300	-0.40186700
P	0.98077600	1.72750800	-1.03223100
C	-2.13560900	5.01947400	-2.10771400
C	-0.80189000	5.38877100	-1.91422000
C	0.15266700	4.42822500	-1.57836400
C	-0.21596900	3.08208800	-1.41980000
C	-1.55867900	2.72241500	-1.61674000
C	-2.51096200	3.68367200	-1.96092300
H	1.18654400	4.73167500	-1.45657100
H	-1.86075300	1.68924800	-1.50753400
C	4.49209900	-4.00672600	-3.68873800
C	3.97590600	-4.60238400	-2.53832200
C	3.45647200	-3.81626300	-1.50631900
C	3.45121100	-2.41886200	-1.61165900
C	3.95489100	-1.82731500	-2.78537700
C	4.48028500	-2.61315200	-3.80887500
H	3.03745600	-4.29706400	-0.62943200
H	3.94038300	-0.74614700	-2.89279400
C	2.09154500	-3.79108800	3.50995200
C	3.34615000	-3.72241400	2.89613200
C	3.50215400	-3.01002500	1.70818800
C	2.40137000	-2.37029300	1.11520900
C	1.15076600	-2.43645800	1.74031700
C	0.99857100	-3.14476000	2.93330600
H	4.48058400	-2.94709900	1.23910100
H	0.30589500	-1.91622500	1.30528400
C	4.97572400	3.36129800	-2.73125600
C	4.49961900	3.88200900	-1.52572600
C	3.30045500	3.41482400	-0.98728400

C	2.57193600	2.40977700	-1.63860300
C	3.05629400	1.89515100	-2.85092400
C	4.24919300	2.37150200	-3.39720000
H	2.94838600	3.81161000	-0.04079800
H	2.49543500	1.11228200	-3.35606800
H	3.36725000	-0.98868200	5.50390300
C	2.06000100	1.04316100	1.54726100
C	1.01113700	1.61250300	0.81760300
C	-0.25672000	1.79616900	1.44659400
H	-1.06926300	2.23947700	0.88261200
C	-0.48506700	1.40662600	2.74039800
H	-1.46615200	1.54273600	3.18630600
C	0.54095800	0.78715900	3.49808800
C	1.83049600	0.61256600	2.90144300
H	3.81573100	-0.19768200	3.22994900
C	2.84061000	-0.03090200	3.67143800
C	2.58529700	-0.47952100	4.94750000
H	1.12402900	-0.65198000	6.54486300
C	1.31114800	-0.29605500	5.53520400
H	-0.67304600	0.47313400	5.25456300
C	0.31276200	0.32771300	4.82218200
H	7.10274300	4.52220000	2.55488000
C	6.14875200	0.68969300	0.16718100
H	7.18106200	0.60173400	-0.16356900
C	5.21192100	-0.22466800	-0.24369600
H	5.51385200	-1.03662200	-0.89500900
C	3.85330700	-0.12696100	0.16823600
C	3.46117400	0.90523700	1.01931800
C	4.43430700	1.86085300	1.47213100
C	5.79026300	1.75938700	1.02464300
H	7.76308300	2.64226800	1.08176900
C	6.73823100	2.73447200	1.43384300
C	6.37042800	3.77913700	2.25107900
H	4.74381900	4.70684000	3.34804700
C	5.03162500	3.88306900	2.70048700
H	3.07011600	3.04153800	2.67554600
C	4.09207400	2.94775500	2.32652300
H	-2.87535800	5.76750400	-2.38149100
H	4.89424000	-4.62056300	-4.49018800
H	1.97181100	-4.33889900	4.44095200
H	5.91235700	3.72252300	-3.14751000
H	-0.49988300	6.42636300	-2.03242500
H	-3.53970400	3.37781700	-2.11859700
H	3.96823300	-5.68478600	-2.44050000

H	4.87476200	-2.13873500	-4.70375700
H	4.61449100	1.96400600	-4.33629400
H	5.06840000	4.63760500	-0.99126100
H	0.02604700	-3.18238000	3.41571100
H	4.20266000	-4.21652000	3.34741900
Pd	0.50167900	-0.61837700	-1.44896000

3

C	1.54540400	1.83498900	-0.26484400
C	0.19893300	2.37665800	-0.44192600
C	1.47948500	-0.76478400	-0.21415000
C	-1.03639000	1.68388300	-0.29662400
C	0.14485800	-1.18975700	-0.10716600
H	2.29469800	2.62480000	-0.28593600
C	0.16621000	3.73823700	-0.82821800
H	1.10690800	4.27355000	-0.93372400
C	-1.02272000	4.40453900	-1.09587700
H	-1.00404800	5.44913600	-1.39489500
C	-2.22329100	2.38152100	-0.58700400
C	-2.23250300	3.71941600	-0.98125000
H	-3.17407800	1.86311000	-0.49514900
H	-3.17398300	4.22090700	-1.18859800
C	2.53010700	-1.71371000	-0.35239300
C	-0.10017100	-2.57513200	-0.21988900
C	0.93089500	-3.50108100	-0.39660500
C	2.26047700	-3.07467300	-0.44949200
H	3.06937000	-3.79255600	-0.55853200
H	0.69726200	-4.55974100	-0.47366100
H	-1.12265000	-2.93807000	-0.16031000
C	2.07810100	0.58626500	-0.18457300
C	3.54749800	0.37341100	-0.20186600
C	3.81231500	-1.00814300	-0.33459600
C	4.60556200	1.27960500	-0.13424600
C	5.12021400	-1.48410100	-0.40651800
H	4.42599900	2.34577500	-0.02238100
H	5.31872000	-2.54769600	-0.51102900
C	6.17443100	-0.56911600	-0.33882700
C	5.91759100	0.80103700	-0.20111300
H	6.74693200	1.50078600	-0.14334700
H	7.20067900	-0.92251400	-0.39081600
Si	-1.26057400	-0.05491300	0.40032300
C	-1.29434700	0.05298400	2.32315800
C	-1.59271000	-1.33363900	2.93119800
C	0.09900100	0.51324300	2.80905400

C	-2.33372200	1.08595900	2.80898300
H	-2.58223200	-1.71101500	2.65086000
H	-0.85226000	-2.07766900	2.61393300
H	-1.55826200	-1.27999200	4.02910400
H	0.36777100	1.49632500	2.40637900
H	0.10295700	0.59150900	3.90597900
H	0.88678600	-0.19209600	2.52390000
H	-2.30194500	1.16175000	3.90561200
H	-2.13008400	2.08289100	2.40168300
H	-3.36011800	0.82160600	2.53268600
C	-2.84532300	-0.76729700	-0.35533900
C	-2.81140900	-1.11666400	-1.72080300
C	-4.06258100	-0.94373200	0.32530000
C	-3.93716700	-1.61661900	-2.37517000
H	-1.88524700	-1.00401000	-2.28008200
C	-5.19493600	-1.44499400	-0.32289200
H	-4.14036900	-0.69163300	1.37758500
C	-5.13516000	-1.78215300	-1.67539200
H	-3.88016300	-1.87849300	-3.42869700
H	-6.12193800	-1.57231600	0.23055500
H	-6.01458800	-2.17245400	-2.18117600

TS18

C	1.24603800	-2.26221700	1.03854500
C	0.73291300	-1.14799700	0.35521400
C	-0.64871400	-0.93095000	0.21564700
C	-1.52131300	-1.93631700	0.74370200
C	-0.99971900	-3.03601200	1.45330300
C	0.37321700	-3.19251200	1.60497500
Si	-1.26112600	0.54398700	-0.81494300
H	2.31876100	-2.41560300	1.10848500
H	-1.68830900	-3.77189800	1.85675500
H	0.76880200	-4.05217300	2.14000400
C	-0.00225000	1.95736800	-0.62243500
C	-0.32979900	3.23162200	-1.12116300
C	1.26207200	1.78415700	0.00239000
C	0.56428200	4.29861500	-1.03458600
H	-1.29759300	3.40073500	-1.58521000
C	2.16452700	2.87881900	0.06757600
H	1.23399500	1.23419400	1.19613900
C	1.82141900	4.12429500	-0.44222800
H	0.28243100	5.27105500	-1.43071600
H	3.13620500	2.73400600	0.53428300
H	2.51820900	4.95586900	-0.38021300

C	-2.93141100	-1.90690900	0.54598200
C	-4.13641100	-1.94264100	0.38823000
C	-5.54395500	-1.90194800	0.18578800
C	-6.34785100	-3.02643400	0.45949900
C	-6.15089700	-0.72166200	-0.28965200
C	-7.72500800	-2.96863100	0.26027300
H	-5.88079400	-3.93608300	0.82483800
C	-7.52860800	-0.67495600	-0.48401800
H	-5.53360100	0.14451000	-0.49506100
C	-8.32003400	-1.79466800	-0.21132500
H	-8.33626000	-3.84158700	0.47268100
H	-7.98628800	0.24075900	-0.84879700
H	-9.39491200	-1.75355600	-0.36537400
Pd	2.18353200	-0.04505800	-0.42727100
O	3.48757200	-1.72668600	-1.17124400
S	4.71689600	-0.86194500	-1.37079300
O	4.30624900	0.58034600	-1.24678900
O	5.60490200	-1.22464400	-2.46613500
C	5.67645500	-1.18083400	0.19656300
F	4.86929400	-1.02787300	1.27024900
F	6.69147800	-0.32022500	0.30717400
F	6.15119600	-2.42802100	0.20478400
C	-2.86632400	1.29760500	-0.14248800
C	-3.70415000	2.10349000	-0.93580800
C	-3.19581100	1.17787500	1.21999600
C	-4.81142700	2.76461400	-0.39587100
H	-3.50274600	2.21994500	-1.99605400
C	-4.30302400	1.82631100	1.76687500
H	-2.58781900	0.54792300	1.86282300
C	-5.11462200	2.62678100	0.95929900
H	-5.43921900	3.37876500	-1.03653200
H	-4.53800500	1.70063000	2.82065700
H	-5.97917300	3.13172800	1.38176500
C	-1.39957700	-0.00223000	-2.66545900
C	-1.35157400	1.19817500	-3.63566300
C	-0.21443500	-0.93176200	-3.01038700
C	-2.71744300	-0.78178900	-2.87127700
H	-2.18501000	1.89617200	-3.49668000
H	-0.41977400	1.76527300	-3.53630800
H	-1.40986800	0.83504100	-4.67144700
H	-0.19880800	-1.83183800	-2.38794900
H	-0.28922300	-1.25013300	-4.05981900
H	0.75380900	-0.43055400	-2.88867000
H	-2.78788200	-1.12309300	-3.91399800

H	-2.77303800	-1.66584700	-2.22767100
H	-3.60115400	-0.16894300	-2.66159600
N	1.11671600	1.01252200	2.62975300
C	2.36720500	0.36075400	3.07297500
C	0.79300600	2.27733000	3.31718500
H	0.33992400	0.35161300	2.67888300
H	3.07760500	1.15643200	3.32137500
H	2.78021300	-0.17790100	2.21356100
H	1.52344400	3.01655100	2.96591800
H	0.93026400	2.16735900	4.40249600
C	-0.62243600	2.74443400	2.99837100
H	-1.36833500	2.03247100	3.36835600
H	-0.81618500	3.70931300	3.47768600
H	-0.77027100	2.86036300	1.92140000
C	2.16691600	-0.59358700	4.24814400
H	1.49563500	-1.41132800	3.96040500
H	3.12402000	-1.03440000	4.54679200
H	1.74185900	-0.08163300	5.11933000

INT26

C	1.02851300	-2.29707000	-1.71965500
C	0.63560500	-1.01308400	-1.28453700
C	-0.71676700	-0.75723400	-0.97404200
C	-1.64306800	-1.85084700	-1.05132200
C	-1.21603300	-3.13055800	-1.45195900
C	0.11186100	-3.34390100	-1.80241600
Si	-1.32430100	1.02468000	-0.75766600
H	2.06623500	-2.49464100	-1.97055000
H	-1.94066000	-3.93791200	-1.49422600
H	0.43890100	-4.32659600	-2.13285900
C	0.13547700	2.14387600	-0.34746400
C	-0.15616000	3.41724800	0.19257700
C	1.48019300	1.82663300	-0.60253500
C	0.83827800	4.35412900	0.45637200
H	-1.18529600	3.67998900	0.42119900
C	2.48644700	2.78338600	-0.35462100
H	1.83116000	-0.16197100	1.10539700
C	2.16807300	4.03620100	0.17114400
H	0.57968000	5.32231300	0.87737200
H	3.52657900	2.54623200	-0.55401800
H	2.96060400	4.75594100	0.36222500
C	-3.02512700	-1.71748400	-0.73086300
C	-4.20908900	-1.67773300	-0.45685600
C	-5.58321800	-1.55367100	-0.11118600

C	-6.50066500	-2.58050900	-0.41116800
C	-6.04138600	-0.39277600	0.54475500
C	-7.84245100	-2.44556200	-0.06349300
H	-6.14902900	-3.47444400	-0.91743900
C	-7.38487900	-0.26887700	0.88806000
H	-5.33594100	0.39535200	0.77864600
C	-8.28944300	-1.29126700	0.58653900
H	-8.54224700	-3.24225300	-0.30089800
H	-7.72682800	0.63005000	1.39416100
H	-9.33725400	-1.18966100	0.85579800
Pd	2.30135800	0.08622600	-1.10523300
O	3.90648500	-1.75433900	-0.82183700
S	5.04620700	-0.81249800	-0.55844500
O	4.62427000	0.58878000	-0.89269000
O	6.37600900	-1.23393600	-0.98138100
C	5.11789400	-0.78069200	1.31010700
F	4.03459000	-0.12125000	1.81217500
F	6.20973900	-0.15573500	1.74251700
F	5.09004900	-2.02305700	1.81349200
C	-2.49154400	1.14773100	0.74164400
C	-3.35092800	2.24317300	0.94632700
C	-2.43281300	0.18740600	1.77032900
C	-4.09139100	2.38766900	2.12373100
H	-3.45452200	3.00198800	0.17685800
C	-3.16986500	0.31811100	2.94786700
H	-1.83425100	-0.71071300	1.63175500
C	-3.99912600	1.42717400	3.13205000
H	-4.74436800	3.24775900	2.24822200
H	-3.11045100	-0.45119700	3.71379400
H	-4.57709300	1.53345300	4.04600100
C	-2.09886400	1.63297900	-2.42236100
C	-2.20861800	3.17321600	-2.46786000
C	-1.14082700	1.19013600	-3.55299000
C	-3.49506000	1.02738700	-2.66846400
H	-2.90718900	3.56929400	-1.72137500
H	-1.24150700	3.66216500	-2.31600400
H	-2.58816300	3.48196100	-3.45238800
H	-1.07200800	0.09962800	-3.62619100
H	-1.50453600	1.56935700	-4.51872200
H	-0.12548700	1.57718200	-3.40291800
H	-3.90629800	1.41419800	-3.61231000
H	-3.46247700	-0.06274300	-2.74375000
H	-4.20153500	1.28015700	-1.86878200
N	1.23840400	-0.66713000	1.80406300

C	1.66506500	-2.11710300	1.82394300
C	1.25421800	0.03592300	3.13044900
H	0.30663000	-0.60385000	1.37450600
H	2.46863400	-2.19480200	2.55859600
H	2.08966300	-2.32513900	0.84097800
H	2.27380500	-0.06462700	3.50761100
H	0.57909500	-0.51535700	3.79139500
C	0.84695300	1.49664600	2.99202700
H	-0.17613200	1.59234200	2.61974100
H	0.89990700	1.97251300	3.97635100
H	1.51168000	2.03471700	2.30996000
C	0.48708000	-3.03141600	2.12616500
H	-0.26278300	-2.97015300	1.32967100
H	0.83682500	-4.06700300	2.17336400
H	0.01270000	-2.79464200	3.08540500

TS19

C	0.90416500	-1.56820900	-2.20103600
C	0.41706300	-0.59620500	-1.31723500
C	-0.93014800	-0.49589300	-0.96253400
C	-1.84892700	-1.32879600	-1.66979000
C	-1.37311800	-2.25920600	-2.61671600
C	-0.01145400	-2.39093300	-2.86426100
Si	-1.41280000	0.75683600	0.36910400
H	1.97048900	-1.71915600	-2.34617300
H	-2.08990100	-2.89111500	-3.13208300
H	0.34634200	-3.14786500	-3.55729100
C	0.11627300	1.03257000	1.46467200
C	-0.10437900	1.64879600	2.71219400
C	1.45498300	0.72716500	1.09991100
C	0.94575300	1.96704300	3.57217400
H	-1.11932500	1.88025800	3.02437300
C	2.51233700	1.07535100	1.97564700
H	1.92166400	-0.55550900	0.69706800
C	2.26143600	1.67260700	3.20559300
H	0.73671700	2.43698000	4.53004300
H	3.52781200	0.81201400	1.70017500
H	3.08490700	1.90056200	3.87757600
C	-3.25572800	-1.24651100	-1.46647200
C	-4.46210400	-1.19773100	-1.32396000
C	-5.86263500	-1.11049600	-1.08759500
C	-6.78992700	-1.54724200	-2.05442000
C	-6.33632000	-0.58416300	0.13139900
C	-8.15729100	-1.45574300	-1.80579900

H	-6.42567200	-1.95368100	-2.99314600
C	-7.70539000	-0.49809000	0.36928600
H	-5.62318500	-0.25657900	0.87824100
C	-8.61996500	-0.93133000	-0.59522900
H	-8.86449400	-1.79458600	-2.55809800
H	-8.05931300	-0.09327000	1.31377800
H	-9.68759700	-0.86237800	-0.40478700
Pd	1.78597500	0.79483300	-0.99161700
O	4.63057700	-0.44273700	0.26899900
S	3.92699800	-1.73458400	0.10749700
O	3.96327700	-2.35164700	-1.22269000
O	2.52991900	-1.72355900	0.74347200
C	4.80192900	-2.91171100	1.25328300
F	6.07049800	-3.05206200	0.85209200
F	4.20229400	-4.10391500	1.24020200
F	4.78997800	-2.42494500	2.49893700
C	-2.73054800	0.06938700	1.53826200
C	-3.59652200	0.88624900	2.28850400
C	-2.78746200	-1.31814900	1.76930500
C	-4.47893300	0.34631600	3.22863900
H	-3.59489900	1.96226600	2.14369500
C	-3.67320600	-1.86556000	2.69772800
H	-2.13820400	-1.98342300	1.20611300
C	-4.52180100	-1.03385200	3.43250700
H	-5.13597000	1.00309900	3.79335300
H	-3.70267900	-2.94167700	2.84622800
H	-5.21203800	-1.45896800	4.15636400
C	-1.93820000	2.42844500	-0.46217200
C	-1.83317400	3.61727100	0.51748300
C	-1.00886200	2.72147100	-1.65994300
C	-3.38639500	2.31596100	-0.98845400
H	-2.48729500	3.50968400	1.38947700
H	-0.81120100	3.75120900	0.88869100
H	-2.12807500	4.54587500	0.00772400
H	-1.06208400	1.93559300	-2.42103200
H	-1.29639800	3.67105600	-2.13450700
H	0.04171000	2.81504500	-1.34898400
H	-3.67934900	3.25546700	-1.47949600
H	-3.49108700	1.50927600	-1.72089000
H	-4.10710000	2.12116200	-0.18766500
N	3.47653800	2.30159100	-1.17352400
C	4.16255000	2.13821300	-2.48545300
C	3.15410900	3.73245800	-0.94020000
H	4.11198400	1.96862800	-0.44490700

H	5.06843400	2.76401900	-2.50420100
H	3.48459000	2.53848100	-3.24952800
H	2.42078600	4.01875100	-1.70337600
H	4.05369600	4.34438900	-1.11452000
C	2.59770900	4.02130200	0.44819300
H	3.30478500	3.73193800	1.23201200
H	2.40406800	5.09514600	0.54569100
H	1.66448400	3.48220700	0.62828000
C	4.52322000	0.69032100	-2.80126000
H	3.63276700	0.05685800	-2.89341600
H	5.06018500	0.64630000	-3.75520000
H	5.14773700	0.25133800	-2.02079100

INT27

C	0.90165100	-2.20208600	-1.39006100
C	0.40364900	-1.00907200	-0.83547400
C	-0.97600500	-0.83375000	-0.60846200
C	-1.85960300	-1.85081300	-1.07385300
C	-1.34839100	-3.03031500	-1.65495300
C	0.02140400	-3.21095900	-1.79333300
Si	-1.55408700	0.76279000	0.24188600
H	1.97130300	-2.35838000	-1.51316900
H	-2.04417000	-3.79553900	-1.98570700
H	0.40978700	-4.13361000	-2.21764900
C	-0.08256700	1.34654300	1.28349000
C	-0.30647100	2.00317000	2.51260100
C	1.24955200	1.12030700	0.90506200
C	0.74718000	2.38756800	3.34053900
H	-1.32582400	2.19609300	2.83657200
C	2.31632000	1.47327700	1.74397800
H	2.39886000	-0.96360200	0.61855300
C	2.06102700	2.10808200	2.96168200
H	0.54265100	2.88483700	4.28524700
H	3.34281100	1.27454400	1.45303400
H	2.89116600	2.38117800	3.60904100
C	-3.27614100	-1.71451400	-0.99768900
C	-4.48793400	-1.62644500	-0.95376600
C	-5.89709300	-1.46554000	-0.83578600
C	-6.78213400	-2.17383800	-1.67253500
C	-6.42268100	-0.58795700	0.13449700
C	-8.15844500	-2.00424400	-1.54157400
H	-6.37815300	-2.85046400	-2.41964200
C	-7.80015400	-0.42678500	0.25685700
H	-5.74267000	-0.04949000	0.78359000

C	-8.67247400	-1.13116500	-0.57827100
H	-8.83245900	-2.55451600	-2.19271200
H	-8.19380700	0.25049000	1.01025100
H	-9.74689700	-1.00193300	-0.47883700
Pd	1.70011300	0.50824300	-0.94902000
O	4.90817200	-0.02127800	0.15371700
S	4.47083200	-1.41731300	0.24861600
O	4.47749700	-2.25914700	-0.94240800
O	3.09860100	-1.54877000	1.05609900
C	5.52554800	-2.24107800	1.54970900
F	6.77437000	-2.28140900	1.08229800
F	5.08743500	-3.47584700	1.77417700
F	5.48923500	-1.53145700	2.67423600
C	-2.93173200	0.42844600	1.50035800
C	-3.80143800	1.43501000	1.96017800
C	-3.03771900	-0.83878000	2.10347700
C	-4.73788300	1.19010300	2.96902400
H	-3.75687900	2.43150200	1.53143300
C	-3.97602500	-1.09475600	3.10376600
H	-2.38529100	-1.64389600	1.77662600
C	-4.83101000	-0.07989700	3.54034000
H	-5.39627100	1.98894900	3.30142700
H	-4.04251100	-2.08784800	3.54042900
H	-5.56338500	-0.27809700	4.31857700
C	-2.06550600	2.10259900	-1.06310500
C	-1.92467000	3.52044300	-0.46679400
C	-1.13803300	2.01413200	-2.29431600
C	-3.51707400	1.87652500	-1.53934300
H	-2.57457600	3.68423400	0.39996600
H	-0.89661700	3.72324300	-0.14556500
H	-2.19679500	4.27358800	-1.22091100
H	-1.19463000	1.03360300	-2.77949600
H	-1.42305600	2.77648600	-3.03470900
H	-0.08783600	2.18916200	-2.02483900
H	-3.78853400	2.63707400	-2.28640700
H	-3.64184000	0.89275700	-2.00305800
H	-4.24161200	1.94253600	-0.72161900
N	3.19021600	2.07236000	-1.69945100
C	3.63631200	1.66198800	-3.05848600
C	2.79216500	3.50428300	-1.71173600
H	3.97454300	1.94698400	-1.05566500
H	4.45711400	2.31576800	-3.39266300
H	2.79230100	1.83920500	-3.73582000
H	1.91000300	3.58300900	-2.35726700

H	3.59141400	4.09635200	-2.18642500
C	2.47986000	4.07376000	-0.33401800
H	3.31671300	3.93122600	0.35883900
H	2.29342800	5.14975600	-0.42182300
H	1.60061300	3.60199900	0.10740000
C	4.07350100	0.20301600	-3.13087900
H	3.25645500	-0.48626100	-2.88041100
H	4.40050300	-0.03529000	-4.14877600
H	4.89591900	-0.00499800	-2.44338000

TS20

C	1.78210200	-1.25615200	-0.79354300
C	2.55889400	-2.29379600	-1.34649300
C	0.48931100	-1.10057200	-1.34080900
C	2.12690600	-3.04919600	-2.44241600
H	3.54166100	-2.50342100	-0.94372700
C	0.10784700	-1.73725100	-2.53008900
C	0.92204800	-2.73610200	-3.07199000
H	2.76167200	-3.83791100	-2.83597500
H	-0.83637200	-1.49207300	-3.00564300
H	0.61521700	-3.25894400	-3.97372100
C	2.41927400	1.55324600	-1.15916900
C	1.16457100	1.73374500	-1.79848600
C	3.46199400	2.38550200	-1.58965600
C	0.99626000	2.65187100	-2.85186000
C	3.29742600	3.31706900	-2.61991600
C	2.06652800	3.44264100	-3.26194400
H	0.02280600	2.75203000	-3.32213300
H	4.13617200	3.93731100	-2.92220400
H	1.93529900	4.15329700	-4.07234800
H	4.43401700	2.32002200	-1.11709800
Pd	-1.19440600	-0.81304700	-0.19774700
Si	2.61659300	0.18308500	0.15910800
C	-0.04217900	1.11276800	-1.31692000
C	-1.22766700	1.18214200	-0.87404400
C	-2.32295500	2.11351500	-0.65413600
C	-2.39908700	2.85036000	0.53981200
C	-3.30648000	2.28435300	-1.64279300
C	-3.45257900	3.74166800	0.73993400
H	-1.62979200	2.71994600	1.29394900
C	-4.35611800	3.17819600	-1.43350300
H	-3.24385600	1.71319300	-2.56419700
C	-4.43544400	3.90338700	-0.24100500
H	-3.50441200	4.31351800	1.66201400

H	-5.11216600	3.30891100	-2.20213800
H	-5.25550700	4.59669900	-0.08007500
N	-3.13134300	-0.77962700	1.02165000
H	-3.18725100	-1.77749900	1.23046100
C	-4.38966900	-0.40524100	0.31338900
C	-4.54792600	-1.07749300	-1.04147400
H	-5.24689700	-0.64734000	0.95856100
H	-4.37504100	0.67892200	0.19011000
H	-5.48344600	-0.75036700	-1.50665100
H	-4.58322500	-2.16834300	-0.95540200
H	-3.72317400	-0.80723400	-1.70953400
C	-3.06884300	-0.06339000	2.32903000
C	-1.81532500	-0.37553500	3.12819800
H	-3.11132900	1.00392800	2.10166700
H	-3.97004200	-0.30587700	2.91142000
H	-1.83234500	0.17482200	4.07337900
H	-0.91643500	-0.07025200	2.58702400
H	-1.73628800	-1.44153800	3.36701300
C	4.47232600	-0.17662200	0.57821700
C	5.02806600	1.01495200	1.40002400
C	4.61684100	-1.44505600	1.45757300
C	5.35836400	-0.36327300	-0.67896400
H	5.00105300	1.96213200	0.85116600
H	4.47489200	1.16099600	2.33321900
H	6.07717900	0.82187300	1.66156200
H	4.16441000	-2.33837900	1.01421700
H	5.68274400	-1.66290300	1.60826400
H	4.18215100	-1.30887700	2.45146900
H	6.40312200	-0.49427300	-0.36637900
H	5.08597500	-1.24404500	-1.26609900
H	5.32810400	0.49223600	-1.35722800
C	1.74594200	0.80203400	1.72911400
C	1.84091600	0.12126700	2.95981500
C	1.12294900	2.06553000	1.74550600
C	1.34544600	0.66965000	4.14407000
H	2.31416900	-0.85288000	3.00876900
C	0.61832300	2.61788200	2.92576100
H	1.04536700	2.64279300	0.82959300
C	0.73116300	1.92315900	4.13117600
H	1.44387400	0.11912400	5.07566400
H	0.15796100	3.60261300	2.90518000
H	0.35346000	2.35790300	5.05244600
N	-1.07708700	-3.18184300	0.20360500
H	-0.27189200	-3.38183800	-0.39290400

C	-0.72709300	-3.60850100	1.58133200
C	0.56459500	-2.97385800	2.06832400
H	-1.56340900	-3.33186800	2.23344200
H	-0.64871400	-4.70567800	1.61936800
H	0.78098000	-3.29576700	3.09216000
H	0.48889700	-1.88620700	2.05720800
H	1.40987100	-3.26015100	1.43290000
C	-2.22216500	-3.97910100	-0.31011800
H	-2.08673700	-5.03369000	-0.02704100
H	-3.12675600	-3.63719900	0.20715900
C	-2.40283200	-3.88434700	-1.81951800
H	-1.51528000	-4.25264400	-2.34425400
H	-3.25633400	-4.49741100	-2.12641300
H	-2.58533200	-2.85710500	-2.14072200

INT28

C	-1.51700700	1.49467400	-1.02313500
C	-1.50424700	2.85632400	-1.31456000
C	-0.42384800	0.71184300	-1.50450100
C	-0.46763700	3.46216200	-2.05804000
H	-2.32292800	3.48708500	-0.98667800
C	0.60150000	1.30547900	-2.28910400
C	0.56558900	2.69331700	-2.56263800
H	-0.51680200	4.52555000	-2.27536500
H	1.26987100	0.66536100	-2.86139100
H	1.32687900	3.13336400	-3.20005300
C	-2.82160700	-1.12330600	-1.14308300
C	-1.53936000	-1.59760600	-1.52335300
C	-3.93156600	-1.92656300	-1.45159400
C	-1.40039500	-2.83527900	-2.16810300
C	-3.79081700	-3.15528600	-2.09926700
C	-2.52074600	-3.61287100	-2.45223200
H	-0.41263800	-3.17961700	-2.45704500
H	-4.67015900	-3.75096500	-2.32679200
H	-2.40234900	-4.56684300	-2.95806100
H	-4.92965600	-1.59780600	-1.18694000
Pd	1.84748400	0.56176600	-0.37235900
Si	-2.89261900	0.49326000	-0.16194200
C	-0.34621200	-0.75735100	-1.25481600
C	0.85237700	-1.14845900	-0.77428900
C	1.25894500	-2.49630100	-0.37679700
C	0.62376000	-3.14125600	0.70176900
C	2.26870200	-3.17861900	-1.07893100
C	0.99417800	-4.43460100	1.06631900

H	-0.15831800	-2.61658200	1.24212100
C	2.62995600	-4.47659800	-0.71665800
H	2.75588100	-2.68641500	-1.91682300
C	1.99740400	-5.10544800	0.35982300
H	0.49541500	-4.92347700	1.89853100
H	3.40241600	-4.99815800	-1.27462300
H	2.28082400	-6.11490800	0.64279300
N	3.26928100	-0.24365200	1.09318800
H	3.68112600	0.64214400	1.39221200
C	4.37678600	-1.09248100	0.55798200
C	5.03551600	-0.53297300	-0.69303600
H	5.12137500	-1.22816200	1.35499400
H	3.94386800	-2.07113900	0.34491500
H	5.84138700	-1.20313400	-1.00945600
H	5.47469800	0.45536200	-0.52374100
H	4.31362500	-0.45754800	-1.51324800
C	2.68532700	-0.89147000	2.30894200
C	1.50998600	-0.13519600	2.90316700
H	2.37004500	-1.89228300	2.00975100
H	3.48796900	-1.00718200	3.05090900
H	1.16074900	-0.65112400	3.80170800
H	0.66759600	-0.09137600	2.20631200
H	1.77837600	0.88633100	3.19235600
C	-4.60131400	1.36765100	-0.14742300
C	-5.63345100	0.48057800	0.59098500
C	-4.54555100	2.70562900	0.62728500
C	-5.06705300	1.62747800	-1.59591800
H	-5.83162700	-0.46623400	0.08195300
H	-5.31171400	0.24968600	1.61300400
H	-6.59184600	1.01313000	0.65794500
H	-3.85859200	3.43624200	0.18887900
H	-5.54173000	3.16849300	0.62437900
H	-4.26076400	2.55800000	1.67433200
H	-6.05633400	2.10502500	-1.59598500
H	-4.38049000	2.29350400	-2.13270100
H	-5.14710900	0.70005100	-2.17397700
C	-2.34860100	0.12020100	1.60954100
C	-2.00114300	1.15256500	2.50133800
C	-2.36064900	-1.19656500	2.10613500
C	-1.69047000	0.88609600	3.83624700
H	-1.97818100	2.18275400	2.15480900
C	-2.04515700	-1.47063300	3.43969800
H	-2.62924000	-2.01676000	1.44470200
C	-1.71464700	-0.42842600	4.30902600

H	-1.43469700	1.70191500	4.50732300
H	-2.07011800	-2.49488300	3.80254600
H	-1.48193200	-0.63821700	5.34952700
N	2.59748100	2.73773600	0.02616300
H	1.98433300	3.23143900	-0.62569200
C	2.28062300	3.24495700	1.38557500
C	0.78318600	3.21340100	1.66199200
H	2.82295500	2.62607800	2.11056100
H	2.66465000	4.26956600	1.49870200
H	0.57828500	3.56964400	2.67645900
H	0.38077700	2.20241500	1.56890400
H	0.24219400	3.85789700	0.95996200
C	3.99749300	3.03726000	-0.36547700
H	4.24672600	4.07372900	-0.09384400
H	4.65565400	2.39345700	0.22960300
C	4.23841500	2.82518500	-1.85582000
H	3.64402700	3.52760300	-2.45107400
H	5.29213700	2.99822600	-2.09514300
H	3.97885800	1.80821200	-2.16357100

TS21

C	-1.98072000	-0.04494300	1.70232100
C	-2.48901000	-0.18611600	3.00366300
C	-0.67601300	0.47644300	1.57748500
C	-1.73520800	0.17133200	4.12393600
H	-3.48818500	-0.58231100	3.15260200
C	0.07035000	0.89604500	2.69029200
C	-0.45798300	0.71608300	3.96754100
H	-2.15223900	0.04082500	5.11869500
H	1.04915400	1.34638300	2.55784200
H	0.12378800	1.01020700	4.83677300
C	-2.85414700	1.45545000	-0.64274100
C	-1.66143300	2.21848700	-0.54960900
C	-3.96460000	2.07300900	-1.24102500
C	-1.61553000	3.53971500	-1.03139700
C	-3.92070900	3.38486000	-1.71604500
C	-2.74027800	4.12153300	-1.60685300
H	-0.68615800	4.09768700	-0.96119300
H	-4.80341300	3.82744000	-2.16921500
H	-2.69179100	5.14307900	-1.97354800
H	-4.89349800	1.52293200	-1.34139400
Pd	0.53153100	-0.26407600	0.08487000
O	1.80225500	-2.44061500	0.90196400
S	2.72908100	-2.22015600	-0.24071900

O	2.16810500	-1.15546600	-1.16895900
O	3.29363700	-3.38824800	-0.91341800
C	4.16685400	-1.31382300	0.52520600
F	3.71210500	-0.26684700	1.24186500
F	4.98556900	-0.84160000	-0.42859700
F	4.86061900	-2.11698700	1.33457800
Si	-2.90534000	-0.30058900	0.07661500
C	-0.41371300	1.67638500	-0.02089100
C	0.86442600	1.74991500	-0.21680600
C	2.08360100	2.47790600	-0.34828100
C	2.13973500	3.80813700	0.13001100
C	3.23064600	1.89902300	-0.93199900
C	3.31400800	4.54270000	0.00759100
H	1.26192500	4.24004900	0.60190100
C	4.40040700	2.64281100	-1.03816900
H	3.18659300	0.87440100	-1.28132600
C	4.44654300	3.96196100	-0.57446300
H	3.35201500	5.56427400	0.37517900
H	5.28245200	2.18678900	-1.47788400
H	5.36525300	4.53568900	-0.65953100
C	-1.85177400	-1.44753500	-0.98996000
C	-1.15412300	-2.53118500	-0.40975800
C	-1.74469100	-1.26471000	-2.38395600
C	-0.37433100	-3.39074300	-1.19214500
H	-1.21093500	-2.70620200	0.66216100
C	-0.96567800	-2.12009900	-3.16144200
H	-2.25494600	-0.42859000	-2.85712600
C	-0.27429000	-3.18022000	-2.56557000
H	0.18809200	-4.18728800	-0.71663900
H	-0.88045700	-1.95078200	-4.23163600
H	0.35785400	-3.82648300	-3.16709500
C	-4.66048800	-1.05104500	0.26322700
C	-4.52005600	-2.41207000	0.98755300
H	-5.50596800	-2.89074800	1.07112800
H	-3.86695000	-3.09733200	0.43541800
H	-4.11707000	-2.31405600	2.00095800
C	-5.25664400	-1.33314300	-1.13628800
H	-6.22619800	-1.84019700	-1.03063200
H	-5.43118500	-0.42138700	-1.71766100
H	-4.60445300	-1.98405600	-1.72926700
C	-5.62059700	-0.14231200	1.05990700
H	-6.60270400	-0.62737200	1.15381600
H	-5.25820400	0.05964600	2.07347800
H	-5.77763700	0.82607800	0.57377000

INT29

C	-1.65016000	-1.57223800	1.16020300
C	-1.41904000	-2.86200900	1.62065300
C	-0.89075300	-0.51156100	1.74902700
C	-0.44207500	-3.14309000	2.60139600
H	-1.98528300	-3.69319800	1.21299900
C	0.07387000	-0.78385000	2.76231500
C	0.29841800	-2.12242500	3.16689800
H	-0.28063200	-4.17047700	2.91463700
H	0.48319800	0.03461800	3.34889600
H	1.03556900	-2.32992500	3.93647100
C	-3.41918600	0.66832000	0.48556500
C	-2.44625800	1.47264000	1.13759800
C	-4.71252400	1.19168200	0.34363600
C	-2.76770300	2.76159800	1.57952700
C	-5.03598600	2.47198500	0.80094600
C	-4.05825400	3.26174400	1.40689000
H	-2.00687600	3.36448600	2.06488500
H	-6.04635500	2.85249000	0.67713400
H	-4.30118100	4.26180300	1.75583200
H	-5.48705600	0.60144100	-0.13528600
Pd	1.24293200	-0.19602100	0.83501400
O	2.57806000	-1.99131200	0.06784600
S	3.38531900	-1.05244100	-0.78322500
O	2.74914200	0.32686200	-0.69073400
O	3.76221900	-1.49610600	-2.12105700
C	4.96462700	-0.83180900	0.17766300
F	4.67276300	-0.40711500	1.41647900
F	5.74484900	0.07138400	-0.41978900
F	5.61617600	-1.99480500	0.25899400
Si	-2.78401400	-0.96690100	-0.22946100
C	-1.08759700	0.91335900	1.31535200
C	0.09010100	1.41417700	0.90989900
C	0.54188900	2.67104000	0.33919100
C	0.69050300	3.81034400	1.15268900
C	0.84495800	2.75642700	-1.03383300
C	1.10500500	5.01902100	0.59769500
H	0.48178900	3.73494500	2.21621700
C	1.25945600	3.96816800	-1.57883900
H	0.75354200	1.87271500	-1.65431100
C	1.38867700	5.10059200	-0.76876500
H	1.21101500	5.89578400	1.23067700
H	1.48491200	4.02795000	-2.63987100

H	1.71532300	6.04318700	-1.19954600
C	-1.64021800	-0.54210600	-1.67070500
C	-0.45472200	-1.26595300	-1.90212000
C	-1.93616400	0.53155000	-2.52919800
C	0.41098700	-0.92488100	-2.94389200
H	-0.18164100	-2.09047000	-1.24738000
C	-1.08219100	0.86875500	-3.58191900
H	-2.83079000	1.12721300	-2.36070500
C	0.09468200	0.14386500	-3.78670900
H	1.33806500	-1.47300100	-3.08144300
H	-1.32627800	1.70718100	-4.22948600
H	0.77109300	0.41621300	-4.59250000
C	-4.12209100	-2.21555000	-0.78935200
C	-3.43552300	-3.48948100	-1.33518700
H	-4.19475500	-4.18003100	-1.72903900
H	-2.74213900	-3.25776200	-2.15173600
H	-2.87554000	-4.03333100	-0.56787900
C	-4.94633300	-1.61024100	-1.94945800
H	-5.66754700	-2.35315300	-2.31882500
H	-5.51866100	-0.72655100	-1.65053900
H	-4.30557700	-1.32343000	-2.79130700
C	-5.05248200	-2.58383800	0.38376800
H	-5.81481200	-3.30475800	0.05523900
H	-4.50011200	-3.04263500	1.21288800
H	-5.57596700	-1.70681900	0.78218400

TS22

C	-1.60948700	-2.16300600	-0.00031700
C	-1.20602500	-3.35805500	-0.62046200
C	-0.60938800	-1.22932600	0.35007800
C	0.12634300	-3.58489300	-0.96839800
H	-1.94349000	-4.11604200	-0.86661700
C	0.74807700	-1.42397700	-0.02695500
C	1.08249200	-2.59362600	-0.72909000
H	0.41228900	-4.51497200	-1.45356900
H	2.10518000	-2.74609600	-1.05924100
C	-3.28416600	-0.42650800	1.66000200
C	-2.06708600	0.27699600	1.86162600
C	-4.31174800	-0.27758300	2.60326300
C	-1.92727400	1.09523400	2.99586700
C	-4.16663900	0.54957300	3.71785700
C	-2.96868300	1.23963800	3.90915800
H	-0.98768200	1.60826000	3.16964700
H	-4.97831000	0.64747900	4.43408500

H	-2.83674800	1.87794400	4.77902300
H	-5.24443500	-0.81810700	2.47691200
Pd	1.61158800	0.45264700	-0.37824800
O	3.00844900	-1.55023000	1.46086000
S	4.21903000	-1.05750000	0.61942000
O	5.14883300	-0.23810300	1.38343000
O	3.76010000	-0.56951900	-0.71173400
C	5.09471900	-2.66201700	0.24792100
F	5.50752100	-3.21861500	1.38407400
F	6.14303400	-2.40219800	-0.53476400
F	4.26884500	-3.50137000	-0.38372100
Si	-3.34797300	-1.44779100	0.08480700
C	-0.91653700	0.09333700	0.93355200
C	-0.03929100	1.07020600	0.58096400
C	-0.23084100	2.51264900	0.78610500
C	0.69669300	3.28716400	1.50823900
C	-1.34067600	3.15811100	0.20720700
C	0.51742300	4.66338700	1.65335200
H	1.55276000	2.79304500	1.95814900
C	-1.51359500	4.53414700	0.34948700
H	-2.05674700	2.56737200	-0.35577300
C	-0.58637000	5.29304900	1.07025200
H	1.23769600	5.24349900	2.22461700
H	-2.37588300	5.01559600	-0.10467200
H	-0.72313200	6.36553400	1.17850800
C	-3.42239900	-0.19428500	-1.33907300
C	-2.67637100	-0.37643300	-2.51716900
C	-4.18847800	0.98015100	-1.22339000
C	-2.69586300	0.57367900	-3.54100800
H	-2.05321000	-1.26120100	-2.62651800
C	-4.21132100	1.93538700	-2.24268100
H	-4.75538300	1.16336800	-0.31298100
C	-3.46183700	1.73394100	-3.40460800
H	-2.10631800	0.41332800	-4.44033700
H	-4.80702100	2.83788000	-2.12793600
H	-3.47232700	2.47786900	-4.19719000
C	-4.80532200	-2.68334400	-0.07204000
C	-4.72472000	-3.41578200	-1.43132300
H	-5.60485800	-4.06278900	-1.55790000
H	-4.70839200	-2.71076000	-2.27087900
H	-3.84117200	-4.05555400	-1.51547100
C	-6.14934600	-1.91947100	-0.04811300
H	-6.98062600	-2.62497500	-0.19137400
H	-6.32792500	-1.39858000	0.89747700

H	-6.20379900	-1.17666700	-0.85260000
C	-4.76050600	-3.71104800	1.07656600
H	-5.59101600	-4.42615400	0.98445900
H	-3.82620100	-4.28557200	1.06906200
H	-4.84371900	-3.23069600	2.05851800
H	2.00894400	-1.34176500	0.91621600
N	2.26234700	2.40459100	-1.21097900
H	1.74236600	3.11826500	-0.69664000
C	3.71624400	2.66154800	-1.02261000
C	4.08383100	2.87814800	0.44064500
H	4.00509100	3.54400100	-1.61430900
H	4.25386500	1.79867900	-1.42574700
H	5.16211700	3.04388300	0.52862300
H	3.56800400	3.75366100	0.85128600
H	3.83621900	2.00483500	1.04936600
C	1.87442600	2.49270900	-2.64481800
C	0.36466800	2.43057800	-2.85422600
H	2.37337600	1.66717100	-3.16535000
H	2.27256700	3.42851100	-3.06748100
H	0.13588700	2.52616300	-3.92106400
H	-0.05618900	1.48670100	-2.49639900
H	-0.14344400	3.24285500	-2.32355700

INT30

C	-1.65815100	-2.17207200	0.12232300
C	-1.21622300	-3.40691100	-0.39062700
C	-0.69054200	-1.18273200	0.39019300
C	0.12246300	-3.61590700	-0.71226400
H	-1.92868800	-4.20721800	-0.56804000
C	0.65875100	-1.34515300	-0.01907100
C	1.04306500	-2.56258500	-0.58882700
H	0.44609600	-4.57688500	-1.10563000
H	2.05824500	-2.70221100	-0.94766400
C	-3.39235900	-0.34054700	1.60529000
C	-2.18715300	0.38658600	1.80020300
C	-4.44974200	-0.15072600	2.50706300
C	-2.09026600	1.26452800	2.89444000
C	-4.34690300	0.73843800	3.57759200
C	-3.16024400	1.44842900	3.76652300
H	-1.16138100	1.79499600	3.07161500
H	-5.18114100	0.86815400	4.26223000
H	-3.05933500	2.13417000	4.60394900
H	-5.37283800	-0.70823900	2.38241300
Pd	1.57777000	0.45357800	-0.32672700

O	3.14809800	-1.51577600	1.56651700
S	4.31299500	-1.07068500	0.58419400
O	5.29857600	-0.26286600	1.27924900
O	3.74640600	-0.61855700	-0.70482800
C	5.10207100	-2.72806400	0.23595400
F	5.57231100	-3.23767700	1.36951100
F	6.09882600	-2.53485600	-0.62654000
F	4.20475100	-3.55811700	-0.29414300
Si	-3.39702300	-1.46003100	0.09796500
C	-1.00774700	0.16124300	0.91822400
C	-0.09265600	1.11037200	0.58228900
C	-0.26022500	2.56130500	0.74116600
C	0.65403100	3.34150400	1.47408200
C	-1.33303700	3.21045600	0.09888200
C	0.49973600	4.72532500	1.56673500
H	1.48096800	2.84559400	1.97374900
C	-1.48206800	4.59360400	0.19024300
H	-2.03870000	2.61545300	-0.47333300
C	-0.56681900	5.35783700	0.92078000
H	1.21002000	5.30948400	2.14656600
H	-2.31580400	5.07717900	-0.31250000
H	-0.68425200	6.43596600	0.98807900
C	-3.40006800	-0.28569100	-1.39618900
C	-2.57387000	-0.51479400	-2.51106200
C	-4.16876700	0.89252300	-1.38214600
C	-2.51698500	0.39452900	-3.56986600
H	-1.94483700	-1.40153200	-2.53971000
C	-4.11695900	1.80663400	-2.43760200
H	-4.79613400	1.11381700	-0.52115100
C	-3.28706400	1.55966700	-3.53421200
H	-1.86490000	0.19884200	-4.41766000
H	-4.71628900	2.71332000	-2.40077100
H	-3.23773400	2.27253700	-4.35352600
C	-4.84690000	-2.70371100	-0.04711900
C	-4.70214900	-3.50700500	-1.36026900
H	-5.56505000	-4.17748800	-1.48435400
H	-4.66630900	-2.84709900	-2.23516800
H	-3.80301600	-4.13032500	-1.37688800
C	-6.19281800	-1.94738700	-0.11987800
H	-7.01542800	-2.66295700	-0.26421100
H	-6.41326500	-1.38144400	0.79057200
H	-6.21404600	-1.24516800	-0.96163100
C	-4.84613500	-3.66830300	1.15575000
H	-5.67031200	-4.39148800	1.06866100

H	-3.91063700	-4.23766200	1.21693400
H	-4.97058800	-3.13645200	2.10637100
H	2.23338700	-1.33263900	1.13209000
N	2.35540200	2.41215800	-1.13555300
H	1.82564900	3.13921800	-0.65116500
C	3.79965500	2.63736200	-0.87212800
C	4.09222100	2.82972500	0.61182400
H	4.14372700	3.51867100	-1.43625100
H	4.34031700	1.76764900	-1.25677200
H	5.16966000	2.94027600	0.76807300
H	3.59435700	3.72638800	0.99797300
H	3.75964800	1.96847900	1.19796800
C	2.04211700	2.50179100	-2.58588700
C	0.54207800	2.47312100	-2.86634700
H	2.54384900	1.66008900	-3.07780000
H	2.48213200	3.42429700	-2.99731900
H	0.36533400	2.56848900	-3.94319700
H	0.08336400	1.54082500	-2.52362700
H	0.02947100	3.29970500	-2.36250900

TS23

C	1.91179400	-1.48007900	-1.49771900
C	1.44930000	-2.60026100	-2.21270900
C	1.09532500	-0.33430600	-1.50315300
C	0.20135100	-2.61321400	-2.83867500
H	2.06057100	-3.49555800	-2.26234600
C	-0.21501100	-0.41478200	-2.00882600
C	-0.68095600	-1.53471900	-2.67783600
H	-0.11861700	-3.49089100	-3.39334700
H	-0.40853100	1.20918500	-2.04841800
H	-1.70853600	-1.59388500	-3.01816200
C	3.81755400	0.38446200	-0.34064400
C	2.87769900	1.36446700	-0.76145100
C	5.15683100	0.77545200	-0.19069400
C	3.32010300	2.66354700	-1.06847100
C	5.57978800	2.07717700	-0.46277900
C	4.65681700	3.01985300	-0.91686400
H	2.61406400	3.39643500	-1.44159100
H	6.62540900	2.34671200	-0.33973600
H	4.97624700	4.02896200	-1.16260000
H	5.89666800	0.04987800	0.12931700
Pd	-1.42487800	0.74528000	-0.80848000
O	-3.04190500	-0.72780400	-0.88040800
S	-3.12311600	-1.73593200	0.25749700

O	-3.22557200	-1.07178000	1.57740900
O	-2.19616900	-2.86635500	0.14523100
C	-4.82404800	-2.41137200	-0.07325300
F	-5.72686700	-1.41895500	-0.00691700
F	-5.13338600	-3.33613500	0.84095700
F	-4.87825500	-2.96349800	-1.28995400
Si	3.18505500	-1.38326700	-0.11470200
C	1.45158500	0.99905900	-0.95430300
C	0.37180100	1.83008800	-0.82248100
C	0.27697700	3.20589300	-0.33756900
C	0.96362700	3.60941000	0.82509600
C	-0.54971000	4.13890600	-0.98886500
C	0.83378900	4.90858200	1.30812300
H	1.58800500	2.89029800	1.34444200
C	-0.67665300	5.43984300	-0.50298400
H	-1.09821000	3.82893800	-1.87446000
C	0.01331000	5.82935800	0.64789900
H	1.36584200	5.20124900	2.20916500
H	-1.31762100	6.14789600	-1.02110200
H	-0.09130300	6.84044400	1.03116700
N	-2.65425600	1.71427500	0.78070100
H	-3.13682700	0.86375400	1.09175700
C	-3.66603200	2.66324100	0.25352300
C	-4.52575900	2.06205200	-0.85545200
H	-4.30914800	2.99249500	1.08461500
H	-3.12606800	3.54614600	-0.10543200
H	-5.30955200	2.77373200	-1.13754600
H	-4.99849100	1.12905500	-0.53461700
H	-3.92998400	1.83567300	-1.74583800
C	-1.96555800	2.26536200	1.97514400
C	-0.97769200	1.27196000	2.57266200
H	-1.46757300	3.19093500	1.67873800
H	-2.72789400	2.53199200	2.72363900
H	-0.52352600	1.69062900	3.47705200
H	-0.17238000	1.03012900	1.87205300
H	-1.47518300	0.33540900	2.83445900
C	4.53137500	-2.74641800	-0.09948600
C	5.45158900	-2.59057600	1.13276300
C	3.83869000	-4.12445600	0.02419200
C	5.36498300	-2.70149600	-1.39580100
H	6.02667100	-1.65903700	1.12552300
H	4.87993400	-2.62300600	2.06719200
H	6.17721300	-3.41618700	1.15952500
H	3.22361200	-4.36745100	-0.84727000

H	4.59856500	-4.91399000	0.11378700
H	3.19638800	-4.17825900	0.91065700
H	6.11504400	-3.50556900	-1.39555000
H	4.73674400	-2.83597200	-2.28488200
H	5.89815100	-1.75074900	-1.50997700
C	2.14483700	-1.46194300	1.46164400
C	0.86339200	-2.04769600	1.45855100
C	2.61878100	-0.92047100	2.67147700
C	0.09081500	-2.10430500	2.61996600
H	0.43806600	-2.44818000	0.54269900
C	1.85217200	-0.97892400	3.83743400
H	3.59299500	-0.43553900	2.70296300
C	0.58853200	-1.57544900	3.81296300
H	-0.90410400	-2.53587300	2.57282400
H	2.23693000	-0.55377200	4.76142500
H	-0.01298000	-1.61285900	4.71775400

INT31

C	1.88104900	-1.70273500	-1.36972100
C	1.38362600	-2.91647200	-1.82099600
C	0.99754700	-0.57138700	-1.41975700
C	0.03861600	-3.05012500	-2.22988900
H	2.00861400	-3.80358600	-1.81106400
C	-0.40744900	-0.76011300	-1.62271700
C	-0.87203200	-2.01487600	-2.03587100
H	-0.30829200	-4.00752300	-2.61215200
H	-0.07093600	1.91223400	-2.23185200
H	-1.93450000	-2.18412200	-2.16595600
C	3.81081700	0.31274800	-0.61249600
C	2.78264000	1.20750100	-1.03119700
C	5.13059600	0.77406400	-0.59692300
C	3.13516800	2.51009000	-1.44595900
C	5.46132600	2.07080800	-1.00103000
C	4.45834300	2.93676800	-1.43616900
H	2.36775900	3.19123600	-1.79133600
H	6.49829300	2.39594100	-0.98690600
H	4.70308300	3.94159200	-1.76788300
H	5.92975900	0.11180300	-0.28227200
Pd	-1.52603100	0.65618700	-0.84629000
O	-3.27902900	-0.68342300	-0.74956600
S	-3.44541800	-1.43953700	0.56068500
O	-4.24453200	-0.68424300	1.54416100
O	-2.20978800	-2.08199900	1.03745200
C	-4.52648500	-2.83582400	-0.02292200

F	-5.67665500	-2.36540100	-0.51835000
F	-4.79584700	-3.66287300	0.99311700
F	-3.89442400	-3.52830400	-0.98572600
Si	3.25623000	-1.41994100	-0.11775500
C	1.37610900	0.77986300	-1.16873200
C	0.26795900	1.74934000	-1.19753400
C	0.34931300	2.99026500	-0.39399200
C	0.89722100	2.97503100	0.90364100
C	-0.16015200	4.20354200	-0.88814400
C	0.94582900	4.13696200	1.66853000
H	1.27437400	2.04226700	1.31409100
C	-0.11947400	5.36575700	-0.11732200
H	-0.59139100	4.22979600	-1.88671200
C	0.43670800	5.33873600	1.16424100
H	1.36989900	4.10163100	2.66842500
H	-0.52049200	6.29278900	-0.51856200
H	0.46721900	6.24227700	1.76659700
N	-2.93455400	2.05262200	0.29027900
H	-3.62784800	1.33725300	0.52509100
C	-3.60983900	3.07101000	-0.54534000
C	-4.22643700	2.46419800	-1.80308900
H	-4.38835000	3.57693600	0.04822300
H	-2.86132100	3.82692300	-0.80478900
H	-4.78878900	3.22724000	-2.35265100
H	-4.90707700	1.64376600	-1.55184800
H	-3.45376700	2.05818800	-2.46529200
C	-2.45316700	2.62216600	1.57300400
C	-1.83000000	1.55553900	2.46665500
H	-1.72810300	3.40332800	1.33701200
H	-3.29644200	3.10436200	2.09283500
H	-1.47345800	2.00944800	3.39798200
H	-0.97459200	1.07916100	1.97804900
H	-2.55501400	0.77315200	2.70957000
C	4.62711600	-2.74868200	-0.01008200
C	5.63520700	-2.39518000	1.10761400
C	3.97963600	-4.10085800	0.37243700
C	5.35785500	-2.88499400	-1.36098200
H	6.18450900	-1.46805400	0.91397600
H	5.13928000	-2.29357800	2.07945200
H	6.38127300	-3.19737000	1.19870600
H	3.31153400	-4.48359100	-0.40461300
H	4.76360100	-4.85604600	0.52568700
H	3.40347800	-4.02633800	1.30205600
H	6.12653600	-3.66874000	-1.30156400

H	4.66801100	-3.15878500	-2.16854200
H	5.85692600	-1.95387800	-1.65434700
C	2.34913600	-1.18695000	1.52621400
C	1.02769700	-1.63374900	1.71732600
C	2.94619100	-0.43446200	2.55721000
C	0.32861000	-1.34367000	2.89125000
H	0.50775300	-2.18330200	0.93830600
C	2.25463800	-0.14857800	3.73595400
H	3.95453900	-0.04451700	2.43093000
C	0.94296100	-0.60249900	3.90264900
H	-0.70018200	-1.67582900	2.98384600
H	2.73391300	0.43668000	4.51708900
H	0.39680200	-0.36682900	4.81249000

TS24

C	-2.27282500	0.48789600	-0.99236700
C	-2.27286300	1.38834000	-2.06715100
C	-1.03616800	0.02629400	-0.46921200
C	-1.08024700	1.85085900	-2.62194800
H	-3.22003100	1.74825000	-2.46190400
C	0.15347900	0.54221300	-1.00620400
C	0.13800800	1.43180200	-2.08358600
H	-1.09357300	2.54647600	-3.45743000
H	1.06959400	1.81965900	-2.48638300
C	-3.33316600	-0.50426100	1.53950500
C	-1.98840300	-0.88776600	1.75474100
C	-4.20484100	-0.44286300	2.63716900
C	-1.55860000	-1.18828700	3.05794300
C	-3.77252800	-0.75335600	3.92697200
C	-2.44244400	-1.12413100	4.13426000
H	-0.51986300	-1.45056500	3.23084300
H	-4.46228600	-0.69455200	4.76474500
H	-2.08716400	-1.34930600	5.13652400
H	-5.23638100	-0.13479000	2.48003800
Si	-3.87905300	-0.08797600	-0.20722100
C	-1.02947000	-1.00926400	0.61605800
C	-0.27410700	-2.13091700	0.52497000
C	0.62254900	-2.44923700	-0.60340400
C	0.25970700	-3.49617300	-1.46386000
C	0.98088800	-3.74219200	-2.63127100
H	-0.62709700	-4.08354700	-1.24085800
C	2.49607600	-1.95377500	-2.07732300
C	2.09320500	-2.95521800	-2.95293100
H	0.66727300	-4.53980500	-3.29979000

H	3.38566200	-1.37471800	-2.30609300
H	2.64405000	-3.13593100	-3.87189800
Pd	1.89893800	0.31374900	-0.13440900
H	-0.44522200	-2.92189300	1.25354900
C	-5.08614900	1.36297500	-0.16007200
C	-4.56975200	2.62517600	0.19825900
C	-6.46669100	1.27588000	-0.41257800
C	-5.39312000	3.74642100	0.29993400
H	-3.50540800	2.73440600	0.39310100
C	-7.29707700	2.39531300	-0.31354100
H	-6.91187800	0.32715500	-0.69428500
C	-6.76187300	3.63356800	0.04327700
H	-4.96708200	4.70734400	0.57671700
H	-8.36071100	2.29872900	-0.51662100
H	-7.40608900	4.50573500	0.11999200
C	-4.55031100	-1.64916300	-1.10786700
C	-5.01370900	-1.27519500	-2.53123700
C	-3.40385100	-2.67920400	-1.21812400
C	-5.70468400	-2.29891900	-0.31635300
H	-5.84050600	-0.55668300	-2.52722700
H	-4.19449700	-0.83615900	-3.11410900
H	-5.35672900	-2.17224600	-3.06733000
H	-3.04672500	-2.99454300	-0.23130800
H	-3.75847100	-3.57604800	-1.74748800
H	-2.54585600	-2.28158400	-1.77139500
H	-6.03593200	-3.21953900	-0.81885900
H	-5.39044900	-2.56957500	0.69876300
H	-6.57998900	-1.64665800	-0.22806500
S	3.70337900	2.22364200	0.97477500
C	4.79337500	2.55604900	-0.49979000
F	4.39884000	1.79255000	-1.53980200
F	6.06123200	2.24298800	-0.20773400
F	4.72543400	3.83782900	-0.85971300
O	2.31213400	2.47324800	0.45005300
O	3.88499300	0.73705600	1.15367300
O	4.18083700	3.08654100	2.04622400
C	1.79830900	-1.68773900	-0.86827400
H	2.65576900	-1.68515400	0.11380600
N	3.75638500	-2.09123200	1.02798100
H	4.01758800	-1.23365000	1.51717300
C	3.15678000	-3.07277800	1.94357800
C	2.27743700	-2.36066400	2.96800600
H	3.94068900	-3.66093300	2.44344700
H	2.56322300	-3.76910400	1.33605200

H	1.74069300	-3.08644700	3.58737100
H	2.87932400	-1.72519500	3.62760300
H	1.54425400	-1.72507100	2.46318400
C	4.87081900	-2.57178800	0.19463300
C	5.64911400	-1.40691300	-0.41588300
H	4.44221500	-3.20893200	-0.59009900
H	5.54269900	-3.20301500	0.79524600
H	6.42755300	-1.78863200	-1.08440200
H	4.99841800	-0.73707600	-0.98360000
H	6.12525900	-0.79979100	0.36028700

INT32

C	-2.25584300	0.36081100	-1.21569300
C	-2.32681500	1.11155200	-2.39730100
C	-0.99728500	-0.11559100	-0.75000600
C	-1.17971300	1.41046400	-3.12857100
H	-3.29176900	1.47711200	-2.74085300
C	0.16669000	0.22919600	-1.47539000
C	0.05756400	0.96770200	-2.66389500
H	-1.24407800	1.98936400	-4.04680900
H	0.95412200	1.21657200	-3.22535300
C	-3.18725200	-0.26083500	1.46867000
C	-1.85968100	-0.72201000	1.63295200
C	-3.98367200	-0.03206700	2.60104900
C	-1.39450400	-0.95256900	2.94308400
C	-3.50513600	-0.25988600	3.89088100
C	-2.20146900	-0.73034300	4.05687600
H	-0.38165500	-1.31207400	3.09854500
H	-4.13681800	-0.07142900	4.75466200
H	-1.80705400	-0.91392500	5.05329400
H	-4.99829200	0.33672600	2.46639400
Si	-3.82719700	-0.02426200	-0.27601000
C	-0.95839400	-0.99677400	0.46488900
C	-0.21703100	-2.13900000	0.53220500
C	0.72548700	-2.71093100	-0.43598200
C	0.73084700	-4.11625300	-0.57402000
C	1.59350700	-4.75256000	-1.45993000
H	0.02967100	-4.70496600	0.01506600
C	2.51173100	-2.59793600	-2.07104900
C	2.48492100	-3.98721300	-2.21728500
H	1.57089700	-5.83420500	-1.56210800
H	3.22364100	-2.02119600	-2.65601500
H	3.16508600	-4.47021600	-2.91474300
Pd	2.02861300	-0.02132400	-0.85124000

H	-0.42728400	-2.79292100	1.37899000
C	-4.96903800	1.47983900	-0.32515800
C	-4.37955500	2.75351500	-0.19053000
C	-6.36956500	1.42399500	-0.43840300
C	-5.15150800	3.91507300	-0.16820900
H	-3.29806300	2.83792700	-0.11411600
C	-7.14913200	2.58352400	-0.41771500
H	-6.87030200	0.46773400	-0.54923500
C	-6.54159300	3.83230600	-0.28188800
H	-4.66931100	4.88401000	-0.06635900
H	-8.22982700	2.50979900	-0.51014500
H	-7.14610200	4.73560700	-0.26722500
C	-4.62478500	-1.65224800	-0.91756500
C	-5.17973600	-1.43408600	-2.34064100
C	-3.52748400	-2.73949300	-0.97492900
C	-5.74098400	-2.14722300	0.02615600
H	-5.97781300	-0.68381600	-2.36780900
H	-4.39133800	-1.10729300	-3.02974600
H	-5.59392400	-2.37358000	-2.73471800
H	-3.11186800	-2.95006900	0.01687400
H	-3.95285300	-3.67662000	-1.36252500
H	-2.69650100	-2.45390100	-1.62888300
H	-6.13772200	-3.10843800	-0.33195200
H	-5.36496000	-2.30328500	1.04441900
H	-6.58613400	-1.45328500	0.08858900
S	4.17443000	1.63580200	0.39024900
C	5.65934100	1.96180500	-0.68210400
F	5.48235900	1.38227900	-1.87383300
F	6.75297600	1.45759500	-0.10484100
F	5.81201000	3.27688700	-0.84829700
O	3.01120000	2.15818200	-0.38886900
O	4.10730500	0.11637400	0.42859500
O	4.43416800	2.25052300	1.69603000
C	1.65736100	-1.94424000	-1.16839100
H	1.34727900	-0.79596500	1.75951800
N	2.14141600	-0.48901300	2.34837000
H	2.87565500	-0.21134000	1.66000000
C	1.74924600	0.71045100	3.17266800
C	0.95225000	1.72450800	2.36204500
H	2.68483600	1.14088400	3.53870900
H	1.16737900	0.33321300	4.01831900
H	0.68916800	2.55984700	3.01883700
H	1.52991400	2.11965400	1.52460700
H	0.02555100	1.28859300	1.97984100

C	2.68130600	-1.64930000	3.13093000
C	3.25644500	-2.71154900	2.20045800
H	1.86231300	-2.03461100	3.74643000
H	3.44739500	-1.24014900	3.79600800
H	3.66271100	-3.53293600	2.79878400
H	2.49403900	-3.11439400	1.52810000
H	4.06116600	-2.29288000	1.58865000

TS25

C	2.29415000	0.00982700	-1.10390100
C	2.27493700	-0.48373500	-2.41327800
C	1.06729300	0.31554100	-0.45015900
C	1.07032300	-0.66126700	-3.10370200
H	3.21328700	-0.72371700	-2.90815000
C	-0.15524200	0.05929300	-1.12735500
C	-0.13191600	-0.37987200	-2.46673900
H	1.07405000	-1.02234700	-4.12963400
H	-1.07042300	-0.51504200	-2.99764000
C	3.43417900	0.36730700	1.56335800
C	2.09253000	0.66406300	1.90482200
C	4.35468900	0.07953700	2.58286400
C	1.72403100	0.65178600	3.26454300
C	3.98015100	0.08623000	3.92611100
C	2.65543900	0.37373500	4.26253200
H	0.68908300	0.83453000	3.53811600
H	4.70750300	-0.14193700	4.70079100
H	2.34082300	0.36532200	5.30309300
H	5.38188200	-0.16216700	2.31692500
Si	3.91520300	0.38911600	-0.24470700
C	1.05593500	0.97505900	0.87810100
C	0.14123900	1.95228100	1.16130600
C	-0.92149800	2.40109400	0.27934300
C	-1.29948200	3.75929400	0.27936800
C	-1.54889900	1.50141700	-0.62931200
C	-2.20383500	4.25773100	-0.65233500
H	-0.84697100	4.43019300	1.00676400
C	-2.42277700	2.04005500	-1.60598100
C	-2.74732400	3.40000700	-1.61834600
H	-2.47128200	5.31044200	-0.64388400
H	-2.85224800	1.38136100	-2.35627200
H	-3.43840500	3.78481200	-2.36417400
Pd	-1.79152300	-0.42903400	-0.04441800
H	0.28759900	2.53516600	2.06817000
C	5.15491500	-0.99121600	-0.60713700

C	4.66959400	-2.30584800	-0.75649900
C	6.54701600	-0.80437000	-0.68530300
C	5.53139400	-3.38160800	-0.97325300
H	3.59859600	-2.48809000	-0.71202500
C	7.41615500	-1.87645800	-0.90212800
H	6.96978800	0.18962800	-0.57974800
C	6.90995100	-3.16895800	-1.04684100
H	5.12805400	-4.38483100	-1.08724600
H	8.48749500	-1.70076800	-0.95977900
H	7.58421200	-4.00443500	-1.21717300
C	4.52611500	2.14218600	-0.75457300
C	5.02382800	2.12318000	-2.21408300
C	3.33015500	3.11582500	-0.64646400
C	5.64139600	2.64892100	0.18405900
H	5.88714600	1.46183900	-2.34969200
H	4.23566200	1.78873600	-2.90009200
H	5.32572800	3.13352400	-2.52687000
H	2.93534500	3.16500900	0.37459600
H	3.64847900	4.12977400	-0.92964100
H	2.50494500	2.82773800	-1.30669600
H	5.92076300	3.67807400	-0.08529000
H	5.31353900	2.65667800	1.23011900
H	6.55336500	2.04441300	0.12691400
N	-1.72326400	-2.65586700	0.50046700
H	-0.87102800	-2.96087000	0.02718900
C	-1.53873900	-2.87037400	1.95528700
C	-0.29937300	-2.15169500	2.47721400
H	-1.47670600	-3.94969100	2.17336200
H	-2.43757100	-2.48698000	2.44948000
H	-0.16314500	-2.35021500	3.54552900
H	0.60780000	-2.48080800	1.95574200
H	-0.38696100	-1.07181100	2.33155800
C	-2.85425200	-3.44439000	-0.03612600
C	-2.95790800	-3.33204900	-1.55411300
H	-3.76430400	-3.05901400	0.43255300
H	-2.75503000	-4.50244900	0.25837800
H	-3.78956900	-3.94292300	-1.92178700
H	-3.12647300	-2.29417800	-1.85547800
H	-2.03940000	-3.68075600	-2.04184700
S	-5.05719000	0.22833800	0.89031800
C	-5.63603700	-0.53485700	-0.71724800
F	-4.71808800	-0.32576600	-1.66929100
F	-6.78997900	0.00764000	-1.08670500
F	-5.78953400	-1.84785200	-0.53370700

O	-3.86547600	-0.53350100	1.28344400
O	-4.67168800	1.69329700	0.39117400
O	-6.20325000	0.33788300	1.76712700
H	-3.79760200	1.71772100	-0.09625100

INT33

C	-2.00773200	1.18504400	-0.80547500
C	-2.29747100	2.29452700	-1.62804200
C	-0.69312600	1.01643100	-0.33416300
C	-1.31546800	3.20927500	-1.98375400
H	-3.31529500	2.45001800	-1.97674500
C	0.30518300	1.96721900	-0.68617000
C	-0.00535900	3.04524400	-1.50136000
H	-1.55548800	4.05336800	-2.62622000
H	0.75241100	3.77509200	-1.77229700
C	-2.45337000	-1.20324000	0.87306500
C	-1.05360000	-1.15142700	1.10690800
C	-3.20829100	-2.21607200	1.49273100
C	-0.46580600	-2.20142900	1.84456600
C	-2.61889100	-3.20605100	2.27252800
C	-1.22956000	-3.20917800	2.41852200
H	0.60759200	-2.24175800	1.95936500
H	-3.22730100	-3.97689700	2.73812600
H	-0.73724700	-3.99886900	2.98022600
H	-4.28678400	-2.23182000	1.35332100
Si	-3.31749800	-0.06470700	-0.34183400
C	-0.21040100	-0.03683400	0.59924600
C	1.09439000	0.19601800	0.95338800
C	1.95760100	-0.28348800	2.03452400
C	3.26130100	-0.75419900	1.75727800
C	4.14144100	-1.07247100	2.79398900
H	3.56534900	-0.90754500	0.72572800
C	2.45978300	-0.44638800	4.41345000
C	3.74693700	-0.91861600	4.12302300
H	5.13319800	-1.44962700	2.55833500
H	2.14685400	-0.32601900	5.44737000
H	4.43185100	-1.16593300	4.92936100
Pd	2.11074600	1.70767700	0.14479900
H	1.58976600	-0.62789400	-0.80219000
C	-4.77448500	0.81420000	0.48607000
C	-4.61293000	2.11610300	0.99670700
C	-6.03023400	0.20162200	0.66024600
C	-5.65559000	2.77638100	1.65028500
H	-3.65940700	2.62409700	0.87742300

C	-7.07662300	0.85530300	1.31343400
H	-6.20369600	-0.80111700	0.27993700
C	-6.89147700	2.14719400	1.81039100
H	-5.50290700	3.78258400	2.03308300
H	-8.03602200	0.35766300	1.43199500
H	-7.70519000	2.65951900	2.31752400
C	-3.86182400	-1.03852600	-1.92215200
C	-4.82571500	-0.17517500	-2.76370600
C	-2.59786400	-1.34592300	-2.75605800
C	-4.54897600	-2.37950600	-1.58827900
H	-5.74270900	0.07421200	-2.21774100
H	-4.35815800	0.76381100	-3.08262600
H	-5.11505300	-0.71715900	-3.67601000
H	-1.87302500	-1.94777100	-2.19890000
H	-2.87506600	-1.91145100	-3.65788800
H	-2.09162000	-0.43030200	-3.08135500
H	-4.81681100	-2.89839800	-2.52026400
H	-3.89037400	-3.04339000	-1.01917400
H	-5.47659400	-2.25184200	-1.01755800
S	1.62726600	-2.54239200	-1.87340400
C	2.71815100	-3.52711000	-0.71935300
F	2.65021900	-4.81347500	-1.05718900
F	2.30150100	-3.37642400	0.54115800
F	3.98308400	-3.10562600	-0.81454200
O	2.06899900	-2.85298100	-3.22015300
O	0.25966800	-2.73951200	-1.41673400
O	2.13657400	-1.05861200	-1.52879000
C	1.57771200	-0.12889600	3.38727000
H	0.57865200	0.23472800	3.60778400
N	3.54496600	3.28001200	-0.66384800
H	4.43977400	3.04656900	-0.22432000
C	3.74250600	3.15520600	-2.13286200
C	4.29850000	1.78718200	-2.51553400
H	4.41634900	3.95282400	-2.48410100
H	2.76904900	3.31335600	-2.60623300
H	4.46256200	1.74000100	-3.59708500
H	5.26299800	1.60077400	-2.02481900
H	3.60726200	0.98434300	-2.23999100
C	3.21213100	4.66635800	-0.24915300
C	3.15961800	4.80261700	1.26897400
H	2.23862800	4.91162900	-0.68365900
H	3.94771900	5.36943500	-0.67123500
H	2.93242800	5.83686400	1.54782200
H	2.38630000	4.15170800	1.69131700

H	4.12168100	4.53637700	1.72538700
TS26			
C	-2.00832300	1.11918800	-0.86394100
C	-2.30480200	2.21326900	-1.69398400
C	-0.68192000	0.95190600	-0.40614100
C	-1.32217100	3.12784800	-2.06341700
H	-3.32461100	2.36600700	-2.03759800
C	0.31347600	1.90714100	-0.76360700
C	-0.01424400	2.98329600	-1.57929600
H	-1.56744200	3.95846300	-2.72143800
H	0.73623500	3.71624300	-1.85991100
C	-2.45984400	-1.17307100	0.92637800
C	-1.04949300	-1.14827700	1.10393800
C	-3.21378800	-2.13199800	1.62243700
C	-0.45372000	-2.18392800	1.85884500
C	-2.61325900	-3.10030800	2.42306000
C	-1.21905600	-3.14240500	2.50782300
H	0.62192000	-2.25767300	1.91523800
H	-3.22075100	-3.83190600	2.94926700
H	-0.72588200	-3.92496400	3.07764500
H	-4.29685200	-2.12838600	1.52402700
Si	-3.32681600	-0.10044100	-0.34372800
C	-0.20160100	-0.09401100	0.51301500
C	1.17713900	0.02377700	0.73109300
C	2.00008900	-0.32261300	1.90063100
C	3.32117300	-0.79464600	1.72816700
C	4.16176300	-0.97702100	2.82871700
H	3.66696900	-1.05348600	0.73257000
C	2.40388700	-0.21584700	4.30283000
C	3.70975400	-0.69012700	4.11666300
H	5.16874600	-1.35595200	2.67524100
H	2.04596600	0.01084400	5.30382200
H	4.36413700	-0.83519900	4.97182200
Pd	2.11967300	1.68905500	0.06132400
H	1.68055400	-0.53970700	-0.42960200
C	-4.77588600	0.82146300	0.44490500
C	-4.59692400	2.12863200	0.93623800
C	-6.04381100	0.23294700	0.61342900
C	-5.63534700	2.81719800	1.56650300
H	-3.63380400	2.61899200	0.81993300
C	-7.08593700	0.91546500	1.24362200
H	-6.23033300	-0.77210900	0.24591100
C	-6.88373400	2.21173500	1.72188600

H	-5.46991900	3.82675200	1.93461700
H	-8.05529500	0.43684100	1.35825900
H	-7.69414700	2.74630400	2.21079700
C	-3.85394200	-1.15743600	-1.87178800
C	-4.81623600	-0.33872600	-2.75865800
C	-2.58413700	-1.50205000	-2.68228400
C	-4.53767300	-2.47990500	-1.46528500
H	-5.73949300	-0.06893600	-2.23338900
H	-4.35007500	0.58662400	-3.11782600
H	-5.09396400	-0.92473700	-3.64662900
H	-1.84791400	-2.05902200	-2.09480200
H	-2.85643900	-2.12291400	-3.54810500
H	-2.08826300	-0.60284800	-3.06414400
H	-4.80125100	-3.04887900	-2.36838100
H	-3.87682000	-3.10964300	-0.86110200
H	-5.46669100	-2.32594700	-0.90317700
S	1.71737600	-2.47345800	-1.78499300
C	2.69273100	-3.62314800	-0.68972100
F	2.46782700	-4.89185300	-1.03794700
F	2.32976600	-3.45835500	0.59533400
F	4.00460000	-3.36633600	-0.79030800
O	2.09802400	-2.81167000	-3.15163000
O	0.32912900	-2.62019600	-1.33914100
O	2.31327500	-1.10538100	-1.35878900
C	1.56254900	-0.02883200	3.21327800
H	0.55122900	0.34109000	3.35444900
N	3.46320400	3.38443500	-0.58990900
H	4.33623100	3.19813400	-0.08805100
C	3.77455800	3.28993500	-2.04260800
C	4.41607100	1.95196200	-2.39933000
H	4.43633900	4.12162300	-2.33180700
H	2.83250600	3.41454600	-2.58495600
H	4.66275500	1.93004800	-3.46586900
H	5.34863700	1.79979800	-1.84004200
H	3.74316500	1.11358700	-2.18802300
C	3.01736200	4.74104000	-0.18466600
C	2.83444600	4.84461600	1.32562500
H	2.06943600	4.93808600	-0.69366200
H	3.74206500	5.49224100	-0.53625100
H	2.52301500	5.85791600	1.59998100
H	2.07137100	4.13966600	1.67300400
H	3.77062900	4.62686800	1.85536100

INT34

C	-1.92940800	1.17930700	-0.89356900
C	-2.15821200	2.25070800	-1.75541800
C	-0.60779100	0.97635900	-0.39806800
C	-1.12094400	3.11892600	-2.12278000
H	-3.15962100	2.43986500	-2.13271100
C	0.44898200	1.87178500	-0.76428400
C	0.16563200	2.94601400	-1.60996400
H	-1.32259100	3.93821800	-2.80952500
H	0.94680600	3.64334300	-1.89601200
C	-2.49333600	-1.02846900	0.95753300
C	-1.08253800	-1.01880400	1.17154600
C	-3.27481000	-1.94468400	1.67124300
C	-0.51711800	-2.02239100	1.99679100
C	-2.70327200	-2.88525000	2.52954600
C	-1.31358800	-2.94212700	2.66241600
H	0.55478600	-2.09939100	2.09262600
H	-3.33530300	-3.58616000	3.06846400
H	-0.85022000	-3.70346300	3.28262700
H	-4.35457100	-1.93617100	1.54582900
Si	-3.30532900	0.02311300	-0.36926100
C	-0.20557200	-0.04214900	0.53720200
C	1.24129100	-0.03066900	0.76125900
C	1.95056100	-0.20711100	2.04023700
C	3.22242300	-0.82247400	2.02539700
C	3.98372700	-0.89800800	3.19370400
H	3.57423200	-1.26618200	1.09814000
C	2.23064400	0.23758500	4.41593500
C	3.49294600	-0.37224300	4.38974000
H	4.95582700	-1.38322900	3.16925300
H	1.84538600	0.64743600	5.34602300
H	4.08386400	-0.43767700	5.29922900
Pd	2.24750300	1.58773100	0.02696700
H	1.68369900	-0.63523200	-0.05896500
C	-4.72789500	1.01535500	0.37598200
C	-4.51850100	2.33311600	0.82463400
C	-6.01126600	0.46363100	0.55340400
C	-5.54408700	3.06811200	1.42268400
H	-3.54271700	2.79567400	0.70087900
C	-7.04009900	1.19316000	1.15140700
H	-6.22083000	-0.54792100	0.21715400
C	-6.80832200	2.49941200	1.58754100
H	-5.35602700	4.08486600	1.75825600
H	-8.02220200	0.74354900	1.27341000
H	-7.60853300	3.07029000	2.05125600

C	-3.83806800	-1.06235000	-1.87388700
C	-4.78765700	-0.24429600	-2.77566500
C	-2.57572100	-1.44633200	-2.67786400
C	-4.54563100	-2.36049700	-1.43169900
H	-5.71014300	0.04571000	-2.26028100
H	-4.30840600	0.66868500	-3.14951100
H	-5.06692800	-0.84248100	-3.65452600
H	-1.83489200	-1.98994500	-2.08468600
H	-2.86322700	-2.08815200	-3.52289300
H	-2.07167900	-0.56583400	-3.09045000
H	-4.82573800	-2.94260300	-2.32084000
H	-3.89218000	-2.99097900	-0.82032900
H	-5.46795200	-2.17667300	-0.86710300
S	1.77410200	-2.49575300	-1.77577500
C	2.09901200	-3.89359200	-0.59085300
F	1.21164500	-4.88481000	-0.74995400
F	2.00010400	-3.45260600	0.68959200
F	3.33196200	-4.39363100	-0.75137400
O	2.00524500	-3.06566900	-3.10695000
O	0.38198200	-2.10552400	-1.44053700
O	2.78763700	-1.48533500	-1.32254300
C	1.47018800	0.32700900	3.25637200
H	0.49482800	0.80619400	3.27356500
N	3.74065000	3.07361600	-0.80595000
H	4.60956400	2.82908000	-0.32234100
C	3.96803700	2.80979900	-2.25503300
C	4.49443600	1.39824700	-2.49961200
H	4.67220900	3.55627800	-2.65579700
H	3.00979200	2.95363000	-2.76421700
H	4.67567600	1.25214800	-3.56956300
H	5.44888200	1.24036000	-1.97978700
H	3.78949300	0.62661800	-2.17044200
C	3.47493100	4.50276700	-0.51407900
C	3.34835400	4.75743400	0.98406600
H	2.54482700	4.77305300	-1.02349700
H	4.27398100	5.12755600	-0.94358200
H	3.16890500	5.82080800	1.17451100
H	2.51749100	4.18156600	1.40633200
H	4.26648000	4.47267800	1.51340600

INT35

C	2.56757300	-1.02305200	-1.03363200
C	2.96416300	-2.26474200	-1.55652600
C	1.19491600	-0.72909800	-1.06621800

C	2.02294900	-3.17516200	-2.04893400
H	4.01670400	-2.53742000	-1.55640900
C	0.23685600	-1.66102000	-1.48246600
C	0.65011500	-2.89508200	-1.98334100
H	2.35691200	-4.12298400	-2.46472400
H	-0.06186200	-3.64149700	-2.33087200
C	2.44424600	1.04963100	1.01199600
C	1.05783200	1.09730400	0.71385700
C	2.87766900	1.58683400	2.23455600
C	0.15064400	1.63622800	1.64094900
C	1.97471700	2.13049200	3.14931100
C	0.60919400	2.14315400	2.85346400
H	-0.90987000	1.65352600	1.42481200
H	2.33256900	2.52757000	4.09569700
H	-0.10713800	2.54113000	3.56610900
H	3.93564700	1.55450100	2.48535900
Si	3.66555700	0.24658300	-0.18355000
C	0.58299400	0.54805600	-0.58047200
C	-0.36733000	1.13353900	-1.40771100
Pd	-1.51388900	-0.92407200	-0.91118700
C	5.00147800	-0.65326400	0.79800200
C	4.64378900	-1.84888700	1.45366400
C	6.32060700	-0.19366500	0.96159800
C	5.56064400	-2.55294300	2.23452200
H	3.63365000	-2.23771300	1.34905400
C	7.24371400	-0.89414600	1.74186200
H	6.64390400	0.72191600	0.47684900
C	6.86563800	-2.07625400	2.38003600
H	5.25769500	-3.47252100	2.72868100
H	8.25712700	-0.51604100	1.84982400
H	7.58264800	-2.62278800	2.98715600
C	4.33052400	1.52131400	-1.45837100
C	5.37917800	0.84951300	-2.36950400
C	3.15213800	2.00303500	-2.33383700
C	4.93821500	2.75182100	-0.75196300
H	6.25488000	0.49957900	-1.81236300
H	4.95462700	-0.01294000	-2.89881000
H	5.73185200	1.56074700	-3.13031400
H	2.37826600	2.50515800	-1.74248400
H	3.51247400	2.72633100	-3.07910700
H	2.67785200	1.17666800	-2.87490000
H	5.26246400	3.49186000	-1.49773400
H	4.20688900	3.23929600	-0.09644900
H	5.81381200	2.50335100	-0.14249700

S	-3.48356800	0.44303900	1.21377300
C	-5.21465500	-0.09048800	1.63703300
F	-6.11065000	0.54803200	0.87691800
F	-5.47962900	0.15201000	2.92357100
F	-5.34856000	-1.41955900	1.42015700
O	-3.42996900	0.01230500	-0.24506700
O	-3.45002300	1.89504900	1.41298900
O	-2.61392900	-0.38304400	2.07379000
N	-2.44129700	-2.86065700	-0.68084500
H	-1.83206400	-3.50475300	-1.18615200
C	-2.46997100	-3.29835000	0.74862500
C	-1.09388900	-3.25839400	1.40119200
H	-2.88627800	-4.31664400	0.77904100
H	-3.15334900	-2.63196300	1.27513600
H	-1.15003300	-3.72192800	2.39176000
H	-0.34660000	-3.79963800	0.80871400
H	-0.76194600	-2.22477000	1.53036500
C	-3.79440900	-2.91699000	-1.30131300
C	-3.75635100	-2.59039000	-2.78915100
H	-4.41646400	-2.20230800	-0.76094700
H	-4.20889600	-3.92337500	-1.14036600
H	-4.75662900	-2.70437600	-3.21974700
H	-3.42747500	-1.55923000	-2.95528600
H	-3.07708300	-3.26010600	-3.33180700
C	-1.03944100	2.44673200	-1.25985500
C	-2.36642000	2.59175400	-1.69371600
C	-0.35937400	3.57851400	-0.77911700
C	-3.00810800	3.82563000	-1.61662600
H	-2.90994600	1.72000800	-2.04142700
C	-0.99865800	4.81472700	-0.71621600
H	0.67099800	3.49129500	-0.45247200
C	-2.32752100	4.94160500	-1.12742300
H	-4.04514300	3.91082700	-1.92842100
H	-0.45712400	5.67967800	-0.34264800
H	-2.82860600	5.90379800	-1.06544600
H	-0.43826600	0.71032400	-2.41244600

TS27

C	-2.62130900	-1.18438800	0.04714300
C	-2.88061600	-2.52279500	-0.21431300
C	-1.27784400	-0.69906600	-0.07597300
C	-1.85534000	-3.38680700	-0.63957300
H	-3.89635700	-2.90262600	-0.13691700
C	-0.21903100	-1.60159700	-0.42637900

C	-0.55296200	-2.92107700	-0.77284000
H	-2.08550600	-4.42598000	-0.86485600
H	0.21804900	-3.59870700	-1.11951800
C	-3.21346500	1.65594800	0.16098900
C	-1.80099800	1.82893400	0.01850600
C	-4.05113000	2.77827400	0.16488000
C	-1.31064900	3.15995500	-0.01284100
C	-3.54451300	4.07419400	0.07262100
C	-2.16171800	4.25677100	0.01412300
H	-0.24966200	3.34659900	-0.06527600
H	-4.21621500	4.92839200	0.06506500
H	-1.73968300	5.25697100	-0.02003100
H	-5.12622700	2.63454800	0.24788900
Si	-3.96224500	-0.00636300	0.57796100
C	-0.87046700	0.68264500	-0.01593500
C	0.59694200	0.85155100	0.01131300
C	1.28458300	1.91270500	-0.76058500
C	2.32662100	2.66964900	-0.19760800
C	3.00085500	3.62113000	-0.96040200
H	2.61999600	2.48357200	0.82976700
C	1.62356800	3.07821000	-2.87169700
C	2.64963100	3.83574500	-2.29547000
H	3.81575600	4.18229800	-0.51282600
H	1.35449900	3.22781200	-3.91418400
H	3.18014200	4.57587900	-2.88844600
Pd	1.61922600	-0.92525000	-0.43048400
H	0.94387700	0.74891200	1.05489800
C	-5.53779100	-0.31910900	-0.40487700
C	-5.41649600	-0.70532400	-1.75497500
C	-6.83618100	-0.15193400	0.11018800
C	-6.54046700	-0.91245400	-2.55495300
H	-4.42902100	-0.85434100	-2.18532900
C	-7.96520500	-0.35880600	-0.68573300
H	-6.97953000	0.13847800	1.14598900
C	-7.81949300	-0.73914800	-2.02067900
H	-6.41891300	-1.21091800	-3.59297800
H	-8.95708900	-0.22508400	-0.26187600
H	-8.69701900	-0.90160100	-2.64093000
C	-4.15905400	-0.12964500	2.49230700
C	-4.81849400	-1.47852700	2.84815600
C	-2.74946000	-0.07399800	3.12445800
C	-4.98978900	1.03621900	3.06788600
H	-5.83241100	-1.56528900	2.44165500
H	-4.23166600	-2.32502700	2.47080200

H	-4.88690000	-1.58804500	3.93979800
H	-2.22603300	0.85737000	2.87657700
H	-2.83120000	-0.12288900	4.21917900
H	-2.11936500	-0.90977500	2.80205200
H	-5.04672800	0.94543200	4.16190700
H	-4.53574800	2.00722000	2.84102900
H	-6.01915600	1.05332300	2.69368300
S	4.25321200	-0.10156000	1.12172200
C	5.69504200	1.06588900	0.97195400
F	6.41917200	1.03657600	2.09669500
F	5.26531500	2.32310600	0.77425000
F	6.47652100	0.71416900	-0.05664300
O	4.85401400	-1.41943000	1.41417200
O	3.37795700	0.49250800	2.14797200
O	3.67851100	-0.03188500	-0.27905000
C	0.95412600	2.12150700	-2.11540900
H	0.16681300	1.52091800	-2.56460500
N	2.87877100	-2.80056300	-0.72310500
H	3.72422100	-2.36291500	-0.34697400
C	2.63333100	-4.00515800	0.10872100
C	2.31834600	-3.65567300	1.55936900
H	3.51884000	-4.65773100	0.05859300
H	1.80642400	-4.56559300	-0.34084900
H	2.22464100	-4.57384800	2.15042500
H	3.11378700	-3.04056200	1.98949000
H	1.37786900	-3.10011300	1.62816800
C	3.14085300	-3.14625700	-2.13925000
C	3.54076300	-1.92621400	-2.96500800
H	2.22690700	-3.59840800	-2.54333500
H	3.93066700	-3.91291400	-2.19103200
H	3.81013900	-2.23371400	-3.98141300
H	2.71672100	-1.20634300	-3.02770100
H	4.39326500	-1.40812600	-2.51503800

TS28

C	1.13177700	-2.30332400	-1.86088600
C	1.37399800	-1.13132900	-1.12706000
C	2.63574800	-0.91667300	-0.53189200
C	3.54147900	-2.02613600	-0.49270200
C	3.25995400	-3.21146200	-1.19711400
C	2.08107900	-3.32480800	-1.92271000
Si	3.21519400	0.77803600	0.13135300
H	0.17458200	-2.46132700	-2.34805700
H	3.97309900	-4.02882400	-1.16144800

H	1.86687600	-4.23179800	-2.48153400
C	2.15016600	2.10024900	-0.75133700
C	2.54924000	3.45076200	-0.71122800
C	1.03059000	1.75312800	-1.56053200
C	1.89147100	4.43071100	-1.45387800
H	3.40964900	3.74978000	-0.12104200
C	0.34451500	2.78361300	-2.26227200
H	1.32796500	0.89640700	-2.51443100
C	0.77923500	4.10007300	-2.23819900
H	2.24211300	5.45888200	-1.41891200
H	-0.51098500	2.51202900	-2.87853000
H	0.25715900	4.86825700	-2.80152500
C	4.74194700	-1.97350300	0.27276800
C	5.77934200	-1.94609800	0.90708600
C	7.01007100	-1.81374900	1.61201200
C	7.55668900	-2.89503700	2.32984300
C	7.69610900	-0.58158300	1.58715700
C	8.76177900	-2.74344500	3.01134100
H	7.02905500	-3.84388000	2.34649700
C	8.90021100	-0.44265600	2.27219100
H	7.27973200	0.24769700	1.02639300
C	9.43577100	-1.51892200	2.98570000
H	9.17686700	-3.58175600	3.56362800
H	9.42399300	0.50888800	2.24671100
H	10.37564600	-1.40517000	3.51844800
P	-1.90810100	1.66244700	0.30068900
P	-1.61708900	-1.75523100	-0.05352300
C	0.93556800	-5.49776300	0.99078200
C	-0.10614500	-5.62690200	0.07190000
C	-0.91050500	-4.52997000	-0.24545100
C	-0.68025300	-3.28704600	0.35969700
C	0.37305800	-3.16731600	1.28002100
C	1.17311300	-4.26164200	1.59716700
H	-1.69494000	-4.64916100	-0.98305100
H	0.58488700	-2.20768300	1.73235800
C	-1.84341100	6.30218500	0.25395600
C	-3.01173700	5.65009200	-0.14361800
C	-3.05698000	4.25489300	-0.19640500
C	-1.92146900	3.49713900	0.12880500
C	-0.75407500	4.16157900	0.53182700
C	-0.71594000	5.55242000	0.59698000
H	-3.98333900	3.76682900	-0.47997600
H	0.13381600	3.59146900	0.78389000
C	-2.28795400	1.57643000	4.92780500

C	-3.16479800	2.36156200	4.17317100
C	-3.07406100	2.37476000	2.78377500
C	-2.11489600	1.58409500	2.12982400
C	-1.24058800	0.80328600	2.89286300
C	-1.32323300	0.80008700	4.28577900
H	-3.75035900	2.99912100	2.20888800
H	-0.50082100	0.18855000	2.39588300
C	-4.23550900	-2.85499600	-3.72359900
C	-4.42482800	-3.52029000	-2.50928500
C	-3.64725200	-3.19114200	-1.40060700
C	-2.65910900	-2.19727200	-1.49819500
C	-2.49421600	-1.52021800	-2.71238900
C	-3.27261300	-1.84990100	-3.82176300
H	-3.82496600	-3.68888800	-0.45180700
H	-1.78329700	-0.70402200	-2.76844600
H	-7.33086700	1.51236600	3.46888600
C	-3.90644400	-0.66937200	1.24136400
C	-2.83814800	-1.56685300	1.32873400
C	-2.60068900	-2.25920600	2.54801700
H	-1.79155400	-2.97611100	2.61102100
C	-3.37912500	-2.03205800	3.65595000
H	-3.17710400	-2.56647200	4.58070000
C	-4.44025100	-1.09555000	3.62109500
C	-4.72392900	-0.41994500	2.39102100
H	-6.01533700	1.04575300	1.44759500
C	-5.79003800	0.52267400	2.37006100
C	-6.52439500	0.78550300	3.50448600
H	-6.82349100	0.33730600	5.60741000
C	-6.23654200	0.11865900	4.72007300
H	-4.98770200	-1.32206000	5.70105800
C	-5.21704900	-0.80411900	4.77339500
H	-8.39882300	-1.63654200	-2.96276000
C	-4.75167700	1.16343800	-2.58125500
H	-4.93255500	1.58211500	-3.56816200
C	-3.70049500	1.61162100	-1.82343400
H	-3.05149100	2.38833300	-2.21644200
C	-3.44964400	1.08154200	-0.52259700
C	-4.23100700	0.03532300	-0.04172200
C	-5.35897800	-0.42317600	-0.80864500
C	-5.62082900	0.15410000	-2.09255700
H	-6.90721300	0.14070800	-3.83002600
C	-6.72477400	-0.30633900	-2.85602500
C	-7.55235700	-1.29547400	-2.37382600
H	-7.95290100	-2.65018000	-0.72922900

C	-7.29857800	-1.86948400	-1.10660900
H	-6.04327800	-1.90793600	0.61726500
C	-6.22712900	-1.45132800	-0.34787200
H	1.56428400	-6.35141600	1.22708700
H	-1.81368200	7.38703000	0.30154900
H	-2.35836400	1.57277100	6.01173000
H	-4.85079700	-3.10738100	-4.58206100
H	-0.29371000	-6.58302500	-0.40871600
H	1.99095800	-4.14232200	2.30175900
H	-3.89676200	6.22466700	-0.40238700
H	0.19865200	6.04931700	0.90779900
H	-3.14118600	-1.30673500	-4.75358500
H	-5.19415500	-4.28100900	-2.41934500
H	-0.63652600	0.18713200	4.86266500
H	-3.92274300	2.96150100	4.66770100
Pd	-0.16163100	0.16118700	-0.63545900
C	4.97017900	1.18013300	-0.47924200
C	5.59080100	0.45145400	-1.51041200
C	5.67437300	2.28946500	0.02849200
C	6.85289600	0.79516100	-1.99605200
H	5.08905400	-0.41089700	-1.93792300
C	6.93585100	2.64593200	-0.45396700
H	5.24528000	2.89174100	0.82411300
C	7.53309000	1.89366600	-1.46673500
H	7.30864000	0.19997800	-2.78291700
H	7.45233600	3.50475400	-0.03357200
H	8.51845000	2.15983500	-1.83894900
C	3.04734500	0.90211200	2.07200100
C	2.30191500	-0.35823800	2.55389300
C	4.40573800	0.94765300	2.80265800
C	2.21640500	2.13948200	2.47232600
H	1.34007700	-0.46028800	2.04532200
H	2.87885800	-1.26945500	2.36293000
H	2.10795000	-0.29560200	3.63423600
H	4.94998700	1.87877100	2.62473500
H	4.23639800	0.87737000	3.88641200
H	5.05843200	0.11974800	2.51442000
H	2.10525600	2.18019200	3.56480500
H	2.68656400	3.07775700	2.15542100
H	1.20817200	2.10972100	2.04603400
N	1.76947100	0.36531300	-3.79082100
C	0.58416600	-0.24198100	-4.42938500
C	2.42232600	1.41231200	-4.60730800
H	2.43155800	-0.36336000	-3.52129000

H	0.03366200	0.56676200	-4.92298000
H	-0.04869000	-0.62301700	-3.62821700
H	1.75349500	2.28100100	-4.58748500
H	2.49782700	1.07847500	-5.65107200
C	3.79487000	1.78948800	-4.06733800
H	4.48209700	0.93740100	-4.09135600
H	4.22965600	2.58510300	-4.68041200
H	3.73654900	2.14646300	-3.03699000
C	0.91469700	-1.36611800	-5.40950100
H	1.43434100	-2.17944000	-4.89000300
H	-0.00563700	-1.77575300	-5.83966200
H	1.54769400	-1.01917400	-6.23307100

INT36

C	1.13127600	-0.14452800	-2.91038900
C	1.37899200	0.12198900	-1.54965700
C	2.64704000	-0.21175800	-1.01058200
C	3.50904700	-1.05078300	-1.78209000
C	3.21916900	-1.32828400	-3.13238200
C	2.06009500	-0.82206000	-3.70782900
Si	3.21260000	0.50341800	0.66597200
H	0.17297900	0.11682500	-3.35185600
H	3.90136300	-1.94825400	-3.70554200
H	1.83665200	-1.02348300	-4.75249800
C	2.23203600	2.13976100	0.76739000
C	2.85501500	3.34515500	1.16484900
C	0.89687900	2.19565600	0.30114800
C	2.20979900	4.57899900	1.05999800
H	3.87506400	3.32692500	1.53672100
C	0.26347900	3.45087000	0.18517600
H	1.96818100	2.84197900	-1.45818500
C	0.91145000	4.63440000	0.54710900
H	2.71941500	5.48791400	1.36884700
H	-0.75940700	3.50775600	-0.18010300
H	0.39649500	5.58776700	0.45311100
C	4.65558600	-1.65427000	-1.18870400
C	5.62915700	-2.15418400	-0.65780600
C	6.79305300	-2.64889100	-0.00176700
C	7.28925800	-3.93767100	-0.27836400
C	7.46443500	-1.83606100	0.93578900
C	8.42870800	-4.40329400	0.37312900
H	6.77351100	-4.56210500	-1.00161500
C	8.60289400	-2.31276900	1.58021800
H	7.08955500	-0.83990600	1.14267300

C	9.08769400	-3.59438600	1.30358300
H	8.80404900	-5.39916800	0.15523100
H	9.11482700	-1.68003700	2.29992200
H	9.97609200	-3.96149500	1.80965400
P	-1.90535500	0.92053500	1.47240800
P	-1.64370300	-1.19000700	-1.28458500
C	0.91952600	-4.47694100	-3.34618200
C	-0.14791700	-3.91709300	-4.04900500
C	-0.95863300	-2.94913500	-3.45145800
C	-0.70878900	-2.52990600	-2.13752400
C	0.37206900	-3.09567900	-1.44196100
C	1.17736900	-4.06380600	-2.03684900
H	-1.76712400	-2.51214800	-4.02565000
H	0.60149500	-2.75959700	-0.43925000
C	-1.72034100	4.48450900	4.45494400
C	-2.95274500	4.11559700	3.91170300
C	-3.02805900	3.07549000	2.98429900
C	-1.86694600	2.39569000	2.57841500
C	-0.63520800	2.76877900	3.13842700
C	-0.56381800	3.80453400	4.06947900
H	-3.99581100	2.79847000	2.57824500
H	0.27350500	2.26017100	2.84241400
C	-2.43745400	-2.43532000	4.63548200
C	-3.24762000	-1.29802900	4.69061400
C	-3.10370900	-0.28804900	3.74210200
C	-2.15511800	-0.41280400	2.71476800
C	-1.34450400	-1.55287800	2.67007800
C	-1.48258100	-2.55910400	3.62575100
H	-3.73308000	0.59354400	3.80219200
H	-0.61492800	-1.65945700	1.87858700
C	-4.18807400	0.83659100	-4.60033600
C	-4.43539300	-0.49521800	-4.25792500
C	-3.68360800	-1.11396000	-3.26028700
C	-2.66433100	-0.41039400	-2.59879200
C	-2.43678200	0.93039100	-2.93801400
C	-3.19047700	1.55050600	-3.93449400
H	-3.90695500	-2.13792100	-2.97518000
H	-1.69345800	1.49296600	-2.38207100
H	-7.30522300	-1.48825300	3.56765400
C	-3.90803000	-1.37735900	0.42067900
C	-2.86648200	-2.06880800	-0.20435800
C	-2.63541100	-3.43352500	0.12171700
H	-1.84098100	-3.97675700	-0.37617700
C	-3.39983100	-4.07741700	1.06389600

H	-3.20430200	-5.11975600	1.30291400
C	-4.44338800	-3.40140500	1.74167600
C	-4.71631800	-2.03739800	1.40230200
H	-5.98866300	-0.33698500	1.84162200
C	-5.77129400	-1.37067800	2.08623500
C	-6.50608200	-2.01616100	3.05500900
H	-6.81352000	-3.85848300	4.16137000
C	-6.22722500	-3.36254200	3.39320600
H	-4.99589900	-5.07285900	2.99808500
C	-5.21756300	-4.03864300	2.74732500
H	-8.38822100	0.97871900	-3.19192000
C	-4.76866200	2.65670400	-0.87395000
H	-4.95806100	3.66104900	-1.24495600
C	-3.72267700	2.42332100	-0.01873100
H	-3.09491200	3.25239600	0.29092000
C	-3.45525900	1.11563600	0.48604300
C	-4.22990500	0.04160700	0.05475800
C	-5.35787700	0.27607500	-0.80785700
C	-5.62505800	1.60130300	-1.27879400
H	-6.91052700	2.84154900	-2.49662600
C	-6.72475900	1.82924700	-2.14635000
C	-7.54490700	0.79324600	-2.53297000
H	-7.93778700	-1.33313200	-2.37389200
C	-7.28821900	-0.51768600	-2.06851400
H	-6.03514600	-1.78321600	-0.89542600
C	-6.22068600	-0.77137400	-1.23517600
H	1.55199200	-5.22379000	-3.81767700
H	-1.66351800	5.29460200	5.17655800
H	-2.55239500	-3.22032200	5.37734400
H	-4.78449800	1.31903800	-5.36908300
H	-0.35189800	-4.22901700	-5.06966300
H	2.01629200	-4.47722900	-1.48452500
H	-3.85954100	4.63308100	4.21228300
H	0.40010100	4.08234800	4.48603200
H	-3.01612900	2.59658700	-4.17339000
H	-5.23085200	-1.04525600	-4.75118400
H	-0.84902200	-3.43993800	3.57305400
H	-3.99727400	-1.19998900	5.47004000
Pd	-0.18331200	0.54466400	-0.23313300
C	5.02654000	1.07702700	0.62606100
C	5.78668600	1.17338500	-0.55334300
C	5.64027600	1.52133600	1.81483100
C	7.09592500	1.65812400	-0.54782300
H	5.36074800	0.84774600	-1.49624600

C	6.94929200	2.00938100	1.83246000
H	5.09005800	1.49559700	2.75191900
C	7.68573000	2.07213200	0.64802600
H	7.65980000	1.70019300	-1.47608400
H	7.39212400	2.33605900	2.76958700
H	8.70785000	2.44037500	0.65679500
C	2.88060300	-0.73308400	2.13278400
C	2.11478200	-1.94403900	1.56443700
C	4.17220600	-1.27212300	2.78291600
C	2.00838900	-0.05450700	3.20822400
H	1.20361200	-1.62338300	1.05283200
H	2.72268600	-2.50425600	0.84512700
H	1.82703700	-2.62772200	2.37597500
H	4.72445200	-0.50433500	3.33071700
H	3.91222400	-2.05807600	3.50603200
H	4.85229300	-1.71146700	2.04715200
H	1.81795700	-0.74817500	4.03910300
H	2.48606300	0.84095100	3.62529700
H	1.03545300	0.24189100	2.80477200
N	2.09711100	3.01501000	-2.47311400
C	0.72791600	3.20556700	-3.07368600
C	3.05518900	4.15725700	-2.67793300
H	2.48173700	2.12742500	-2.82320500
H	0.39460500	4.20092300	-2.77110300
H	0.09932300	2.46828000	-2.57629100
H	2.62965200	4.99861900	-2.12538600
H	3.05232900	4.39635100	-3.74381000
C	4.44780000	3.80465100	-2.18115800
H	4.86965600	2.96078700	-2.73637900
H	5.11042600	4.66375900	-2.32176800
H	4.43996100	3.54837600	-1.11934300
C	0.72458300	3.01170500	-4.58257400
H	1.11196100	2.02147600	-4.84476000
H	-0.30710400	3.06820700	-4.94309500
H	1.30546200	3.77417100	-5.11039600

TS29

C	-1.12969800	-1.83269100	3.44599600
C	-1.68330800	-1.77861200	2.15817700
C	-2.63415100	-0.80399900	1.78370200
C	-2.81159800	0.28088000	2.68979400
C	-2.25561300	0.22428900	3.98357100
C	-1.46984700	-0.85431500	4.37858800
Si	-3.93163100	-1.20731600	0.43526400

C	-3.38571200	-2.86603300	-0.29619700
C	-2.22786200	-3.52098200	0.14827800
C	-4.16056400	-3.53558000	-1.26207100
C	-3.80754300	-4.80607000	-1.71477200
C	-2.68033200	-5.45544900	-1.20378800
C	-1.88160000	-4.81347200	-0.25917600
H	-0.41675100	-2.60801000	3.70486100
H	-2.42496700	1.05431500	4.66171000
H	-1.05307700	-0.88577900	5.38054800
H	-1.93139400	-2.96595900	1.46839800
H	-5.03426200	-3.04837900	-1.68559800
H	-4.40840700	-5.29070800	-2.47954300
H	-2.39679000	-6.43621600	-1.57259000
H	-0.96689600	-5.28105300	0.08950500
O	-0.18248900	-4.54036100	-3.18489100
S	0.46784400	-3.32399300	-2.68620600
O	1.70987100	-2.88074500	-3.33847000
O	0.58170700	-3.28909300	-1.17104400
C	-0.75137500	-1.94713900	-3.06269800
F	-0.56337700	-1.49521100	-4.30642700
F	-0.57368800	-0.90968900	-2.21049700
F	-2.01365000	-2.36785300	-2.94038900
C	-4.06215500	0.05083800	-0.95149200
C	-5.24842000	0.20266200	-1.69489400
C	-2.93528400	0.79023900	-1.35449200
C	-5.30833800	1.05576900	-2.79941500
H	-6.14292300	-0.34457000	-1.41463900
C	-2.98781700	1.63800300	-2.46183000
H	-2.00100100	0.70161700	-0.80749900
C	-4.17435200	1.77290900	-3.18533400
H	-6.23718000	1.15675200	-3.35523500
H	-2.10767900	2.19677700	-2.75629200
H	-4.21169500	2.43727800	-4.04465300
C	-5.60071200	-1.51763000	1.39459700
C	-6.31887200	-0.19966500	1.75566100
C	-6.58379200	-2.39574400	0.58476500
C	-5.27399100	-2.28799500	2.69633300
H	-5.73047300	0.41949900	2.43601000
H	-6.54134100	0.40657200	0.87056600
H	-7.27284600	-0.42450100	2.25445400
H	-6.17976400	-3.39301300	0.38912600
H	-7.51019300	-2.52426900	1.16246800
H	-6.86767300	-1.95281800	-0.37636700
H	-6.20621600	-2.55039000	3.21647700

H	-4.73801400	-3.22354500	2.49167700
H	-4.66609500	-1.69602100	3.38785000
C	-3.45747200	1.47209300	2.25742700
C	-3.90281600	2.50899600	1.80406200
C	-4.41477100	3.68665200	1.19337900
C	-4.97824100	3.61149600	-0.09650200
C	-4.31870300	4.93886200	1.83298700
C	-5.42239300	4.76774600	-0.73101700
H	-5.04143300	2.65183500	-0.59331800
C	-4.76515000	6.08971700	1.18714000
H	-3.88264500	4.99688600	2.82582300
C	-5.31525400	6.00889200	-0.09657100
H	-5.84141700	4.69725000	-1.73074900
H	-4.68120700	7.05239800	1.68388900
H	-5.65755400	6.90981200	-0.59835500
P	1.61311600	-1.26888200	1.25404900
P	1.17002000	1.81790400	-1.24825700
C	-1.79776500	5.25574200	-2.30089800
C	-0.89071100	4.82184000	-3.26820600
C	0.05182900	3.83507200	-2.96287000
C	0.09012700	3.25222000	-1.68607000
C	-0.85160100	3.68251700	-0.72988300
C	-1.77047100	4.68741000	-1.02483200
H	0.75212400	3.51221700	-3.72585700
H	-0.87237600	3.22125100	0.25474100
C	3.81973700	-4.59876500	3.66346900
C	4.49184400	-3.41998100	3.32973700
C	3.84068400	-2.42371400	2.60361600
C	2.50161900	-2.58205100	2.21031600
C	1.84386500	-3.77725200	2.53636800
C	2.49588800	-4.77754800	3.26054800
H	4.37597000	-1.51997100	2.33543600
H	0.82287800	-3.93749600	2.19931900
C	0.79596900	2.19576100	4.23285000
C	1.73508400	1.22128800	4.57348300
C	2.00779600	0.17101100	3.69639000
C	1.34035700	0.08556200	2.46542700
C	0.37252600	1.04941700	2.14872700
C	0.11439700	2.10692300	3.01793200
H	2.74638700	-0.57151000	3.97370000
H	-0.18189200	0.96719500	1.21994300
C	3.94466900	1.07843800	-4.89065200
C	3.99165200	2.32248500	-4.25113800
C	3.15911200	2.58264900	-3.16425200

C	2.26227500	1.60105300	-2.71007500
C	2.22508000	0.35885000	-3.35652100
C	3.06193600	0.09651500	-4.44161400
H	3.21481500	3.54082800	-2.65391100
H	1.57934500	-0.42642200	-2.99345500
H	6.34985100	1.00787500	4.00905500
C	3.27010600	1.68264700	0.61694400
C	2.30316300	2.51852000	0.05338200
C	2.08364500	3.80099600	0.62804900
H	1.36600700	4.47256000	0.17160200
C	2.74355100	4.20181300	1.76417400
H	2.54339100	5.17973400	2.19653300
C	3.68411200	3.35193000	2.39537400
C	3.98687300	2.09288500	1.78434600
H	5.26726600	0.35223600	1.89701800
C	4.98386700	1.27668500	2.38762000
C	5.59673800	1.65155100	3.56231900
H	5.74664300	3.16082500	5.11723700
C	5.25980300	2.87655700	4.18828400
H	4.08252800	4.66494100	4.06631200
C	4.33309900	3.71195000	3.60588800
H	7.92677600	0.56540200	-3.29529700
C	4.36702300	-1.85014900	-1.63117300
H	4.58835200	-2.69896100	-2.27133800
C	3.31434000	-1.91641600	-0.75905400
H	2.71989600	-2.81973400	-0.71621900
C	2.95462200	-0.80456000	0.06027200
C	3.64722200	0.39998100	-0.06405600
C	4.79487300	0.46109400	-0.93674600
C	5.16097100	-0.68066500	-1.71803800
H	6.54659800	-1.49044600	-3.16297900
C	6.29473000	-0.61503700	-2.56954600
C	7.05775400	0.52758000	-2.64391400
H	7.30020300	2.56505400	-1.94027600
C	6.70233900	1.65990500	-1.87497100
H	5.33169300	2.51556000	-0.48660100
C	5.59690600	1.63184400	-1.05399600
H	-2.53088600	6.02238700	-2.53653900
H	4.33005900	-5.37789700	4.22307600
H	0.59417800	3.01950900	4.91239200
H	4.60824700	0.87538200	-5.72721400
H	-0.90870200	5.25302300	-4.26609200
H	-2.47837100	5.01135000	-0.27030200
H	5.52768500	-3.27928400	3.62651600

H	1.97120300	-5.69906200	3.49766900
H	3.02440400	-0.88516400	-4.90406500
H	4.69306100	3.08137400	-4.58812400
H	-0.63829800	2.84428100	2.75335100
H	2.27308900	1.28569100	5.51486100
Pd	-0.46460100	-2.34166200	0.50442300

INT37

C	-2.41567300	-3.14789600	2.63843000
C	-3.00802900	-2.59732500	1.47826900
C	-3.19061900	-1.18880400	1.31399000
C	-2.72104100	-0.35786900	2.38409000
C	-2.13833700	-0.92941400	3.52527300
C	-1.98359700	-2.31306000	3.65401500
Si	-4.35804200	-0.58167400	-0.09665300
C	-4.09422300	-1.91820100	-1.39601400
C	-2.81949600	-2.50041500	-1.44851200
C	-5.03720600	-2.35006600	-2.34907400
C	-4.73032000	-3.35555400	-3.26618600
C	-3.46928900	-3.95225100	-3.25147800
C	-2.49846400	-3.51996900	-2.34093500
H	-2.31176300	-4.22436800	2.72491500
H	-1.77548000	-0.27214200	4.30800600
H	-1.51513800	-2.71953700	4.54478200
H	-3.50247600	-3.28026400	0.79482000
H	-6.01993500	-1.89136200	-2.38477300
H	-5.47530500	-3.67215700	-3.99157800
H	-3.22082900	-4.73465000	-3.96412000
H	-1.49732600	-3.93366100	-2.38847900
O	0.18529700	-2.81712300	-3.47276900
S	0.28392500	-1.38019100	-3.17318300
O	1.52866000	-0.69764300	-3.53923600
O	-0.18133800	-1.01602000	-1.76902600
C	-0.99753800	-0.52487600	-4.22594700
F	-0.81467800	-0.85331500	-5.51274100
F	-0.86764900	0.80302100	-4.09797300
F	-2.24210900	-0.86701800	-3.87084700
C	-3.83145400	1.05319000	-0.87444800
C	-4.77602400	1.93984100	-1.42607600
C	-2.46978400	1.34770300	-1.07623400
C	-4.37972500	3.07391400	-2.14124300
H	-5.83842100	1.75506900	-1.30464600
C	-2.06831800	2.47614300	-1.78980800
H	-1.70047200	0.68453800	-0.69296700

C	-3.02272200	3.34607100	-2.32044900
H	-5.13259000	3.74058900	-2.55508500
H	-1.01314700	2.67150700	-1.93666300
H	-2.70370100	4.22727600	-2.87012100
C	-6.12360300	-0.53830700	0.69741400
C	-6.25770500	0.71744600	1.58864400
C	-7.26672800	-0.54378600	-0.34355900
C	-6.30523200	-1.79036800	1.58668800
H	-5.49700300	0.74564800	2.37514200
H	-6.16724200	1.64631700	1.01641500
H	-7.24221900	0.72094000	2.07874500
H	-7.33189700	-1.50410600	-0.86396500
H	-8.22817000	-0.39029100	0.16747200
H	-7.17382800	0.24174100	-1.10031100
H	-7.32401500	-1.80894400	1.99931600
H	-6.16284200	-2.71954800	1.02040100
H	-5.60905500	-1.80049700	2.43234200
C	-2.83419800	1.05717100	2.33426700
C	-2.90571200	2.26984700	2.34056500
C	-3.00789300	3.68624900	2.29962300
C	-3.61824700	4.31587200	1.19689700
C	-2.49116600	4.47511200	3.34766400
C	-3.71045900	5.70407000	1.15165000
H	-3.99540100	3.70929700	0.38310100
C	-2.58503500	5.86389200	3.28926500
H	-2.02045200	3.98724800	4.19627000
C	-3.19598500	6.48236300	2.19316200
H	-4.17495800	6.17939200	0.29228100
H	-2.18095800	6.46572400	4.09860700
H	-3.26561100	7.56579000	2.15043800
P	0.84116400	-1.90438800	1.18152300
P	2.12711100	1.83926700	-0.97391400
C	-0.27766000	5.83513100	-0.83148500
C	0.53294100	5.53758500	-1.92844600
C	1.31663600	4.38128100	-1.93531800
C	1.29134700	3.48643500	-0.85099200
C	0.44675200	3.78903000	0.23255300
C	-0.31108200	4.95795000	0.25416700
H	1.95171100	4.17322000	-2.79092800
H	0.38322300	3.10821500	1.07466100
C	1.69872500	-6.24913300	2.64723600
C	2.59289500	-5.22568400	2.97223600
C	2.34359500	-3.91734000	2.55920500
C	1.18136600	-3.60241200	1.83475900

C	0.30263400	-4.64309800	1.49883100
C	0.55726900	-5.95638300	1.90041200
H	3.05966600	-3.13994400	2.79762600
H	-0.57979400	-4.42979200	0.90310200
C	0.78285000	1.10345300	4.71312800
C	1.20490000	-0.20377700	4.95884500
C	1.26980600	-1.13044500	3.91671400
C	0.91591900	-0.75726700	2.61201700
C	0.46488900	0.55196700	2.38147800
C	0.41089800	1.47866200	3.42030600
H	1.58791400	-2.14206200	4.13334900
H	0.13398800	0.83917200	1.38778200
C	5.75944200	2.82513500	-3.71827800
C	5.63181900	3.48800900	-2.49280500
C	4.54789900	3.21171100	-1.66177000
C	3.57980100	2.26735500	-2.04293400
C	3.71146500	1.60944000	-3.27312800
C	4.79935100	1.89040200	-4.10499000
H	4.45679900	3.72562100	-0.70865300
H	2.97958000	0.86338700	-3.56240000
H	5.54116700	-2.21644900	4.23319300
C	3.40902700	0.39297400	1.05560200
C	2.96119300	1.66225000	0.68506500
C	3.12683900	2.74477400	1.59369500
H	2.79647000	3.73562700	1.30216300
C	3.65857000	2.55693100	2.84629600
H	3.74469500	3.39287600	3.53703300
C	4.11408500	1.27902800	3.25542700
C	4.03900800	0.19396600	2.32450600
H	4.60806300	-1.86262000	1.97714700
C	4.59397800	-1.05883200	2.70510800
C	5.12145500	-1.25075800	3.96339100
H	5.54668500	-0.35597400	5.89620300
C	5.13540500	-0.19207300	4.90382400
H	4.68623800	1.87548600	5.25348300
C	4.65418900	1.04817700	4.54823100
H	7.28367900	-1.14140300	-3.50982900
C	3.29630500	-2.79194300	-1.87997800
H	3.23149900	-3.53473500	-2.66943000
C	2.31683000	-2.71984400	-0.92860700
H	1.49096800	-3.42229000	-0.97757500
C	2.32155300	-1.71074900	0.08045600
C	3.33709700	-0.75896000	0.09517100
C	4.41830900	-0.87086300	-0.85247600

C	4.38291600	-1.88362300	-1.86198700
H	5.37241400	-2.71894900	-3.59074500
C	5.42894800	-1.95632800	-2.81804900
C	6.49014800	-1.08134400	-2.76986800
H	7.38111900	0.59673400	-1.72263100
C	6.54739200	-0.09817500	-1.75477700
H	5.58681300	0.78032800	-0.06798900
C	5.53913600	0.00579500	-0.82357600
H	-0.88251700	6.73793300	-0.82012800
H	1.89868800	-7.26952700	2.96269600
H	0.73981100	1.82538100	5.52421900
H	6.60729600	3.03735000	-4.36509300
H	0.56725900	6.21127900	-2.78119400
H	-0.93337000	5.17789300	1.11321200
H	3.49377500	-5.44757900	3.53815200
H	-0.13364100	-6.74791600	1.62262100
H	4.89832300	1.36503300	-5.05106100
H	6.37745800	4.21795100	-2.18667500
H	0.05872500	2.48636100	3.22365500
H	1.49314800	-0.50598400	5.96170700
Pd	-1.31524100	-2.00029500	-0.19066600

TS30

C	2.12817200	0.79741600	-0.60612700
C	2.58296900	-0.53588600	-1.00165600
C	4.25814000	2.22121600	-0.65451600
C	3.71157500	-1.18681700	-0.41337700
C	5.34864400	1.35917200	-0.40175000
C	1.81334200	-1.23652500	-1.95039900
H	1.00101400	-0.70873700	-2.43525800
C	2.05145300	-2.56803300	-2.26335500
H	1.42218000	-3.07326300	-2.99026100
C	3.89887800	-2.54926400	-0.72029500
C	3.07988000	-3.24604800	-1.60792100
H	4.73599400	-3.07695000	-0.27352700
H	3.26025400	-4.29952000	-1.80280400
C	6.63273400	1.77598600	-0.80135500
C	6.84966600	2.98881500	-1.45126900
C	5.76380500	3.81874900	-1.73189800
H	5.90717400	4.75737900	-2.25983200
H	7.85499400	3.27845100	-1.74406300
H	7.48245400	1.12921700	-0.60650900
C	2.83944800	1.92763700	-0.31452100
C	1.99323200	3.04644100	0.15630800

C	2.46373400	4.15604200	0.86580800
C	-0.23822600	4.00328300	0.15469900
H	3.51488400	4.21202200	1.13070800
H	-1.28091900	3.99267100	-0.12538600
C	0.24994100	5.12244600	0.84301900
C	1.59059000	5.18787400	1.21626000
H	1.96542700	6.04908100	1.76166600
H	-0.42673400	5.94008500	1.07451300
Si	5.16909900	-0.31020400	0.45493300
C	5.02358400	-0.03708200	2.35008800
C	6.17980200	0.85676200	2.85193900
C	3.69753800	0.69226800	2.65589700
C	5.04705000	-1.39194700	3.08770300
H	7.16576900	0.41187700	2.68469300
H	6.17379100	1.83610800	2.35992100
H	6.07600500	1.02657900	3.93311600
H	2.83445700	0.16782000	2.24050500
H	3.55667700	0.77523700	3.74390400
H	3.69364900	1.70978300	2.25033700
H	4.82163300	-1.24812600	4.15482200
H	4.30672200	-2.08629900	2.68279400
H	6.02266600	-1.88182300	3.02779500
C	6.71267700	-1.29842000	-0.04039600
C	6.88734900	-1.58669800	-1.41139200
C	7.73818900	-1.70022600	0.83280900
C	8.01937300	-2.24918900	-1.88282500
H	6.12275400	-1.28890200	-2.12499600
C	8.87617000	-2.36676900	0.36847900
H	7.66745700	-1.49373400	1.89450100
C	9.01947800	-2.64474500	-0.99030400
H	8.12285500	-2.45592600	-2.94478600
H	9.64945500	-2.66554200	1.07118900
H	9.90365000	-3.16180900	-1.35310800
C	4.48727800	3.44071400	-1.33117800
H	3.64975300	4.09214900	-1.55827800
C	0.62028200	2.95306800	-0.16607600
H	0.98431100	1.77187100	-1.12979000
Pd	-0.15332500	0.92713700	-0.22175800
P	-0.85761600	-1.33796100	0.31390300
P	-2.48763200	1.53909700	-0.56188200
C	-2.56594900	4.83764000	-3.83181000
C	-3.46553400	4.91463900	-2.76758100
C	-3.46519100	3.93510800	-1.77201800
C	-2.55506700	2.87006300	-1.83099100

C	-1.64586900	2.80540000	-2.90069800
C	-1.65675800	3.77824400	-3.89845900
H	-4.15997800	4.01855300	-0.94378100
H	-0.92312400	1.99539200	-2.94940200
C	2.14788600	-3.63452100	2.98941300
C	1.79085800	-2.31214200	3.26589600
C	0.95123900	-1.62164200	2.39677300
C	0.40264300	-2.26243600	1.27251400
C	0.80566500	-3.57068700	0.97543400
C	1.67967600	-4.24758300	1.82831700
H	0.70858800	-0.58189500	2.60023800
H	0.45637200	-4.06353500	0.07737500
C	-2.20219300	-4.11480900	-3.14545400
C	-1.76698000	-2.81628100	-3.42054100
C	-1.36110800	-1.98128800	-2.38184000
C	-1.37996700	-2.43454800	-1.05620700
C	-1.85023900	-3.72965400	-0.78438300
C	-2.24874600	-4.56705100	-1.82564700
H	-1.06318600	-0.96158400	-2.59790500
H	-1.92256500	-4.07857600	0.24127300
C	-4.59782300	3.02961300	3.27341500
C	-5.34746900	2.82555900	2.11265800
C	-4.72420800	2.38365900	0.94707700
C	-3.33864300	2.15654600	0.93047500
C	-2.59137500	2.36285500	2.10022500
C	-3.22079200	2.79718700	3.26623000
H	-5.31954800	2.18097000	0.06162300
H	-1.52179500	2.17599400	2.09932500
H	-6.03077000	-5.02558400	-0.44781500
C	-3.92684700	-0.89512400	-0.51438300
C	-3.56087800	0.21668400	-1.27326600
C	-3.91549200	0.28046200	-2.65038200
H	-3.64443300	1.14837400	-3.23825000
C	-4.60768500	-0.74298100	-3.24942900
H	-4.87378400	-0.67532900	-4.30121700
C	-4.98913800	-1.89347000	-2.51649400
C	-4.65571700	-1.96895900	-1.12586400
H	-4.80416700	-3.20615600	0.65053800
C	-5.05169100	-3.12872900	-0.40160700
C	-5.73705900	-4.15012200	-1.01977400
H	-6.59955100	-4.88665600	-2.87058600
C	-6.05936200	-4.07264900	-2.39600300
H	-5.93421300	-2.89546300	-4.18402000
C	-5.69064700	-2.96649400	-3.12709600

H	-7.64117200	-0.13576200	4.39643200
C	-3.17990000	-1.09935500	3.73249500
H	-2.99927200	-1.16010700	4.80272600
C	-2.15126500	-1.32638800	2.85266200
H	-1.18171800	-1.58587700	3.25295200
C	-2.34469900	-1.25010300	1.44450700
C	-3.62383600	-0.97793700	0.95061300
C	-4.71961600	-0.77212100	1.85958200
C	-4.48456800	-0.80569600	3.27058200
H	-5.35510200	-0.58950300	5.23822100
C	-5.55637600	-0.56404400	4.17039600
C	-6.82533300	-0.31315300	3.70180100
H	-8.07257700	-0.09719600	1.94077500
C	-7.06887300	-0.29183800	2.30785800
H	-6.25367300	-0.47635700	0.34951200
C	-6.04631300	-0.50973300	1.41202300
H	-2.56792100	5.60220900	-4.60313800
H	2.81196600	-4.16987500	3.66165000
H	-2.52306200	-4.76449400	-3.95412200
H	-5.08878300	3.35985200	4.18407200
H	-4.16902300	5.73994400	-2.70668200
H	-0.94922600	3.71570600	-4.72016900
H	2.19159600	-1.80801100	4.13919600
H	1.98657000	-5.26022300	1.58329400
H	-2.63662600	2.94547300	4.16969100
H	-6.42131000	2.98383100	2.12152100
H	-2.61671100	-5.56373500	-1.60260700
H	-1.75887300	-2.44669200	-4.44161700

INT38

C	2.23820500	0.39002700	-1.06451100
C	2.82379600	-0.95195500	-1.18605800
C	4.20348000	1.89795600	-1.29135300
C	3.97025100	-1.38873000	-0.46312300
C	5.31945400	1.27472300	-0.69157200
C	2.10734700	-1.88068900	-1.96662500
H	1.24549600	-1.53897100	-2.52834900
C	2.47357700	-3.21897400	-2.03815700
H	1.90012900	-3.90372500	-2.65734300
C	4.29464700	-2.75669400	-0.52886900
C	3.56522300	-3.66746100	-1.29414400
H	5.15753900	-3.11978500	0.02116300
H	3.85390900	-4.71489700	-1.31359600
C	6.60192000	1.68431100	-1.10801900

C	6.78736300	2.64125200	-2.10373200
C	5.67609700	3.20103900	-2.73525400
H	5.80127200	3.92209600	-3.53823100
H	7.79176900	2.93293000	-2.39755500
H	7.47627300	1.22709400	-0.65615300
C	2.78294200	1.63126000	-0.91185900
C	1.98956000	2.76746100	-0.35848000
C	2.64001000	3.99844400	-0.11688100
C	0.09437600	3.66090400	0.88708500
H	3.66614500	4.12357800	-0.43861600
H	-0.90165400	3.56038200	1.30293500
C	0.75921500	4.87415200	1.09758100
C	2.03610200	5.04368900	0.57784800
H	2.58025100	5.97110900	0.73071000
H	0.27188700	5.66818800	1.65691200
Si	5.15501800	-0.21799800	0.46064100
C	4.55772800	0.19344200	2.24427200
C	5.39361100	1.34604600	2.84243800
C	3.07764700	0.63344300	2.25284600
C	4.68248500	-1.07923200	3.11155800
H	6.46130100	1.11410000	2.90679700
H	5.29120800	2.26087700	2.24667400
H	5.04660300	1.57220200	3.86081900
H	2.42996400	-0.09410300	1.75401500
H	2.73000800	0.73208100	3.29238200
H	2.93531400	1.60429300	1.77247200
H	4.29543700	-0.88285500	4.12235100
H	4.09816800	-1.90442100	2.69079400
H	5.71390700	-1.42464400	3.21848200
C	6.86384600	-1.04617800	0.43676800
C	7.30441400	-1.61667300	-0.77701600
C	7.77460200	-1.04596100	1.50835100
C	8.57649100	-2.17251000	-0.90786500
H	6.64149400	-1.62669000	-1.63863800
C	9.05177800	-1.60040400	1.38561200
H	7.50161300	-0.60509100	2.46047600
C	9.45579400	-2.16858800	0.17782600
H	8.88248100	-2.60576800	-1.85647400
H	9.72938500	-1.58488400	2.23511200
H	10.44818100	-2.60033800	0.08045700
C	4.39775300	2.83515300	-2.32475700
H	3.53021300	3.28573900	-2.79937400
C	0.66763400	2.62045600	0.15477800
H	1.13713200	0.37380600	-1.21786500

Pd	-0.24077100	0.78113300	0.06913700
P	-1.10901500	-1.49202200	0.29231100
P	-2.35905700	1.69829000	-0.21178700
C	-2.09612000	5.70861800	-2.52845100
C	-2.98485400	5.59688700	-1.45963300
C	-3.09286700	4.39616200	-0.75361300
C	-2.30451400	3.29600700	-1.11459700
C	-1.39672500	3.42180500	-2.18090200
C	-1.30229600	4.61584000	-2.88993900
H	-3.77391200	4.33738000	0.08713600
H	-0.74423000	2.59205700	-2.43674800
C	2.00454500	-3.73410400	2.89096300
C	1.46108500	-2.51514000	3.30528800
C	0.53543800	-1.85692900	2.50013300
C	0.10869000	-2.43001000	1.28688300
C	0.67463700	-3.64162800	0.86904000
C	1.62237300	-4.28406900	1.66745400
H	0.13961600	-0.89511200	2.81782400
H	0.39721600	-4.07712800	-0.08284700
C	-2.06798700	-3.86095200	-3.56000600
C	-1.58201900	-2.55392800	-3.63646800
C	-1.28003500	-1.85417600	-2.46939300
C	-1.45610500	-2.45749400	-1.21658000
C	-1.96136000	-3.76490600	-1.14534900
C	-2.25865900	-4.46437300	-2.31424900
H	-0.94022900	-0.82457200	-2.52745100
H	-2.13330400	-4.22947200	-0.17838100
C	-4.62273800	2.34136300	3.76722100
C	-5.28825800	2.52522100	2.55338500
C	-4.61285100	2.33322700	1.34963200
C	-3.25596200	1.96978900	1.35344000
C	-2.59371500	1.78464700	2.57614500
C	-3.27671600	1.96882900	3.77749400
H	-5.14897300	2.43342600	0.41070300
H	-1.54948500	1.48450400	2.58352400
H	-6.25775500	-4.50986400	-1.72204500
C	-3.93204500	-0.61645000	-0.75623000
C	-3.39091700	0.57388100	-1.25210400
C	-3.52470200	0.88890100	-2.63505400
H	-3.12073600	1.81721300	-3.01830700
C	-4.18048900	0.04363100	-3.49453800
H	-4.28075300	0.30888000	-4.54388700
C	-4.74250100	-1.17241700	-3.03493900
C	-4.62013800	-1.50858100	-1.64799100

H	-5.09064800	-3.02098700	-0.16358600
C	-5.18290900	-2.73961200	-1.20556500
C	-5.83544900	-3.57634700	-2.08244000
H	-6.47663800	-3.90487900	-4.13001700
C	-5.95766500	-3.23509800	-3.45058200
H	-5.50287400	-1.78552300	-4.96418100
C	-5.41831300	-2.05751800	-3.91527400
H	-8.22201200	-0.47742000	3.74301700
C	-3.81027800	-1.78164000	3.40234100
H	-3.78875900	-2.09211300	4.44389900
C	-2.68933600	-1.92333200	2.62112900
H	-1.79737600	-2.35691300	3.05510600
C	-2.68881200	-1.51542000	1.25955300
C	-3.85628000	-1.00354700	0.69146600
C	-5.04585500	-0.88260000	1.48491900
C	-5.00850600	-1.24802800	2.86907300
H	-6.12370700	-1.35991400	4.71888200
C	-6.17086400	-1.08340900	3.66875400
C	-7.33646900	-0.59412600	3.12516500
H	-8.30975100	0.12752900	1.32604500
C	-7.38490600	-0.25012600	1.75274800
H	-6.32439900	-0.11131000	-0.09153600
C	-6.27118600	-0.38748100	0.95501600
H	-2.01201200	6.64535000	-3.07156300
H	2.73768000	-4.24045200	3.51191800
H	-2.31169800	-4.40397400	-4.46827900
H	-5.15598100	2.47823200	4.70318600
H	-3.59449200	6.44621100	-1.16536100
H	-0.59575300	4.70020100	-3.71033900
H	1.77930500	-2.06416800	4.23992500
H	2.06301600	-5.21604000	1.32664200
H	-2.75939200	1.81383600	4.71957700
H	-6.34067400	2.78993400	2.54210800
H	-2.65369200	-5.47400600	-2.25270500
H	-1.45303900	-2.07382400	-4.60191400

TS31

C	-2.47424000	1.71093700	0.55360600
C	-1.84508200	0.51674300	0.43767700
C	-2.34630700	-0.82677500	0.25540200
C	-3.84406500	1.71785300	1.17430800
C	-3.48624800	-1.23083600	-0.51492600
C	-4.98272800	1.13432400	0.56423000
C	-5.18904800	2.38965900	3.09954100

H	-5.25230100	2.84919600	4.08250100
C	-6.33053000	1.88610600	2.47728300
H	-7.30067400	1.96163100	2.96043800
C	-6.21499300	1.25380900	1.23916100
H	-7.10580900	0.82013300	0.79550900
C	-3.95883200	2.30089900	2.44963000
H	-3.06399200	2.68858500	2.93091900
C	-1.47079400	-3.10987000	0.26527600
H	-0.70805400	-3.83502400	0.54294200
C	-2.55487800	-3.51528900	-0.49219700
H	-2.65375400	-4.55059900	-0.80803000
C	-3.55471300	-2.58246800	-0.85199300
H	-4.41864600	-2.94742800	-1.40224200
C	-1.35663900	-1.76320800	0.69960000
H	-1.33177700	-1.63293500	2.21299100
Si	-4.89964300	-0.03931900	-0.93375700
C	-4.62231500	0.71539600	-2.68359100
C	-6.50370700	-1.05610500	-0.85726600
C	-7.63213600	-0.79446300	-1.65615300
C	-6.63282600	-2.06635900	0.11742200
C	-8.82235600	-1.51002100	-1.50175200
H	-7.59728800	-0.01953700	-2.41411000
C	-7.81619900	-2.78735900	0.27789500
H	-5.79088700	-2.29921700	0.76231500
C	-8.91773400	-2.51141900	-0.53503000
H	-9.67374300	-1.28336800	-2.13792200
H	-7.87928700	-3.56368200	1.03631600
H	-9.84183700	-3.07006100	-0.41439500
Pd	0.12518900	-0.26448900	0.25079300
P	1.74218300	-1.81838800	-0.63014700
P	1.65755100	1.55118300	0.36169700
C	0.18694300	4.86935100	3.27297100
C	0.93462800	5.24231700	2.15626900
C	1.39218500	4.28094300	1.25209900
C	1.09994100	2.92671800	1.45484600
C	0.31627400	2.56690700	2.56278800
C	-0.12627200	3.52274000	3.47330500
H	1.94433800	4.60038300	0.37735300
H	0.04569400	1.52789700	2.69049500
C	-0.76688700	-4.01034600	-3.86891400
C	-0.91106400	-2.63700600	-3.65028200
C	-0.13036900	-2.00105500	-2.68830600
C	0.81025100	-2.72528000	-1.93460400
C	0.95342700	-4.09936500	-2.16446400

C	0.16474500	-4.73712700	-3.12609100
H	-0.27440900	-0.94013100	-2.50014000
H	1.66640500	-4.67927900	-1.58720900
C	3.53424400	-5.03142700	2.18064600
C	2.41000300	-4.29574100	2.56290300
C	1.87966200	-3.33444100	1.70269800
C	2.46909200	-3.10126700	0.45193100
C	3.59726400	-3.84401500	0.07367900
C	4.12444700	-4.80623800	0.93487400
H	1.01180700	-2.75206100	1.99334400
H	4.07127400	-3.65753200	-0.88574300
C	3.41369200	3.41027800	-3.50080100
C	3.94351900	3.77225700	-2.26077600
C	3.42865800	3.21511200	-1.09085600
C	2.36118600	2.30541100	-1.14929200
C	1.84926400	1.93278900	-2.39986200
C	2.37166300	2.48217500	-3.56950900
H	3.87797300	3.46654700	-0.13485500
H	1.05298500	1.19707700	-2.45586000
H	7.54265600	-3.02124600	1.14061600
C	4.00769900	-0.06116400	0.63937900
C	3.11184000	0.81149100	1.26631700
C	3.20416100	1.00762100	2.67316800
H	2.54117600	1.71203500	3.15889600
C	4.12404000	0.32957800	3.43442700
H	4.17586100	0.50293800	4.50671800
C	5.02384000	-0.58876900	2.84224500
C	4.98075500	-0.77216400	1.42235400
H	5.91438800	-1.81339100	-0.23679200
C	5.92281400	-1.66521800	0.83631800
C	6.83586600	-2.34354100	1.61097400
H	7.59068100	-2.70967100	3.61371900
C	6.86369300	-2.16794300	3.01561000
H	5.99243900	-1.15415100	4.69203500
C	5.97546000	-1.30594900	3.61569200
H	7.84149900	2.31745900	-3.63566200
C	4.25807600	-0.58777100	-3.64648800
H	4.33223500	-0.72350900	-4.72255100
C	3.28399600	-1.24466100	-2.93521400
H	2.59227000	-1.89753500	-3.45445700
C	3.16608000	-1.07231100	-1.52843400
C	4.05857800	-0.24374900	-0.85042100
C	5.09614400	0.43028300	-1.57593300
C	5.17959000	0.27027800	-2.99721100

H	6.22771000	0.84374400	-4.79992900
C	6.18069700	0.97068600	-3.72135100
C	7.07704800	1.78927800	-3.07314600
H	7.72179300	2.58191200	-1.15976700
C	7.00790200	1.93919600	-1.66710200
H	5.99946500	1.40991100	0.13682900
C	6.04399000	1.27961700	-0.93821700
H	-0.16285400	5.62292900	3.97262500
H	-1.38209000	-4.51122200	-4.61099200
H	3.95316900	-5.77420800	2.85336100
H	3.82408500	3.83637400	-4.41150900
H	1.15873200	6.28978000	1.97700400
H	-0.72458100	3.21977600	4.32910700
H	-1.64186700	-2.06429100	-4.21449100
H	0.27920400	-5.80488200	-3.29094700
H	1.97267900	2.17764200	-4.53266200
H	4.77556500	4.46727000	-2.20482600
H	5.00382100	-5.37072800	0.63888700
H	1.95325500	-4.46689500	3.53421500
C	-1.91521200	3.00947200	0.09332700
C	-1.03091500	3.02095300	-1.00386300
C	-2.33212400	4.25832700	0.59296900
C	-0.55962000	4.20824700	-1.55677800
H	-0.74739900	2.07591500	-1.44660200
C	-1.85717700	5.44911600	0.04542300
H	-3.03953700	4.31087400	1.41021900
C	-0.96844100	5.43428100	-1.03084900
H	0.12165100	4.16996600	-2.40142300
H	-2.19210400	6.39519400	0.46183800
H	-0.61093600	6.36528100	-1.46185200
C	-5.55556400	1.91730700	-2.94355700
H	-5.39412200	2.71283500	-2.20646800
H	-5.35451800	2.34057100	-3.93786100
H	-6.61701400	1.65168800	-2.91553500
C	-4.85490500	-0.39624300	-3.73287500
H	-4.66456000	-0.00021800	-4.74047600
H	-4.16821500	-1.23918900	-3.57721700
H	-5.87374700	-0.79347700	-3.72083000
C	-3.16948100	1.20677100	-2.83470200
H	-2.97315500	2.07627800	-2.20662200
H	-2.43896100	0.42954800	-2.57804300
H	-2.98620100	1.50986300	-3.87592200
N	-1.68644100	-1.59717400	3.40071900
H	-1.46109200	-2.51706700	3.78948900

C	-3.16726800	-1.38852300	3.43738400
H	-3.44801300	-1.10798400	4.45930200
H	-3.37884100	-0.53568300	2.78608900
C	-3.92712000	-2.62830400	2.98700300
H	-3.73444900	-3.48001300	3.65122400
H	-5.00057800	-2.41926300	3.01624000
H	-3.66164000	-2.91252000	1.96649200
C	0.56634600	-0.77481500	4.07694100
H	0.93657000	-0.73148800	3.04991100
H	1.08343000	-0.00000900	4.64948300
H	0.84265400	-1.74595600	4.50518100
C	-0.93746200	-0.54619900	4.13838100
H	-1.29430600	-0.52349600	5.17546800
H	-1.21955700	0.40043900	3.67078300

INT39

C	-2.47016800	1.59548400	0.37916100
C	-1.84547800	0.40240300	0.16410200
C	-2.40482700	-0.93178200	-0.04749600
C	-3.76748400	1.59132900	1.13758100
C	-3.66387200	-1.35950700	-0.56786400
C	-4.96457900	0.98585400	0.68368100
C	-4.84529900	2.16345000	3.26092600
H	-4.78217000	2.60841400	4.25091500
C	-6.03860000	1.59941000	2.81014200
H	-6.92561900	1.60655800	3.43766600
C	-6.08303500	1.01612800	1.54394100
H	-7.01263900	0.56028900	1.22004100
C	-3.72751600	2.15533600	2.42937100
H	-2.79669100	2.59280800	2.77718100
C	-1.44486500	-3.16313900	-0.29303300
H	-0.60218600	-3.84929900	-0.26133700
C	-2.69233700	-3.61869000	-0.73012600
H	-2.83002400	-4.66668400	-0.98649200
C	-3.75794500	-2.72023800	-0.90434500
H	-4.68183200	-3.10252300	-1.32989100
C	-1.29319500	-1.81094200	0.03590500
H	-1.92800100	-1.75573500	2.02897600
Si	-5.03527800	-0.09880200	-0.87870700
C	-4.72921700	0.78900600	-2.57637200
C	-6.74901300	-0.90828700	-0.80952800
C	-7.87869100	-0.19520100	-1.26002800
C	-6.98552400	-2.14271300	-0.17650800
C	-9.17183600	-0.69939100	-1.11358800

H	-7.75631800	0.78170500	-1.72025500
C	-8.27594000	-2.65774500	-0.02959300
H	-6.15370800	-2.71650000	0.21786600
C	-9.37420900	-1.93896000	-0.50294100
H	-10.02028800	-0.12418900	-1.47433800
H	-8.42249700	-3.61950800	0.45559500
H	-10.37918800	-2.33646700	-0.39118500
Pd	0.15100100	-0.33485700	-0.00203400
P	1.91838400	-1.79479600	-0.73017800
P	1.65955300	1.51336100	0.37865700
C	-0.02837600	4.76709500	3.25210700
C	0.74985600	5.16718200	2.16659300
C	1.26704200	4.22383500	1.27582500
C	0.99934100	2.86057200	1.45290000
C	0.16690900	2.47562000	2.51626300
C	-0.32231000	3.41243000	3.42365200
H	1.85115100	4.56406500	0.43038700
H	-0.10064900	1.43236500	2.61471500
C	0.12563000	-4.15554200	-4.30710000
C	-0.25499700	-2.83470600	-4.05364900
C	0.29498300	-2.14625900	-2.97423200
C	1.24201700	-2.76539000	-2.14083600
C	1.62308000	-4.08791300	-2.40460800
C	1.06260500	-4.77947400	-3.48135200
H	-0.03390100	-1.13267000	-2.75967800
H	2.34641400	-4.58635900	-1.76710200
C	3.39733100	-4.93473000	2.33985600
C	2.15702900	-4.31058100	2.49519600
C	1.72729200	-3.36811900	1.56173200
C	2.53343700	-3.04257500	0.46058300
C	3.77232300	-3.68012400	0.30577400
C	4.20135500	-4.62057900	1.24259600
H	0.76547700	-2.87854100	1.67327400
H	4.41003800	-3.42504000	-0.53496800
C	3.69208700	3.56369300	-3.24474000
C	4.12051200	3.87611500	-1.95294600
C	3.52752900	3.25988400	-0.85191800
C	2.48411400	2.33805800	-1.03139600
C	2.07232200	2.01825200	-2.33283100
C	2.67299500	2.62724200	-3.43391700
H	3.89532100	3.47686100	0.14647500
H	1.29163400	1.27827700	-2.48160800
H	7.66840300	-2.82526700	1.56021900
C	4.02595200	-0.04366900	0.83226300

C	3.03090700	0.75749300	1.40077300
C	2.95242200	0.85698500	2.81933500
H	2.21742200	1.51133500	3.26941100
C	3.80154900	0.15621700	3.63945600
H	3.71782500	0.25324300	4.71945300
C	4.81235300	-0.67571300	3.10082500
C	4.94736300	-0.75427000	1.67780000
H	6.14295300	-1.60828300	0.08014600
C	6.00896800	-1.54590500	1.15327000
C	6.86522800	-2.23029200	1.98585300
H	7.39169100	-2.71455500	4.03613500
C	6.71021300	-2.16706700	3.39148800
H	5.58195900	-1.33278300	5.01260300
C	5.70401300	-1.40222100	3.93453900
H	8.16422200	2.61428800	-2.97145400
C	4.68343600	-0.37886200	-3.42807100
H	4.85678700	-0.46563900	-4.49775400
C	3.66902400	-1.09026300	-2.83597900
H	3.04816600	-1.73624400	-3.44483400
C	3.41778000	-0.98464700	-1.43946400
C	4.22230400	-0.16224300	-0.65103300
C	5.30091400	0.56837900	-1.25121700
C	5.51783600	0.47268400	-2.66367100
H	6.70711700	1.15065200	-4.33791600
C	6.55915300	1.22942200	-3.26388300
C	7.36821400	2.04229600	-2.50347800
H	7.81169300	2.76892300	-0.50827500
C	7.16694700	2.12973000	-1.10483100
H	6.01438900	1.49774000	0.57535200
C	6.16089800	1.41442500	-0.49526000
H	-0.41711600	5.50431500	3.94855500
H	-0.31042300	-4.69722600	-5.14168000
H	3.73761700	-5.66085000	3.07250900
H	4.16287200	4.03651500	-4.10166700
H	0.95680300	6.22089100	2.00421300
H	-0.94343800	3.08917500	4.25550300
H	-0.99122400	-2.34555700	-4.68519900
H	1.35870400	-5.80718100	-3.67224700
H	2.35159900	2.36347800	-4.43735600
H	4.93409800	4.57898500	-1.80288800
H	5.17038700	-5.09567300	1.12297100
H	1.52944400	-4.55590600	3.34834000
C	-1.92725500	2.90170600	-0.07298500
C	-1.01929600	2.93354600	-1.15268800

C	-2.38457900	4.14487000	0.41003400
C	-0.55242800	4.13054700	-1.68714700
H	-0.69754700	1.99610300	-1.58750500
C	-1.92107900	5.34517900	-0.12638400
H	-3.11586700	4.18502000	1.20714300
C	-0.99754200	5.34940700	-1.17284800
H	0.15479400	4.10664700	-2.51091000
H	-2.29028200	6.28394300	0.27775400
H	-0.64427600	6.28716400	-1.59247900
C	-5.09940100	2.28391700	-2.46955400
H	-4.47625500	2.80346200	-1.73282700
H	-4.95167800	2.77984400	-3.43925300
H	-6.14780200	2.43451200	-2.18331200
C	-5.56784600	0.11330000	-3.68656800
H	-5.32361800	0.56935300	-4.65621000
H	-5.34941400	-0.95940600	-3.76567500
H	-6.64505800	0.21747700	-3.53811900
C	-3.24790500	0.66884800	-3.00229400
H	-2.57483300	1.14394300	-2.28971400
H	-2.94029200	-0.37825800	-3.10956600
H	-3.10651200	1.16257500	-3.97420600
N	-2.26153000	-1.72871500	3.02389200
H	-2.00970100	-2.63550800	3.43134200
C	-3.76635000	-1.57301900	3.03535400
H	-4.04349200	-1.25410200	4.04318700
H	-3.99336500	-0.76351500	2.34159100
C	-4.44725400	-2.87415000	2.64474900
H	-4.27735900	-3.65997600	3.39083500
H	-5.52476500	-2.70022700	2.57596700
H	-4.10209600	-3.22261500	1.66752200
C	-0.02609800	-0.91770200	3.79011900
H	0.41199400	-0.91452600	2.78817500
H	0.47423200	-0.14143500	4.37498400
H	0.18942700	-1.88121200	4.26790400
C	-1.52059400	-0.63419400	3.74436900
H	-1.95389000	-0.56684900	4.74619600
H	-1.75904400	0.28141700	3.19894300

TS32

P	-0.72831600	-1.44570000	-0.66492100
P	-2.61185900	1.44137000	-0.46419800
C	-4.06659100	4.76825500	-3.34645900
C	-4.11843000	4.99076500	-1.97001000
C	-3.72547600	3.99024300	-1.07680800

C	-3.27345700	2.75561900	-1.55811700
C	-3.21433800	2.54159900	-2.94742200
C	-3.61656500	3.53724400	-3.83552800
H	-3.75514100	4.18366700	-0.01023400
H	-2.84079000	1.59634700	-3.33415100
C	2.66424000	-4.60468500	-0.46383300
C	2.65274200	-3.63050400	-1.46306600
C	1.65630800	-2.65422000	-1.47731500
C	0.65926400	-2.64047700	-0.49426000
C	0.67502000	-3.62689200	0.50814500
C	1.67505300	-4.59883200	0.52248500
H	1.65653700	-1.90685400	-2.25804500
H	-0.08505000	-3.63695600	1.28238500
C	-3.68467700	-3.83008200	-3.31744800
C	-3.34651600	-2.51486200	-3.63990400
C	-2.46404000	-1.80336200	-2.82682000
C	-1.91655000	-2.40020600	-1.68334200
C	-2.24497400	-3.73004000	-1.37686600
C	-3.13045300	-4.43661200	-2.18705800
H	-2.20469700	-0.77659700	-3.07020200
H	-1.81598500	-4.21191000	-0.50452500
C	-2.60828000	3.03358400	3.87584500
C	-3.82234900	2.83048100	3.21337200
C	-3.83233700	2.36330000	1.90075100
C	-2.62233900	2.10229400	1.23713700
C	-1.40824700	2.30638500	1.90645900
C	-1.40400000	2.77256100	3.22071000
H	-4.77838100	2.17902400	1.39926000
H	-0.47272900	2.08026300	1.41074400
H	-5.27202600	-5.26150500	1.38293600
C	-3.75797400	-1.01548100	0.32764600
C	-3.89515600	0.10850600	-0.48959700
C	-4.95653000	0.16538700	-1.43377000
H	-5.08843800	1.04858400	-2.04633300
C	-5.82343900	-0.88966700	-1.58629200
H	-6.62530500	-0.83199200	-2.31789000
C	-5.68774500	-2.06445700	-0.80737800
C	-4.65542200	-2.12013100	0.18353100
H	-3.75936500	-3.35322600	1.72627600
C	-4.53467700	-3.29987100	0.97009300
C	-5.38088200	-4.36791200	0.77501300
H	-7.05300900	-5.16451600	-0.35700400
C	-6.39370200	-4.31340600	-0.21360600
H	-7.32059800	-3.13100900	-1.74336900

C	-6.54367600	-3.18362800	-0.98507000
H	-4.05607400	-0.22160000	6.49193400
C	-0.71368500	-0.89173500	3.38298700
H	0.05707900	-0.81239600	4.14387200
C	-0.35975000	-1.12426200	2.07853300
H	0.69123100	-1.21120200	1.82442100
C	-1.35401400	-1.25644000	1.06356900
C	-2.69542800	-1.06267500	1.38186000
C	-3.08267900	-0.83780600	2.74819600
C	-2.07381300	-0.76057600	3.76090600
H	-1.67257500	-0.47481800	5.86595700
C	-2.45143200	-0.53296300	5.10978900
C	-3.77613600	-0.39058800	5.45620000
H	-5.82099000	-0.34838800	4.73649800
C	-4.77703600	-0.46335700	4.45922400
H	-5.21971300	-0.71954100	2.38876100
C	-4.44050600	-0.67407500	3.14016900
H	-4.37035900	5.54937700	-4.03718800
H	3.43967800	-5.36537300	-0.45131100
H	-4.37604700	-4.38375300	-3.94597700
H	-2.60461500	3.38581000	4.90317300
H	-4.46208500	5.94672700	-1.58542300
H	-3.56911900	3.35868500	-4.90592400
H	3.42812300	-3.61531100	-2.22280300
H	1.67781200	-5.35372800	1.30358000
H	-0.45845300	2.92049800	3.73537800
H	-4.76101300	3.01775200	3.72590900
H	-3.39438900	-5.45827700	-1.93178200
H	-3.77248700	-2.04019100	-4.51911500
C	2.14266800	1.77685400	0.10288200
C	3.12482200	0.56545500	2.18015600
C	2.56233100	0.93428900	-1.05615700
C	4.31339400	-0.07950500	1.74991600
C	3.85140800	0.37676000	-1.23035000
C	6.26154000	-1.17222800	-0.31244400
C	7.59684400	-1.12361900	-0.74946300
C	5.64915500	-2.44150200	-0.24856900
C	8.29035300	-2.28378500	-1.10649400
H	8.11835800	-0.17533300	-0.81620200
C	6.33461400	-3.60247300	-0.60342300
H	4.62044400	-2.52680800	0.08967600
C	7.66115700	-3.52673800	-1.03574300
H	9.32266900	-2.21351800	-1.43831400
H	5.83612700	-4.56630700	-0.53825100

H	8.19998100	-4.42893500	-1.31208100
C	6.16039900	1.97435300	0.22459200
C	7.29834200	1.82572900	1.25939200
C	6.72962700	2.34526600	-1.16350400
C	5.24648700	3.13292400	0.68049500
H	6.90337600	1.59498100	2.25636400
H	8.01203300	1.03857800	0.99721300
H	7.86008900	2.76702400	1.33708400
H	5.92908600	2.47729900	-1.90146300
H	7.28002200	3.29422800	-1.09991000
H	7.42144100	1.59580000	-1.55968900
H	5.83842400	4.05559900	0.76053400
H	4.43688200	3.32309400	-0.03219500
H	4.79840200	2.94123900	1.66176900
C	3.23718600	-0.24035800	-3.53676900
H	3.52756800	-0.65740600	-4.49706100
C	1.61417600	0.78404400	-2.09322600
C	1.94014700	0.22958100	-3.33245400
H	1.19256200	0.16700000	-4.11814200
C	4.15026400	-0.20152200	-2.48069700
H	5.13780100	-0.62641100	-2.63539000
H	0.85645300	1.93540500	-2.12489000
C	2.62132700	0.29554300	3.47099700
H	1.73017500	0.82226400	3.80356400
C	4.91655700	-0.99709100	2.63044400
C	4.38634500	-1.28312500	3.88855600
H	4.88479600	-1.99607800	4.53920500
C	3.22894600	-0.62821200	4.31324100
H	2.81459200	-0.82317500	5.29875500
H	5.82973800	-1.49973200	2.32692300
Pd	-0.41902700	0.85040800	-1.26978900
C	1.33759800	2.98848400	-0.26559900
C	0.34691700	2.92234300	-1.26754100
C	1.57936200	4.23097700	0.34210800
C	-0.33214500	4.06239800	-1.70233300
C	0.86520300	5.36282500	-0.05462300
H	2.35233200	4.31793200	1.09934500
C	-0.07662900	5.28784400	-1.08464300
H	-1.05991100	3.99748700	-2.50226200
H	1.07183700	6.31728600	0.42129000
H	-0.60847300	6.17748900	-1.40891300
Si	5.18248800	0.32315700	0.11919200
C	2.38154700	1.57766900	1.42394300
H	1.87959200	2.28780700	2.07961300

INT40

P	-0.68576500	-1.50703200	-1.05552900
P	-2.59263900	1.31272600	-0.25568300
C	-5.48358800	3.77792400	-2.91249100
C	-5.18278000	4.23609200	-1.62958900
C	-4.33480600	3.50134700	-0.79704100
C	-3.78090600	2.29579900	-1.24597100
C	-4.07640800	1.84764600	-2.54566500
C	-4.92796900	2.57893400	-3.37039100
H	-4.09197500	3.88482500	0.18700300
H	-3.62450000	0.93320700	-2.91848700
C	2.39881900	-4.58798900	-2.66677800
C	1.40454200	-4.02954300	-3.47586500
C	0.52743100	-3.08548100	-2.94942500
C	0.61051500	-2.69933100	-1.59901900
C	1.58723800	-3.28906800	-0.78839100
C	2.48595000	-4.21570400	-1.32647400
H	-0.23795100	-2.65549400	-3.59016400
H	1.66319300	-3.04526400	0.26319000
C	-4.25493600	-4.24430500	-2.15893300
C	-4.15816200	-2.96434200	-2.70508100
C	-3.10425300	-2.12620000	-2.33441500
C	-2.14355000	-2.56293800	-1.41685600
C	-2.23382400	-3.86124100	-0.88858800
C	-3.29071300	-4.69164100	-1.24991200
H	-3.02609300	-1.12875800	-2.75627200
H	-1.47951800	-4.21793800	-0.19388200
C	-1.98831400	3.36628600	3.83771200
C	-3.26951400	3.00520300	3.41180500
C	-3.44432400	2.40050300	2.17005500
C	-2.33837000	2.18480200	1.32788700
C	-1.05834800	2.54484600	1.75885900
C	-0.88798600	3.12703400	3.01571700
H	-4.43612400	2.08254100	1.86130500
H	-0.19880400	2.34068500	1.13336200
H	-3.52882000	-5.28925400	3.10620500
C	-3.00666600	-1.15442500	1.09249400
C	-3.57197000	-0.16845900	0.27987900
C	-4.92089500	-0.29900000	-0.15151700
H	-5.37220600	0.47472400	-0.75909000
C	-5.66700600	-1.40132100	0.18588900
H	-6.69327800	-1.48866900	-0.16126600
C	-5.11553500	-2.44291500	0.96986500

C	-3.77338200	-2.30835900	1.45032900
H	-2.21134500	-3.27526800	2.60373900
C	-3.22621600	-3.36377000	2.23278000
C	-3.96450400	-4.49197300	2.51091100
H	-5.85908200	-5.52019500	2.25465700
C	-5.28939800	-4.62379500	2.02758100
H	-6.86851300	-3.70825300	0.90237300
C	-5.85215100	-3.61718000	1.27650800
H	-0.74653200	0.44660600	6.67715600
C	1.01463800	-0.51592000	2.52808500
H	2.01606300	-0.27228000	2.86698100
C	0.80115600	-0.90356700	1.22983800
H	1.63663400	-0.93255900	0.54147200
C	-0.50808500	-1.22398300	0.76114300
C	-1.60292900	-1.02872000	1.60057600
C	-1.39620800	-0.63582200	2.96801400
C	-0.06468000	-0.39754900	3.43815400
H	1.16646600	0.18343600	5.11446500
C	0.14777500	-0.00377100	4.78466700
C	-0.91465300	0.14820000	5.64636100
H	-3.06928700	0.05206000	5.86765500
C	-2.23352100	-0.07833400	5.18620600
H	-3.48801600	-0.61006900	3.54432700
C	-2.47059800	-0.45258500	3.88195900
H	-6.14014000	4.35438200	-3.55754700
H	3.09398800	-5.31429900	-3.07799400
H	-5.07645500	-4.89578300	-2.44257100
H	-1.84861500	3.81621900	4.81626800
H	-5.60060300	5.17314300	-1.27335600
H	-5.14872600	2.22108500	-4.37183100
H	1.31706600	-4.32299300	-4.51832600
H	3.25376600	-4.63837800	-0.68714300
H	0.11037700	3.37245300	3.36015800
H	-4.12809800	3.17433300	4.05505700
H	-3.36510400	-5.68612500	-0.82076000
H	-4.90178400	-2.61452500	-3.41543600
C	1.91615600	2.35954800	-0.65564300
C	3.13584900	2.03738700	1.68094700
C	2.21535200	1.22199500	-1.56626000
C	4.05500700	0.96371400	1.57532100
C	3.19294600	0.20853700	-1.33978200
C	5.03093600	-1.60914100	0.30161900
C	6.06674300	-2.29615600	-0.35823600
C	4.28722400	-2.33495700	1.25460500

C	6.34978800	-3.63660500	-0.08224100
H	6.67419800	-1.78544500	-1.09781000
C	4.56924000	-3.67048100	1.54447200
H	3.48308400	-1.84887800	1.79853800
C	5.60479100	-4.32746500	0.87455000
H	7.15975500	-4.13569700	-0.60715100
H	3.98392800	-4.19611700	2.29466100
H	5.83207300	-5.36567400	1.10073900
C	6.03780400	1.24039800	-0.77076600
C	7.27587300	1.08380600	0.13805100
C	6.39146000	0.84211800	-2.21980100
C	5.60901800	2.72650800	-0.78064100
H	7.06084200	1.38742000	1.16977900
H	7.64542400	0.05272300	0.16279000
H	8.09358600	1.72042800	-0.22709200
H	5.53572500	0.95696100	-2.89443400
H	7.19629500	1.48946300	-2.59437800
H	6.74620300	-0.19016300	-2.30724800
H	6.42412900	3.34366000	-1.18293100
H	4.72799600	2.89427300	-1.41148400
H	5.38012500	3.09638900	0.22444300
C	2.60678200	-0.85750800	-3.49270200
H	2.77926000	-1.65757200	-4.20246300
C	1.49440200	1.16879500	-2.80626500
C	1.68559300	0.14333300	-3.74560800
H	1.13238000	0.17668300	-4.67984800
C	3.33662800	-0.80679500	-2.30267300
H	4.06391900	-1.59345300	-2.12749100
H	0.95760200	2.04294200	-3.15292500
C	2.93255700	2.62491900	2.95217400
H	2.25926900	3.47342400	3.03428400
C	4.70051700	0.51970700	2.74454500
C	4.45808400	1.08751900	3.99586200
H	4.97503900	0.71326700	4.87478800
C	3.56535900	2.15555100	4.09655500
H	3.37448300	2.62929300	5.05534900
H	5.41366600	-0.29637200	2.67811300
Pd	-0.64807400	0.91518500	-1.52343800
C	0.93358100	3.36431900	-1.19483700
C	-0.35774700	2.97073000	-1.60811500
C	1.31272800	4.70909300	-1.31745400
C	-1.20821000	3.91025100	-2.18849900
C	0.43738500	5.65482600	-1.85435800
H	2.31252400	5.00422600	-1.00959500

C	-0.81677100	5.25129600	-2.30430000
H	-2.17914000	3.62047900	-2.56707000
H	0.74828100	6.69174400	-1.94395000
H	-1.49759200	5.96930400	-2.75390800
Si	4.58318300	0.20188300	-0.05424200
C	2.33157700	2.64024700	0.61542800
H	1.87449500	3.55756600	0.97985900

TS3-cf1

C	2.11376500	-0.95901700	-1.34360600
C	2.73942000	-1.68703600	-2.37543300
C	0.82337800	-0.46477500	-1.63308900
C	2.15598500	-1.85508200	-3.63450600
H	3.71680900	-2.12214800	-2.21243100
C	0.28326400	-0.51862200	-2.92520500
C	0.94184700	-1.23502500	-3.92590300
H	2.67424100	-2.43277100	-4.39500900
H	-0.66245100	-0.03085800	-3.14050500
H	0.50468100	-1.30944500	-4.91797200
C	3.06364600	1.62425900	-0.43302400
C	1.85104100	2.19892000	-0.88641500
C	4.18980600	2.46377200	-0.41314500
C	1.80819800	3.52972300	-1.35078400
C	4.14947400	3.78572000	-0.85895800
C	2.95424200	4.31709300	-1.34374200
H	0.86243300	3.93830100	-1.69417200
H	5.04907300	4.39423200	-0.82927500
H	2.90929300	5.34021700	-1.70643000
H	5.13194800	2.08620000	-0.03518500
Pd	-0.69976900	-0.31007600	-0.27172700
O	-3.45515500	-2.46421400	0.93175900
S	-3.77157100	-1.01841300	1.03698100
O	-2.54633200	-0.13493500	0.94322700
O	-4.70851100	-0.59952100	2.07501100
C	-4.65175800	-0.69039200	-0.57944300
F	-3.75618400	-0.62938300	-1.59691100
F	-5.31836800	0.47245500	-0.54848100
F	-5.51630000	-1.67094500	-0.84812900
Si	3.11838400	-0.20795000	0.09726200
C	0.54754700	1.56878600	-0.77886700
C	-0.68324800	1.75501900	-0.53326700
C	-1.71738100	2.70542600	-0.18713900
C	-1.36630300	3.84439200	0.56252900
C	-3.04853500	2.51818100	-0.58104700

C	-2.34304500	4.77381400	0.91125500
H	-0.33294300	3.98678300	0.86569900
C	-4.01979700	3.45111500	-0.22849200
H	-3.30794100	1.64006000	-1.15322600
C	-3.67126000	4.57825700	0.51935200
H	-2.06910700	5.64884300	1.49435300
H	-5.05091800	3.28430300	-0.52465700
H	-4.43211500	5.30063800	0.80164800
N	-0.78239300	-2.53091100	-0.03349000
H	-1.75889300	-2.62909600	0.27245200
C	0.05524200	-3.03133600	1.08415300
C	-0.45106700	-2.51866100	2.42830000
H	0.03173200	-4.13225500	1.07801200
H	1.09037900	-2.72703200	0.90085200
H	0.14103100	-2.95299700	3.23760900
H	-1.50002700	-2.79391700	2.57176400
H	-0.37039100	-1.43079100	2.49839700
C	-0.63282200	-3.33984200	-1.26798700
C	-1.81158800	-3.13817700	-2.21544100
H	0.31345400	-3.07883100	-1.74791200
H	-0.57239600	-4.40242400	-0.98754500
H	-1.67827400	-3.75244600	-3.11243200
H	-1.90090200	-2.09534000	-2.52559000
H	-2.75221600	-3.42564300	-1.73337300
C	4.93693900	-0.89696600	0.14263000
C	5.67849500	-0.33415100	1.38158400
C	4.95853100	-2.44341600	0.25987300
C	5.74742500	-0.50870600	-1.12032100
H	5.74481000	0.75880200	1.37732200
H	5.19469400	-0.62455300	2.31852500
H	6.70696900	-0.72182500	1.40159800
H	4.40937200	-2.94861800	-0.53966500
H	5.99835700	-2.79714600	0.21576000
H	4.54763600	-2.79706200	1.20944000
H	6.76806500	-0.90748900	-1.03235700
H	5.32022200	-0.91107100	-2.04230200
H	5.83127200	0.57191900	-1.25536300
C	2.36730800	-0.27339300	1.84186500
C	2.64093400	-1.31880600	2.74543500
C	1.61074300	0.80876700	2.33477500
C	2.20524600	-1.27989800	4.07020100
H	3.20382200	-2.18688200	2.42140900
C	1.14471200	0.84102200	3.65074900
H	1.38058600	1.64934800	1.69120400

C	1.44933800	-0.19983700	4.52777600
H	2.44420500	-2.10210400	4.73980400
H	0.54958600	1.68503700	3.98852300
H	1.09714700	-0.17271900	5.55526100

TS3-cf2

C	-1.64308300	-0.10771200	-1.13351800
C	-2.39488600	-0.68195400	-2.17848000
C	-0.31820100	0.22220100	-1.44123700
C	-1.86076700	-0.87372500	-3.45337800
H	-3.42653100	-0.96521200	-1.99358100
C	0.20386700	0.14399700	-2.73312500
C	-0.57118700	-0.43322000	-3.74261400
H	-2.46531900	-1.33898900	-4.22676100
H	1.21364700	0.47941600	-2.94978000
H	-0.15850900	-0.54331800	-4.74170600
C	-2.04078600	2.35033200	0.50657800
C	-0.77519100	2.85676500	0.12833000
C	-2.99202500	3.27955200	0.96735100
C	-0.51911000	4.24437100	0.17149200
C	-2.73353800	4.64858800	1.02668900
C	-1.49149200	5.13384100	0.61292100
H	0.45808400	4.61061000	-0.13057300
H	-3.49897000	5.33183500	1.38449000
H	-1.27667900	6.19867000	0.63928000
H	-3.97286400	2.92212100	1.26811200
Pd	1.26787700	0.03250400	-0.16205200
O	0.58215600	-2.03782300	0.20891000
S	1.08137700	-3.20152900	-0.63042500
O	0.37119900	-3.40555900	-1.89298400
O	2.56425000	-3.25797400	-0.66075000
C	0.58031600	-4.60570700	0.48249300
F	-0.74733300	-4.60012500	0.66732400
F	0.93741100	-5.77392600	-0.06052100
F	1.17791700	-4.48572400	1.67951500
Si	-2.53045800	0.51554900	0.41544200
C	0.38806100	2.05483600	-0.22070400
C	1.65922400	2.05670200	-0.28069300
C	2.93108000	2.73919900	-0.21562400
C	3.64980700	3.03742900	-1.38576100
C	3.47508500	3.08336200	1.03591200
C	4.89289800	3.66207500	-1.30292600
H	3.23115800	2.76696300	-2.35010100
C	4.71815500	3.70889500	1.11008000

H	2.91575900	2.85238600	1.93727200
C	5.43230800	3.99469000	-0.05716600
H	5.44330800	3.88589200	-2.21234600
H	5.13131700	3.97068300	2.08015500
H	6.40411900	4.47619700	0.00377900
C	-2.18439500	-0.29629600	2.12843600
C	-4.37441800	0.45731000	-0.03556900
C	-5.23481300	-0.57766600	0.37399500
C	-4.90191600	1.41854300	-0.92137600
C	-6.56093100	-0.64255500	-0.06126500
H	-4.87338800	-1.35602400	1.03783900
C	-6.22554200	1.36231400	-1.35896100
H	-4.26821300	2.22651000	-1.27762700
C	-7.06179800	0.33054100	-0.92668200
H	-7.19987200	-1.45499600	0.27527600
H	-6.60278100	2.12147500	-2.03956500
H	-8.09330100	0.28291100	-1.26604200
C	-3.25453600	0.19488300	3.13144700
H	-4.26709200	-0.11871000	2.86194200
H	-3.03564800	-0.21200800	4.12909200
H	-3.25602500	1.28899000	3.21892100
C	-2.19437400	-1.83710500	2.04423300
H	-1.43164700	-2.20692800	1.35596000
H	-1.98721400	-2.26376100	3.03681200
H	-3.16266000	-2.23577100	1.72167700
C	-0.81039300	0.16064600	2.66134000
H	0.00324900	-0.14711200	1.99928400
H	-0.75469900	1.24926600	2.77757600
H	-0.62331500	-0.29311500	3.64537300
N	3.25990200	-0.71395200	0.58394700
H	3.11790500	-1.70039100	0.33402100
C	4.45196200	-0.26270600	-0.17521100
C	4.26967000	-0.43737100	-1.67937100
H	5.32267300	-0.84678500	0.16077100
H	4.64697400	0.78247100	0.07754600
H	5.20075400	-0.18857100	-2.20017800
H	3.99256200	-1.46856800	-1.91972600
H	3.48332100	0.22380700	-2.05773600
C	3.46355700	-0.63391500	2.05305300
C	2.59516900	-1.64043900	2.80322700
H	3.25165200	0.39322100	2.37064400
H	4.52330300	-0.82700300	2.28042300
H	2.75502600	-1.53853000	3.88212300
H	1.53463300	-1.49884300	2.59120800

H	2.84856000	-2.66489800	2.51174700
TS3-cf3			
C	-1.94290800	-0.42850100	-1.16365100
C	-2.83923500	-0.95735500	-2.11548700
C	-0.74393900	0.11892400	-1.66846800
C	-2.59638700	-0.87831100	-3.48883300
H	-3.76535100	-1.41145900	-1.77792600
C	-0.54728800	0.31381800	-3.04354800
C	-1.46977700	-0.20050800	-3.95696200
H	-3.31036500	-1.30405700	-4.18865800
H	0.34373200	0.82216900	-3.40093700
H	-1.29959200	-0.08019500	-5.02387300
C	-2.46844200	1.88846300	0.51993700
C	-1.33817300	2.53399000	-0.03098800
C	-3.48943900	2.70384200	1.03840400
C	-1.27470200	3.94109500	-0.09054200
C	-3.42301700	4.09665400	0.99299200
C	-2.31260400	4.71597600	0.41650900
H	-0.39580900	4.41501300	-0.51750100
H	-4.23469900	4.69351600	1.39981000
H	-2.24954100	5.79947300	0.36516700
H	-4.36602100	2.23617900	1.47779100
Pd	1.07565000	-0.10851200	-0.75549800
O	3.71914700	-2.75635000	-0.07053300
S	3.88966800	-1.45380700	0.61482600
O	5.22212700	-1.08287100	1.08376200
O	3.17219100	-0.32107600	-0.08817400
C	2.85972000	-1.66459800	2.15233100
F	3.44360900	-2.49667000	3.01467000
F	2.65693600	-0.48269800	2.76173900
F	1.65119100	-2.17687500	1.82053800
Si	-2.61559900	-0.00162400	0.56740800
C	-0.12050900	1.86041800	-0.45964400
C	1.14428600	1.94583100	-0.39833900
C	2.33768700	2.73547200	-0.23729100
C	2.54556600	3.83190000	-1.09864200
C	3.27473900	2.45689700	0.77498500
C	3.66921400	4.63884100	-0.94135500
H	1.82501300	4.03341900	-1.88632100
C	4.39188200	3.27375400	0.92429600
H	3.12191000	1.60364900	1.42156200
C	4.59431300	4.36109000	0.06952100
H	3.82479000	5.48194100	-1.60874300

H	5.11335300	3.05074500	1.70462300
H	5.47344500	4.98852200	0.18748900
C	-1.81365100	-0.59298600	2.22607800
C	-4.46261300	-0.44066400	0.49698500
C	-5.01680900	-1.57260300	1.12180900
C	-5.32859100	0.34371500	-0.29292000
C	-6.36804400	-1.89951500	0.98207400
H	-4.39402200	-2.21922200	1.73085600
C	-6.67958300	0.02597000	-0.43581500
H	-4.94025700	1.21712900	-0.81006000
C	-7.20515500	-1.09822200	0.20513700
H	-6.76429000	-2.78014200	1.48105700
H	-7.32073200	0.65433100	-1.04880200
H	-8.25713700	-1.34886900	0.09664800
C	-2.77482100	-0.15492200	3.35993400
H	-3.74240700	-0.66341200	3.32169700
H	-2.31605400	-0.38401400	4.33197800
H	-2.96255300	0.92544700	3.33564500
C	-1.57864000	-2.11484600	2.30994800
H	-0.79407400	-2.43779400	1.62263900
H	-1.24209000	-2.38136200	3.32180600
H	-2.47570500	-2.70655000	2.09980800
C	-0.46588700	0.11858500	2.46705400
H	0.27330700	-0.13066900	1.70367700
H	-0.57454300	1.20817300	2.48600000
H	-0.04779200	-0.19522700	3.43301800
N	1.17987000	-2.24420000	-1.41995200
H	1.98374300	-2.56342100	-0.86740400
C	0.02185300	-3.11628200	-1.09036000
C	0.44773400	-4.53198500	-0.70017400
H	-0.65547100	-3.11807500	-1.95027700
H	-0.53243600	-2.65686800	-0.27217900
H	-0.43043500	-5.14469700	-0.46712200
H	1.00293400	-5.02685300	-1.50445700
H	1.09102100	-4.50281000	0.18648400
C	1.57624400	-2.37110700	-2.84769500
C	2.88356300	-1.64911200	-3.15928200
H	0.75688900	-1.96573200	-3.44900800
H	1.67394600	-3.43716400	-3.09998700
H	3.15240400	-1.81250300	-4.20882500
H	2.79261400	-0.57059900	-2.98992400
H	3.69410700	-2.01718900	-2.52504300

TS4-cf1

C	1.75724900	0.80241500	-1.10281200
C	2.62807100	1.06373300	-2.18051800
C	0.37879500	1.06385900	-1.32526100
C	2.18857900	1.64677100	-3.37067100
H	3.68408100	0.82647600	-2.08099900
C	-0.05996700	1.68846300	-2.50724500
C	0.84181300	1.98643800	-3.52489300
H	2.89964000	1.85196700	-4.16626800
H	-1.11040200	1.93470400	-2.62045400
H	0.49278400	2.46257300	-4.43754200
C	1.63491200	-0.47360900	1.92474400
C	0.25983900	-0.18328600	2.13585800
C	2.25036600	-1.34913200	2.83195600
C	-0.46519300	-0.77910100	3.17900500
C	1.54231900	-1.91363200	3.89718600
C	0.18512800	-1.63152500	4.06678800
H	-1.52773600	-0.58896300	3.26281100
H	2.04755100	-2.58882700	4.58243600
H	-0.37326800	-2.09153000	4.87673800
C	-0.37229000	0.64358600	1.14917700
C	-0.47560900	1.64121800	0.34338600
H	3.29571400	-1.61231700	2.69512200
Pd	-0.87178700	-0.39761200	-0.55507000
O	-3.80770500	-2.47411700	-0.82521100
S	-3.38192600	-2.23688200	0.57394900
O	-3.89679200	-3.12474700	1.61459600
O	-1.89783600	-1.96973900	0.68704400
C	-4.11601200	-0.56450800	0.98143900
F	-5.43763900	-0.65372000	1.14000200
F	-3.58157400	-0.06742700	2.11913300
F	-3.86656400	0.32937000	0.00096400
Si	2.65804800	0.29736900	0.51969800
C	-1.03587300	2.98509900	0.28551700
C	-2.24660900	3.22448500	0.96247300
C	-0.40182900	4.03754000	-0.39463700
C	-2.80202200	4.50205100	0.96525100
H	-2.74484600	2.39535200	1.45421000
C	-0.95938800	5.31420500	-0.37805900
H	0.52570400	3.85020900	-0.92481000
C	-2.15950800	5.54930700	0.29888400
H	-3.74002000	4.67856900	1.48399400
H	-0.45728200	6.12665100	-0.89581800
H	-2.59530500	6.54457100	0.30230300
C	3.88595800	-1.04008800	-0.01685300

C	5.23087900	-0.80317200	-0.35170300
C	3.40192200	-2.35468100	-0.16941700
C	6.05670700	-1.82902100	-0.81929300
H	5.65200100	0.19199900	-0.24793400
C	4.21919200	-3.38313900	-0.63851200
H	2.37218900	-2.58236100	0.09196200
C	5.55199100	-3.12176900	-0.96589200
H	7.09376400	-1.61711100	-1.06686000
H	3.81702400	-4.38752700	-0.74413000
H	6.19280900	-3.92074500	-1.32952500
C	3.50282400	1.87074200	1.26694600
C	4.48897600	1.42732400	2.37117500
H	4.94848900	2.31094400	2.83671400
H	3.98071900	0.86694100	3.16401500
H	5.29826500	0.79908600	1.98375000
C	4.25060700	2.71820300	0.21694300
H	3.57779700	3.07891800	-0.56830200
H	4.69736600	3.59781600	0.70200800
H	5.06508500	2.17258900	-0.27201200
C	2.42011300	2.76376200	1.91373300
H	1.71258900	3.15354200	1.17542000
H	1.84685100	2.22920600	2.67896600
H	2.89442500	3.62861700	2.39936600
N	-1.43333500	-1.59667400	-2.35802200
H	-2.19810100	-2.14898700	-1.95131000
C	-1.98796300	-0.86342100	-3.51676900
C	-3.22435800	-0.05344200	-3.13838200
H	-2.24454700	-1.58159200	-4.31155100
H	-1.19697100	-0.21583700	-3.90982200
H	-3.63027300	0.44593000	-4.02508700
H	-3.99629900	-0.70034300	-2.71188200
H	-2.98855800	0.70689300	-2.38749300
C	-0.32869700	-2.50558500	-2.74509300
C	0.01115500	-3.49211000	-1.63078500
H	0.53994900	-1.88449200	-2.99415200
H	-0.60799500	-3.05971700	-3.65532700
H	0.85055600	-4.12611800	-1.93581600
H	0.28389100	-2.97257000	-0.70734800
H	-0.84572300	-4.13375200	-1.39925700

TS4-cf2

C	1.07019700	-0.03605200	1.84587200
C	1.20450100	0.20049000	3.22964900
C	-0.07591000	0.53817000	1.23643400

C	0.33229900	1.02115200	3.94795200
H	2.01760300	-0.26138000	3.77216700
C	-0.92852000	1.40114800	1.93823800
C	-0.72177500	1.65330700	3.29367800
H	0.48768900	1.16894300	5.01314500
H	-1.78614500	1.83554200	1.44279000
H	-1.40688700	2.30236800	3.83179600
C	2.08561300	-2.03602900	-0.46523400
C	1.29075400	-1.52499300	-1.53278700
C	2.57552900	-3.33973300	-0.61637000
C	1.13713700	-2.23842500	-2.72962700
C	2.37882000	-4.07654000	-1.79029800
C	1.69728200	-3.50827500	-2.86522500
H	0.56744700	-1.79884700	-3.54104000
H	2.77768800	-5.08416400	-1.86681400
H	1.57660500	-4.05769100	-3.79455900
C	0.55706000	-0.31183600	-1.27035200
C	0.41215300	0.87860400	-0.81264500
H	3.13120900	-3.80440200	0.18904500
Pd	-1.16043600	-0.48953600	-0.17743200
O	-5.23000800	-0.58989100	2.13951400
S	-4.37510200	-0.42126400	0.96713000
O	-4.81479100	-1.04348800	-0.30652200
O	-2.90595300	-0.64723400	1.24536200
C	-4.42592000	1.40290300	0.58963800
F	-5.63122000	1.76657000	0.14782000
F	-3.51326800	1.71133000	-0.36277200
F	-4.12952900	2.12574600	1.68322500
Si	2.56544900	-0.80785900	0.92102700
C	0.66452500	2.27028600	-1.14370700
C	1.17908800	2.52365800	-2.43245500
C	0.46953100	3.34945800	-0.26843400
C	1.50413700	3.81807900	-2.82184000
H	1.32685000	1.69055600	-3.11200600
C	0.78143900	4.64604900	-0.67132300
H	0.09713200	3.17031600	0.73095500
C	1.30252600	4.88664500	-1.94386600
H	1.91093000	3.99349300	-3.81374000
H	0.62328300	5.47068200	0.01803500
H	1.54738700	5.89944000	-2.25167700
C	3.41476300	0.63435400	0.03179600
C	4.06297200	0.46231500	-1.20454900
C	3.44087200	1.91535300	0.61097200
C	4.70392800	1.52733500	-1.84042100

H	4.05782000	-0.51242600	-1.68613300
C	4.07955200	2.98408500	-0.01990600
H	2.93336700	2.08869100	1.55696400
C	4.71084100	2.79275200	-1.24984700
H	5.19260100	1.37057600	-2.79894600
H	4.06723000	3.96879300	0.43924900
H	5.19931900	3.62594200	-1.74812200
C	3.92440200	-1.55896200	2.08836500
C	4.54976500	-0.48077600	3.01129300
H	5.39482300	-0.92250300	3.55789800
H	4.93645200	0.36584700	2.43427100
H	3.86294300	-0.08199700	3.76059100
C	5.10427500	-2.05706900	1.21107400
H	5.90345700	-2.43729100	1.86273200
H	4.83864500	-2.86257000	0.52453800
H	5.52718300	-1.24168300	0.61381300
C	3.38220400	-2.72245600	2.94534900
H	4.18505500	-3.14455000	3.56663800
H	2.58045900	-2.40103700	3.61954700
H	2.97980000	-3.53871700	2.33453800
N	-2.34474200	-1.85081900	-1.52840100
H	-3.26605600	-1.71315300	-1.09296500
C	-2.47887800	-1.42602600	-2.93922300
C	-2.98546100	0.00858100	-3.05862400
H	-3.16453000	-2.11195600	-3.46144200
H	-1.49945800	-1.52776000	-3.41710600
H	-3.15179600	0.25986600	-4.11197900
H	-3.92700200	0.13232800	-2.51635800
H	-2.26076400	0.71758000	-2.64545000
C	-1.99655400	-3.28467200	-1.40059200
C	-1.89105100	-3.71447800	0.06035200
H	-1.04387800	-3.44802800	-1.91339000
H	-2.75698600	-3.88946600	-1.91941000
H	-1.73228200	-4.79657800	0.12267900
H	-1.04883200	-3.21772400	0.55632100
H	-2.80016000	-3.46071600	0.61432100

TS4-cf3

C	-1.16489000	0.20974600	1.69598600
C	-1.53040100	0.23647500	3.05493300
C	-0.76330000	-1.06359300	1.19444300
C	-1.64175500	-0.92173200	3.83219400
H	-1.75869900	1.18198100	3.52811800
C	-0.94193500	-2.23712200	1.94575100

C	-1.39711700	-2.17145200	3.26149600
H	-1.94625800	-0.84339200	4.87225100
H	-0.70303400	-3.19617600	1.49650900
H	-1.52157300	-3.08167000	3.84226200
C	-0.33008200	2.10513700	-0.79415100
C	0.05343900	1.04569900	-1.67021200
C	0.24066600	3.35860100	-1.05337300
C	0.91485800	1.25585400	-2.75771000
C	1.09244500	3.57595700	-2.14067400
C	1.41303800	2.53067600	-3.00570200
H	1.21814100	0.41055400	-3.36394500
H	1.51680700	4.56329900	-2.29965300
H	2.08751000	2.69414200	-3.84031100
C	-0.34063400	-0.27600200	-1.28119800
C	-1.12546400	-1.16158300	-0.77990100
H	0.04057100	4.19342100	-0.39400800
Pd	0.98612600	-1.04863700	0.10816500
O	4.99462200	-0.38140200	-2.23738700
S	4.12667100	-0.38852900	-1.06131500
O	4.65032700	-1.02394500	0.17457900
O	2.69903400	-0.78523700	-1.35858200
C	3.95669400	1.41455100	-0.57040500
F	4.93057300	1.75952100	0.28263900
F	2.77359000	1.63319000	0.04330000
F	4.02626000	2.21045000	-1.64311100
Si	-1.61180400	1.72032100	0.57210100
C	-2.13875800	-2.12495600	-1.18121900
C	-2.10920900	-2.58469500	-2.51329500
C	-3.15891900	-2.57120900	-0.32706500
C	-3.08481700	-3.46171800	-2.97725800
H	-1.30950500	-2.24801500	-3.16579300
C	-4.13310500	-3.44819300	-0.79837700
H	-3.19898000	-2.21101500	0.69243500
C	-4.10017500	-3.89676000	-2.12041700
H	-3.04970700	-3.80992900	-4.00565700
H	-4.92506400	-3.77640300	-0.13102300
H	-4.85980000	-4.58463100	-2.48155000
C	-3.19697500	1.15425100	-0.30005500
C	-3.42231000	1.39380600	-1.66690800
C	-4.20677300	0.49235400	0.42239600
C	-4.60119400	0.97872400	-2.28971300
H	-2.66173000	1.89664500	-2.25849400
C	-5.39193400	0.08505200	-0.19202100
H	-4.05917500	0.27289900	1.47751900

C	-5.58980500	0.32311400	-1.55317800
H	-4.74639900	1.16545600	-3.35069500
H	-6.15334300	-0.43078300	0.38767600
H	-6.50599600	-0.00380200	-2.03772800
C	-2.08486600	3.31873800	1.56628100
C	-3.29931300	3.11119300	2.50686400
H	-3.57692800	4.07833000	2.94920000
H	-4.17221800	2.73807600	1.96179900
H	-3.11057800	2.42865000	3.33791100
C	-2.55985200	4.39397400	0.55180900
H	-2.86539000	5.29772700	1.09756300
H	-1.79980300	4.69494400	-0.16996300
H	-3.42868500	4.04217100	-0.01619200
C	-0.88866000	3.84582300	2.38773000
H	-1.15879500	4.77991200	2.90078400
H	-0.57407600	3.12943700	3.15619100
H	-0.01155100	4.05489700	1.76581100
N	2.37798100	-1.83040500	1.67784000
H	3.27383600	-1.55637400	1.25129700
C	2.27621200	-1.15723600	2.99339900
C	2.51810900	0.34576900	2.88645900
H	3.00996200	-1.60228000	3.68426000
H	1.28018700	-1.35793400	3.39985200
H	2.49399400	0.79706100	3.88448800
H	3.49216600	0.55902100	2.43478800
H	1.74905900	0.82673700	2.27543300
C	2.39789100	-3.30470600	1.80453600
C	2.59516500	-3.98492500	0.45241300
H	1.45640600	-3.61822000	2.26935500
H	3.20742300	-3.59690800	2.49186600
H	2.70676200	-5.06659500	0.58566900
H	1.74136700	-3.80280200	-0.21033700
H	3.49064500	-3.59776900	-0.04403700

TS11-cf1

C	-3.21368700	-0.69158000	-1.19871100
C	-3.83547400	-1.45174100	-2.21573300
C	-2.02115100	-0.04263200	-1.54980700
C	-3.32219500	-1.52870000	-3.50900700
H	-4.74988800	-1.98941800	-1.99029500
C	-1.54544100	-0.03366000	-2.86610700
C	-2.18667100	-0.79392200	-3.84693400
H	-3.82483500	-2.13766800	-4.25482800
H	-0.66204700	0.54064100	-3.13248500

H	-1.79992600	-0.80442300	-4.86282100
C	-4.54051500	1.56902500	0.10291500
C	-3.55482600	2.44164500	-0.41149000
C	-5.80796600	2.11437400	0.37383000
C	-3.87670200	3.78547400	-0.70645500
C	-6.11683600	3.44960300	0.11363900
C	-5.14887400	4.28333100	-0.44766900
H	-3.11264600	4.43848600	-1.11587300
H	-7.10964000	3.83105800	0.33448400
H	-5.37790300	5.31943900	-0.67985300
H	-6.58217700	1.47120100	0.78155100
Si	-4.23873400	-0.28299300	0.35427700
C	-2.13268700	2.16489500	-0.55416400
C	-0.99488700	2.70594200	-0.62119700
C	-0.32365100	3.99066200	-0.51606800
C	0.55995100	4.46500700	-1.49602900
C	-0.65849400	4.82342600	0.56961900
C	1.11594300	5.73888600	-1.38274600
H	0.80013500	3.84508500	-2.34919500
C	-0.10301900	6.09430100	0.67442400
H	-1.34440000	4.45794400	1.32578400
C	0.79068100	6.55451400	-0.29754100
H	1.79933200	6.09375000	-2.14873200
H	-0.36115700	6.72280900	1.52146600
H	1.22645200	7.54571400	-0.21079500
C	-3.56992800	-0.50680500	2.15977000
C	-5.88517900	-1.19439300	0.12367200
C	-6.19789000	-2.39274400	0.79216600
C	-6.81172700	-0.73450500	-0.83538600
C	-7.37987500	-3.09042200	0.53228700
H	-5.51856500	-2.79883800	1.53400600
C	-7.99553500	-1.42437800	-1.09914000
H	-6.60449500	0.17515100	-1.39267600
C	-8.28476200	-2.60579300	-0.41275500
H	-7.59311300	-4.01012900	1.07049500
H	-8.69050000	-1.04048000	-1.84114900
H	-9.20635800	-3.14459700	-0.61478400
P	1.80624600	1.33207800	0.49446900
P	0.38428600	-1.70704400	-0.32115400
C	-1.81735700	-5.41070200	-2.07416600
C	-0.51586500	-5.13425600	-2.49661100
C	0.15511100	-4.00425500	-2.02616000
C	-0.47653900	-3.12292600	-1.13203300
C	-1.77308700	-3.42817400	-0.69422300

C	-2.44111200	-4.55724000	-1.16362800
H	1.17254400	-3.82624600	-2.35405700
H	-2.26780500	-2.78378100	0.01645100
C	1.32304800	4.66088800	3.68754500
C	2.28568400	4.82010200	2.69001100
C	2.44815500	3.84712100	1.70196100
C	1.64048400	2.70351400	1.70269900
C	0.65509100	2.56141300	2.69467400
C	0.50304700	3.52933200	3.68579700
H	3.18390200	4.00035200	0.92156700
H	0.00381300	1.69348700	2.69293200
C	4.55013600	2.66618800	-2.99201500
C	5.04342600	2.65280500	-1.68488000
C	4.22028800	2.26221700	-0.63030000
C	2.88432700	1.90141700	-0.87081400
C	2.40510900	1.89903100	-2.18666200
C	3.23175200	2.28265100	-3.24169200
H	4.62530600	2.20937600	0.37610600
H	1.38827200	1.57641600	-2.38510400
C	1.21070500	-3.66357900	3.80335300
C	1.44600300	-4.38225900	2.62831400
C	1.21338100	-3.79245800	1.38824800
C	0.75721800	-2.46582000	1.31087100
C	0.51808600	-1.75517500	2.49304800
C	0.74293100	-2.35081100	3.73368900
H	1.38746700	-4.36370300	0.48230000
H	0.16092700	-0.73347200	2.44421900
H	7.67921400	-0.40243500	-1.50638400
C	3.17382400	-1.20907700	-0.73739900
C	1.93384200	-1.49335800	-1.30009300
C	1.77328600	-1.45677400	-2.71843000
H	0.78767500	-1.60239000	-3.14723000
C	2.84719300	-1.24657700	-3.54447000
H	2.71068400	-1.23271700	-4.62292600
C	4.14710100	-1.04558800	-3.01272200
C	4.31486500	-1.00733800	-1.59104300
H	5.76578500	-0.70854600	-0.00550900
C	5.61758900	-0.75706800	-1.07749600
C	6.69205800	-0.58287000	-1.92215500
H	7.37754000	-0.49148800	-3.97911500
C	6.52179600	-0.63155500	-3.32511000
H	5.12559300	-0.88411900	-4.93348400
C	5.27107400	-0.85263800	-3.85667100
H	5.75883600	-4.85144000	3.60573100

C	3.80261800	-0.67353600	3.49885400
H	3.98669500	-0.52148100	4.55932900
C	3.13490100	0.28396700	2.77441200
H	2.79802600	1.18297100	3.27492500
C	2.87688900	0.10605600	1.38779100
C	3.34932200	-1.03842000	0.74032500
C	4.03088200	-2.05248800	1.48561000
C	4.24191200	-1.87404300	2.89070000
H	5.02439000	-2.75724400	4.70365500
C	4.87265000	-2.90417600	3.63744200
C	5.27977800	-4.06785900	3.02595000
H	5.40194700	-5.16726900	1.15985700
C	5.07719900	-4.24634700	1.63560200
H	4.31579800	-3.41467200	-0.17819400
C	4.47155200	-3.26468700	0.88430000
H	-2.33623000	-6.29030600	-2.44416400
H	1.20361900	5.41914800	4.45609500
H	5.19826800	2.95530600	-3.81388400
H	1.39052300	-4.12736600	4.76883500
H	-0.01308400	-5.80256200	-3.18993800
H	-3.45062200	-4.76189000	-0.81843700
H	2.91030200	5.70841000	2.67205400
H	-0.25912400	3.40310900	4.44960300
H	0.55732800	-1.78544500	4.64225500
H	1.81521600	-5.40209600	2.67686300
H	2.85068300	2.26458200	-4.25876400
H	6.07642600	2.92404700	-1.48929300
Pd	-0.41526900	0.60019600	-0.34880400
C	-4.76207000	-0.22836800	3.10889300
H	-5.56156400	-0.96792000	3.01275900
H	-4.41218800	-0.24994900	4.15052900
H	-5.19854600	0.76187900	2.93163500
C	-2.98629000	-1.90044300	2.46350400
H	-2.06047500	-2.08224200	1.91373900
H	-2.73462800	-1.97579400	3.53085400
H	-3.67570100	-2.71961300	2.23809400
C	-2.48243800	0.54255700	2.46659700
H	-1.61492200	0.42170900	1.80863300
H	-2.84610900	1.56806600	2.34282100
H	-2.13632200	0.42977600	3.50495600

TS12-cf1

C	2.14677000	1.38496300	-1.46175500
C	2.06994200	0.12348200	-1.65102900

C	2.78335000	-1.08310900	-1.98279800
C	1.97840400	1.55392500	0.63873400
C	3.58018500	-1.63871900	-0.95314200
C	2.96376900	0.74749500	1.25964000
C	2.33800500	3.36031200	2.22083000
H	2.10841600	4.36780200	2.55618400
C	3.23541200	2.55526400	2.92087600
H	3.72790200	2.92468100	3.81585400
C	3.55078800	1.28869000	2.42931800
H	4.32689500	0.72627400	2.93877100
C	1.72918000	2.86103600	1.07239200
H	1.07089000	3.49970100	0.50440200
C	3.55002000	-2.72848300	-3.57528200
H	3.52989500	-3.15349100	-4.57419300
C	4.37645600	-3.27518200	-2.59139000
H	5.01524100	-4.12206300	-2.82560800
C	4.38858200	-2.73357200	-1.30422200
H	5.06005700	-3.16331500	-0.56656500
C	2.75204100	-1.62892300	-3.27305100
H	2.11231100	-1.18202100	-4.02735800
C	2.97087600	-2.23802400	2.10902300
Si	3.71964500	-0.97486700	0.83619100
C	5.58598200	-0.74490300	1.05053000
C	6.44082400	-1.75320900	1.53125100
C	6.18093800	0.45084000	0.60262200
C	7.82567500	-1.57455900	1.57413400
H	6.03256400	-2.69636400	1.88216000
C	7.56306000	0.63529200	0.64008700
H	5.55472300	1.25538600	0.22301500
C	8.39027400	-0.37848700	1.12925300
H	8.46136400	-2.36868100	1.95649700
H	7.99496200	1.56878400	0.28910500
H	9.46697900	-0.23701400	1.16252500
C	2.36345100	2.68029100	-2.07395500
C	1.71383100	2.94002100	-3.29729600
C	3.20320000	3.66023500	-1.51885900
C	1.89504100	4.15983000	-3.94428800
H	1.07033400	2.17614700	-3.72401300
C	3.38386200	4.87580000	-2.17440100
H	3.70991300	3.46235700	-0.58134000
C	2.72700600	5.13251800	-3.38147200
H	1.39109500	4.35055900	-4.88751600
H	4.04082700	5.62518300	-1.74290900
H	2.86767700	6.08468800	-3.88476500

P	-1.03881300	-1.36068800	-1.18787000
P	-1.46878200	1.53990700	0.75525600
C	-0.83427200	6.01849200	-0.29885800
C	-1.22018700	5.67202800	0.99720100
C	-1.45368700	4.33496100	1.33092500
C	-1.30357600	3.33230500	0.36460800
C	-0.92865400	3.69151600	-0.94197100
C	-0.69296900	5.02408500	-1.27186500
H	-1.73186800	4.07634700	2.34717500
H	-0.78642300	2.92237700	-1.69431500
C	0.92248000	-5.11422500	-3.12835300
C	-0.09627200	-4.44248800	-3.80345200
C	-0.69345300	-3.31196100	-3.24080000
C	-0.27094400	-2.83203000	-1.99093300
C	0.78998600	-3.49018900	-1.34578000
C	1.36655400	-4.63126200	-1.89595900
H	-1.48861300	-2.81437200	-3.78250700
H	1.17968600	-3.10399300	-0.41420300
C	-3.91920900	0.17680300	-4.46935600
C	-4.22447200	-1.00377700	-3.78694200
C	-3.37435400	-1.47137900	-2.78627700
C	-2.21483300	-0.75555100	-2.45146800
C	-1.91091600	0.42338800	-3.14619000
C	-2.76011800	0.88772800	-4.15142900
H	-3.62132100	-2.38326900	-2.25239200
H	-1.00994700	0.97596500	-2.89463600
C	-1.64984300	1.35927100	5.37829700
C	-2.79953900	1.68805900	4.65629100
C	-2.76054800	1.73825300	3.26309500
C	-1.56807900	1.45525400	2.57976400
C	-0.41362700	1.13802800	3.31110600
C	-0.45670700	1.08939500	4.70423600
H	-3.65766200	1.98993700	2.70586100
H	0.51769700	0.93992300	2.79455500
H	-7.20158400	-2.95195100	-0.91461400
C	-3.70190700	-0.12528300	0.22358700
C	-3.17288100	1.16036600	0.14678900
C	-3.93069400	2.19782400	-0.47009900
H	-3.53282700	3.20321700	-0.50991000
C	-5.16298900	1.94897400	-1.01830200
H	-5.72147800	2.75420100	-1.48871600
C	-5.72256400	0.64884300	-0.98814700
C	-4.99503900	-0.40065700	-0.34172700
H	-5.04229400	-2.51525000	0.15513900

C	-5.57205400	-1.70308300	-0.32833100
C	-6.78463400	-1.94909300	-0.93315900
H	-8.45290800	-1.11494100	-2.04515400
C	-7.49605300	-0.90672500	-1.57530300
H	-7.51111700	1.17652000	-2.08283200
C	-6.97438600	0.36638500	-1.59586400
H	-4.78218400	-2.82219300	5.70294800
C	-1.99228900	-3.60732200	2.11404400
H	-1.61702700	-4.52465100	2.56069200
C	-1.52868400	-3.20501200	0.88657500
H	-0.79850200	-3.82282900	0.38192200
C	-1.99502000	-2.01069200	0.26760800
C	-3.00086400	-1.26818700	0.89483500
C	-3.49968600	-1.68050800	2.17853800
C	-2.96383400	-2.84906000	2.80943600
H	-3.01729400	-4.12718100	4.55361500
C	-3.43990000	-3.23974100	4.08951900
C	-4.42174500	-2.51603900	4.72524100
H	-5.75606300	-0.81072000	4.59777200
C	-4.97333300	-1.37337200	4.09697900
H	-4.96609700	-0.09536100	2.39170400
C	-4.52926800	-0.96951900	2.85860900
H	-0.63918500	7.05712800	-0.54981100
H	1.37737400	-5.99878900	-3.56471800
H	-4.58547800	0.54257500	-5.24533800
H	-1.68459400	1.31408500	6.46305400
H	-1.33204900	6.44118400	1.75617800
H	-0.37245700	5.27915800	-2.27735900
H	-0.43872900	-4.80014400	-4.77039500
H	2.18142900	-5.12349700	-1.37488400
H	0.44235100	0.83826100	5.25976400
H	-3.72969500	1.89725300	5.17655200
H	-2.52025400	1.80577300	-4.68062300
H	-5.13229800	-1.55199200	-4.01901200
Pd	0.42879200	0.41223300	-0.32958900
C	3.25080000	-3.70034100	1.69554300
H	2.85181000	-3.93850000	0.70513900
H	4.32030100	-3.93630100	1.68049700
H	2.78120100	-4.38436200	2.41583700
C	1.44450100	-2.03151500	2.19266700
H	1.18929500	-1.07127300	2.64667700
H	0.95148600	-2.05849000	1.21712200
H	0.98176200	-2.81680700	2.80534200
C	3.54305000	-2.01029000	3.52753700

H	3.28507600	-1.01894100	3.91442600
H	3.11066600	-2.74699000	4.21901500
H	4.63099400	-2.11545100	3.57049100

TS33

C	3.31458100	-0.54703700	-1.13715300
C	4.11896400	-1.13780900	-2.14027200
C	2.12572100	0.06119400	-1.56759900
C	3.75567000	-1.13900100	-3.48552600
H	5.06456400	-1.59224200	-1.86612700
C	1.78896900	0.13333000	-2.92624100
C	2.58782500	-0.48959400	-3.88678700
H	4.39969300	-1.61478500	-4.21981400
H	0.89775100	0.66438100	-3.24842000
H	2.30388200	-0.45159800	-4.93510500
C	4.63568900	1.65167700	0.00865600
C	3.63181600	2.49447800	-0.53592700
C	5.95150300	2.13744000	-0.01404700
C	3.96276600	3.75455400	-1.07666800
C	6.27763200	3.39374200	-0.53079900
C	5.27868300	4.20645700	-1.06341000
H	3.17557400	4.37792100	-1.48889000
H	7.31159200	3.72678600	-0.52813400
H	5.51883900	5.18135500	-1.47740000
H	6.75786400	1.51589600	0.35447500
Pd	0.37362800	0.66021100	-0.52972500
Si	4.19868200	-0.13023800	0.50118700
C	2.20329400	2.25007900	-0.51531800
C	1.05484500	2.74466400	-0.37672400
C	0.38525900	4.00458800	-0.09618000
C	0.26145500	4.95571400	-1.12374900
C	-0.05170600	4.32780800	1.19732500
C	-0.29482900	6.20414700	-0.85718900
H	0.58725900	4.70164400	-2.12683300
C	-0.61023300	5.57842500	1.45548600
H	0.05976100	3.60802500	1.99751500
C	-0.73538200	6.51918900	0.43099900
H	-0.39134400	6.92905700	-1.65995800
H	-0.94122100	5.81769900	2.46202600
H	-1.17152200	7.49285200	0.63460200
P	-0.32316000	-1.64884900	-0.38379900
P	-1.98016500	1.34779300	-0.15586400
C	-2.89473600	4.91028400	-2.98527000
C	-3.34627000	4.96367200	-1.66660400

C	-3.06863600	3.92022400	-0.78045600
C	-2.32504600	2.81469000	-1.20749900
C	-1.84532900	2.78292700	-2.52848000
C	-2.13707800	3.81721200	-3.41499900
H	-3.41377300	3.98649000	0.24460700
H	-1.24329900	1.94287400	-2.86517100
C	2.57551500	-5.28335100	-0.33618700
C	1.69126800	-5.12459900	0.73135200
C	0.82485500	-4.02971300	0.77389500
C	0.84797500	-3.06630500	-0.24715200
C	1.71751400	-3.25365100	-1.33515300
C	2.57584900	-4.35037400	-1.37594500
H	0.12959000	-3.94631800	1.60036600
H	1.71143400	-2.55822300	-2.16564900
C	-2.67678100	-3.23652500	-4.04888300
C	-2.45319100	-4.06598600	-2.94634900
C	-1.76198700	-3.58405800	-1.83810700
C	-1.30429000	-2.25613700	-1.81329300
C	-1.52383900	-1.43432700	-2.92433200
C	-2.20753100	-1.92254900	-4.03838300
H	-1.58055300	-4.23853300	-0.99132000
H	-1.17030300	-0.40975100	-2.91140500
C	-3.17818500	2.22825700	4.22669700
C	-4.14410700	2.29598100	3.21899400
C	-3.79175600	2.04670000	1.89378900
C	-2.46074200	1.74521300	1.56243900
C	-1.50223600	1.66293500	2.58021200
C	-1.85835700	1.90734800	3.90588700
H	-4.55563600	2.05879400	1.12167100
H	-0.48417000	1.38386400	2.33787500
H	-5.45984900	-5.25325800	-0.12792800
C	-3.46062500	-1.07763200	-0.07140900
C	-3.29979200	0.15542200	-0.70645800
C	-4.09572800	0.46081900	-1.84486100
H	-4.00686900	1.42688900	-2.32401800
C	-4.98028200	-0.45631700	-2.35879400
H	-5.57388600	-0.20483200	-3.23402600
C	-5.12400400	-1.73854200	-1.77688000
C	-4.37044900	-2.04742400	-0.59962600
H	-3.95580100	-3.58607500	0.87239900
C	-4.52095900	-3.33797500	-0.01908900
C	-5.36152500	-4.27148000	-0.58217700
H	-6.75872300	-4.71134200	-2.18423500
C	-6.09996300	-3.96425800	-1.75116700

H	-6.54839100	-2.47596600	-3.22833000
C	-5.98446200	-2.72215600	-2.33235200
H	-5.24975800	-1.21859500	5.88828500
C	-1.27313400	-1.68346900	3.59588800
H	-0.70868200	-1.76384600	4.52143700
C	-0.62364800	-1.75392700	2.39031400
H	0.45042300	-1.87525100	2.38137300
C	-1.33708400	-1.65852500	1.15897400
C	-2.70293800	-1.38986200	1.17984700
C	-3.40458100	-1.33599000	2.43446400
C	-2.67790500	-1.50244900	3.65696100
H	-2.79997200	-1.57968700	5.81398900
C	-3.36774100	-1.45233400	4.89583900
C	-4.72864100	-1.24881100	4.93583300
H	-6.52362700	-0.90810400	3.76853900
C	-5.45083000	-1.07439400	3.73222100
H	-5.37492800	-0.96372200	1.60416400
C	-4.80672600	-1.10778200	2.51507900
H	-3.11949500	5.72109300	-3.67218400
H	3.24779100	-6.13610000	-0.36611700
H	-3.21383000	-3.61580100	-4.91337000
H	-3.45933000	2.40798500	5.26011200
H	-3.91362700	5.82202700	-1.31900600
H	-1.76757900	3.77459500	-4.43581500
H	1.66421300	-5.85719000	1.53280800
H	3.24627200	-4.46901600	-2.22205000
H	-1.10787800	1.82922200	4.68725700
H	-5.17664700	2.52141200	3.46826700
H	-2.37835700	-1.27335600	-4.89235100
H	-2.82160100	-5.08720200	-2.94774800
C	5.66492900	-1.31674100	0.68271000
C	6.90948800	-0.98555700	1.24991700
C	5.43897100	-2.67774200	0.38579800
C	7.89304000	-1.95240300	1.47325600
H	7.12294100	0.03475000	1.55203300
C	6.41398900	-3.64942900	0.61173600
H	4.48220600	-2.99172700	-0.02247600
C	7.65082400	-3.28775000	1.14935900
H	8.84573100	-1.66084100	1.90694500
H	6.20439500	-4.68852600	0.37100600
H	8.41484800	-4.04029900	1.32353500
C	3.36417800	-0.19006300	2.24788100
C	2.06653600	0.61962800	2.37960000
C	3.09734700	-1.65959000	2.63812700

C	4.38835600	0.40977100	3.24229600
H	2.21817400	1.68131300	2.16070500
H	1.28688500	0.25364600	1.70357700
H	1.67784000	0.53947000	3.40584900
H	4.02482500	-2.23192400	2.72905900
H	2.58687500	-1.70350400	3.61153100
H	2.47230300	-2.17736500	1.90322600
H	3.96907600	0.38605400	4.25798700
H	5.32454600	-0.15638900	3.26540300
H	4.62268800	1.45501800	3.00688800

TS34

C	-2.36395800	-0.59203700	1.72128600
C	-1.96114100	0.59450900	1.47716700
C	-2.41342400	1.93128100	1.17359400
C	-2.02794000	-1.63817800	0.01613300
C	-3.15239500	2.06506500	-0.03158900
C	-3.02997400	-1.14984200	-0.85922500
C	-2.57736700	-3.94624100	-0.50295600
H	-2.39958900	-5.00889800	-0.36731700
C	-3.56381900	-3.49501500	-1.38361200
H	-4.17891800	-4.20738000	-1.92604500
C	-3.78061300	-2.12673500	-1.55158700
H	-4.58454300	-1.81074400	-2.21043200
C	-1.82055700	-3.01738200	0.20158100
H	-1.06738300	-3.35629600	0.90651000
C	-2.66986700	4.28005800	1.68092600
H	-2.48577300	5.12674100	2.33579400
C	-3.42037300	4.43965700	0.51462900
H	-3.83045500	5.41225600	0.25800400
C	-3.66989400	3.34169700	-0.31336700
H	-4.30515200	3.48385900	-1.18206600
C	-2.17688200	3.02286800	2.02085500
H	-1.62611500	2.87512200	2.94137500
Si	-3.57116000	0.66282000	-1.26857300
Pd	-0.37469300	-0.34904400	0.42535500
P	1.30733100	1.28899700	1.13493800
P	1.27003900	-1.66590800	-0.77829200
C	-0.62097400	-4.76708000	-3.69206000
C	0.37083300	-5.17813000	-2.80165400
C	0.96995100	-4.26040000	-1.93580400
C	0.57928900	-2.91240200	-1.94710600
C	-0.44403600	-2.51879500	-2.82554300
C	-1.02731000	-3.43105300	-3.70039000

H	1.73204500	-4.60820600	-1.24925000
H	-0.80798100	-1.50050900	-2.80797400
C	0.20168500	2.61466600	5.45106900
C	0.02818400	1.28901000	5.04288000
C	0.36387300	0.90848700	3.74362000
C	0.89687100	1.84469500	2.84115200
C	1.08158300	3.16876400	3.26333500
C	0.73025700	3.55074100	4.55998100
H	0.21095500	-0.11894600	3.42661900
H	1.48407600	3.90772500	2.57905200
C	1.62345000	5.29780400	-1.15589200
C	0.42152800	4.58670200	-1.12306400
C	0.34968000	3.36887000	-0.44847900
C	1.47897600	2.85154600	0.20122000
C	2.67565000	3.58159600	0.18646200
C	2.74788700	4.79537600	-0.49722900
H	-0.58721300	2.82859100	-0.41517300
H	3.55108800	3.19773500	0.69874200
C	4.03752100	-4.15668200	1.97212500
C	4.35641600	-4.01983900	0.61851700
C	3.54102300	-3.25948500	-0.21697400
C	2.39470400	-2.62924400	0.29447900
C	2.08110400	-2.77222100	1.65321700
C	2.90061100	-3.53262100	2.48876800
H	3.80378200	-3.13964600	-1.26356000
H	1.20347300	-2.27346700	2.05713700
H	6.34471000	3.73777600	-1.85265600
C	3.26811700	0.32263900	-1.20758500
C	2.29562800	-0.49629300	-1.78821400
C	1.94029900	-0.30142200	-3.15290800
H	1.21642600	-0.95554600	-3.62017200
C	2.50640400	0.69904600	-3.90215200
H	2.21144900	0.83304200	-4.93983000
C	3.49458000	1.55074400	-3.35177200
C	3.91042200	1.33776000	-1.99825900
H	5.31819000	1.98995300	-0.47944000
C	4.96359100	2.15116700	-1.49034800
C	5.54097100	3.13306700	-2.26318200
H	5.55984700	4.14402600	-4.18486600
C	5.09922700	3.36189500	-3.58852700
H	3.76200100	2.73400200	-5.14217800
C	4.09886000	2.58154600	-4.12003600
H	8.36661200	-2.43252300	1.01739400
C	4.72838300	-0.24812600	2.82354400

H	5.10459300	-0.38881200	3.83363500
C	3.53524300	0.39805300	2.61933800
H	2.98637600	0.76711700	3.47600200
C	3.01160700	0.58625500	1.30864500
C	3.73805400	0.13493300	0.20540200
C	4.99998400	-0.52219100	0.40356600
C	5.48605200	-0.73744700	1.73275500
H	7.05791300	-1.59360500	2.94623700
C	6.70693500	-1.43552400	1.92971900
C	7.43297800	-1.90103800	0.85758700
H	7.54312100	-2.04505900	-1.30401000
C	6.96421100	-1.68095400	-0.46002800
H	5.43575000	-0.85774100	-1.69705400
C	5.78208500	-1.01055300	-0.68182600
H	-1.08133200	-5.48300800	-4.36687700
H	-0.07108700	2.91421700	6.45880900
H	1.68364600	6.24204700	-1.68950600
H	4.67910200	-4.74319000	2.62331300
H	0.68600800	-6.21749500	-2.77761700
H	-1.81278400	-3.10132900	-4.37396700
H	-0.37210900	0.55368900	5.73553200
H	0.87021300	4.58167100	4.87223800
H	2.65445100	-3.63088000	3.54218900
H	5.25083500	-4.48635900	0.21789500
H	3.68593700	5.34164800	-0.52228100
H	-0.46267400	4.97528400	-1.62014700
C	-3.10269900	-1.39466200	2.67525900
C	-2.86889300	-1.16707100	4.04545100
C	-4.10000100	-2.30708000	2.28457200
C	-3.61157600	-1.84966300	5.00577300
H	-2.11431500	-0.44429300	4.33635600
C	-4.84383400	-2.97630500	3.25235300
H	-4.30344000	-2.46784300	1.23305200
C	-4.59755600	-2.75799300	4.61165500
H	-3.42446300	-1.67011500	6.06057500
H	-5.62140900	-3.66943200	2.94503500
H	-5.17662600	-3.29018300	5.36080600
C	-5.45811800	0.58566700	-1.23746600
C	-6.30319700	0.65158800	-2.35784300
C	-6.05897400	0.40229900	0.02488300
C	-7.69073800	0.54111100	-2.22666700
H	-5.88846300	0.79134200	-3.35096000
C	-7.44126100	0.28681100	0.16176100
H	-5.43763300	0.34897400	0.91735300

C	-8.26219600	0.35724200	-0.96745500
H	-8.32269100	0.59903000	-3.10886000
H	-7.87880400	0.14550700	1.14647900
H	-9.34041500	0.27088200	-0.86480700
C	-2.82065700	1.09348600	-3.00557100
C	-1.29024600	1.24572800	-2.86499000
C	-3.11684300	-0.03228700	-4.02385200
C	-3.37026400	2.41973700	-3.57918900
H	-1.02290900	2.17909600	-2.36598800
H	-0.82398700	0.43630800	-2.29222700
H	-0.81110000	1.26106400	-3.85352900
H	-4.18876800	-0.17276300	-4.19724700
H	-2.66106000	0.21890400	-4.99157400
H	-2.71064800	-0.99593400	-3.70769000
H	-2.95944700	2.58230600	-4.58542700
H	-4.46153500	2.42848500	-3.66598800
H	-3.07296900	3.27895900	-2.97053600