

Supporting Information

Insight into the Mechanism of the Arylation of Arenes via Norbornene Relay Palladation through *meta*- to *para*-Selectivity

Shengnan Liu, Qiong Wang, Fang Huang, Wenjuan Wang, Chong Yang, Jianbiao Liu* and
Dezhan Chen*

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

Table of Contents

I. Catalytically active species considered by computations.....	S2
II. Possible CMD mechanisms.....	S3
III. Possible C-H activation pathway.....	S4
IV. Free energy profiles for the norbornene insertion.....	S4
V. Free energy profiles for the NBE relay palladation through <i>para</i> - to <i>meta</i> -position....	S6
VI. Distortion-interaction analysis.....	S8
VII. Calculated energies and imaginary frequencies.....	S9
VIII. Cartesian coordinates of all the structures.....	S14

I. Catalytically active species considered by computations.

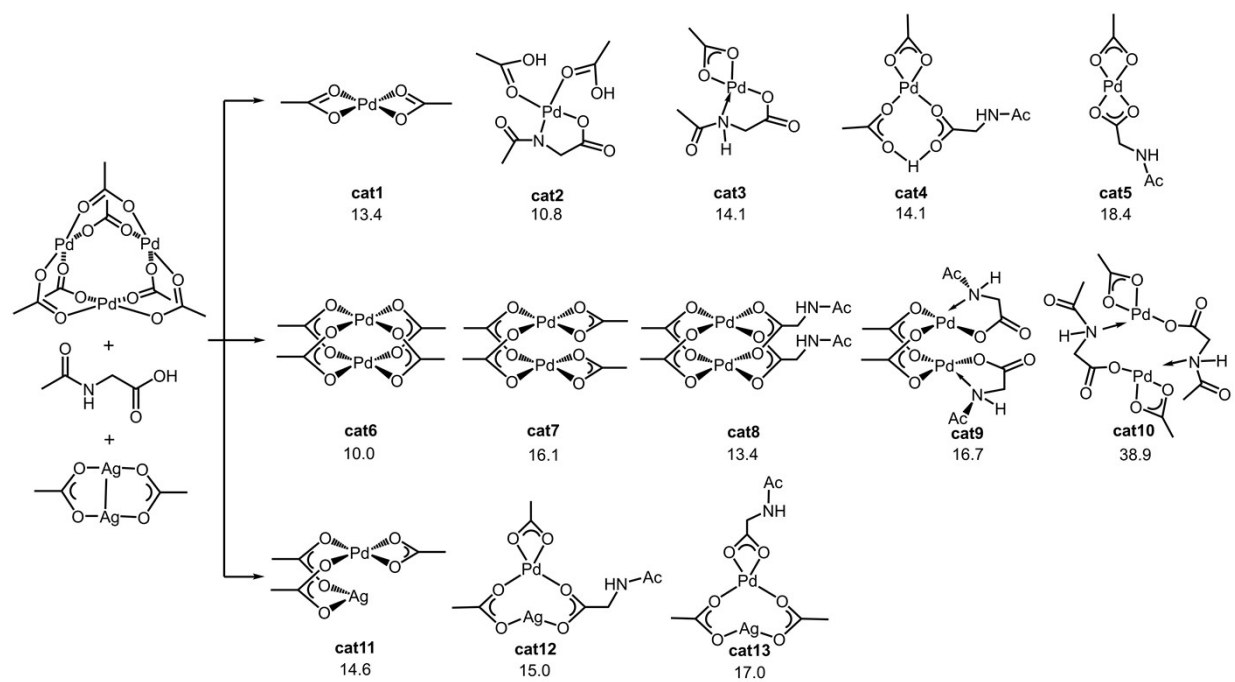


Fig. S1 Reaction free energies for decomposition of palladium trimer to monomer or dimer (in kcal/ mol).

II. Possible CMD mechanisms.

Scheme S1 Possible CMD mechanisms.

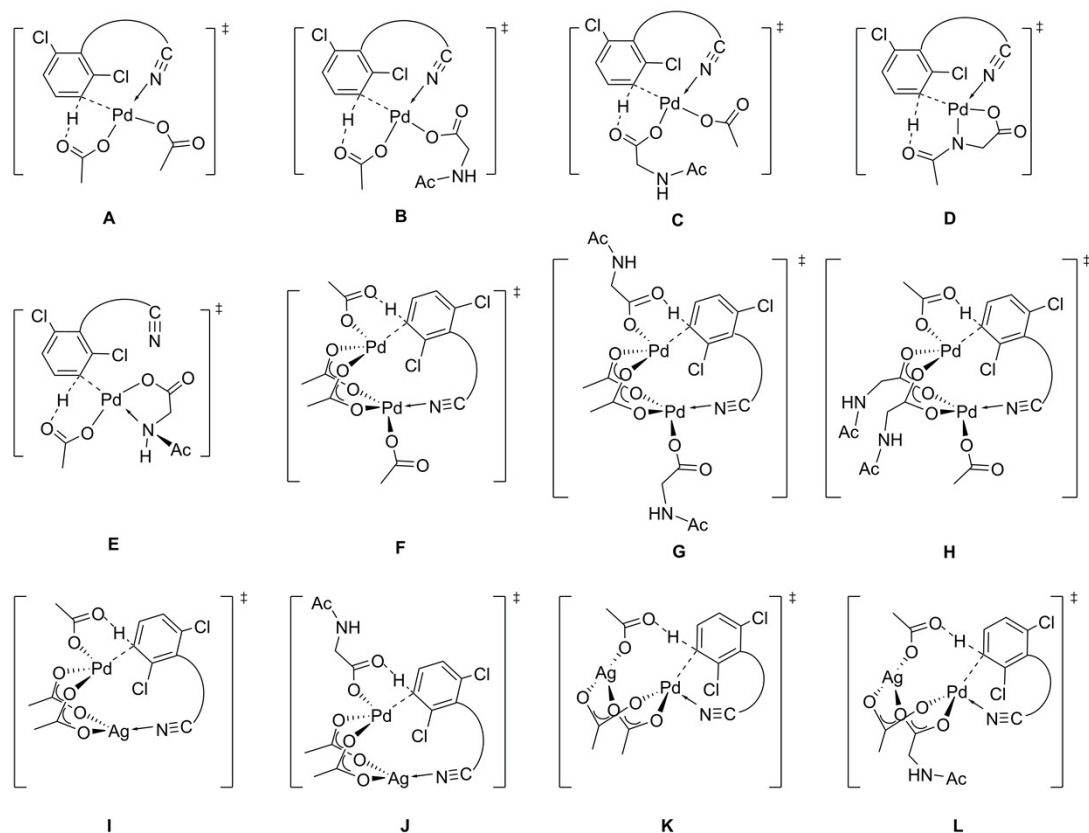


Table S1 Activation free energies (activation energies) for possible CMD mechanisms (in kcal/mol).

	A	B	C	D	E	F
meta	30.2	31.8	33.8	24.3	38.8	33.4
para	34.6	36.5	40.3	26.6	39.3	34.8

Table S2 Activation free energies (activation energies) for possible CMD mechanisms (in kcal/mol).

	G	H	I	J	K	L
meta	32.0	34.6	26.9	27.2	35.8	39.2
para	33.6	36.8	28.5	28.6	40.2	40.4

III. Possible C-H activation pathway.

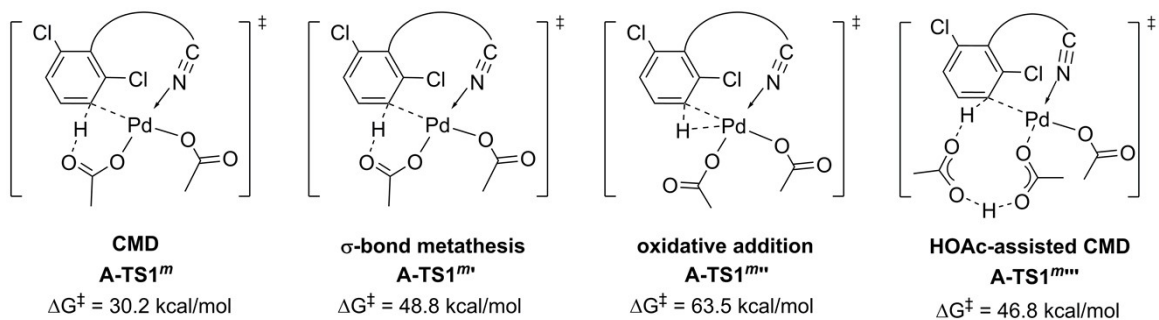


Fig. S2 Four major kinds of mechanisms for Pd catalyzed C-H bond activation.

IV. Free energy profiles for norbornene insertion.

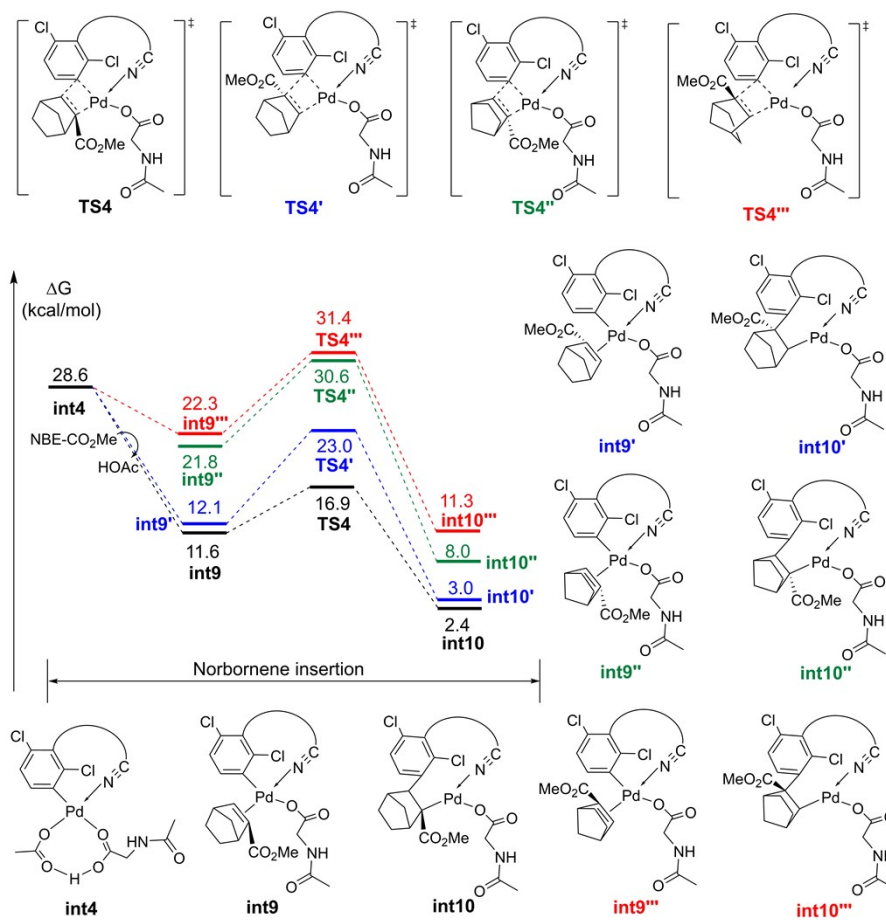


Fig. S3 Free energy profiles for four types of norbornene insertion.

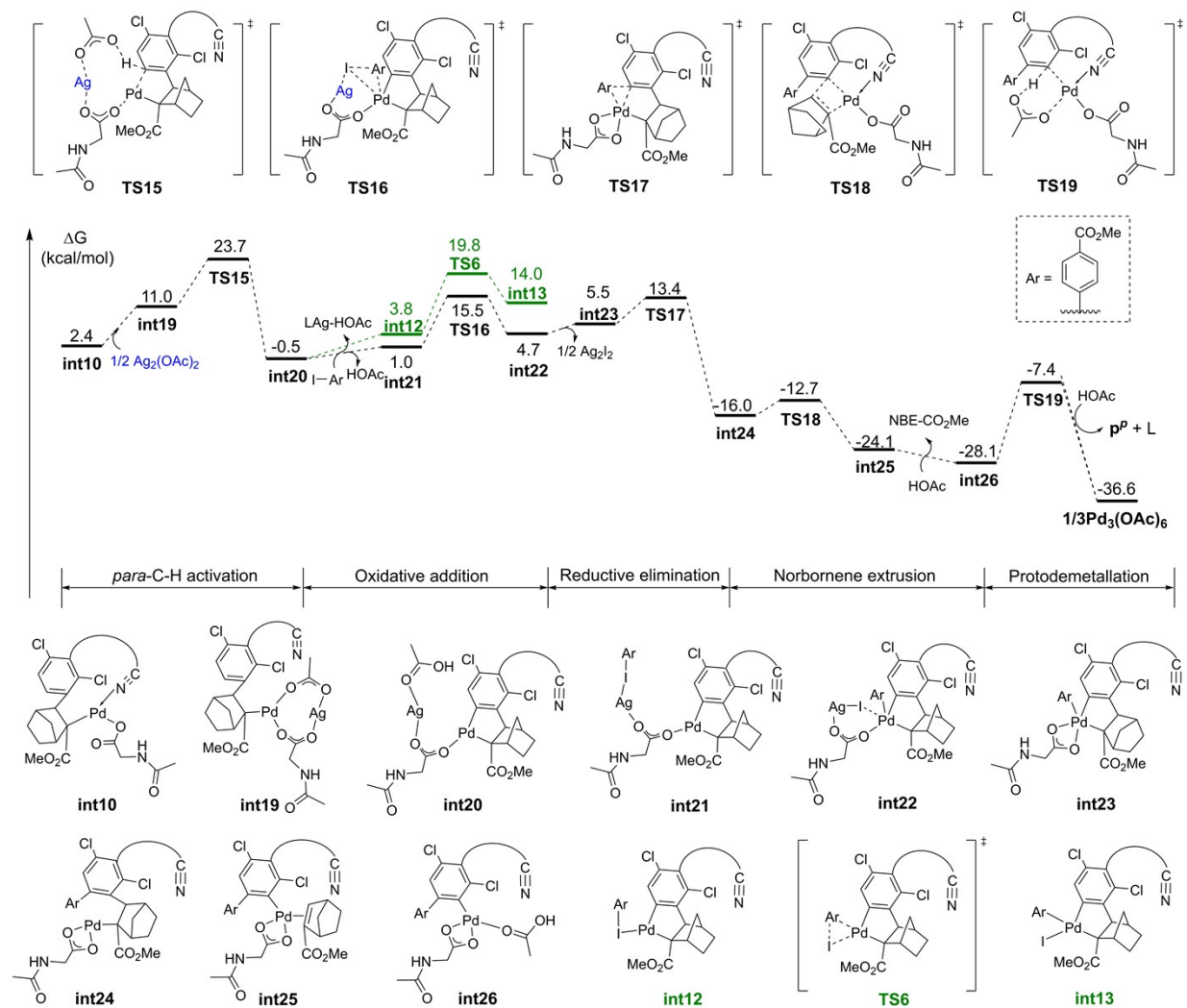


Fig. S4 Free energy profiles for the secondary *para*-C-H arylation.

V. Free energy profiles for the NBE relay palladation through *para*- to *meta*-position.

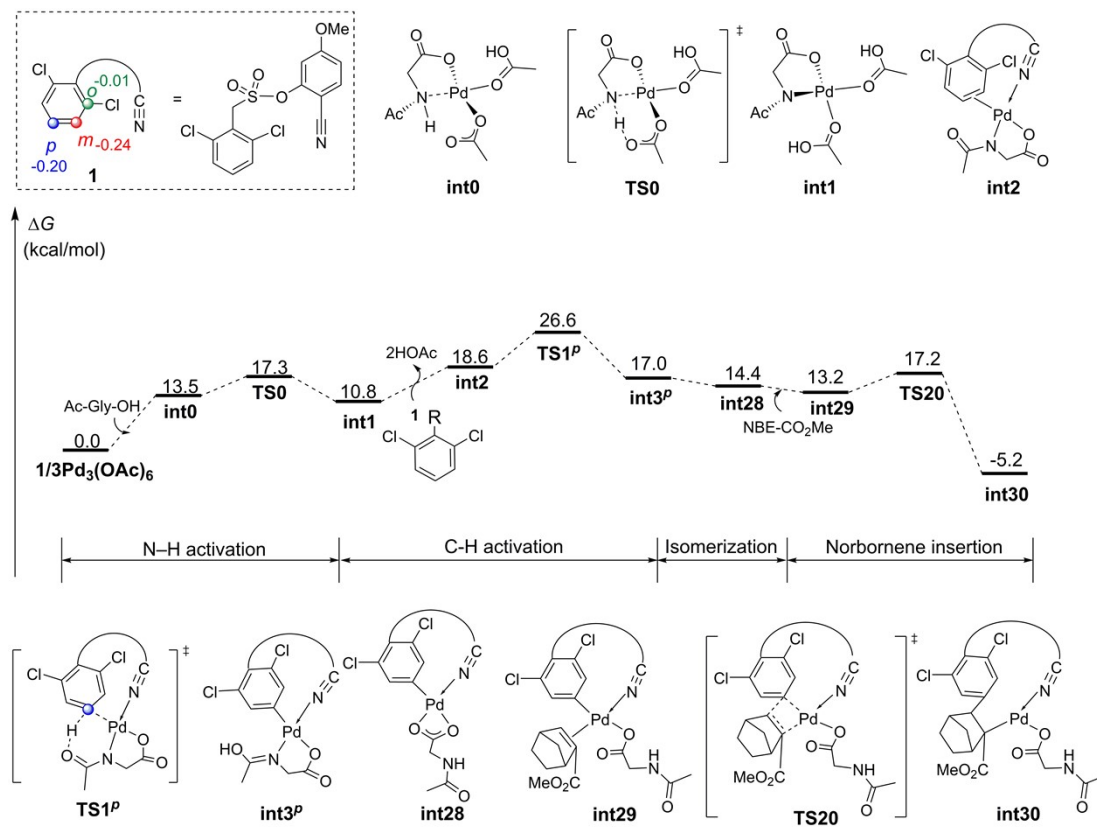


Fig. S5 Free energy profiles for the primary *para*-C-H activation and norbornene insertion.

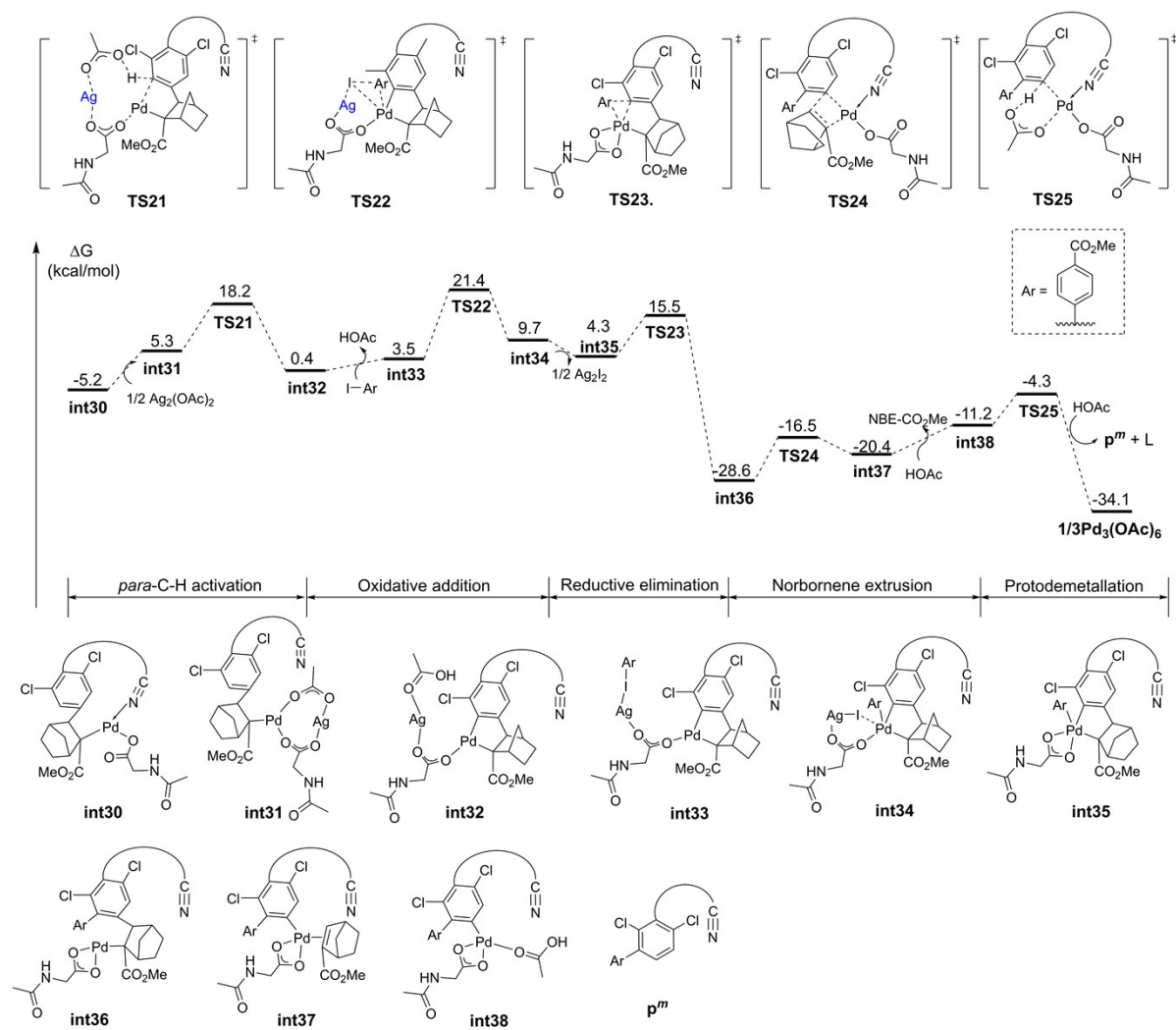


Fig. S6 Free energy profiles for the secondary *meta*-C-H arylation.

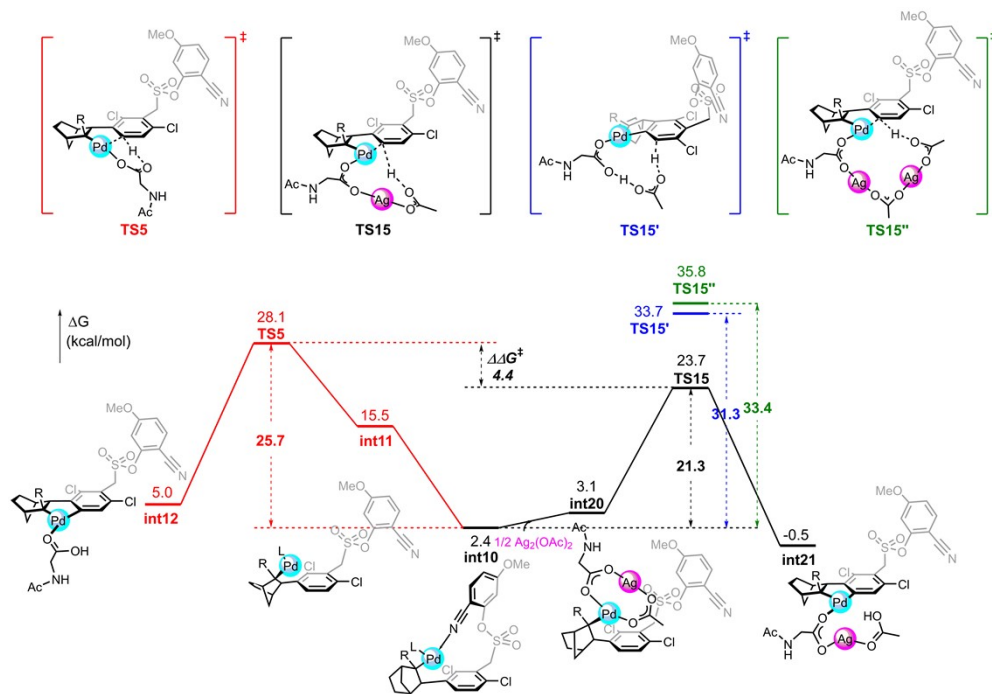


Fig. S7 Free energy profiles for the *para*-C-H activation.

VI. Distortion-interaction analysis.

Table S3 Distortion of substrate part for key transition state **TS1^m** and **TS1^p**.

Energy (kcal/mol)	E _{dist} (Pd)	E _{dist} (sub)	E _{int}
TS1^m	16.2	22.3	-51.5
TS1^p	17.1	24.8	-53.8

VII. Calculated energies and imaginary frequencies

Stationary point	Thermal correction to Gibbs free energy at B3LYP/6-31G(d,p)-SDD (in a.u.) (1)	Single-point energy including solvation energy at M06/6-311++G(d,p)-SDD (in a.u.) (2)	Gibbs free energies (G) (in a.u.) (3)=(1)+(2)+ $aRT*\ln 31.4$ ($a=3.8088*10^{-7}$)	Imaginary frequencies (in cm ⁻¹)
Pd₃(OAc)₆	0.211656	-1754.470024	-1754.254186	
1	0.159334	-2252.016428	-2251.852912	
Ac-Gly-OH	0.067385	-437.0006694	-436.9291024	
NBE-CO₂Me	0.146626	-500.4210651	-500.2702571	
HOAc	0.025068	-229.0417185	-229.0124685	
PhCOOMeI	0.079555	-470.7423397	-470.6586027	
Ag₂OAc₂	0.041734	-750.9684046	-750.9224885	
Ag₂I₂	-0.050943	-316.9586785	-317.0054395	
int0	0.149453	-1021.812607	-1021.658972	
TS0	0.146435	-1021.803411	-1021.652794	809.04 <i>i</i>
int1	0.149567	-1021.817005	-1021.663256	
int2	0.237942	-2815.720934	-2815.478810	
TS1^m	0.234793	-2815.708707	-2815.469732	803.83 <i>i</i>
int3	0.239794	-2815.708968	-2815.490060	
int4	0.234245	-2815.731678	-2815.493250	
int5	0.334959	-3286.485788	-3286.146647	
TS2	0.338759	-3286.456558	-3286.113617	164.48 <i>i</i>
int6	0.347004	-3286.465360	-3286.114174	
int7	0.365183	-3108.210110	-3107.840745	
TS3	0.366947	-3108.201848	-3107.830719	229.39 <i>i</i>

int8	0.367776	-3108.225698	-3107.853740	
int9	0.409997	-3316.174466	-3315.760287	
TS4	0.41006	-3316.165953	-3315.751711	228.38 <i>i</i>
int10	0.410671	-3316.189699	-3315.774846	
int9'	0.408901	-3316.172534	-3315.759451	
TS4'	0.409652	-3316.155906	-3315.742072	239.45 <i>i</i>
int10'	0.410894	-3316.189048	-3315.773972	
int9''	0.409996	-3316.158208	-3315.744030	
TS4''	0.41176	-3316.14594	-3315.730001	249.53 <i>i</i>
int10''	0.413408	-3316.183539	-3315.765949	
int9'''	0.409859	-3316.157253	-3315.743212	
TS4'''	0.408735	-3316.141546	-3315.728629	229.99 <i>i</i>
int10'''	0.411345	-3316.176261	-3315.760734	
int11	0.403354	-3316.161617	-3315.754081	
TS5	0.39979	-3316.137999	-3315.734027	1237.87 <i>i</i>
int12	0.404816	-3316.179781	-3315.770783	
int13	0.407918	-3349.924010	-3349.511910	
TS6	0.41492	-3349.905507	-3349.486405	141.61 <i>i</i>
int14	0.414926	-3349.914772	-3349.495664	
int15	0.466369	-3566.930981	-3566.460430	
TS7	0.46497	-3566.912108	-3566.4429564	196.67 <i>i</i>
int16	0.467803	-3566.968864	-3566.496879	
TS8	0.418271	-3349.906878	-3349.484425	205.03 <i>i</i>
int17	0.420449	-3349.968787	-3349.544157	
TS9	0.473582	-3566.959325	-3566.481561	243.79 <i>i</i>
int18	0.469965	-3566.973548	-3566.499401	
TS10	0.467549	-3566.946605	-3566.474875	228.1 <i>i</i>

int19	0.335959	-3295.575035	-3295.234894	
TS11	0.338381	-3295.561452	-3295.218889	893.03 <i>i</i>
p^p	0.260831	-2710.780861	-2710.515848	
TS12	0.410056	-3316.138565	-3315.724327	213.41 <i>i</i>
TS13	0.427620	-3349.898000	-3349.466198	186.03 <i>i</i>
TS14	0.471577	-3566.894730	-3566.41897	194.32 <i>i</i>
int20	0.440936	-3691.667486	-3691.222368	
TS15	0.432941	-3691.639384	-3691.202261	1202.62 <i>i</i>
int21	0.434640	-3691.679641	-3691.240819	
int22	0.496663	-3933.385390	-3932.884545	
TS16	0.499223	-3933.364846	-3932.861441	172.29 <i>i</i>
int23	0.499497	-3933.382245	-3932.878566	
int24	0.512549	-3774.891331	-3774.374600	
TS17	0.507242	-3774.873347	-3774.361923	195.13 <i>i</i>
int25	0.517007	-3774.930143	-3774.408954	
TS18	0.516767	-3774.924555	-3774.403606	239.31 <i>i</i>
int26	0.51274	-3774.938648	-3774.421726	
int27	0.386701	-3503.561309	-3503.170426	
TS19	0.383503	-3503.525060	-3503.137375	802.10 <i>i</i>
TS1^p	0.234345	-2815.704628	-2815.46610	1055.17 <i>i</i>
int3^p	0.238632	-2815.724142	-2815.481328	
int28	0.231887	-2815.721627	-2815.485558	
int29	0.40727	-3316.169135	-3315.757683	
TS20	0.409662	-3316.165132	-3315.751288	170.7 <i>i</i>
int30	0.416689	-3316.207838	-3315.786967	
int31	0.441067	-3691.676706	-3691.231457	
TS21	0.436184	-3691.651405	-3691.211039	893.02 <i>i</i>

int32	0.440416	-3691.683980	-3691.239382	
int33	0.493961	-3933.378708	-3932.880565	
TS22	0.497716	-3933.353853	-3932.851955	171.59 <i>i</i>
int34	0.496192	-3933.371068	-3932.870694	
int35	0.509453	-3774.890148	-3774.376513	
TS23	0.507348	-3774.870282	-3774.358752	217.84 <i>i</i>
int36	0.509851	-3774.943057	-3774.429024	
TS24	0.513754	-3774.927555	-3774.409619	182.23 <i>i</i>
int37	0.511286	-3774.931380	-3774.415912	
int38	0.387025	-3503.534676	-3503.143469	
TS25	0.38259	-3503.519231	-3503.132459	1090.06 <i>i</i>
p^m	0.260257	-2710.776377	-2710.511938	
TS1^o	0.236781	-2815.595062	-2815.354099	353.61 <i>i</i>
cat1	0.049437	-584.7837400	-584.7301210	
cat3	0.097517	-792.7472656	-792.6455666	
cat4	0.141946	-1021.804216	-1021.658087	
cat5	0.093162	-792.7360964	-792.6387524	
cat6	0.131480	-1169.622482	-1169.486820	
cat7	0.125490	-1169.606839	-1169.477167	
cat8	0.227856	-1585.546735	-1585.314697	
cat9	0.230045	-1585.543681	-1585.309454	
cat10	0.225356	-1585.503606	-1585.274068	
cat11	0.087199	-960.2806502	-960.1892692	
cat12	0.130495	-1168.240074	-1168.105397	
cat13	0.130569	-1168.236995	-1168.102244	
A-TS1^m	0.235778	-2836.796188	-2836.556228	1027.68 <i>i</i>
A-TS1^p	0.234979	-2836.788357	-2836.549196	1085.21 <i>i</i>

B-TS1^m	0.284668	-3044.7591872	-3044.470337	1041.40 <i>i</i>
B-TS1^p	0.279709	-3044.7466665	-3044.462775	1088.06 <i>i</i>
C-TS1^m	0.28467	-3044.755911	-3044.467059	1062.30 <i>i</i>
C-TS1^p	0.28016	-3044.741016	-3044.456674	1067.87 <i>i</i>
E-TS1^m	0.283016	-3044.746363	-3044.459164	900.47 <i>i</i>
E-TS1^p	0.281551	-3044.744057	-3044.458324	1174.90 <i>i</i>
F-TS1^m	0.314200	-3421.620780	-3421.302398	778.64 <i>i</i>
F-TS1^p	0.315869	-3421.620308	-3421.300257	878.58 <i>i</i>
G-TS1^m	0.401395	-3837.543603	-3837.138026	950.65 <i>i</i>
G-TS1^p	0.403224	-3837.542903	-3837.135497	1064.32 <i>i</i>
H-TS1^m	0.408154	-3837.546212	-3837.133876	585.44 <i>i</i>
H-TS1^p	0.410440	-3837.544979	-3837.130357	891.76 <i>i</i>
I-TS1^m	0.267518	-3212.294398	-3212.022698	794.73 <i>i</i>
I-TS1^p	0.269819	-3212.294093	-3212.020092	1068.59 <i>i</i>
J-TS1^m	0.310193	-3420.253266	-3419.938891	1028.49 <i>i</i>
J-TS1^p	0.314281	-3420.255144	-3419.936681	1187.32 <i>i</i>
K-TS1^m	0.269459	-3212.264704	-3211.991063	1221.85 <i>i</i>
K-TS1^p	0.268839	-3212.257126	-3211.984105	1211.94 <i>i</i>
L-TS1^m	0.317344	-3420.223826	-3419.902300	1252.26 <i>i</i>
L-TS1^p	0.312291	-3420.216904	-3419.900431	1225.58 <i>i</i>
A-TS1^{m'}	0.234583	-2836.765293	-2836.526528	1381.36 <i>i</i>
A-TS1^{m''}	0.237306	-2836.744628	-2836.503140	773.14 <i>i</i>
A-TS1^{m'''}	0.284241	-3065.830631	-3065.542207	1121.52 <i>i</i>
TS15'	0.448722	-3545.190461	-3544.737557	1308.68 <i>i</i>
TS15''	0.467411	-4067.115642	-4066.644049	1017.25 <i>i</i>

VIII. Cartesian coordinates of all the structures

Pd₃(OAc)₆

Pd	-1.62114400	0.93251000	0.01274400
C	0.06061200	2.61436300	1.87414600
O	-1.05129900	2.41046000	1.30224400
O	1.17254800	2.05778800	1.62076900
C	2.27447900	-1.27396100	-1.89536700
O	1.53246800	-2.12673500	-1.32275700
O	2.36824700	-0.03434800	-1.64096400
C	3.17821900	-1.80152800	-2.99044100
H	3.43230900	-1.00333900	-3.68893100
H	4.10340000	-2.16517800	-2.53057900
H	2.70065300	-2.63517100	-3.50705700
C	0.07492900	3.66442400	2.96561700
H	-0.91684600	3.77127700	3.40589500
H	0.81278200	3.40409100	3.72623800
H	0.36884100	4.62202600	2.52270600
Pd	-0.00115600	-1.87405300	-0.00000800
C	2.27088900	-1.35105600	1.84997400
O	2.64436500	-0.29058300	1.26411100
O	1.24089600	-2.04848500	1.60285600
C	-0.05734900	2.61457100	-1.87401600
O	-1.16995300	2.05931700	-1.62068700
O	1.05431000	2.40928900	-1.30211300
C	-0.07039600	3.66475800	-2.96538100
H	0.92154200	3.77055800	-3.40554800
H	-0.80845500	3.40531000	-3.72610500
H	-0.36330600	4.62263900	-2.52241200
C	3.14412900	-1.82231700	2.99433200
H	2.86200000	-1.26855300	3.89607500
H	2.99919700	-2.88777400	3.17458800
H	4.19142500	-1.60300200	2.77957800
Pd	1.62229700	0.93050900	-0.01274100
C	-2.27252700	-1.34817200	-1.85003600
O	-2.64470700	-0.28723300	-1.26418500
O	-1.24342000	-2.04688700	-1.60287700
C	-3.14631900	-1.81834900	-2.99441900
H	-2.86328300	-1.26512600	-3.89621100
H	-3.00287900	-2.88403700	-3.17451400
H	-4.19332500	-1.59751100	-2.77981800

C	-2.27611400	-1.27120900	1.89529100
O	-2.36839400	-0.03149200	1.64086400
O	-1.53507200	-2.12487300	1.32275200
C	-3.18054700	-1.79769500	2.99031400
H	-4.10600900	-2.16052200	2.53036800
H	-2.70388200	-2.63172700	3.50713800
H	-3.43395400	-0.99914300	3.68863600

1

C	4.11285000	0.13913700	-1.29927700
C	3.25372200	-0.73512800	-0.64001100
C	2.45864300	-0.32974500	0.45036600
C	2.61206100	1.00477000	0.87416600
C	3.45996600	1.89712900	0.22364200
C	4.20074300	1.46059300	-0.86996400
H	4.69955000	-0.21790400	-2.13709800
H	3.52615300	2.92026000	0.57171100
H	4.85743300	2.15298900	-1.38640700
Cl	3.21615600	-2.40313000	-1.19301800
C	1.51762800	-1.27589700	1.13062500
H	1.89201800	-2.30164500	1.13553600
H	1.28114600	-0.97423400	2.15086100
S	-0.11780400	-1.46910000	0.32454900
O	-0.87175300	-2.46062100	1.09114000
O	-0.02382300	-1.56932100	-1.12550800
O	-0.70583700	0.06302000	0.70832000
C	-1.88097000	0.47408200	0.08775900
C	-1.84304800	1.65504800	-0.66886000
C	-3.06332900	-0.23699300	0.27906700
C	-3.04807000	2.11800500	-1.23557300
C	-4.24235700	0.23237400	-0.31310000
H	-3.03758800	-1.13541100	0.87980200
C	-4.22927100	1.41978800	-1.06692500
H	-3.03423600	3.03326200	-1.81693500
H	-5.15721300	1.76713500	-1.50642100
C	-0.62615900	2.37761100	-0.86241500
N	0.34483400	2.99486400	-1.03699600
O	-5.44242300	-0.38350100	-0.20413600
C	-5.51911900	-1.60651400	0.52473500
H	-6.55828000	-1.92799200	0.45443300
H	-4.86841900	-2.37265000	0.08819400

H	-5.25417900	-1.46059300	1.57844400
Cl	1.75417200	1.59702300	2.28773100

Ac-Gly-OH

C	-0.57374600	-0.63531700	-0.00011700
H	-0.55227300	-1.29769600	-0.87509600
H	-0.55213300	-1.29778100	0.87479200
N	0.53574300	0.28565100	-0.00014900
H	0.30585700	1.26976100	-0.00014900
C	-1.86971500	0.14326000	0.00000900
O	-2.93874800	-0.67577600	0.00004400
H	-3.72660600	-0.10600400	0.00014500
O	-1.95318900	1.35323200	0.00006600
C	1.82245600	-0.16780100	-0.00000200
O	2.08454100	-1.36513400	0.00009700
C	2.89875600	0.90546200	0.00003400
H	2.50423200	1.92499200	-0.00013200
H	3.53157000	0.76757700	0.88075500
H	3.53182000	0.76738800	-0.88047700

NBE-CO₂Me

C	-0.03547000	0.37621500	0.19916300
C	0.77029300	-0.86557000	0.56589300
C	2.23460500	0.80800900	0.15551900
C	0.84223000	1.36804500	-0.04702400
C	1.96123000	-0.20218900	1.29804600
H	2.79710900	-0.88660200	1.48150000
H	1.67102300	0.28217100	2.23466800
C	1.47236300	-1.33569000	-0.75283500
H	1.99493800	-2.28332300	-0.58723200
H	0.75415700	-1.49143500	-1.56177800
C	2.47907100	-0.17942800	-1.04229400
H	3.51389500	-0.53641500	-1.02524500
H	2.31181500	0.30221500	-2.00919300
H	0.22240800	-1.64678700	1.09219300
H	3.03139300	1.53904900	0.30473700
C	-1.48956000	0.47704600	-0.01313300
O	-2.09286900	1.49572200	-0.29298100
O	-2.09991300	-0.72625600	0.14781500
C	-3.52210100	-0.71553800	-0.04255800
H	-3.77479100	-0.38152200	-1.05215600

H	-3.84903500	-1.74358700	0.11346600
H	-4.00295800	-0.04687500	0.67603900
H	0.59633200	2.35198700	-0.43033200

HOAc

O	0.78023900	-1.04527000	-0.00000400
C	0.09207200	0.12522500	-0.00000800
O	0.64297700	1.20278900	-0.00000200
C	-1.39655200	-0.11148600	-0.00000800
H	-1.68169100	-0.69375700	-0.88104500
H	-1.68170800	-0.69334000	0.88131600
H	-1.91660300	0.84532600	-0.00018200
H	1.72115500	-0.80081200	0.00005600

PhCOOMeI

C	-1.31131700	-1.04915000	-0.00015400
C	-1.94552200	0.19957800	-0.00005400
C	-1.17416300	1.36823500	0.00007600
C	0.21737100	1.29906200	0.00008900
C	0.82924500	0.04500900	-0.00001300
C	0.08039000	-1.13161900	-0.00013000
H	-1.90691700	-1.95478300	-0.00024700
H	-1.68151700	2.32716900	0.00016500
H	0.81017500	2.20661800	0.00018400
H	0.56844000	-2.09922200	-0.00020300
I	2.97673400	-0.08198100	0.00001600
C	-3.42935000	0.34353100	-0.00005500
O	-4.01528100	1.40850400	-0.00022800
O	-4.06225600	-0.85102100	0.00012400
C	-5.49708800	-0.78408000	0.00016600
H	-5.85741400	-0.25986700	-0.88840400
H	-5.83943600	-1.81873800	0.00041600
H	-5.85734800	-0.25945200	0.88851600

Ag₂OAc₂

O	2.11755400	1.13880700	-0.00660200
C	2.68289500	-0.00023200	-0.00555000
O	2.11746700	-1.13921400	-0.00638900
C	4.20004000	-0.00009200	0.03506900
H	4.51867100	0.00570800	1.08321800
H	4.59573400	-0.90066100	-0.43621200

H	4.59546200	0.89575600	-0.44545400
Ag	0.00006500	1.39028200	-0.00596200
O	-2.11760200	-1.13927000	-0.00644500
C	-2.68289700	-0.00022200	-0.00567300
O	-2.11742000	1.13875100	-0.00665100
C	-4.20003600	0.00018000	0.03512600
H	-4.51856500	0.00824900	1.08329200
H	-4.59532600	0.89517100	-0.44712100
H	-4.59595700	-0.90122400	-0.43434300
Ag	-0.00006600	-1.39014200	-0.00570800
Ag₂I₂			
Ag	0.00000000	-1.43075600	0.00000000
I	-2.43911000	0.00004300	0.00000000
Ag	0.00002900	1.43076500	0.00000000
I	2.43908400	-0.00005100	0.00000000
int0			
Pd	-0.17950000	-0.24602900	0.06686800
O	2.34597900	-1.40985400	-1.32312800
C	2.39698600	-3.62241400	-0.38599900
C	1.82020400	-2.22868300	-0.55072000
O	0.77837300	-2.00618900	0.20187200
C	1.00220200	2.03324500	-1.15404700
C	-0.44604600	2.44902900	-0.83215800
O	-1.12667700	1.53658700	-0.13803300
O	-0.90369500	3.50367200	-1.20783800
H	1.65320500	2.90906100	-1.10362900
H	1.01732800	1.67009000	-2.18625400
H	3.03849700	-3.85841900	-1.23575100
H	2.99875700	-3.64501500	0.52875700
H	1.60247000	-4.36411000	-0.28262500
N	1.49958300	0.92203600	-0.29838000
H	2.04955900	0.18499700	-0.81042600
C	2.15261000	1.23676400	0.96519800
O	3.00861500	0.49250900	1.37885800
C	1.69015600	2.48276000	1.68444700
H	2.13867500	2.48461100	2.67751100
H	2.01239900	3.38364600	1.15118700
H	0.60025300	2.51628000	1.76435200
C	-3.11590600	-0.83780600	0.26934000

C	-4.30113700	-1.73912500	0.46429900
H	-4.94992400	-1.68077100	-0.41426800
H	-3.97218900	-2.76437400	0.62546000
H	-4.88234300	-1.38987300	1.32290500
O	-1.95930700	-1.30389500	0.34372200
O	-3.41234700	0.40999200	0.03144100
H	-2.58869300	0.99175700	-0.08182400

TS0

Pd	-0.24542200	-0.25805700	0.04207000
O	2.46869600	-1.36258600	-1.04744200
C	2.32321800	-3.68068500	-0.51486900
C	1.76234100	-2.28143300	-0.51259400
O	0.63047800	-2.10654800	0.03753700
C	1.10067500	1.90313900	-1.13074600
C	-0.29317000	2.45735700	-0.77973100
O	-1.05505900	1.57957100	-0.11425400
O	-0.66468500	3.56458400	-1.09512200
H	1.82530600	2.71934800	-1.12968000
H	1.04824500	1.52007400	-2.15654600
H	2.85446600	-3.86741200	-1.45012400
H	3.04558700	-3.76096400	0.30447300
H	1.53238600	-4.41496000	-0.36240100
N	1.49705900	0.78342900	-0.25121500
H	2.05402500	-0.26937000	-0.75500200
C	2.14910000	1.06334300	0.98957000
O	2.42088700	0.14594700	1.74110300
C	2.52874500	2.49814000	1.30530400
H	2.96615500	2.51477500	2.30303200
H	3.26363000	2.87880200	0.58768600
H	1.66035300	3.16383000	1.27351800
C	-3.22100400	-0.62935200	0.26575100
C	-4.47370900	-1.43512400	0.46071400
H	-5.16585600	-1.24057800	-0.36299600
H	-4.23500600	-2.49595900	0.51680800
H	-4.96579900	-1.11351700	1.38375500
O	-2.10627100	-1.19273700	0.28076800
O	-3.41678400	0.64873700	0.09627500
H	-2.54878600	1.16447500	-0.02056600

int1

Pd	0.20952800	0.02928200	0.15306700
O	-1.15859000	2.68508200	-0.95184800
C	-0.11000200	4.26642800	0.51778700
C	-0.47888100	2.86265500	0.08446600
O	-0.03427300	1.92245600	0.84261000
C	-1.58636100	-2.11558900	0.64588400
C	-0.29222900	-2.76905900	0.13299900
O	0.60943700	-1.89233900	-0.30483900
O	-0.12420100	-3.96744100	0.15186900
H	-1.56531200	-2.16903800	1.74235400
H	-2.42341600	-2.72416600	0.30038400
H	0.90128300	4.48782800	0.15992600
H	-0.80251100	4.98907800	0.08498400
H	-0.10065300	4.34124600	1.60693600
N	-1.67692100	-0.71604100	0.21083700
H	-2.05379400	1.56297300	-0.86218000
C	-2.79354700	-0.22379900	-0.25459100
O	-2.90864900	0.95542500	-0.78346700
C	-4.09769400	-0.99080100	-0.23016800
H	-4.90348100	-0.30245700	-0.48218800
H	-4.08462800	-1.79636300	-0.97199800
H	-4.28985400	-1.43436900	0.74955300
C	3.19855700	-0.20706100	-0.22691600
C	4.59537100	0.34338800	-0.28668500
H	5.00404000	0.18095000	-1.28851100
H	4.59314800	1.40625300	-0.05049800
H	5.23089600	-0.20146200	0.41707600
O	2.23816200	0.55209000	0.02234500
O	3.10789300	-1.48730300	-0.45273500
H	2.14491500	-1.81591300	-0.41091400

int2

C	-1.58393100	2.45896200	-1.29496400
C	-0.25751600	2.75953800	-1.04897300
C	0.37440400	2.46851300	0.19413000
C	-0.42455700	1.88398000	1.18166400
C	-1.79118400	1.59184100	0.97554600
C	-2.36392800	1.88558300	-0.27291200
H	-2.02870900	2.71902200	-2.24811700
H	-2.44618100	1.31643400	1.79580000

H	-3.44100800	1.81820300	-0.36619400
Cl	0.63085800	3.59991900	-2.30344500
C	1.80424600	2.84893500	0.44506500
H	2.06359100	3.79902500	-0.02775600
H	2.03999900	2.90289700	1.50791000
S	3.06926200	1.71602200	-0.24187100
O	4.38182000	2.28387000	0.04534000
O	2.73194200	1.23308600	-1.57397100
O	2.80537900	0.43675100	0.83877300
C	3.19429000	-0.82079100	0.40027000
C	2.21099800	-1.68922300	-0.10305700
C	4.52261800	-1.21095900	0.50861000
C	2.58735700	-2.99197200	-0.49144100
C	4.88312400	-2.50761200	0.10893600
H	5.23961700	-0.50200700	0.90051400
C	3.90518300	-3.39395600	-0.38641200
H	1.83297000	-3.67101500	-0.87354300
H	4.21321100	-4.39057900	-0.68095400
C	0.86895100	-1.24020600	-0.19931100
N	-0.22288400	-0.85670200	-0.25516100
O	6.13822600	-2.99498800	0.16699400
C	7.18722300	-2.14920200	0.63833200
H	8.09619900	-2.74771300	0.58177400
H	7.29408100	-1.26029400	0.00660100
H	7.01496400	-1.84473300	1.67702800
Cl	0.21964700	1.54529400	2.77432700
Pd	-2.25122600	-0.60384100	-0.10048000
C	-4.76244900	-1.97008800	-0.55979500
H	-5.47746100	-2.49130100	0.08509800
H	-5.27818800	-1.76651400	-1.51011000
N	-4.24629200	-0.75079000	0.05596900
C	-3.63828400	-2.95956400	-0.86068900
O	-2.40729000	-2.51106300	-0.63644800
O	-3.84822700	-4.07902700	-1.28169800
C	-5.02271000	0.04053000	0.83431200
O	-4.59250300	1.03156000	1.44664100
C	-6.50903400	-0.30660700	0.93912000
H	-6.97019500	-0.47984000	-0.03789800
H	-6.65684100	-1.21150900	1.53934200
H	-7.00574000	0.52637000	1.43624700

TS1^m

C	-0.85034800	2.91068000	-1.78303700
C	0.31146800	3.09967500	-1.03705400
C	0.52061300	2.46653400	0.20749500
C	-0.53923300	1.67611200	0.69171600
C	-1.71870000	1.42789400	-0.03569900
C	-1.83964900	2.07314300	-1.28372400
H	-0.96754500	3.42228600	-2.73121400
H	-2.82198500	1.35507200	0.59872600
H	-2.75085100	1.93077200	-1.85772600
Cl	1.50630400	4.21064700	-1.67487100
C	1.80878300	2.63064600	0.95660400
H	2.23711500	3.62930600	0.84531700
H	1.71633500	2.39471700	2.01633600
S	3.17106900	1.55535000	0.36193200
O	4.35886600	1.83702500	1.16328500
O	3.24757600	1.49606700	-1.09162200
O	2.51445800	0.08560400	0.89521600
C	3.01094300	-1.07545200	0.32532700
C	2.09594100	-1.92132300	-0.32773800
C	4.35227100	-1.41956500	0.45032300
C	2.55742800	-3.14678000	-0.85380100
C	4.79675600	-2.63132600	-0.09957400
H	5.01751600	-0.74397700	0.97089000
C	3.88931800	-3.49494100	-0.74617500
H	1.85414600	-3.80922200	-1.34647800
H	4.26157400	-4.42953400	-1.14950600
C	0.73349600	-1.53707900	-0.42596700
N	-0.37540200	-1.20583700	-0.47929800
O	6.07343700	-3.05981800	-0.04628200
C	7.05518600	-2.23216300	0.57802500
H	7.99769200	-2.77111300	0.48343200
H	7.13491800	-1.26233500	0.07442400
H	6.82791700	-2.07813900	1.63902600
Cl	-0.41873700	0.97185900	2.29933000
Pd	-2.33927000	-0.71291500	-0.21470500
C	-5.08578900	-1.66676500	-0.18049300
H	-5.72463400	-1.97498900	0.65460600
H	-5.74070900	-1.48739700	-1.04394600
N	-4.29285500	-0.48421000	0.14559000
C	-4.18156000	-2.86076300	-0.53015300

O	-2.88310800	-2.61589000	-0.55437200
O	-4.66214700	-3.95145600	-0.76953000
C	-4.78705500	0.56282200	0.78941300
O	-4.06824500	1.55821100	1.12243100
C	-6.25757500	0.60760500	1.15869100
H	-6.89376500	0.38060500	0.29842800
H	-6.47620700	-0.13222500	1.93635600
H	-6.49349000	1.60075300	1.53889100

int3

C	-0.70473800	2.84317600	-1.80194400
C	0.36397800	3.12212500	-0.95538400
C	0.55600700	2.41746400	0.24769300
C	-0.42768400	1.46248000	0.58164100
C	-1.45347400	1.06508300	-0.28741600
C	-1.56963000	1.79783500	-1.48197900
H	-0.82846800	3.41209500	-2.71655600
H	-3.10632800	1.59040200	0.70465300
H	-2.35326300	1.53869700	-2.18899800
Cl	1.46999800	4.40578100	-1.42327700
C	1.79734600	2.58905100	1.06683500
H	2.21870200	3.59460600	1.00525600
H	1.67093600	2.30785300	2.11170300
S	3.18921000	1.54506400	0.47051300
O	4.32705700	1.72875600	1.36842400
O	3.36247700	1.61851000	-0.97408000
O	2.47507700	0.04510800	0.82573800
C	3.00062400	-1.10340500	0.26514000
C	2.08675500	-2.03004900	-0.27745100
C	4.36504800	-1.37566700	0.29652000
C	2.57851700	-3.25045800	-0.78945200
C	4.83367700	-2.58292700	-0.24140500
H	5.03303700	-0.65314100	0.74504600
C	3.93151900	-3.52257900	-0.77935300
H	1.87722800	-3.97055700	-1.19685600
H	4.32375900	-4.45176600	-1.17594600
C	0.69724900	-1.73855300	-0.29902900
N	-0.43330200	-1.48501900	-0.30618800
O	6.13372600	-2.93799600	-0.27187000
C	7.11025200	-2.03297000	0.24372500
H	8.07269600	-2.52201100	0.09414300

H	7.09427000	-1.08076900	-0.29812300
H	6.95617700	-1.84988900	1.31321800
Cl	-0.36691000	0.71517800	2.18657300
Pd	-2.33480000	-0.78805700	-0.15650900
C	-5.17314700	-1.40856100	-0.34866300
H	-6.04690400	-1.48805200	0.30276400
H	-5.53131700	-1.26667900	-1.37633500
N	-4.30739500	-0.28018100	0.03168700
C	-4.42115000	-2.75940500	-0.30363200
O	-3.12289200	-2.68199900	-0.18835000
O	-5.07268200	-3.78553500	-0.39959300
C	-4.81053000	0.79737700	0.53730300
O	-4.04458500	1.81056600	0.91983000
C	-6.27768400	1.04183000	0.75904100
H	-6.84968200	0.83860200	-0.14982700
H	-6.65857100	0.38270700	1.54607300
H	-6.42949300	2.07720100	1.06254200

int4

C	-0.31861800	2.87070900	-1.61755500
C	0.74576200	3.13390800	-0.76099100
C	0.96632100	2.36728100	0.39813200
C	0.02104200	1.35954100	0.68300600
C	-0.97085500	0.98266800	-0.22491200
C	-1.14092000	1.77120500	-1.36773100
H	-0.47082200	3.49080700	-2.49369200
H	-1.92087700	1.52233100	-2.08124100
Cl	1.81641400	4.47066200	-1.16215700
C	2.21512100	2.50673900	1.21008000
H	2.63947700	3.51244500	1.18369200
H	2.10502800	2.17996400	2.24356700
S	3.59303000	1.48282100	0.54392100
O	4.73998600	1.59410800	1.44200800
O	3.75718500	1.63749000	-0.89520300
O	2.86130200	-0.03290100	0.81397300
C	3.36755200	-1.15534700	0.19373400
C	2.43584700	-2.07309300	-0.33937900
C	4.73381300	-1.41870300	0.15083800
C	2.91478700	-3.26899200	-0.91923700
C	5.18659000	-2.60072700	-0.45217500
H	5.41771900	-0.70869100	0.59519300

C	4.26798300	-3.52926200	-0.98246400
H	2.20190100	-3.98036300	-1.32192300
H	4.64857900	-4.43902500	-1.43178900
C	1.04371200	-1.80023100	-0.29278500
N	-0.09263800	-1.56876000	-0.24688000
O	6.48571900	-2.94151200	-0.55599100
C	7.47946600	-2.04559100	-0.05570300
H	8.43706300	-2.52001200	-0.26927100
H	7.42929200	-1.07531500	-0.56193300
H	7.37586300	-1.90252100	1.02577800
Cl	0.08841700	0.54036200	2.24665300
Pd	-1.93229500	-0.75377600	-0.09488800
C	-5.84122800	-1.56272000	0.18466700
H	-6.01051100	-2.17008300	1.08445100
H	-6.17674400	-2.17736800	-0.65840200
N	-6.57604700	-0.31759200	0.22197900
C	-4.35434200	-1.32528800	0.06316200
O	-3.54810100	-2.29295300	0.00264600
O	-3.90452600	-0.11699600	0.03484600
C	-8.55672500	1.09305500	-0.01484900
H	-7.84947800	1.90524500	0.17419400
H	-9.04594300	1.26114300	-0.97808900
H	-9.33486300	1.11352600	0.75311500
H	-6.03723700	0.52991300	0.32715900
O	-8.56364400	-1.30764600	-0.23816400
C	-7.91799000	-0.28734200	-0.02646500

int5

C	-2.60145300	-2.54275500	-2.63193300
C	-3.31890100	-2.86698900	-1.48473200
C	-2.88894100	-2.46169800	-0.20739000
C	-1.65456300	-1.78259300	-0.14127600
C	-0.96835400	-1.34318500	-1.27408200
C	-1.46167200	-1.74502300	-2.52159100
H	-2.95810200	-2.87261900	-3.60116400
H	-0.96201300	-1.41660800	-3.42964100
Cl	-4.78977600	-3.81326900	-1.67164300
C	-3.75861500	-2.61159500	1.00061900
H	-4.41894800	-3.48023000	0.95323800
H	-3.20573400	-2.62073300	1.93930200
S	-4.95452600	-1.22354900	1.17917600

O	-5.66514400	-1.37910300	2.44632500
O	-5.68247900	-0.95511400	-0.05363600
O	-3.80360800	0.01727800	1.37256100
C	-4.19584100	1.33148300	1.21701100
C	-3.32767200	2.18429300	0.50241500
C	-5.36271800	1.82224800	1.79630400
C	-3.66449800	3.55071900	0.38178800
C	-5.68853600	3.17714500	1.64211400
H	-5.98941500	1.14779100	2.36350700
C	-4.82892500	4.04188700	0.93532100
H	-2.99601000	4.21043100	-0.16069100
H	-5.10286400	5.08623700	0.84191600
C	-2.13067700	1.68411300	-0.07568700
N	-1.14804400	1.27641100	-0.53923100
O	-6.79933200	3.74553000	2.15097100
C	-7.73094000	2.92925900	2.86185400
H	-8.54615000	3.59381000	3.14742100
H	-8.11806300	2.12472500	2.22692000
H	-7.27660900	2.50089800	3.76244400
Cl	-0.94569800	-1.44472700	1.44458300
Pd	0.41384700	0.10816900	-1.19002500
C	2.90182600	3.36280000	-2.49822100
H	2.36910300	4.12058900	-3.08588100
H	3.78212600	3.08781600	-3.09028300
N	3.30692300	3.87918100	-1.20534200
C	1.99126500	2.13929000	-2.37012100
O	1.78479400	1.71925000	-1.15251100
O	1.51647500	1.62443800	-3.38493200
C	4.26183300	4.84082600	-1.07822000
O	4.83180700	5.33645800	-2.04527400
C	4.58012300	5.26497000	0.35013400
H	4.00741400	4.72590000	1.11038000
H	5.64753100	5.11337700	0.53289300
H	4.38342200	6.33600200	0.45149300
H	2.85230300	3.46461500	-0.40443600
C	4.93873500	-2.37594200	1.74881200
C	5.33905400	-1.09512600	2.14932800
C	4.89464100	0.02845900	1.44188200
C	4.05872100	-0.10988200	0.33410500
C	3.67976500	-1.39732000	-0.03783700
C	4.09810800	-2.53597200	0.64674100

H	5.27988800	-3.24482300	2.29945800
H	5.21502500	1.01126100	1.77079800
H	3.69405200	0.75757300	-0.20540300
H	3.77869700	-3.52596900	0.34136900
I	2.41393200	-1.65425400	-1.77176100
C	6.23428900	-0.86796800	3.32262200
O	6.59508300	0.22760800	3.70372300
O	6.60232700	-2.02202000	3.91956700
C	7.46654100	-1.87386000	5.05869500
H	6.97779500	-1.28147800	5.83597800
H	7.66188400	-2.88589300	5.41235400
H	8.39768200	-1.37954700	4.77143900

TS2

C	1.66384000	-1.52921700	3.42901200
C	2.58488400	-2.13785900	2.58393500
C	2.37752100	-2.19957100	1.19465800
C	1.15473600	-1.68688700	0.70262800
C	0.25259100	-0.98743400	1.51221200
C	0.53267600	-0.92402300	2.88407800
H	1.84972100	-1.49397600	4.49637500
H	-0.13370200	-0.38039100	3.54448600
Cl	4.02587700	-2.83869700	3.30621200
C	3.45668800	-2.66944800	0.26875200
H	4.10926700	-3.42041300	0.71875700
H	3.08716000	-3.03287500	-0.68914100
S	4.64295700	-1.33201500	-0.16661300
O	5.61562900	-1.86192100	-1.11872200
O	5.07704700	-0.57361700	0.99857300
O	3.54265100	-0.36275500	-1.02978800
C	3.84701700	0.96298100	-1.26512100
C	2.80623300	1.89965200	-1.09495000
C	5.10263800	1.36093000	-1.71383300
C	3.05933900	3.25870500	-1.38482500
C	5.33746300	2.71876200	-1.97426900
H	5.86931800	0.61246200	-1.86009300
C	4.30605500	3.66594900	-1.81279000
H	2.26062700	3.98122300	-1.25736400
H	4.51695200	4.70651400	-2.02994800
C	1.52811200	1.48422800	-0.63833300
N	0.48130500	1.13843000	-0.27685400

O	6.51844800	3.20941600	-2.39776800
C	7.62137800	2.31722000	-2.56233100
H	8.45816700	2.93954900	-2.87887300
H	7.87117600	1.81773700	-1.61975300
H	7.41295600	1.56641300	-3.33297600
Cl	0.78181400	-1.93688800	-1.00342700
Pd	-1.12638000	0.33591100	0.83568100
C	-2.54576900	4.33031200	0.92699400
H	-1.75936400	5.08223100	0.80656700
H	-3.04828400	4.56855200	1.87426200
N	-3.46454700	4.38516100	-0.19143400
C	-1.89776900	2.95828900	1.08165800
O	-2.33933500	2.01272000	0.30546100
O	-1.00616000	2.79065400	1.92444300
C	-3.89300600	5.57040300	-0.70803100
O	-3.56438900	6.65259500	-0.23222200
C	-4.81698300	5.46511800	-1.91385900
H	-4.99144000	4.43884300	-2.24929600
H	-5.77768100	5.92323700	-1.66220100
H	-4.38784500	6.04253100	-2.73713300
H	-3.68879800	3.50342300	-0.62819400
C	-2.71472300	-3.17911600	-1.25225100
C	-3.42822100	-2.51701000	-2.26137300
C	-3.77437200	-1.16928100	-2.09640000
C	-3.42420300	-0.47886200	-0.93772900
C	-2.67879200	-1.15534200	0.02967600
C	-2.34215000	-2.50504700	-0.09173300
H	-2.45372500	-4.22425000	-1.37256200
H	-4.33296500	-0.67299700	-2.88317100
H	-3.69540400	0.55944900	-0.79812800
H	-1.80165000	-3.01812500	0.69342500
I	-3.13817700	-0.55515100	2.36967200
C	-3.85681900	-3.19582000	-3.51664200
O	-4.47910400	-2.65500500	-4.41003400
O	-3.47626900	-4.49250800	-3.55779000
C	-3.86133800	-5.20479000	-4.74440100
H	-3.41863000	-4.74263600	-5.63022400
H	-3.48618200	-6.21950600	-4.61280400
H	-4.94846300	-5.20756600	-4.85510600

int6

C	-1.02063400	-2.11561000	-3.29192600
C	-1.80295200	-2.84435900	-2.40512100
C	-1.58167600	-2.79066000	-1.01887300
C	-0.47909500	-2.02715200	-0.56084600
C	0.25335100	-1.20241900	-1.42609000
C	-0.03262300	-1.26882700	-2.79525400
H	-1.20887800	-2.17320500	-4.35774600
H	0.50751200	-0.63983800	-3.49134000
Cl	-3.08318700	-3.84615100	-3.07161900
C	-2.54726600	-3.41696800	-0.05956500
H	-3.03928600	-4.30207800	-0.46750600
H	-2.11327100	-3.65478700	0.91022800
S	-3.97512600	-2.32081600	0.32463000
O	-4.85085800	-3.01338700	1.26649300
O	-4.51790300	-1.67942000	-0.86522200
O	-3.10330900	-1.14643900	1.19116200
C	-3.66050300	0.10501900	1.37917800
C	-2.82129300	1.22089400	1.17806000
C	-4.97290600	0.26702600	1.80850200
C	-3.32860100	2.52028400	1.40912200
C	-5.46624800	1.56430200	2.01519300
H	-5.58244100	-0.60971700	1.97966600
C	-4.63653300	2.68621100	1.81856200
H	-2.67790200	3.37420700	1.24281000
H	-5.05042900	3.67294800	1.99136700
C	-1.48560100	1.04101100	0.74070100
N	-0.38601800	0.88054900	0.40665500
O	-6.72573300	1.83129800	2.41574300
C	-7.63634700	0.74836500	2.60464800
H	-8.58342500	1.20621100	2.88998200
H	-7.76938900	0.17600300	1.67992800
H	-7.29903900	0.07995100	3.40507900
Cl	-0.07329200	-2.15212600	1.14518200
Pd	1.24162500	0.51025500	-0.89177100
C	0.52049600	4.41614000	-1.89927400
H	-0.52749600	4.48642800	-2.19430500
H	1.13687900	4.73213400	-2.74661200
N	0.76863700	5.29988500	-0.77658000
C	0.82443200	2.95016400	-1.59733600
O	1.68488300	2.66343700	-0.69957000

O	0.22193000	2.04705200	-2.24196700
C	-0.04421100	5.24411900	0.32064800
O	-1.08635800	4.59145900	0.32063000
C	0.40914500	6.04696300	1.52599200
H	1.21761100	6.74746000	1.30188600
H	-0.44597200	6.59806500	1.92343100
H	0.74838900	5.35567500	2.30406600
H	1.70729300	5.64967700	-0.65334200
C	3.90318300	-1.92897700	1.52605100
C	4.15923000	-1.05520600	2.59213100
C	3.57217300	0.21549400	2.60041300
C	2.73323700	0.61542400	1.55878600
C	2.47963500	-0.27716200	0.51892100
C	3.06409700	-1.54168700	0.48102600
H	4.36526400	-2.90962600	1.51079300
H	3.78428300	0.88432800	3.42814900
H	2.29615000	1.60803700	1.56130000
H	2.87847000	-2.21859200	-0.34349300
I	3.24570700	0.19267300	-2.59302700
C	5.04739800	-1.41795400	3.73063500
O	5.29168100	-0.69039500	4.67429800
O	5.56502600	-2.66286400	3.60785300
C	6.43516300	-3.06948300	4.67393800
H	5.90380900	-3.06416900	5.62911800
H	6.75869100	-4.07923500	4.42108300
H	7.29456000	-2.39816900	4.74748700

int7

C	0.43200000	3.08842500	-1.73559600
C	1.44620600	3.25365000	-0.79871900
C	1.48057900	2.49718200	0.38685000
C	0.39149100	1.62943300	0.61964700
C	-0.59498500	1.36982100	-0.33582300
C	-0.55030400	2.12234700	-1.51583900
H	0.43481100	3.68243100	-2.64271400
H	-1.28897600	1.94937700	-2.29263700
Cl	2.69023600	4.45283200	-1.13190200
C	2.67178200	2.51351400	1.29289200
H	3.18471500	3.47755100	1.31530500
H	2.44870300	2.19165800	2.30941200
S	4.00604200	1.37712700	0.73284400

O	5.05413400	1.35149500	1.75092600
O	4.34272200	1.55831400	-0.67301800
O	3.11437000	-0.06599500	0.86050400
C	3.57256200	-1.19522200	0.21142200
C	2.62351500	-1.96707800	-0.48981000
C	4.90202700	-1.59961900	0.29794000
C	3.04475200	-3.16426000	-1.10798700
C	5.30252500	-2.77867500	-0.34547000
H	5.59571000	-0.99755800	0.86870100
C	4.36452700	-3.56330900	-1.04537700
H	2.31569300	-3.76499700	-1.64078300
H	4.70265600	-4.47544600	-1.52307900
C	1.26519500	-1.55528800	-0.55914700
N	0.15685900	-1.21795600	-0.60552400
O	6.56626100	-3.24965800	-0.33534000
C	7.57759700	-2.49992900	0.33778100
H	8.50395200	-3.05433200	0.18783400
H	7.67778800	-1.49570900	-0.08884700
H	7.36799300	-2.42379600	1.41084200
Cl	0.27691300	0.80273200	2.17706700
Pd	-1.69858200	-0.34496100	-0.25141900
C	-2.94124900	-2.64063000	-1.44397400
O	-2.50558100	-2.28399900	-0.26677900
O	-2.98179500	-1.90865800	-2.43723200
C	-3.82937700	0.09780900	0.42114600
C	-4.86369100	0.22936300	-0.69456900
C	-3.76160500	2.20602600	-0.57742100
C	-3.15495200	1.31248900	0.48870700
C	-4.14369200	1.18161500	-1.66896400
H	-4.81816000	1.59993400	-2.42292600
H	-3.29852500	0.69785800	-2.16334200
C	-5.94421600	1.19584500	-0.09977100
H	-6.79195300	1.26286100	-0.78833000
H	-6.33052700	0.84813300	0.86183100
C	-5.18207600	2.55510500	-0.00390800
H	-5.64809300	3.32347300	-0.62832600
H	-5.13286800	2.94852500	1.01581500
H	-5.24356800	-0.70495600	-1.09996100
H	-3.16769600	3.07232200	-0.86872600
H	-2.67690300	1.68201700	1.38848200
O	-5.01464200	-1.64910400	1.44529700

C	-3.97920700	-0.80353600	1.60793200
O	-3.29615800	-0.75194800	2.61041000
C	-5.21862000	-2.57614700	2.52536700
H	-6.10135700	-3.15396100	2.25238900
H	-4.34778400	-3.22736100	2.62862700
H	-5.38124400	-2.04339100	3.46541200
C	-3.42709800	-4.08597700	-1.49761400
H	-2.64075200	-4.76186100	-1.14857000
H	-4.28289100	-4.21104200	-0.82653000
H	-3.71877500	-4.34777800	-2.51558000

TS3

C	0.09097900	3.01806400	-1.83616800
C	1.14789900	3.20014800	-0.95015400
C	1.22034500	2.48992400	0.26358500
C	0.12860700	1.65583400	0.58523400
C	-0.94141200	1.41817600	-0.29902800
C	-0.92180400	2.12116100	-1.51583700
H	0.07155600	3.56540000	-2.77167800
H	-1.71739600	1.96557000	-2.23455300
Cl	2.37936100	4.37526600	-1.37758900
C	2.43169200	2.57902300	1.14168200
H	2.88820300	3.57138400	1.13279900
H	2.23991000	2.27733500	2.17052900
S	3.82372200	1.51060500	0.60154200
O	4.89576600	1.62762400	1.58756000
O	4.10757200	1.63360800	-0.82206400
O	3.04703200	0.02281000	0.83813600
C	3.59416000	-1.09489300	0.22980000
C	2.74274100	-1.88368600	-0.56620700
C	4.91833900	-1.45997000	0.45315600
C	3.25539100	-3.06772700	-1.13746300
C	5.41347300	-2.62795100	-0.14380600
H	5.53196200	-0.83416100	1.08691100
C	4.57185600	-3.43316700	-0.93642500
H	2.60146600	-3.68603200	-1.74264800
H	4.98003200	-4.33629800	-1.37516500
C	1.38860200	-1.49937800	-0.76392600
N	0.28114900	-1.18255600	-0.90520200
O	6.68112400	-3.06750400	-0.00298700
C	7.59662100	-2.29443500	0.77244600

H	8.54565300	-2.82853700	0.72703600
H	7.72110600	-1.28916200	0.35457400
H	7.26970500	-2.21993900	1.81595900
Cl	0.10719300	0.85645000	2.14985100
Pd	-1.69352100	-0.55931900	-0.40630100
C	-3.03018200	-2.72172600	-1.66589100
O	-2.32227200	-2.52910800	-0.58806100
O	-3.33490500	-1.84716900	-2.48350100
C	-3.48993000	0.04214700	0.49479100
C	-4.73135900	0.23730700	-0.38751500
C	-3.69505300	2.25291000	-0.29614800
C	-2.82286800	1.32931500	0.54743800
C	-4.23609400	1.29821400	-1.38565800
H	-5.04937900	1.74692900	-1.96470700
H	-3.48990000	0.89242900	-2.07026100
C	-5.71620800	1.08797600	0.47119500
H	-6.67276900	1.18880700	-0.05157600
H	-5.92417500	0.63742100	1.44501800
C	-4.98094400	2.46101100	0.57420500
H	-5.57622800	3.27314500	0.14571600
H	-4.74207700	2.74372000	1.60429300
H	-5.13980600	-0.67620000	-0.81203700
H	-3.22127600	3.18234400	-0.61400400
H	-2.42048800	1.66448200	1.49814800
O	-4.51589500	-1.74701300	1.62233900
C	-3.55695400	-0.80363900	1.72945800
O	-2.86069900	-0.66667700	2.71846600
C	-4.60706800	-2.65715800	2.72983700
H	-5.44193600	-3.31803200	2.49731500
H	-3.68136400	-3.22941400	2.82587500
H	-4.79145100	-2.11638500	3.66147200
C	-3.48571300	-4.16729900	-1.84206200
H	-2.63029200	-4.84538800	-1.77174400
H	-4.17820400	-4.43422300	-1.03716300
H	-3.98235900	-4.29110600	-2.80530600
int8			
C	-0.61047000	2.77771500	-1.78484000
C	0.60585600	3.01312100	-1.16926100
C	0.87263900	2.56357400	0.14515700
C	-0.17821500	1.93343800	0.84095500

C	-1.46374200	1.70509900	0.26425200
C	-1.62407300	2.13022000	-1.07638300
H	-0.78501400	3.12366400	-2.79646500
H	-2.59319400	2.05375800	-1.54611500
Cl	1.78762100	3.95904300	-2.04929700
C	2.20489200	2.81861100	0.78836600
H	2.60632800	3.79927000	0.52000600
H	2.16738700	2.73346200	1.87292300
S	3.58299800	1.70945900	0.30567900
O	4.69895400	1.98060100	1.20826400
O	3.79138600	1.65737000	-1.13531800
O	2.87289400	0.24433900	0.76204800
C	3.45042700	-0.89164000	0.20800100
C	2.75634500	-1.57197400	-0.80763200
C	4.66930700	-1.35223200	0.69188000
C	3.31494200	-2.75790600	-1.32744100
C	5.21663000	-2.52465700	0.15034300
H	5.16053800	-0.78907100	1.47380200
C	4.52802200	-3.22592700	-0.85884300
H	2.78200200	-3.29743000	-2.10258700
H	4.97088200	-4.13369100	-1.25236000
C	1.50355100	-1.07562700	-1.25749500
N	0.46217200	-0.66417800	-1.57329800
O	6.39377600	-3.05891400	0.53783600
C	7.15643000	-2.38835000	1.54020600
H	8.06063600	-2.98295400	1.67012000
H	7.42685000	-1.37505200	1.22239000
H	6.61116800	-2.34202900	2.48994400
Cl	0.08544000	1.48983900	2.51271700
Pd	-1.55465100	-0.41449300	-0.72493600
C	-2.97947500	-2.36833600	-2.17012700
O	-2.05280700	-2.34314200	-1.24826900
O	-3.53341700	-1.37842200	-2.65339300
C	-3.04243800	-0.24407100	0.69737100
C	-4.53185800	-0.21592800	0.31806000
C	-4.03527600	1.95446400	0.76350800
C	-2.69456600	1.22188400	1.07497900
C	-4.66450000	1.13714900	-0.39538400
H	-5.70854400	1.42062000	-0.56764900
H	-4.15097300	1.14416000	-1.35572400
C	-5.33204200	0.07629300	1.62567300

H	-6.40142300	-0.07144900	1.44248300
H	-5.05407600	-0.58569900	2.44922300
C	-5.00704300	1.57977800	1.91311000
H	-5.90909200	2.19767000	1.85924000
H	-4.56303600	1.73859900	2.90104200
H	-4.86863700	-1.08896200	-0.23642000
H	-3.92154000	3.03165100	0.60984700
H	-2.43837700	1.30656000	2.13230000
O	-3.36402200	-2.42320200	1.56078700
C	-2.60432600	-1.30873000	1.65997400
O	-1.67388700	-1.21570400	2.44403500
C	-2.93113700	-3.53526600	2.35689300
H	-3.66856300	-4.32046700	2.18953900
H	-1.94114900	-3.86912000	2.03603700
H	-2.89076700	-3.26441800	3.41496100
C	-3.34158300	-3.78344200	-2.61110900
H	-2.44393800	-4.32079200	-2.93044000
H	-3.76773500	-4.33417800	-1.76662800
H	-4.06381800	-3.74751100	-3.42754500

int9

C	-1.57714700	-3.31820200	-1.67142200
C	-2.58732400	-3.21926100	-0.72086100
C	-2.42131400	-2.45655700	0.44976900
C	-1.15135400	-1.87558800	0.65573900
C	-0.14416200	-1.88238200	-0.31363500
C	-0.38660100	-2.61659800	-1.48030600
H	-1.73671700	-3.90791000	-2.56716500
H	0.36124500	-2.64069100	-2.26645900
Cl	-4.08625700	-4.08989900	-1.01690600
C	-3.56943600	-2.16617800	1.36490000
H	-4.29832300	-2.97816700	1.41325500
H	-3.26373400	-1.88620000	2.37220900
S	-4.59860600	-0.75510900	0.78484900
O	-5.58982100	-0.44838200	1.81316800
O	-4.99296400	-0.88910300	-0.61112300
O	-3.38272400	0.43413200	0.85736300
C	-3.56271000	1.61541200	0.16501000
C	-2.45912300	2.11496700	-0.55745800
C	-4.75827800	2.32576200	0.22585900
C	-2.58577100	3.35376500	-1.22338000

C	-4.86947500	3.54125900	-0.46404600
H	-5.57494200	1.92823000	0.81283500
C	-3.77346200	4.05507700	-1.18588700
H	-1.73639100	3.74470800	-1.77302700
H	-3.88702900	5.00227000	-1.70007300
C	-1.23794800	1.39123800	-0.60135800
N	-0.24187000	0.79792800	-0.62641000
O	-5.98487800	4.29742000	-0.48054200
C	-7.14386800	3.83704200	0.21517500
H	-7.91020400	4.59237100	0.04200800
H	-7.48437300	2.87207200	-0.17637400
H	-6.95256700	3.75082700	1.29078300
Cl	-0.82076000	-1.07135400	2.19367500
Pd	1.34320300	-0.49220200	-0.25355800
C	3.99759100	2.75193700	-1.42012200
H	3.69446900	3.32351500	-2.30464600
H	5.05530300	2.50306700	-1.56932700
N	3.81415200	3.52939400	-0.20941500
C	3.19969900	1.44301600	-1.39188000
O	2.58644500	1.21102200	-0.26609500
O	3.19377300	0.71464700	-2.38399100
C	4.39116400	4.74981400	-0.04115700
O	5.12910700	5.25325600	-0.88292600
C	4.06156600	5.45691800	1.26794600
H	3.57058000	6.40743200	1.04024900
H	3.41801400	4.87609400	1.93503300
H	4.99522200	5.69200700	1.78627900
C	3.32450700	-1.45782600	0.36790100
C	4.24148100	-1.90566500	-0.76867100
C	2.66075500	-3.51139100	-0.51726300
C	2.35690700	-2.44525200	0.51886400
C	3.25550700	-2.67133800	-1.67030800
H	3.76117100	-3.28437600	-2.42278800
H	2.54846600	-1.99952700	-2.16275400
C	5.05056100	-3.09822100	-0.15455800
H	5.82193100	-3.41618400	-0.86225200
H	5.55357500	-2.82523700	0.77652900
C	3.96149300	-4.20082900	0.03226000
H	4.18149200	-5.09080100	-0.56512700
H	3.85166500	-4.52439800	1.07154200
H	4.83390900	-1.12266300	-1.23371600

H	1.84798200	-4.20041800	-0.74599600
H	3.18500700	3.12956000	0.47283800
H	1.83059600	-2.63334400	1.44779300
O	4.97758100	-0.05203400	1.24641800
C	3.76107600	-0.57115500	1.49530700
O	3.13163900	-0.38112300	2.51584600
C	5.48718400	0.84807400	2.24632100
H	6.52128000	1.04384000	1.96458200
H	4.91068800	1.77598200	2.23584600
H	5.43097900	0.39531000	3.23835500

TS4

C	-1.27830200	-3.18463500	-1.95930300
C	-2.35085700	-3.12203600	-1.07528400
C	-2.23650300	-2.48296600	0.17454900
C	-0.96131700	-1.99808700	0.53401400
C	0.14084700	-2.01893300	-0.34289700
C	-0.06152500	-2.61787800	-1.59816500
H	-1.40184100	-3.66454300	-2.92339200
H	0.75253800	-2.64903800	-2.31208600
Cl	-3.84902800	-3.89935900	-1.55146300
C	-3.43338700	-2.28140700	1.05361400
H	-4.14025800	-3.11282600	1.00348600
H	-3.17533500	-2.08772100	2.09381300
S	-4.48202900	-0.85559100	0.56475600
O	-5.54557000	-0.71288300	1.55595400
O	-4.78630900	-0.84640300	-0.85980500
O	-3.33091300	0.35813200	0.84502800
C	-3.55109200	1.59811100	0.26806300
C	-2.50275800	2.15832700	-0.48613800
C	-4.73870600	2.29158700	0.47962200
C	-2.67265900	3.45047800	-1.02798600
C	-4.89612100	3.56361000	-0.08924100
H	-5.51141900	1.83288100	1.08157600
C	-3.85269300	4.14187100	-0.83941200
H	-1.86486500	3.89177500	-1.60154200
H	-4.00004200	5.13125700	-1.25664000
C	-1.29254800	1.43754900	-0.67276400
N	-0.30397600	0.84399100	-0.80481400
O	-6.00803000	4.31470700	0.04050900
C	-7.11774900	3.78777700	0.76795700

H	-7.89444500	4.55038400	0.71306700
H	-7.48336600	2.85872000	0.31662700
H	-6.85641900	3.60868600	1.81717500
Cl	-0.73472700	-1.31945600	2.13828100
Pd	1.41060100	-0.32867400	-0.33293400
C	4.15857100	2.76018100	-1.54988500
H	3.94426500	3.22504400	-2.51908200
H	5.21949300	2.48338100	-1.57591000
N	3.88728400	3.68096600	-0.46362700
C	3.33349000	1.47367600	-1.44019600
O	2.56616600	1.40648200	-0.39061100
O	3.44357300	0.61169500	-2.31370800
C	4.48262400	4.89991000	-0.38389300
O	5.29198700	5.29808800	-1.21699300
C	4.07972900	5.74932100	0.81609600
H	4.97474600	5.98178000	1.40011300
H	3.67382100	6.69833300	0.45483100
H	3.34270800	5.27193900	1.46840000
C	2.95674200	-1.46885900	0.51221600
C	4.10196100	-1.94206000	-0.39517700
C	2.54519900	-3.59198500	-0.42643700
C	1.95892700	-2.52143500	0.48791700
C	3.33807800	-2.75331300	-1.45608800
H	3.99884700	-3.36955200	-2.07361400
H	2.73966800	-2.11092900	-2.10456300
C	4.80398100	-3.08845900	0.39408900
H	5.69910300	-3.41364400	-0.14543600
H	5.12112500	-2.78040500	1.39348200
C	3.71674700	-4.20737000	0.41241000
H	4.06630500	-5.12056000	-0.07878900
H	3.40150100	-4.48476100	1.42318000
H	4.75269200	-1.15267300	-0.76204600
H	1.83336500	-4.32931600	-0.79854100
H	3.21877600	3.36009100	0.22248300
H	1.47017100	-2.79102100	1.41873200
O	4.43866300	-0.12733900	1.74954900
C	3.25103300	-0.76444900	1.80296000
O	2.53590800	-0.76723700	2.78769600
C	4.79118100	0.61889200	2.92594800
H	5.76557600	1.05730600	2.71270400
H	4.05188800	1.40050400	3.11575700

H	4.84574100	-0.03790600	3.79779500
int10			
C	-0.48416400	-2.91799000	-2.19759100
C	-1.75656700	-2.86518500	-1.65572600
C	-1.96962500	-2.58088400	-0.28633100
C	-0.83118500	-2.43249600	0.53030400
C	0.50252700	-2.51996300	0.02648400
C	0.62315200	-2.74561100	-1.36651300
H	-0.34973900	-3.12841200	-3.25173800
H	1.60111500	-2.89612800	-1.79870800
Cl	-3.10047300	-3.24042300	-2.71124600
C	-3.36013100	-2.51475000	0.27598400
H	-4.01568000	-3.26786200	-0.16890900
H	-3.37813100	-2.62250500	1.35903700
S	-4.30459500	-0.97334100	-0.03114900
O	-5.52171500	-1.04008000	0.77279400
O	-4.36468600	-0.61651000	-1.44219500
O	-3.23480400	0.10713500	0.71138200
C	-3.40304400	1.44036400	0.35764500
C	-2.46159600	2.03263200	-0.50273200
C	-4.46343200	2.16623000	0.88669600
C	-2.60229500	3.40022300	-0.81755300
C	-4.59429700	3.52216800	0.55083500
H	-5.15872400	1.66100900	1.54332600
C	-3.65392400	4.13355400	-0.30202000
H	-1.87694200	3.86962700	-1.47303900
H	-3.77660900	5.18421500	-0.53875000
C	-1.37905400	1.25799600	-0.99831800
N	-0.48287000	0.60410700	-1.34890600
O	-5.58372400	4.32070300	1.00034000
C	-6.58393000	3.76529800	1.85383400
H	-7.27348400	4.58120400	2.06981500
H	-7.12329800	2.95160100	1.35615500
H	-6.14782000	3.39888000	2.79025900
Cl	-1.06863500	-2.21657600	2.24954400
Pd	1.29478100	-0.39673600	-0.52280400
C	4.18169600	2.55325800	-1.69852700
H	4.17389300	2.81535400	-2.76288600
H	5.22671800	2.33506200	-1.44843800
N	3.67407900	3.64533400	-0.89126200

C	3.37190000	1.26488700	-1.51938500
O	2.38597500	1.35887700	-0.67034600
O	3.68812900	0.26141300	-2.15696000
C	4.26301900	4.87031800	-0.88591700
O	5.25067000	5.13296800	-1.56599100
C	3.61605100	5.90572500	0.02672600
H	3.34098900	6.77876400	-0.57142300
H	2.72914700	5.53964000	0.55226500
H	4.35405000	6.23715100	0.76282800
C	2.56064300	-1.27188100	0.85028800
C	3.99406100	-1.69468300	0.49057200
C	2.83164700	-3.64583800	0.51585800
C	1.75783900	-2.59742900	0.93631800
C	3.76177600	-2.87776800	-0.45985000
H	4.68091100	-3.43652300	-0.66565300
H	3.34135800	-2.56091900	-1.41310200
C	4.57143300	-2.44278200	1.73307300
H	5.64486100	-2.60672400	1.59372600
H	4.45182800	-1.87981100	2.66164100
C	3.78426300	-3.79493100	1.73116000
H	4.45656600	-4.64529700	1.57960300
H	3.24109900	-3.97305000	2.66482700
H	4.61750500	-0.88751500	0.11305400
H	2.40748100	-4.59014400	0.16236300
H	2.86943100	3.43126600	-0.31995800
H	1.40850200	-2.78013500	1.95379300
O	3.46987800	0.50715900	2.11919300
C	2.40081100	-0.31064400	1.99383200
O	1.43109500	-0.24326600	2.73108900
C	3.35809700	1.51852200	3.13115800
H	4.29660200	2.07151200	3.09752900
H	2.51549900	2.18100900	2.91746300
H	3.21223900	1.06770500	4.11614600

int9'

C	-1.01556600	-3.37976900	-1.77845600
C	-1.98398100	-3.37861600	-0.78043700
C	-1.84627000	-2.58931000	0.37585000
C	-0.63997300	-1.86816400	0.51477900
C	0.31570800	-1.78350900	-0.50003700
C	0.10074200	-2.55254100	-1.64974300

H	-1.15399300	-3.99163600	-2.66291300
H	0.82332500	-2.51957700	-2.45898000
Cl	-3.39322000	-4.40870100	-0.99895200
C	-2.97538000	-2.41733200	1.34317400
H	-3.61183900	-3.30118600	1.42366800
H	-2.65575100	-2.10360200	2.33609600
S	-4.17068400	-1.12315000	0.81198500
O	-5.14296400	-0.92022300	1.88363200
O	-4.60998400	-1.30101300	-0.56565800
O	-3.08020000	0.17965300	0.83513000
C	-3.41544700	1.35117800	0.18455400
C	-2.41652000	1.95952000	-0.60287000
C	-4.66057900	1.95019300	0.35206400
C	-2.69764200	3.19854200	-1.21885100
C	-4.92712500	3.16635000	-0.29256800
H	-5.39240200	1.46726400	0.98508400
C	-3.93520500	3.79186000	-1.07403400
H	-1.92797000	3.67657400	-1.81492500
H	-4.16703700	4.73820800	-1.54855100
C	-1.14709300	1.34287300	-0.76382000
N	-0.11229100	0.83687500	-0.89512700
O	-6.10283100	3.82037200	-0.20836900
C	-7.16477800	3.23973000	0.54904000
H	-8.00731600	3.92345900	0.44648100
H	-7.44082700	2.25534100	0.15508200
H	-6.89513500	3.14965800	1.60748600
Cl	-0.34261200	-0.99883300	2.02391800
Pd	1.64029600	-0.23789700	-0.60088800
C	3.19635000	3.81418700	-0.83450900
H	2.78366600	4.03629300	-1.82573300
H	4.27002700	3.64628000	-0.98630700
N	2.95268200	4.89827500	0.08991000
C	2.55619600	2.52974700	-0.29190200
O	1.95567700	2.53949200	0.78812900
O	2.72831500	1.50959000	-1.07188100
C	3.31271100	6.18018200	-0.18047600
O	3.89059600	6.50135500	-1.21545900
C	2.95789500	7.20040500	0.89413900
H	2.41158400	6.77658100	1.74142500
H	3.87969100	7.66122400	1.26071900
H	2.35719100	7.99389700	0.44117300

C	3.13174800	-1.90595600	0.15055100
C	3.31208200	-1.93095800	1.66953900
C	4.47150100	-0.14380800	0.89381700
C	3.83782400	-0.80381800	-0.31215300
C	3.42721900	-0.42622000	1.99538000
H	3.81982000	-0.24636300	3.00121900
H	2.50271200	0.13929900	1.86281300
C	4.80328900	-2.37254600	1.86448500
H	5.00128100	-2.52689500	2.92941700
H	5.03152700	-3.31045100	1.35146800
C	5.60365100	-1.15293600	1.30837900
H	6.22882400	-0.69440000	2.08021500
H	6.25750100	-1.41519700	0.47146500
H	2.58155500	-2.51834400	2.22268500
H	4.80286700	0.88334400	0.75288000
H	2.44362000	4.63311900	0.92402100
H	4.20435800	-0.69341700	-1.32697800
O	2.65410000	-4.19925500	0.07045300
C	2.96255100	-3.12961800	-0.68867400
O	3.12608200	-3.18068200	-1.89240800
C	2.50494900	-5.44121200	-0.64128600
H	2.32851700	-6.19652700	0.12376600
H	1.65529600	-5.38349400	-1.32541000
H	3.40918800	-5.66877900	-1.21033000

TS4'

C	-0.85622700	-3.11132900	-2.00472100
C	-1.93513000	-3.07241800	-1.12806200
C	-1.85458400	-2.42047600	0.12065000
C	-0.60141100	-1.88877900	0.49028400
C	0.51320400	-1.90575700	-0.37065200
C	0.34608200	-2.52639900	-1.62376700
H	-0.95807800	-3.59871300	-2.96750500
H	1.19030900	-2.58101200	-2.30300800
Cl	-3.40252600	-3.90132600	-1.60912400
C	-3.07140500	-2.26459900	0.98342700
H	-3.73735200	-3.12855900	0.92804000
H	-2.83583500	-2.05835600	2.02642200
S	-4.17947000	-0.88987400	0.47880800
O	-5.29813800	-0.84562400	1.41727900
O	-4.41102400	-0.85756100	-0.95910700

O	-3.11990500	0.37297700	0.85459800
C	-3.39359100	1.62259900	0.31649600
C	-2.39848600	2.22430000	-0.47411400
C	-4.58461000	2.27911800	0.60901400
C	-2.62325500	3.52706400	-0.96668500
C	-4.79758400	3.56424200	0.08948200
H	-5.31437600	1.78093900	1.23276800
C	-3.80618400	4.18631100	-0.69473400
H	-1.85574800	4.00379700	-1.56643500
H	-3.99419700	5.18498100	-1.07169100
C	-1.18906900	1.53051200	-0.75160700
N	-0.20189900	0.95935500	-0.96451700
O	-5.91677100	4.28736600	0.29962600
C	-6.97134000	3.71740500	1.07393900
H	-7.76441000	4.46494800	1.08722600
H	-7.34574000	2.79412600	0.61770900
H	-6.64550900	3.51372000	2.10045600
Cl	-0.46424300	-1.10660700	2.05812300
Pd	1.62547300	-0.14719700	-0.71407900
C	3.62705100	3.66013100	-1.03623900
H	3.16448600	4.00467300	-1.96900600
H	4.64542600	3.35039200	-1.30031000
N	3.63474300	4.70272200	-0.03433600
C	2.84914900	2.44965000	-0.50395400
O	2.34233300	2.48507600	0.62617500
O	2.80327500	1.46319700	-1.33669500
C	4.24206200	5.90112100	-0.22929200
O	4.82817600	6.18777600	-1.27015100
C	4.15079400	6.87804400	0.93716000
H	3.59062400	6.49156000	1.79327700
H	5.16331200	7.13531400	1.26091900
H	3.67823100	7.80041900	0.58795600
C	2.46750500	-2.28407800	0.33935300
C	2.67397000	-2.16976500	1.85401500
C	4.06868700	-0.63481800	0.93662800
C	3.30665600	-1.25079900	-0.24019100
C	3.00088200	-0.67518300	2.04907700
H	3.41482000	-0.47302900	3.04236200
H	2.16761400	0.00507600	1.86646500
C	4.10350800	-2.78529200	2.07849100
H	4.27274000	-2.86693900	3.15632600

H	4.21159500	-3.79058600	1.66333700
C	5.05695100	-1.73723300	1.42757300
H	5.75248800	-1.32018000	2.16280900
H	5.65280400	-2.15566800	0.61114700
H	1.90104900	-2.62032900	2.47232700
H	4.52507500	0.33104800	0.72562700
H	3.14602800	4.46360600	0.81976200
H	3.83117900	-1.45910100	-1.17185900
O	1.86038000	-4.56304000	0.52940500
C	2.47728100	-3.66967200	-0.26721600
O	3.00251600	-3.95584800	-1.32332500
C	1.82902200	-5.91349900	0.03209200
H	1.33557700	-6.49874300	0.80720800
H	1.26450500	-5.95931600	-0.90252500
H	2.84201900	-6.28165100	-0.14521900

int10'

C	2.03040900	-1.92674400	-2.22292800
C	1.22840800	-2.87086100	-1.62395000
C	0.87287800	-2.78604100	-0.24813100
C	1.43077300	-1.74762900	0.51230600
C	2.31196400	-0.76601800	-0.04623300
C	2.55719100	-0.87730500	-1.44893800
H	2.29078000	-2.01373900	-3.27093600
H	3.35010400	-0.28272000	-1.89109700
Cl	0.70884800	-4.23186800	-2.59481700
C	-0.02031500	-3.82556100	0.36771500
H	0.17458500	-4.81915700	-0.04323200
H	0.07005600	-3.86733000	1.45149800
S	-1.82288100	-3.64880600	0.07967900
O	-2.49467100	-4.63974500	0.91537700
O	-2.15813800	-3.51429900	-1.33144000
O	-2.01598300	-2.13151000	0.79303200
C	-3.17024400	-1.43931500	0.44050200
C	-3.07400700	-0.40400500	-0.50418400
C	-4.37278900	-1.75105600	1.06283900
C	-4.23034800	0.34363100	-0.80469600
C	-5.51650900	-1.00541500	0.73941500
H	-4.38924600	-2.55922500	1.78157700
C	-5.43436900	0.04560600	-0.19481000
H	-4.16396200	1.15640600	-1.51917300

H	-6.33231000	0.61061100	-0.41728400
C	-1.81889700	-0.12021400	-1.10489700
N	-0.76980300	0.09428800	-1.55689400
O	-6.73624300	-1.21810500	1.27644100
C	-6.89815900	-2.27420300	2.22150800
H	-7.95169000	-2.26177900	2.50070600
H	-6.64833700	-3.24549400	1.77959400
H	-6.28312100	-2.10735700	3.11346000
Cl	1.02441500	-1.68048200	2.21613700
Pd	1.19725400	0.95368900	-0.98723500
C	-0.95066900	4.68795300	-1.10094100
H	-1.25366400	4.65563800	-2.15432900
H	-0.12981000	5.41310000	-1.04441900
N	-2.05317700	5.06873400	-0.24599000
C	-0.43512300	3.30622700	-0.68037900
O	-0.96808900	2.70199200	0.26017400
O	0.56386700	2.89716300	-1.39260000
C	-2.70376100	6.25396500	-0.37667500
O	-2.41705300	7.07660500	-1.24208900
C	-3.82170700	6.50046300	0.62959400
H	-3.99391800	5.66283000	1.31149100
H	-3.57793300	7.39101400	1.21614800
H	-4.74502700	6.71458900	0.08442000
C	3.27506700	0.26770600	0.64175600
C	3.13313300	0.66598700	2.15104300
C	2.62847600	2.59158000	1.06165200
C	2.89547200	1.60046600	-0.06912400
C	1.97511900	1.68622000	2.12868100
H	1.84890600	2.18469000	3.09577700
H	1.01002800	1.28351000	1.81350200
C	4.32263600	1.60400200	2.50178900
H	4.31891200	1.77814800	3.58226700
H	5.30262700	1.18694900	2.25440100
C	4.00183100	2.91306200	1.71755100
H	3.91140300	3.77250000	2.39005600
H	4.76752700	3.15538200	0.97485500
H	3.05087000	-0.17981600	2.82809000
H	2.06667200	3.47041200	0.74829500
H	-2.27543500	4.39492700	0.47619000
H	3.59545800	1.93674100	-0.83671600
O	4.94274900	-1.37933100	1.01301100

C	4.69532600	-0.22993600	0.35011100
O	5.49824000	0.30562000	-0.38396900
C	6.24817900	-1.94962300	0.80387900
H	6.27170900	-2.85692800	1.40672500
H	6.39914100	-2.18508500	-0.25246900
H	7.02622500	-1.25359800	1.12603300

int9''

C	-1.46065900	-3.41026000	-1.74334900
C	-2.57931500	-3.24786300	-0.93248400
C	-2.52155200	-2.50696100	0.26166900
C	-1.25889300	-1.99289400	0.63278600
C	-0.14500400	-2.04764800	-0.20674900
C	-0.26616800	-2.78010400	-1.39549600
H	-1.53560700	-3.99278000	-2.65470600
H	0.59023000	-2.85506900	-2.06104800
Cl	-4.08097000	-4.01340800	-1.43655200
C	-3.75947800	-2.17336000	1.03478900
H	-4.53427300	-2.93892600	0.95778400
H	-3.57077200	-1.94643100	2.08345200
S	-4.61571400	-0.67907800	0.38756000
O	-5.75687800	-0.38379900	1.25116000
O	-4.76649200	-0.70237300	-1.06116800
O	-3.37710900	0.42378700	0.75589500
C	-3.38517200	1.67464400	0.17097300
C	-2.16466700	2.14796700	-0.35202500
C	-4.52724600	2.46995200	0.16224500
C	-2.11502300	3.45458800	-0.88419900
C	-4.46125900	3.75425000	-0.39631200
H	-5.43795100	2.08089700	0.59684000
C	-3.24587700	4.24535300	-0.91372900
H	-1.17522900	3.82811700	-1.27589200
H	-3.22369500	5.24723400	-1.32635700
C	-1.00680800	1.32509300	-0.33915000
N	-0.06516900	0.65025700	-0.32706400
O	-5.50955300	4.59903700	-0.46623000
C	-6.77810400	4.16892900	0.02781900
H	-7.46179100	4.99767900	-0.15555300
H	-7.13028200	3.27816500	-0.50416100
H	-6.73595800	3.96201800	1.10325500
Cl	-1.08948400	-1.22904000	2.21729700

Pd	1.42933000	-0.76023500	-0.08843300
C	3.75432200	2.91065900	-0.55082500
H	3.40650900	3.09237200	-1.57511600
H	4.77399500	2.51715500	-0.64226200
N	3.72263900	4.12121200	0.23830500
C	2.86051700	1.85045200	0.10619600
O	2.24262000	2.11348200	1.14367000
O	2.86224400	0.72402800	-0.53139600
C	4.40865200	5.23878500	-0.11547400
O	5.09727100	5.29905100	-1.13097600
C	4.26980700	6.42150600	0.83488800
H	3.61097900	6.22835700	1.68615400
H	5.26191400	6.69202400	1.20737100
H	3.88877600	7.28033800	0.27531600
C	3.36632500	-1.98722400	0.02226200
C	4.37860300	-1.68759300	1.14474100
C	2.81131400	-3.06414500	2.03274400
C	2.41679400	-2.83150000	0.57751300
C	4.35990100	-3.08519400	1.83431500
H	4.91644000	-3.11715400	2.77741900
H	4.70378500	-3.89764800	1.18611800
C	3.74644200	-0.82412800	2.27318700
H	4.51939900	-0.59956600	3.01523900
H	3.33926700	0.12136800	1.92067000
C	2.65352000	-1.76250100	2.87071300
H	2.84270700	-1.98455900	3.92576700
H	1.64853000	-1.34695900	2.79215800
H	5.33461000	-1.32029800	0.77629700
H	2.34715100	-3.94683800	2.47614400
H	3.15073600	4.06411300	1.07194200
H	1.79644000	-3.51524100	0.01685100
C	3.68539800	-1.96973900	-1.44063000
O	2.97574900	-2.44725900	-2.30977200
O	4.88021300	-1.41200400	-1.67645700
C	5.26227600	-1.32394800	-3.06176200
H	4.54613600	-0.70757800	-3.60936700
H	6.24738400	-0.85928000	-3.06206500
H	5.30186800	-2.31839400	-3.51238400
TS4''			
C	-1.11304300	-3.33610100	-1.84750300

C	-2.30312600	-3.17855600	-1.14365300
C	-2.33709200	-2.53003600	0.10351100
C	-1.10181600	-2.10303500	0.64889200
C	0.11010000	-2.20011400	-0.05534900
C	0.06652500	-2.84105500	-1.30991300
H	-1.11408100	-3.84077200	-2.80676500
H	0.99557300	-2.98094500	-1.85450600
Cl	-3.76161600	-3.85512500	-1.84595000
C	-3.64417700	-2.26215100	0.78814800
H	-4.37896200	-3.05037800	0.61074800
H	-3.54731600	-2.09340700	1.85947500
S	-4.51823600	-0.77110800	0.16743600
O	-5.75813200	-0.62172900	0.92573100
O	-4.51916700	-0.68169100	-1.28646400
O	-3.40360200	0.36362000	0.74872900
C	-3.45044300	1.64825700	0.23257100
C	-2.26113400	2.17462400	-0.30362100
C	-4.61131100	2.41133500	0.30656100
C	-2.25758700	3.50892100	-0.76267200
C	-4.59285200	3.72686100	-0.17875600
H	-5.49833000	1.97076500	0.74108100
C	-3.40634100	4.27335900	-0.70701700
H	-1.34092400	3.92556500	-1.16541100
H	-3.41989700	5.29718300	-1.06242500
C	-1.09015000	1.37193900	-0.37050100
N	-0.13688700	0.71445200	-0.42004400
O	-5.66139200	4.54973300	-0.16705100
C	-6.90406200	4.05978300	0.33594700
H	-7.61166300	4.88121000	0.22426800
H	-7.25225200	3.19486500	-0.23968200
H	-6.82465300	3.78825700	1.39487600
Cl	-1.13109000	-1.40268900	2.26168500
Pd	1.51880800	-0.59440100	-0.16070000
C	3.80118900	3.01971800	-0.82604800
H	3.42715900	3.21649600	-1.83796800
H	4.80842400	2.60384100	-0.95011000
N	3.82070500	4.22485200	-0.02768400
C	2.90420800	1.97613500	-0.14859700
O	2.33289900	2.24094700	0.91576900
O	2.84693400	0.86094700	-0.80255100
C	4.52407000	5.32844700	-0.39098300

O	5.18556200	5.38224000	-1.42455700
C	4.44113600	6.50481400	0.57403400
H	3.79204700	6.32388000	1.43544700
H	5.44810200	6.73930200	0.93093100
H	4.07797100	7.38123700	0.03020200
C	3.06303400	-1.94211000	0.26632900
C	4.01088000	-1.69313700	1.46769700
C	2.18430400	-2.74942100	2.32317900
C	1.95759200	-2.72356100	0.80589100
C	3.72562500	-3.00470100	2.26237900
H	4.18697700	-3.02825400	3.25593800
H	4.00056000	-3.91696600	1.72232500
C	3.44932200	-0.64581100	2.44985200
H	4.17710600	-0.47749300	3.25123300
H	3.23419000	0.31583500	1.98354500
C	2.16617300	-1.34371600	2.98788100
H	2.19316500	-1.46616000	4.07564300
H	1.26942700	-0.77969900	2.74514400
H	5.03945700	-1.51591600	1.15817200
H	1.58059500	-3.49813800	2.83894700
H	3.27548000	4.17356900	0.82387000
H	1.72919000	-3.67288200	0.33931500
C	3.65230300	-2.31912000	-1.05612200
O	3.12763400	-3.05583900	-1.87871500
O	4.85454800	-1.75113800	-1.24848200
C	5.46139200	-1.99323800	-2.52959900
H	4.82964600	-1.59763400	-3.32807800
H	6.41568300	-1.46847700	-2.50264100
H	5.61263400	-3.06371500	-2.68824100

int10''

C	-0.24217100	-2.93896600	-2.07363200
C	-1.58187600	-2.79268200	-1.78721100
C	-2.03530400	-2.58290100	-0.45916400
C	-1.07278300	-2.55508300	0.56667800
C	0.33209200	-2.61489600	0.31858200
C	0.70259000	-2.84482000	-1.04089400
H	0.08016900	-3.15990600	-3.08422200
H	1.71856800	-3.16398200	-1.24935700
Cl	-2.72328100	-2.98996400	-3.10062400
C	-3.50485000	-2.46661500	-0.17144300

H	-4.10154300	-3.11205900	-0.82059600
H	-3.75037100	-2.68161300	0.86643300
S	-4.25989500	-0.82201600	-0.47303600
O	-5.59411100	-0.83570900	0.11971300
O	-4.05550800	-0.34778600	-1.83513300
O	-3.23958800	0.07738800	0.53101400
C	-3.21636700	1.44848100	0.29873100
C	-2.12497000	1.99949500	-0.39437100
C	-4.23702600	2.24552000	0.80219300
C	-2.05790600	3.39991200	-0.54650200
C	-4.16600600	3.63494300	0.61911600
H	-5.05539200	1.76872500	1.32446500
C	-3.06538300	4.20522900	-0.05060600
H	-1.20120300	3.83280600	-1.05016700
H	-3.03004600	5.28295100	-0.16149200
C	-1.10241800	1.15288600	-0.89478900
N	-0.25845600	0.44826600	-1.27284100
O	-5.09914000	4.50454400	1.05893400
C	-6.25086500	3.99814600	1.73173400
H	-6.86049100	4.86965700	1.97005000
H	-6.82031200	3.31797400	1.08826700
H	-5.97509000	3.48221100	2.65876900
Cl	-1.66728200	-2.59675400	2.22147200
Pd	1.42544400	-0.67781500	-0.45350300
C	3.69285400	2.96755000	-0.94023800
H	3.76917400	2.90871400	-2.03277700
H	4.66032100	2.63215100	-0.54861800
N	3.38289300	4.31047900	-0.50391000
C	2.59487600	2.00953600	-0.46130200
O	1.61782400	2.43878600	0.16305900
O	2.84216200	0.77851400	-0.78035300
C	4.19905400	5.36578200	-0.76219100
O	5.24451700	5.25451700	-1.39629300
C	3.72857100	6.70689800	-0.21256600
H	2.78172100	6.65272300	0.33219900
H	4.49988000	7.10449600	0.45293600
H	3.62295500	7.41037700	-1.04322800
C	2.64354000	-1.75460700	0.81991400
C	3.15357900	-1.04242000	2.09717300
C	1.41350300	-2.31734400	2.82215400
C	1.51281500	-2.72242800	1.32398100

C	2.92307500	-2.17454800	3.13451900
H	3.11925300	-1.85033500	4.16197600
H	3.49643900	-3.08738200	2.93888200
C	2.15558500	0.01082700	2.61857400
H	2.59201300	0.50750300	3.49280100
H	1.91398200	0.78465200	1.88935800
C	0.92597700	-0.85315200	3.01996300
H	0.64027800	-0.69792400	4.06546800
H	0.05160600	-0.60764800	2.41683100
H	4.17176900	-0.67319200	1.99057200
H	0.87697800	-3.04890200	3.42758800
H	2.52937700	4.39391300	0.03323900
H	1.86282100	-3.76206300	1.27504100
C	3.72639900	-2.39047900	-0.00775600
O	3.62850300	-3.45926700	-0.59826400
O	4.85040400	-1.65245200	-0.04412400
C	5.90302200	-2.15631300	-0.88246500
H	5.57235500	-2.20303800	-1.92292400
H	6.72356600	-1.44752400	-0.77594600
H	6.20945200	-3.15453800	-0.56050100

int9'''

C	-1.38623100	-3.46822500	-1.25115000
C	-2.35846100	-3.19517000	-0.29597600
C	-2.15590300	-2.22360300	0.70101300
C	-0.89051900	-1.59630200	0.73469300
C	0.07270200	-1.77688400	-0.26535400
C	-0.20156600	-2.73140900	-1.25037200
H	-1.56852400	-4.22577100	-2.00509400
H	0.51966500	-2.91798700	-2.03867700
Cl	-3.85660500	-4.11599400	-0.35784100
C	-3.26719900	-1.78476900	1.60301200
H	-3.98097800	-2.58046900	1.82686900
H	-2.92003000	-1.32979800	2.53002500
S	-4.34152600	-0.50478900	0.83393300
O	-5.33606700	-0.07758300	1.81503000
O	-4.73879900	-0.84962100	-0.52470700
O	-3.15626800	0.71018000	0.72505500
C	-3.36636400	1.78474600	-0.11457300
C	-2.28513900	2.18807700	-0.92555100
C	-4.56566900	2.49091700	-0.11628800

C	-2.43590500	3.32950300	-1.74283900
C	-4.70208000	3.60553100	-0.95583900
H	-5.36330800	2.16917300	0.53935000
C	-3.62727200	4.02542100	-1.76542400
H	-1.60291700	3.65027200	-2.35894100
H	-3.75971100	4.89888100	-2.39309700
C	-1.06589100	1.46018200	-0.90774900
N	-0.07664900	0.85593800	-0.88062700
O	-5.82265700	4.34902300	-1.04265900
C	-6.95957700	3.98179200	-0.26040000
H	-7.73590500	4.70376400	-0.51308100
H	-7.30285200	2.97149400	-0.50907000
H	-6.73981200	4.04237200	0.81146300
Cl	-0.51289600	-0.51612200	2.07403600
Pd	1.53867800	-0.37483600	-0.45782100
C	3.68989600	3.40921000	-0.17610100
H	2.93438500	3.98593800	-0.72412800
H	4.52096200	3.25860100	-0.87603400
N	4.11943400	4.10178900	1.01684700
C	3.09823100	2.04798300	0.20943100
O	3.02606300	1.71178700	1.39693900
O	2.71924300	1.34851700	-0.81367900
C	4.63561900	5.35969400	0.98291700
O	4.79415800	5.97794500	-0.06619200
C	5.00687800	5.93677200	2.34453400
H	4.13652800	5.97154100	3.00883400
H	5.77277900	5.32484200	2.83322500
H	5.39143500	6.94655800	2.20204900
C	2.95854700	-2.27209500	-0.06787500
C	3.59594600	-2.97559200	-1.28112100
C	4.75296000	-1.05459200	-0.96069900
C	3.66297300	-1.09336300	0.11175900
C	5.07672000	-2.57992700	-1.00428900
H	5.76517300	-2.85411000	-1.81148900
H	5.45753000	-2.97474400	-0.05735100
C	3.33268200	-2.17643300	-2.59146400
H	3.69114200	-2.75151900	-3.45107500
H	2.27120500	-1.97447600	-2.75193600
C	4.16078300	-0.87078500	-2.38829400
H	4.98487800	-0.81178300	-3.10636800
H	3.57425800	0.04219600	-2.47114000

H	3.36522500	-4.03784100	-1.34187900
H	5.57003800	-0.37105500	-0.72647400
H	3.95141100	3.59975100	1.88051600
H	3.67459800	-0.49710300	1.01987400
C	2.32011700	-3.01135800	1.06719700
O	2.18512200	-2.58195400	2.19281400
O	1.98454000	-4.26854500	0.69979600
C	1.40775500	-5.07469300	1.74126200
H	0.46770200	-4.63636300	2.08456800
H	1.23301200	-6.05208000	1.29227500
H	2.09244500	-5.15510600	2.58883700

TS4'''

C	-1.02560500	-3.50662800	-1.51902900
C	-2.00606400	-3.26363900	-0.56466100
C	-1.80170600	-2.34119100	0.48083300
C	-0.52206100	-1.75574300	0.58377300
C	0.48828300	-1.95158200	-0.38816400
C	0.18978100	-2.83778900	-1.43591100
H	-1.21599100	-4.21030600	-2.32123100
H	0.92781200	-3.03487700	-2.20086900
Cl	-3.50381100	-4.16801700	-0.68435700
C	-2.92167200	-1.96731800	1.40534900
H	-3.58627600	-2.80690100	1.62082200
H	-2.57928700	-1.52723800	2.34090200
S	-4.08437600	-0.72870800	0.70946900
O	-5.11269200	-0.46159000	1.71219900
O	-4.44861700	-1.01514700	-0.67174700
O	-3.00721400	0.57576800	0.69299600
C	-3.34587700	1.68400400	-0.06820300
C	-2.40629700	2.13146600	-1.01515500
C	-4.53935500	2.36593200	0.14581000
C	-2.69053700	3.30231100	-1.74936100
C	-4.81272500	3.51353900	-0.61243800
H	-5.22463600	1.99588900	0.89617100
C	-3.87782400	3.98095200	-1.55732500
H	-1.96507300	3.66137100	-2.47112700
H	-4.11161000	4.87824200	-2.11852800
C	-1.18994400	1.41997900	-1.19900200
N	-0.19786100	0.82994000	-1.32541800
O	-5.94064600	4.24343900	-0.49505600

C	-6.93946200	3.82572400	0.43518200
H	-7.75064200	4.54745600	0.34026800
H	-7.31088000	2.82297900	0.19581800
H	-6.55681100	3.84015700	1.46213900
Cl	-0.20091000	-0.68792800	1.94022100
Pd	1.60431300	-0.15422400	-0.65901400
C	3.55979200	3.68130400	-0.33057400
H	3.01609500	4.21368900	-1.12034000
H	4.54540500	3.44341600	-0.74883500
N	3.67344700	4.48609600	0.86482400
C	2.82186000	2.37827100	0.00220800
O	2.42569400	2.16364700	1.15358900
O	2.68432200	1.59535200	-1.01959300
C	4.26421100	5.70832400	0.86822500
O	4.74633500	6.21537700	-0.14178500
C	4.29507500	6.41655200	2.21726800
H	3.80843300	7.39048100	2.11473700
H	3.80833900	5.85640500	3.02055400
H	5.33689700	6.60227500	2.49384000
C	2.48533100	-2.27181500	0.10834300
C	3.30540600	-3.04317100	-0.95766900
C	4.54618600	-1.20314900	-0.47107900
C	3.21516900	-1.03359000	0.28966500
C	4.71223200	-2.74720800	-0.34985500
H	5.52953200	-3.15455500	-0.95555300
H	4.82851200	-3.09601200	0.68105100
C	3.42543300	-2.28410700	-2.31426500
H	3.87400600	-2.95321600	-3.05570200
H	2.46409300	-1.95493300	-2.71214700
C	4.34931600	-1.06807500	-1.99622500
H	5.31500000	-1.16216500	-2.50441600
H	3.91217000	-0.10839300	-2.27212000
H	3.01996900	-4.09045500	-1.04854800
H	5.34947700	-0.58591900	-0.06558500
H	3.26525000	4.06728900	1.69159100
H	3.22686000	-0.56205200	1.26957600
C	2.11100200	-3.07195800	1.34626200
O	2.26287800	-2.68232400	2.48231200
O	1.66245700	-4.30549000	1.03252500
C	1.35486400	-5.14846800	2.15697100
H	0.55162500	-4.70968900	2.75385200

H	1.04041400	-6.10079200	1.73114400
H	2.23507300	-5.27950600	2.79078000

int10'''

C	2.78612400	-2.42159500	-1.87674800
C	1.76724000	-3.06195000	-1.16348400
C	1.21673900	-2.51191000	-0.00136800
C	1.75368500	-1.26210600	0.44581200
C	2.80208600	-0.58518300	-0.25168100
C	3.28812400	-1.22212200	-1.42040100
H	3.19890800	-2.89489900	-2.75969500
H	4.12767000	-0.78331900	-1.94029000
Cl	1.28934600	-4.64760400	-1.72683500
C	0.23903400	-3.30473600	0.82179900
H	0.53107000	-4.35680400	0.87042100
H	0.13915600	-2.92333400	1.83640200
S	-1.49458300	-3.44426400	0.23773000
O	-2.13746900	-4.45801300	1.06873100
O	-1.62297400	-3.47598200	-1.21271400
O	-2.02442800	-1.92982000	0.76572000
C	-3.18649300	-1.45851700	0.16564500
C	-3.07411600	-0.58947200	-0.93239800
C	-4.42175800	-1.82016500	0.68707000
C	-4.24878000	-0.06150700	-1.50052100
C	-5.58302300	-1.29210200	0.10222700
H	-4.44947100	-2.49571900	1.53134500
C	-5.48646600	-0.40960100	-0.99146900
H	-4.17399900	0.62017600	-2.34047200
H	-6.40114300	-0.01286500	-1.41690500
C	-1.77253000	-0.26631600	-1.39483500
N	-0.66705200	-0.05083100	-1.68478700
O	-6.83590400	-1.57081100	0.52113000
C	-7.01180100	-2.46804400	1.61576200
H	-8.08895200	-2.54768600	1.76242100
H	-6.59953900	-3.45794100	1.38895900
H	-6.54783900	-2.07770700	2.52904000
Cl	1.35544800	-0.78366900	2.10155600
Pd	1.02380500	0.92550100	-0.62686200
C	-1.61676500	4.30657400	-0.33468900
H	-1.85044300	4.44099000	-1.39687800
H	-0.89521800	5.09300200	-0.07982500

N	-2.81187700	4.39399100	0.47439500
C	-0.95637700	2.93860500	-0.11892100
O	-1.45167600	2.12365200	0.66743100
O	0.11479900	2.77932200	-0.83002400
C	-3.70542700	5.40938500	0.34784500
O	-3.54563200	6.34012100	-0.43732900
C	-4.92567600	5.32385900	1.25671600
H	-4.95472900	4.42039400	1.87232600
H	-4.93851400	6.19947500	1.91212400
H	-5.82758900	5.36753500	0.64001500
C	3.53489900	0.63701800	0.35460000
C	4.65564300	1.35517000	-0.50023900
C	3.19333400	3.04203000	-0.08152600
C	2.50119200	1.78219300	0.48023000
C	4.68086200	2.72649300	0.22664000
H	5.36814700	3.43275600	-0.25151700
H	4.91289100	2.66608300	1.28990800
C	4.17325400	1.81040500	-1.91341300
H	5.05246900	2.11776400	-2.48959400
H	3.66845100	1.04099500	-2.49624100
C	3.22673500	3.01455600	-1.62406100
H	3.65203800	3.95040500	-2.00284900
H	2.23565800	2.89862600	-2.06297100
H	5.59486500	0.79550400	-0.51742100
H	2.79317500	3.96684200	0.33653700
H	-2.96654800	3.59776400	1.08028100
H	2.09490700	1.91674200	1.48342200
C	4.20170500	0.22686600	1.68190100
O	4.25040300	0.89560200	2.68979300
O	4.80079400	-0.98035100	1.56432200
C	5.49384300	-1.43994400	2.73878200
H	4.79952900	-1.53741800	3.57677100
H	5.91330400	-2.40969000	2.47189800
H	6.28600300	-0.74003900	3.01508400

int11

C	0.74474600	0.65212900	-1.62521900
C	-0.56967900	0.26023700	-1.84199200
C	-0.97072900	-1.08280200	-1.68342500
C	0.02020600	-2.02016100	-1.31179800
C	1.35541700	-1.66749000	-1.06941900

C	1.69021900	-0.30297500	-1.24474000
H	1.05546600	1.68196900	-1.75046300
H	2.74414200	0.01935400	-1.29950200
Cl	-1.70545500	1.48456600	-2.35973900
C	-2.39305800	-1.50724100	-1.89995200
H	-2.95473300	-0.83052900	-2.54476700
H	-2.46153200	-2.52168900	-2.29502900
S	-3.38098800	-1.61977900	-0.35069300
O	-2.53587600	-1.94497900	0.79107200
O	-4.60042400	-2.36749300	-0.63177100
O	-3.77834400	0.01512300	-0.21061900
C	-5.07408600	0.34545800	0.16484200
C	-6.02393700	0.61901500	-0.83168200
C	-5.37276500	0.46660100	1.51756900
C	-7.30942100	1.03172400	-0.43043900
C	-6.65920200	0.87474000	1.89590800
H	-4.59520700	0.24771700	2.23734100
C	-7.62402500	1.15820300	0.91110900
H	-8.05428100	1.24918300	-1.18806300
H	-8.61047400	1.47556200	1.22977600
C	-5.67508200	0.47278000	-2.20843400
N	-5.36810700	0.34651700	-3.32433600
O	-7.06287700	1.02829400	3.17745700
C	-6.13657700	0.75031000	4.22418000
H	-6.67580500	0.93339600	5.15377300
H	-5.80349200	-0.29375100	4.19523800
H	-5.26517300	1.41375600	4.17240100
Cl	-0.43637800	-3.71366700	-1.17704700
Pd	2.86535400	0.04389400	0.77210300
C	2.68539500	4.32314900	0.69201700
H	3.27458700	4.57310400	1.58292200
H	1.63992700	4.52319100	0.95777200
N	3.09772600	5.10703100	-0.45030900
C	2.84639300	2.83588800	0.39136700
O	2.51229900	2.04518500	1.35008300
O	3.26869600	2.45886000	-0.72131500
C	3.07047200	6.46662700	-0.43987700
O	2.68678500	7.10982600	0.53279900
C	3.54618100	7.14197600	-1.71938100
H	3.86298500	6.44080500	-2.49650500
H	2.73699300	7.76517800	-2.11025900

H	4.37987000	7.80691400	-1.47729100
H	3.42539300	4.57198800	-1.24370300
C	3.30804500	-1.93720200	0.48510800
C	4.74536000	-2.18600800	-0.02652100
C	3.43248700	-3.18134700	-1.59147000
C	2.39859100	-2.64293700	-0.55281700
C	4.55171100	-2.11643000	-1.55694100
H	5.44589700	-2.43508300	-2.10237100
H	4.26367200	-1.13182800	-1.93059400
C	5.04936900	-3.70556500	0.15880000
H	6.11292200	-3.88991200	-0.02242400
H	4.82395300	-4.06143700	1.16759300
C	4.15426400	-4.38234800	-0.93235300
H	4.76546000	-4.91013700	-1.67070700
H	3.45272900	-5.10694800	-0.50923300
H	5.49798200	-1.52684900	0.41289200
H	2.99556600	-3.39975500	-2.56867000
H	1.87748000	-3.47844900	-0.08097000
O	3.50075600	-1.10563900	2.63113300
C	3.03526500	-2.22507400	1.93033300
O	2.46039900	-3.13444200	2.46884800
C	3.14679300	-1.00847100	4.03360000
H	3.48631200	-0.02431500	4.35056500
H	2.06723000	-1.11101900	4.15540900
H	3.66005800	-1.79778600	4.58536000

TS5

C	-0.64837500	-1.14476500	-0.20307700
C	0.60469700	-1.21422200	-0.80171100
C	1.12653600	-0.13909900	-1.54248500
C	0.31644600	1.01208000	-1.64134100
C	-0.94703500	1.12563500	-1.04533900
C	-1.45203300	-0.00316500	-0.33569400
H	-1.01837700	-2.00911300	0.33324700
H	-2.70724100	-0.60900700	-0.32643000
Cl	1.49582700	-2.71432200	-0.64164700
C	2.46169800	-0.21881800	-2.21972600
H	2.77936700	-1.24491900	-2.40667300
H	2.47951900	0.34342000	-3.15476200
S	3.85722600	0.53233000	-1.29030800
O	3.42367800	1.65892300	-0.47020000

O	4.99691400	0.65798400	-2.19140700
O	4.12527300	-0.77388600	-0.26400500
C	5.37321500	-0.87847900	0.33802700
C	6.14360200	-2.01109500	0.03471200
C	5.79869800	0.07984300	1.25365100
C	7.37874000	-2.16914100	0.69446400
C	7.03966700	-0.08930500	1.88195400
H	5.15788500	0.92794100	1.45413000
C	7.82397500	-1.22351900	1.60074500
H	7.98313600	-3.04283600	0.47643600
H	8.77565200	-1.33399900	2.10809200
C	5.67806700	-2.97017800	-0.91611100
N	5.30322100	-3.75527600	-1.68919300
O	7.55977000	0.77848400	2.78019300
C	6.82586100	1.95946400	3.09280700
H	7.43770400	2.50789100	3.80938000
H	6.66457700	2.57698300	2.20163900
H	5.85844600	1.71917300	3.54954900
Cl	0.92166700	2.38256200	-2.56902500
Pd	-2.90098200	0.63546100	1.06699700
C	-4.50159600	-3.35465900	1.22747800
H	-5.44198700	-3.12844500	1.74553100
H	-3.88816100	-3.90089900	1.95494400
N	-4.73680300	-4.13826100	0.03617900
C	-3.80490800	-2.04392900	0.90584400
O	-3.50865300	-1.29295100	1.88326200
O	-3.55033500	-1.77397900	-0.31478400
C	-5.41691900	-5.31885400	0.09584000
O	-5.84211500	-5.76997600	1.15382700
C	-5.60646400	-6.03679900	-1.23172800
H	-5.18963800	-5.49895200	-2.08765100
H	-5.13663400	-7.02222600	-1.16846800
H	-6.67560400	-6.19634600	-1.39552400
H	-4.40930400	-3.74707800	-0.83529500
C	-2.77145600	2.40869800	0.09464000
C	-4.10757800	2.70588500	-0.63082900
C	-2.56817400	2.73665100	-2.29654900
C	-1.70709400	2.43257400	-1.02969500
C	-3.88771000	1.99908600	-1.98515500
H	-4.67807300	2.22557600	-2.70836700
H	-3.78778000	0.91369600	-1.90649000

C	-4.07644900	4.20297000	-1.06408100
H	-5.06548200	4.49929800	-1.42780600
H	-3.81785700	4.87582200	-0.24136900
C	-3.01519300	4.21551900	-2.21276400
H	-3.46327600	4.53338900	-3.15917200
H	-2.17810100	4.88857500	-2.00494800
H	-4.99900300	2.43199300	-0.06123000
H	-2.07009700	2.47138100	-3.23081700
H	-0.99103600	3.24335900	-0.85912800
O	-3.40008900	2.57415700	2.30340900
C	-2.51802400	3.14164900	1.36624400
O	-1.70585300	3.97858200	1.66727000
C	-3.23152800	2.99014000	3.67825900
H	-3.97957800	2.43947200	4.24634400
H	-2.22409500	2.75261000	4.02604500
H	-3.40044200	4.06574100	3.75357800

int12

C	0.36307700	1.02139300	-0.55499800
C	-0.86765500	0.95390500	-1.20658600
C	-1.41219500	-0.26621200	-1.64549400
C	-0.62011800	-1.41842900	-1.44157700
C	0.63378400	-1.38759000	-0.82154700
C	1.10937900	-0.13972300	-0.35271200
H	0.71071000	1.98334800	-0.19628000
H	3.52910500	1.39993800	-0.86267700
Cl	-1.71535100	2.46969700	-1.48546500
C	-2.74797400	-0.33896900	-2.31994800
H	-3.04483300	0.60690600	-2.77365100
H	-2.78841700	-1.12956800	-3.07177300
S	-4.15981000	-0.77632200	-1.23240500
O	-3.80237300	-1.78989300	-0.24407100
O	-5.35272200	-0.93653900	-2.05760500
O	-4.24913800	0.70982500	-0.44166200
C	-5.37139600	0.97722000	0.32907300
C	-6.09767200	2.13952600	0.02409000
C	-5.71473100	0.15805700	1.40246000
C	-7.19812800	2.46894400	0.84073600
C	-6.82538900	0.49634100	2.18585400
H	-5.11245900	-0.71782200	1.59996500
C	-7.56290000	1.66055100	1.90225300

H	-7.76382700	3.36765400	0.62015100
H	-8.41239100	1.90342600	2.53048800
C	-5.72453200	2.96911800	-1.07744200
N	-5.43380300	3.66230100	-1.96600600
O	-7.25531300	-0.23138700	3.24323500
C	-6.56248700	-1.43328700	3.57050100
H	-7.09167600	-1.85731100	4.42430300
H	-6.58181300	-2.14541700	2.73753800
H	-5.52211700	-1.23107200	3.85136500
Cl	-1.23601200	-2.97603200	-1.99676400
Pd	2.76537700	-0.15697500	0.73583000
C	4.03256700	4.14567400	0.78005400
H	4.23452400	4.18217400	1.85331200
H	3.16249600	4.77795200	0.57560000
N	5.15889800	4.63202400	0.01851800
C	3.64686700	2.70861000	0.46780400
O	3.13860500	1.97849000	1.32026600
O	3.83098700	2.34006500	-0.78985400
C	6.35041300	3.95598500	0.10238800
O	6.46435900	2.98797900	0.84486500
C	7.48062800	4.47261000	-0.76485400
H	7.25891000	5.42748100	-1.24836400
H	8.37378000	4.58183800	-0.14545900
H	7.70402000	3.72759200	-1.53430000
H	5.01165700	5.32146800	-0.70193900
C	2.74517900	-2.13977600	0.26640200
C	3.96839300	-2.51893200	-0.61360800
C	2.19204700	-3.17586800	-1.86010000
C	1.51217400	-2.58760000	-0.58085000
C	3.42207200	-2.26091100	-2.03207300
H	4.10239700	-2.60593300	-2.81858300
H	3.16548400	-1.21408300	-2.21757500
C	4.09270900	-4.07028500	-0.62221300
H	5.03300300	-4.36413600	-1.10084300
H	4.09477900	-4.50144000	0.38317700
C	2.85688500	-4.51738300	-1.46859100
H	3.16882200	-5.06677200	-2.36269200
H	2.17589100	-5.16409400	-0.90701600
H	4.89384500	-2.00876100	-0.33564100
H	1.51891900	-3.24877200	-2.71536300
H	0.94509200	-3.36817500	-0.06157100

O	3.85791200	-2.01366600	2.32011100
C	2.80017300	-2.63241700	1.67731600
O	2.05918200	-3.40141500	2.24893200
C	4.00081100	-2.31699000	3.71976300
H	4.87959300	-1.76555400	4.05298200
H	3.11375900	-1.99988700	4.27384200
H	4.14398800	-3.39059000	3.86128300

int13

C	-0.12597900	-0.68382900	0.42793500
C	1.11801800	-1.17304700	0.03395400
C	2.01669400	-0.40827300	-0.73107000
C	1.57964600	0.87814800	-1.11512700
C	0.32635900	1.39402500	-0.76529300
C	-0.51809300	0.59925200	0.04345700
H	-0.76571700	-1.31016400	1.03862500
Cl	1.52711900	-2.81621100	0.51963700
C	3.35701600	-0.94761900	-1.13453200
H	3.36015400	-2.03695400	-1.17156600
H	3.71275400	-0.54479000	-2.08303400
S	4.68095400	-0.54148200	0.06836000
O	4.29726600	-0.94175700	1.41896900
O	5.26302000	0.77329200	-0.17163500
O	5.75103600	-1.70933100	-0.53856300
C	7.10409300	-1.52518800	-0.30578900
C	7.94853400	-1.42227800	-1.42210500
C	7.60164500	-1.50600100	0.99507600
C	9.33534000	-1.30780000	-1.19884100
C	8.98119900	-1.36806500	1.19221000
H	6.90568200	-1.59859500	1.81815900
C	9.84661300	-1.27689100	0.08614500
H	10.00036000	-1.23449000	-2.05246600
H	10.91119100	-1.18068500	0.26705100
C	7.40757000	-1.43152400	-2.74420900
N	6.97819200	-1.43775400	-3.82590500
O	9.57355600	-1.32462900	2.40872700
C	8.74998800	-1.37792400	3.57030500
H	9.42917500	-1.29815600	4.41953000
H	8.03692400	-0.54571400	3.59275900
H	8.20362200	-2.32678600	3.63007900
Cl	2.65948800	1.88647700	-2.07530400

Pd	-2.19934100	1.42534400	0.69766700
C	-6.62981600	-2.98139800	0.56583100
C	-6.37521600	-2.86840000	-0.80652100
C	-5.34921300	-2.02977900	-1.25759000
C	-4.57634700	-1.30372600	-0.35241300
C	-4.85388500	-1.43368000	1.00625000
C	-5.86724400	-2.26034200	1.48538800
H	-7.42333600	-3.63209900	0.91444600
H	-5.16578400	-1.95630600	-2.32431000
H	-3.77880800	-0.65481800	-0.69977100
H	-6.06706000	-2.34816500	2.54751700
I	-3.67021400	-0.32567800	2.43562500
C	-7.16258400	-3.61611200	-1.83189000
O	-6.97907600	-3.52664700	-3.02928700
O	-8.10545800	-4.40768200	-1.27868900
C	-8.89904600	-5.15996400	-2.21283700
H	-8.26401600	-5.81697400	-2.81174200
H	-9.59204600	-5.74243200	-1.60644200
H	-9.44244700	-4.48798600	-2.88140100
C	-1.56362500	2.98975800	-0.46451300
C	-2.55647000	3.23509400	-1.63024600
C	-0.57939300	2.87724900	-2.67975600
C	-0.19318900	2.74596700	-1.16960800
C	-2.00439800	2.28633100	-2.71272100
H	-2.49571300	2.41792000	-3.68307100
H	-2.04994200	1.23126200	-2.42945400
C	-2.22431200	4.62405700	-2.25301200
H	-3.00567800	4.90308800	-2.96789300
H	-2.17184100	5.42184900	-1.50629500
C	-0.85819900	4.37138100	-2.96844600
H	-0.93970400	4.54520300	-4.04617400
H	-0.06011900	5.01807000	-2.59150300
H	-3.60803200	3.12273600	-1.35564300
H	0.14909600	2.42466900	-3.35371500
H	0.52634400	3.52441900	-0.89289200
O	-2.83251500	4.07340600	1.18969300
C	-1.57494700	4.01685800	0.62274100
O	-0.65890100	4.70695800	1.01468400
C	-2.96993200	4.98863400	2.29129000
H	-4.01199700	4.92127700	2.60351500
H	-2.30269900	4.70910800	3.11065200

H	-2.73064700	6.00572100	1.97260100
TS6			
C	0.01333300	0.98332100	0.91204600
C	1.29418600	0.60831400	1.31214600
C	1.97422800	-0.47770200	0.73007800
C	1.27838700	-1.19890100	-0.26214800
C	-0.02335500	-0.87462500	-0.67032800
C	-0.63465700	0.25281400	-0.08272800
H	-0.44947400	1.84781500	1.37267100
Cl	2.03877200	1.54516600	2.60117300
C	3.35993200	-0.85470500	1.16525200
H	3.56067100	-0.53935000	2.18909000
H	3.56849900	-1.91954100	1.05987700
S	4.66390900	-0.02502600	0.17795400
O	4.44321500	1.41730000	0.13446000
O	4.98028500	-0.75931400	-1.04088900
O	5.88070100	-0.33552500	1.31406400
C	7.19246100	-0.34097200	0.86470600
C	7.90796100	-1.54522600	0.94650700
C	7.78200700	0.83581500	0.41030700
C	9.26440700	-1.53943700	0.56444400
C	9.12630100	0.81263700	0.01738100
H	7.18274200	1.73588800	0.37551800
C	9.86578000	-0.38171500	0.10418200
H	9.83260600	-2.46098500	0.62865300
H	10.90692400	-0.36943400	-0.19782700
C	7.26851900	-2.73780500	1.40422600
N	6.75444600	-3.71341200	1.77620100
O	9.80043400	1.89021000	-0.44725800
C	9.10164300	3.12449500	-0.58547300
H	9.82495400	3.83083900	-0.99364500
H	8.25482500	3.02879900	-1.27484800
H	8.74260100	3.49140800	0.38350800
Cl	2.07248900	-2.56932500	-1.02871900
Pd	-2.42553900	0.83908100	-0.78957800
C	-6.07882800	-0.14986100	0.84420400
C	-5.73285100	-0.71136000	2.07898900
C	-4.49519900	-0.39516500	2.66223600
C	-3.60227200	0.45882400	2.02430300
C	-3.95170800	0.97105300	0.76876300

C	-5.20170300	0.71786500	0.18985700
H	-7.04381200	-0.37121300	0.40237300
H	-4.24756400	-0.82960200	3.62526500
H	-2.65096400	0.70164100	2.48111200
H	-5.49198900	1.18373700	-0.74515900
I	-3.14605900	3.27911300	0.27368800
C	-6.63869200	-1.62901100	2.82422800
O	-6.37330100	-2.12699800	3.90088500
O	-7.79867500	-1.85365100	2.16729600
C	-8.71814200	-2.73449700	2.83365700
H	-8.99787400	-2.33053500	3.80959300
H	-9.58829100	-2.79928800	2.18078200
H	-8.26962600	-3.72078800	2.97612900
C	-2.15042600	-0.86599900	-1.96630100
C	-3.25173800	-1.91132500	-1.67105900
C	-1.32746000	-3.03272400	-1.24712000
C	-0.81477900	-1.62597600	-1.70077900
C	-2.62828400	-2.68663200	-0.49311400
H	-3.20734100	-3.57442200	-0.21729600
H	-2.47649500	-2.07234500	0.39780600
C	-3.20225900	-2.98565700	-2.79968800
H	-4.07681800	-3.63965700	-2.71890700
H	-3.21886900	-2.54902600	-3.80267200
C	-1.87803600	-3.75837600	-2.49648000
H	-2.07923400	-4.81026400	-2.27049400
H	-1.17374400	-3.73229200	-3.33332800
H	-4.24348700	-1.48303600	-1.51919900
H	-0.58257900	-3.60536700	-0.69325900
H	-0.23578800	-1.71387500	-2.62667600
O	-3.44223100	0.52209600	-3.36333100
C	-2.25153000	-0.16198900	-3.28650200
O	-1.43083100	-0.14098200	-4.17805500
C	-3.63400900	1.29380200	-4.56540800
H	-4.61722800	1.75285800	-4.46698300
H	-2.85895500	2.05833100	-4.65719700
H	-3.59895100	0.64325100	-5.44187200

int14

C	0.12022200	0.48871700	-1.23523800
C	-1.16805900	0.04624400	-1.53195700
C	-1.89617700	-0.78357900	-0.65608400

C	-1.24651100	-1.18822300	0.52761700
C	0.06555000	-0.80282800	0.84927500
C	0.70410400	0.07313100	-0.04262700
H	0.63052200	1.16100900	-1.91331900
Cl	-1.85744000	0.56301700	-3.05863600
C	-3.29688700	-1.21744600	-0.97974900
H	-3.48081200	-1.21780500	-2.05396200
H	-3.55279500	-2.19152800	-0.56263900
S	-4.55663900	-0.06785400	-0.30536400
O	-4.26922000	1.30272600	-0.71482600
O	-4.88469200	-0.37221600	1.08168800
O	-5.79491000	-0.66224400	-1.28866700
C	-7.10018500	-0.50493700	-0.84210700
C	-7.82736000	-1.66096700	-0.52195800
C	-7.66741600	0.76441600	-0.78182100
C	-9.17672000	-1.51192600	-0.14383300
C	-9.00501000	0.88991800	-0.38401500
H	-7.05730900	1.61792100	-1.04617800
C	-9.75760300	-0.25832200	-0.07308400
H	-9.75561400	-2.39595500	0.10019000
H	-10.79306100	-0.13379700	0.22297900
C	-7.20228200	-2.94416700	-0.57717300
N	-6.69265600	-3.98963900	-0.61963800
O	-9.65890200	2.06915500	-0.27954200
C	-8.94429700	3.27294800	-0.54892000
H	-9.65328800	4.08319300	-0.37772400
H	-8.08802200	3.38758900	0.12560400
H	-8.59714900	3.30742600	-1.58840100
Cl	-2.10306500	-2.21979400	1.66057800
Pd	2.38622600	0.94677400	0.56291100
C	6.03127200	-0.54686100	-0.88833300
C	5.72702100	-1.26692900	-2.05074300
C	4.39606300	-1.37187200	-2.46933700
C	3.36609200	-0.77385400	-1.73969200
C	3.69383300	-0.07244300	-0.58183800
C	5.01336100	0.05675200	-0.14687500
H	7.06195100	-0.44899700	-0.56686200
H	4.17594700	-1.92880400	-3.37430100
H	2.34359400	-0.86458500	-2.08179000
H	5.26309500	0.62910000	0.74103100
I	2.85018900	3.37235800	-0.50597000

C	6.77287200	-1.93362100	-2.87816100
O	6.54465000	-2.56959500	-3.88834700
O	8.01579600	-1.75549900	-2.37804700
C	9.07269200	-2.37011400	-3.13296400
H	9.10246000	-1.96842200	-4.14871600
H	9.99220500	-2.13157100	-2.59889400
H	8.92756500	-3.45192200	-3.18610200
C	2.18084400	-0.48140200	2.14395400
C	3.21690300	-1.61830000	2.23598600
C	1.23700000	-2.72050100	2.14128000
C	0.80845000	-1.21812700	2.08666200
C	2.56613600	-2.70937700	1.36169100
H	3.09923300	-3.66409300	1.41656900
H	2.46359700	-2.42402400	0.31302000
C	3.08253400	-2.25650300	3.65366800
H	3.91827500	-2.94465400	3.81616600
H	3.11559500	-1.51819900	4.46017300
C	1.71940400	-3.01621700	3.58019900
H	1.85873600	-4.09202500	3.72389600
H	1.00491400	-2.67566200	4.33544100
H	4.23610400	-1.32416500	1.99000300
H	0.46743600	-3.40303600	1.77976200
H	0.21199300	-0.95690300	2.96779100
O	3.51607800	1.18655800	3.13930800
C	2.28844700	0.59459700	3.19435800
O	1.41636400	0.94680400	3.96052800
C	3.71717200	2.30192400	4.03576600
H	4.75349500	2.60473000	3.89467500
H	3.04017000	3.11890300	3.77704400
H	3.53799700	1.99175300	5.06687800

int15

C	0.03940600	1.01074700	-0.55032200
C	1.20357500	1.44115100	0.08581800
C	1.67945000	0.83021400	1.26275400
C	0.90166700	-0.22132000	1.79042900
C	-0.28746400	-0.66427000	1.19564900
C	-0.68898200	-0.03349200	0.00991300
H	-0.27841200	1.48563100	-1.47255300
Cl	2.05455200	2.80046500	-0.62361100
C	2.93846000	1.28182300	1.93824700

H	3.21292900	2.30641900	1.68629600
H	2.88347000	1.17750700	3.02313000
S	4.43607700	0.29600300	1.53267500
O	4.11095400	-1.09097100	1.21168700
O	5.47978500	0.61089000	2.50198400
O	4.79245400	1.08446400	0.08710700
C	6.08880700	0.99593500	-0.40144200
C	6.79650900	2.19586100	-0.57057800
C	6.62794700	-0.23461800	-0.76765600
C	8.08455600	2.13274900	-1.13860900
C	7.91896300	-0.27347300	-1.31016500
H	6.03318500	-1.12633900	-0.62289600
C	8.64132300	0.91908000	-1.50013600
H	8.64076500	3.05261100	-1.28244000
H	9.63448200	0.86084300	-1.93088300
C	6.21816400	3.44109700	-0.17607600
N	5.75467300	4.46005000	0.14232500
O	8.54765700	-1.41001900	-1.69131900
C	7.88197100	-2.65494700	-1.49982200
H	8.57547500	-3.41943100	-1.85107700
H	7.65344900	-2.82703500	-0.44161800
H	6.95628600	-2.70751300	-2.08538300
Cl	1.44401400	-1.02883100	3.25914700
Pd	-2.17868000	-0.85317400	-1.02321100
C	-5.89226500	1.05683900	-0.36549600
C	-5.59000400	2.36758500	0.02352400
C	-4.25071700	2.75589500	0.14023400
C	-3.21952400	1.85065100	-0.11548900
C	-3.53493700	0.54250000	-0.49073700
C	-4.86899800	0.14393400	-0.62660700
H	-6.92713100	0.75041000	-0.46970500
H	-4.02645600	3.77541000	0.43680200
H	-2.19362300	2.17773800	-0.01411500
H	-5.11974300	-0.85886400	-0.95161000
C	-6.64121900	3.38088300	0.31916100
O	-6.41692000	4.52560600	0.66149900
O	-7.89189500	2.88719000	0.16594900
C	-8.95227600	3.81682800	0.43598600
H	-8.88831200	4.67872000	-0.23291000
H	-9.87712600	3.26612700	0.26449700
H	-8.90112700	4.16991100	1.46904400

C	-2.25566000	-2.15884900	0.64592900
C	-3.52745900	-2.19425500	1.50096600
C	-1.93200700	-1.60044900	2.99961700
C	-1.11645100	-1.81924400	1.68239400
C	-3.26367000	-1.02837700	2.47930100
H	-4.02662000	-0.96100200	3.26158700
H	-3.16871600	-0.05615400	1.99472400
C	-3.46492700	-3.41176400	2.47739100
H	-4.44241400	-3.52080700	2.95829100
H	-3.24508500	-4.34689800	1.96372900
C	-2.37099500	-2.99162400	3.51001000
H	-2.78523700	-2.91500600	4.52018500
H	-1.53666500	-3.69910800	3.55581800
H	-4.45038900	-2.15714400	0.92139700
H	-1.39748700	-0.99842400	3.73558400
H	-0.45565800	-2.68615000	1.81404200
O	-0.99919300	-2.94436900	-1.15574100
C	-1.96326900	-3.34172500	-0.24261900
O	-2.46673000	-4.43653900	-0.27297900
C	-0.69857400	-3.87446700	-2.22176700
H	0.09477300	-3.40459300	-2.80095600
H	-0.36187400	-4.82095300	-1.79640000
H	-1.58903200	-4.03574200	-2.83196300
C	-3.00242800	-0.84169400	-3.45738200
O	-2.10793200	-0.01658600	-3.07820400
O	-3.48442000	-1.68012300	-2.62384300
C	-3.51291400	-0.80192300	-4.87421700
H	-3.90266400	-1.77758700	-5.16941400
H	-4.32950000	-0.07361000	-4.92967200
H	-2.72422900	-0.47714200	-5.55538300

TS7

C	0.37084800	0.96004900	0.75402900
C	-0.81870500	1.41912100	0.19602200
C	-1.27319500	0.96971200	-1.05826400
C	-0.47907600	-0.00145900	-1.70513900
C	0.70624600	-0.51718600	-1.16777300
C	1.13560000	0.01672100	0.06953500
H	0.70983900	1.37239300	1.69646400
Cl	-1.70234600	2.64499600	1.08300500
C	-2.52331500	1.50288200	-1.68786200

H	-2.80348300	2.48695100	-1.31108000
H	-2.45113000	1.53831900	-2.77600400
S	-4.02679200	0.47138100	-1.43706300
O	-3.70001400	-0.93976000	-1.25465800
O	-5.04142700	0.88468600	-2.40011400
O	-4.43915800	1.09572900	0.07291100
C	-5.76716300	1.01305500	0.46890200
C	-6.45182000	2.21743300	0.69161400
C	-6.36251400	-0.22504700	0.69459100
C	-7.77603200	2.15036400	1.16843400
C	-7.68733000	-0.26651900	1.14843000
H	-5.78361600	-1.12068200	0.51329300
C	-8.38783600	0.92972000	1.39090600
H	-8.31584700	3.07279300	1.35258300
H	-9.40856800	0.86865600	1.75098900
C	-5.81306800	3.46962600	0.43741800
N	-5.29644300	4.49194600	0.23115700
O	-8.37110700	-1.40873100	1.39197200
C	-7.72879500	-2.65563600	1.14221200
H	-8.46611100	-3.42244400	1.38103500
H	-7.43203500	-2.74864200	0.09104800
H	-6.84818600	-2.78662000	1.78245500
Cl	-1.00509700	-0.61304600	-3.27146300
Pd	2.56946200	-1.14459200	0.96699000
C	4.33752900	2.60069900	1.13728500
C	4.64917500	3.05972400	-0.14730800
C	4.13551100	2.37801200	-1.25610500
C	3.34079000	1.24686000	-1.09250300
C	3.07383000	0.75963500	0.19402900
C	3.53976300	1.46947600	1.31322500
H	4.71565700	3.12698400	2.00639500
H	4.35269100	2.75745900	-2.24910600
H	2.91298300	0.78073100	-1.96811400
H	3.31685400	1.13277500	2.31921400
C	5.48985200	4.26499700	-0.39454400
O	5.76872000	4.69028100	-1.49884300
O	5.91452800	4.84090300	0.75160300
C	6.73047600	6.01122200	0.58295800
H	6.17932300	6.79003000	0.05014200
H	6.98298800	6.34080700	1.59055000
H	7.63477300	5.77087500	0.01842300

C	2.18226600	-2.48124900	-0.60422900
C	3.44092100	-2.99588100	-1.31225000
C	2.42917500	-1.71458200	-2.89294800
C	1.38441300	-1.75069800	-1.71582800
C	3.81185800	-1.79400300	-2.19614500
H	4.60740400	-2.02983500	-2.91086500
H	4.11359200	-0.91880600	-1.62807800
C	3.00659300	-4.02605400	-2.40942200
H	3.89633100	-4.55056400	-2.77110200
H	2.32262000	-4.78223600	-2.02360300
C	2.38120000	-3.12697100	-3.52743200
H	2.98325700	-3.15340400	-4.44113900
H	1.36460300	-3.42838600	-3.79865900
H	4.20081900	-3.37840100	-0.63034700
H	2.27117900	-0.89944900	-3.60313400
H	0.56269800	-2.39975100	-2.04107300
O	0.20375000	-3.08882100	0.58433200
C	1.41335500	-3.53843900	0.16896900
O	1.80705000	-4.66597300	0.37901200
C	-0.59296900	-4.03977100	1.31215700
H	-1.51928400	-3.51937600	1.55231500
H	-0.79361200	-4.92079300	0.69781100
H	-0.07538600	-4.35156800	2.22257600
C	3.40871800	-1.97476300	3.27274100
O	2.96771500	-0.79486400	3.28095400
O	3.40329200	-2.66008200	2.17744700
C	3.96806700	-2.62344200	4.51191200
H	3.52362000	-3.61311100	4.64645300
H	5.04666900	-2.76480700	4.38802800
H	3.78141100	-2.00014900	5.38704700

int16

C	-0.78945900	1.89068500	0.61385100
C	0.46295500	1.94743200	1.17942100
C	0.95525200	0.88080200	1.97140700
C	0.13968500	-0.25205500	2.08302900
C	-1.12044300	-0.42071300	1.40686900
C	-1.62472100	0.74902600	0.73624700
H	-1.17655300	2.75926900	0.09633000
Cl	1.37058800	3.42776800	0.99370600
C	2.26489800	1.00757500	2.69547500

H	2.56591800	2.04705000	2.82589000
H	2.25139600	0.51216800	3.66746800
S	3.70740100	0.23237000	1.87531700
O	3.41112800	-1.12050400	1.41179500
O	4.89066100	0.48897200	2.68721800
O	3.72339900	1.24454600	0.53909800
C	4.86379900	1.24536400	-0.25967100
C	5.63341600	2.41748000	-0.29904900
C	5.17137600	0.13221800	-1.03637300
C	6.74510600	2.44929100	-1.16471600
C	6.28994000	0.18339700	-1.87890900
H	4.53479100	-0.73915900	-0.96814400
C	7.07271300	1.35113500	-1.93980600
H	7.34742300	3.34984500	-1.21277200
H	7.92847500	1.36715200	-2.60522000
C	5.28950400	3.54509900	0.50774100
N	5.01488800	4.47216400	1.15535000
O	6.68765100	-0.83574400	-2.67455100
C	5.94197500	-2.05014000	-2.65373500
H	6.44550100	-2.71937900	-3.35164600
H	5.93967200	-2.49970100	-1.65395100
H	4.90880200	-1.88998700	-2.98438800
Cl	0.64682500	-1.46692700	3.25024200
Pd	-0.90009500	-0.78620700	-0.95913100
C	-4.75762600	1.89247000	-1.10460800
C	-5.68858500	1.94530600	-0.05823900
C	-5.29184200	1.58585500	1.23526200
C	-3.98897400	1.16157400	1.47788500
C	-3.06229100	1.06950200	0.42808100
C	-3.45420200	1.46831400	-0.86109800
H	-5.05724800	2.18531200	-2.10418700
H	-6.01643700	1.65599400	2.03941800
H	-3.68167100	0.91581300	2.48929500
H	-2.73515600	1.42825100	-1.67413800
C	-7.09874200	2.38925900	-0.25629600
O	-7.92732200	2.45283500	0.63090300
O	-7.36049400	2.71652000	-1.54064300
C	-8.70426500	3.15392300	-1.79969200
H	-8.93528600	4.04993100	-1.21826600
H	-8.74239100	3.36888400	-2.86736300
H	-9.42002000	2.37055400	-1.53869900

C	-1.51510700	-2.47137700	0.04716900
C	-2.86110300	-3.06378500	-0.39429000
C	-3.33476800	-2.03054400	1.57033600
C	-1.79496000	-1.82188600	1.43548000
C	-3.86429600	-2.01845200	0.11702400
H	-4.90084600	-2.36760400	0.05983100
H	-3.79474700	-1.06292200	-0.39647300
C	-3.17442600	-4.25381600	0.56469700
H	-4.03280500	-4.81452900	0.18067700
H	-2.34217000	-4.95492900	0.64444100
C	-3.51966800	-3.53608900	1.91017800
H	-4.55643600	-3.72434100	2.20611300
H	-2.88346900	-3.85821300	2.74112700
H	-2.89829800	-3.32379700	-1.45221000
H	-3.82319600	-1.36478600	2.28202200
H	-1.30619900	-2.37673500	2.23360700
O	0.73986300	-3.04527800	0.56569200
C	-0.34985100	-3.39904400	-0.15363600
O	-0.36394400	-4.35818400	-0.90195600
C	1.90208400	-3.87160000	0.38311500
H	2.68217200	-3.40640700	0.98146700
H	1.69971100	-4.89228800	0.71879700
H	2.18435200	-3.89958200	-0.67236100
C	-0.34840900	-0.33320300	-3.38419900
O	-0.26359700	0.65439200	-2.59837400
O	-0.69764000	-1.48487100	-2.92677200
C	-0.07786500	-0.19510800	-4.85974300
H	0.45023000	-1.07624800	-5.23110100
H	-1.03218300	-0.13062000	-5.39355600
H	0.49815100	0.71030300	-5.05611200

TS8

C	-0.45740000	1.03660800	-1.21198700
C	0.87856100	1.39320100	-1.06368600
C	1.63626600	0.99938400	0.05573900
C	0.98264700	0.18077200	0.99985900
C	-0.35061600	-0.23401100	0.86732000
C	-1.07455700	0.24124500	-0.24628500
H	-1.01057300	1.41606400	-2.06220000
Cl	1.57409800	2.42550500	-2.30041000
C	3.06250700	1.43286900	0.22539600

H	3.26430600	2.36373500	-0.30489100
H	3.36634400	1.53440900	1.26795300
S	4.25470900	0.24067700	-0.50243200
O	3.89750900	-0.05232200	-1.88465500
O	4.58981400	-0.83260600	0.42560300
O	5.55602000	1.32923500	-0.54026700
C	6.80221100	0.87666900	-0.13355500
C	7.20701000	1.09020500	1.19361900
C	7.64473800	0.28737900	-1.07047300
C	8.50725600	0.69693300	1.56606600
C	8.93267000	-0.10212000	-0.67855400
H	7.27817900	0.15403400	-2.07976900
C	9.35828800	0.11038100	0.64619200
H	8.83514300	0.85742800	2.58728400
H	10.36050900	-0.19668800	0.92296800
C	6.30389500	1.68455000	2.12612200
N	5.54898300	2.16753500	2.86923400
O	9.83557600	-0.68334600	-1.50103700
C	9.46260000	-0.94361700	-2.85152700
H	10.32931400	-1.41752800	-3.31268700
H	8.60401800	-1.62319600	-2.90443200
H	9.22780100	-0.01587600	-3.38674300
Cl	1.88008700	-0.35952200	2.41168400
C	-4.24620300	2.95767600	-1.00831400
C	-4.24093800	3.65874700	0.20428600
C	-3.55673500	3.12643100	1.30362400
C	-2.89714700	1.90243600	1.21144700
C	-2.93944100	1.18987800	0.01023600
C	-3.57838800	1.73816400	-1.11432900
H	-4.76482700	3.36633200	-1.86777000
H	-3.54066200	3.69224300	2.22933700
H	-2.34307400	1.53061000	2.06300500
H	-3.58550000	1.21984400	-2.07186000
C	-4.92380000	4.97286000	0.37511200
O	-4.93316400	5.60862900	1.41094200
O	-5.53637600	5.38434100	-0.75619800
C	-6.21954000	6.64511700	-0.65945200
H	-5.51824400	7.44220700	-0.40078700
H	-6.65389900	6.81971300	-1.64346600
H	-7.00011900	6.60048300	0.10382700
C	-2.05655600	-2.11223500	0.98222100

C	-3.08031300	-2.41475700	2.08081300
C	-1.60406500	-1.03038500	3.11698500
C	-0.94082800	-1.32504100	1.72267000
C	-3.12570800	-1.07168600	2.83262400
H	-3.70864600	-1.13203100	3.75726700
H	-3.52093100	-0.25545500	2.23269100
C	-2.39012100	-3.32036700	3.16350500
H	-3.17222100	-3.72241300	3.81451200
H	-1.86838000	-4.16869800	2.72209200
C	-1.45202400	-2.33588000	3.93277700
H	-1.79060000	-2.18438700	4.96245600
H	-0.41490200	-2.68177000	3.97805800
H	-4.02000700	-2.81985600	1.71128800
H	-1.21018600	-0.13886800	3.61006800
H	-0.11415900	-2.02539800	1.90081700
O	-0.65135600	-2.92422800	-0.76389300
C	-1.57017600	-3.29232900	0.15237400
O	-1.91633000	-4.43948700	0.33266100
C	-0.14210700	-3.98851300	-1.59338500
H	0.59187800	-3.51943700	-2.24685100
H	0.32373000	-4.76131900	-0.97834800
H	-0.95569000	-4.42941100	-2.17412600
Pd	-2.84219900	-0.81382600	-0.51215600
I	-4.68325000	-2.45356900	-1.49844900

int17

C	0.10694000	2.40057800	0.41011300
C	1.47938200	2.41677800	0.59074800
C	2.17119000	1.25485100	0.96247300
C	1.39474600	0.09075200	1.13413600
C	-0.00660700	0.01698400	0.93266300
C	-0.64237100	1.22707700	0.57524900
H	-0.39896000	3.32545500	0.16174600
Cl	2.30490200	3.94952300	0.39114400
C	3.65876700	1.27261900	1.17294800
H	4.01348100	2.27138700	1.42813300
H	4.00091500	0.56105600	1.92455900
S	4.58521300	0.84874700	-0.35171400
O	4.23469100	1.77195500	-1.42313000
O	4.62281800	-0.58949700	-0.58463600
O	6.10070100	1.32830400	0.24005000

C	7.18237300	0.48250200	0.04193700
C	7.55587100	-0.40017000	1.06777700
C	7.91016300	0.58144500	-1.13930600
C	8.70455300	-1.19378100	0.88090300
C	9.04602600	-0.22185400	-1.30880300
H	7.57702600	1.28361400	-1.89211500
C	9.43963800	-1.10733700	-0.28783900
H	9.00609000	-1.87889700	1.66564500
H	10.32425800	-1.71464000	-0.44248400
C	6.76967600	-0.48467700	2.25626800
N	6.10911200	-0.54141800	3.21336300
O	9.82769000	-0.21269400	-2.41225900
C	9.47442300	0.64370600	-3.49523100
H	10.22567400	0.47197400	-4.26630300
H	8.48233500	0.39736300	-3.89116600
H	9.49672000	1.69792800	-3.19456700
Cl	2.25781600	-1.35304100	1.64732600
C	-3.88853000	2.69457100	-0.69859500
C	-4.72590100	2.54011000	0.43402400
C	-4.26792900	1.83903200	1.54522100
C	-2.97827100	1.26779900	1.54251200
C	-2.11166600	1.43282600	0.42313100
C	-2.60911700	2.16823800	-0.69957000
H	-4.26078700	3.22914700	-1.56389400
H	-4.91305500	1.74544800	2.41163500
H	-2.58370900	0.84265600	2.45769900
H	-1.96178500	2.30716900	-1.55877400
C	-6.10806700	3.10741300	0.49227800
O	-6.83197100	3.02802300	1.46401400
O	-6.45562600	3.71780000	-0.65690900
C	-7.78479200	4.26897300	-0.68293400
H	-7.89807200	5.02877700	0.09405300
H	-7.89927500	4.70903900	-1.67285700
H	-8.52503800	3.48199200	-0.52226100
C	-1.93940900	-1.80987100	0.26823700
C	-2.56135900	-2.84239600	1.23077100
C	-0.93751300	-1.91604700	2.51086100
C	-0.66198600	-1.35698400	1.05532100
C	-2.47173000	-2.08103200	2.56921700
H	-2.78458300	-2.69157300	3.42233200
H	-3.04789500	-1.15636400	2.58282100

C	-1.56474700	-4.02056000	1.50344600
H	-2.11914800	-4.84216500	1.96671500
H	-1.12737900	-4.40405400	0.58177400
C	-0.51954900	-3.40610700	2.48507600
H	-0.60607300	-3.83990100	3.48663600
H	0.51165500	-3.55034900	2.15547300
H	-3.54403900	-3.18186700	0.91222200
H	-0.47176400	-1.32402000	3.30175300
H	0.10834900	-2.01315400	0.63282100
O	-1.06374100	-1.29353500	-1.87832500
C	-1.60781100	-2.28701900	-1.13503100
O	-1.74594200	-3.41993300	-1.54196000
C	-0.74741100	-1.65044300	-3.23778800
H	-0.31903800	-0.75328700	-3.68334200
H	-0.02843500	-2.47231800	-3.26092200
H	-1.65570100	-1.95071600	-3.76563800
Pd	-3.40244000	-0.38559400	-0.08387600
I	-5.22350500	-1.81101600	-1.38093500

TS9

C	-0.45851400	-2.61750800	-1.69112700
C	0.80234800	-2.50443100	-2.25449900
C	1.47039200	-1.27045400	-2.28916900
C	0.73448100	-0.14614000	-1.86493900
C	-0.56341900	-0.19959000	-1.29135200
C	-1.12158400	-1.50803600	-1.15029000
H	-0.91026700	-3.59861900	-1.60464000
Cl	1.54142700	-3.95416600	-2.90553500
C	2.90567500	-1.18321500	-2.71010600
H	3.16008500	-1.91227400	-3.48252000
H	3.20258800	-0.18856800	-3.03827500
S	4.09303800	-1.60460400	-1.37490400
O	5.44574300	-1.42524600	-1.89788300
O	3.72668700	-2.82364000	-0.66561800
O	3.73085300	-0.29657600	-0.36687700
C	4.19713800	-0.32993100	0.93871700
C	3.25903100	-0.13234800	1.96863800
C	5.55281500	-0.48104900	1.21330500
C	3.72054400	-0.07761200	3.30095800
C	5.98521500	-0.45052600	2.54669200
H	6.24031300	-0.61250500	0.38908400

C	5.06117600	-0.24086900	3.58906600
H	3.00570500	0.09177100	4.09861900
H	5.42737300	-0.20681500	4.60860700
C	1.88049400	0.02989100	1.66528300
N	0.75573100	0.16789100	1.41051000
O	7.27170200	-0.59841000	2.92540400
C	8.26321100	-0.82563400	1.92439100
H	9.20502700	-0.93563000	2.46189300
H	8.05465400	-1.74070500	1.35879900
H	8.33383700	0.02361300	1.23510500
Cl	1.49690900	1.42039400	-2.06703800
Pd	-0.85464400	1.16648000	0.38123200
C	-3.54714100	-2.04920700	1.73128300
C	-4.59779200	-2.71732700	1.09030300
C	-4.51053400	-2.98033100	-0.28332300
C	-3.39482300	-2.57143900	-1.00476700
C	-2.35046300	-1.86921500	-0.37813600
C	-2.43253700	-1.63357700	1.00491700
H	-3.60160600	-1.85753500	2.79657200
H	-5.32835400	-3.50583900	-0.76467000
H	-3.33709000	-2.77843500	-2.06949100
H	-1.61844700	-1.13198400	1.51506800
C	-5.81903900	-3.17802800	1.81148200
O	-6.74647400	-3.76201900	1.28473400
O	-5.78663500	-2.87418800	3.12748100
C	-6.93851200	-3.28593700	3.87988700
H	-7.06078800	-4.37094100	3.83287700
H	-6.75044500	-2.96465900	4.90412500
H	-7.84232300	-2.81268300	3.48819200
C	-2.03217300	2.32450000	-0.88195400
C	-3.56397200	2.32910600	-0.77008700
C	-3.06544400	0.73940400	-2.30444600
C	-1.69924300	1.28153400	-1.87370800
C	-3.91673400	0.85961900	-1.02005400
H	-4.98193700	0.70315800	-1.21788500
H	-3.60663700	0.20766300	-0.20995700
C	-4.06982400	2.96952000	-2.09966500
H	-5.15514300	3.10530700	-2.05241200
H	-3.62775500	3.94946900	-2.29072800
C	-3.68222400	1.89403300	-3.16328800
H	-4.56017600	1.51535000	-3.69561900

H	-2.98399900	2.26961400	-3.91832700
H	-3.94261100	2.79840600	0.13620900
H	-3.04236600	-0.22470000	-2.81396800
H	-1.00043000	1.55974700	-2.65640200
O	-0.26933900	3.82423600	-1.51054400
C	-1.42570200	3.69931600	-0.83349800
O	-1.95851100	4.62034600	-0.24397900
C	0.44289400	5.05427900	-1.27321700
H	-0.17279900	5.91442300	-1.54594800
H	0.71834300	5.10564200	-0.21765900
H	1.33037000	5.00220500	-1.90454400
C	-0.43737100	3.25268000	2.29501900
O	0.59633300	3.46709700	1.65311900
O	-1.30329700	2.31170000	2.03748500
C	-0.83253100	4.13279400	3.47503000
H	0.04488600	4.64872700	3.86911500
H	-1.54986300	4.88046600	3.11994500
H	-1.31847800	3.54878700	4.26016700

int18

C	-0.00215700	-2.70626300	-1.85494700
C	1.22895200	-2.43030100	-2.43071400
C	1.78499100	-1.14245200	-2.38023300
C	0.97404400	-0.13428100	-1.81700500
C	-0.22908300	-0.37967800	-1.14572400
C	-0.70351200	-1.71184900	-1.15231800
H	-0.38512600	-3.72006000	-1.88156600
Cl	2.08706300	-3.74994500	-3.21596100
C	3.20742400	-0.88557000	-2.76408800
H	3.56942800	-1.55138700	-3.55037200
H	3.40722200	0.14999300	-3.03599100
S	4.37760300	-1.23658200	-1.38684600
O	5.72123000	-0.83968900	-1.80355800
O	4.14550200	-2.53852200	-0.77513300
O	3.78300300	-0.05785500	-0.31870500
C	4.16317000	-0.08657900	1.00879300
C	3.15766200	0.13827600	1.97191900
C	5.49298800	-0.25283900	1.38595900
C	3.52498900	0.20111400	3.33374800
C	5.82870900	-0.21564600	2.74643200
H	6.24030900	-0.39446200	0.61744900

C	4.83747300	0.01964200	3.71967500
H	2.75750100	0.39048300	4.07619700
H	5.13070400	0.05799100	4.76230100
C	1.80258000	0.31307300	1.58268800
N	0.69473700	0.45248600	1.26706700
O	7.08209900	-0.37827100	3.21666200
C	8.13938500	-0.63404600	2.29223300
H	9.03812600	-0.75027300	2.89782500
H	7.95759200	-1.55387500	1.72531600
H	8.27270200	0.20422300	1.59894000
Cl	1.53221200	1.53683900	-1.93588300
Pd	-0.95452900	1.05542900	0.13568800
C	-3.14574900	-2.42630000	1.67789600
C	-4.15444800	-3.13010500	1.00668900
C	-4.03296700	-3.35952700	-0.37017600
C	-2.92287200	-2.88904000	-1.06350400
C	-1.91429900	-2.16409700	-0.40474800
C	-2.03966400	-1.94849800	0.97836700
H	-3.22834900	-2.25748100	2.74537500
H	-4.81974400	-3.90844100	-0.87665500
H	-2.83785900	-3.07065200	-2.13127300
H	-1.25833000	-1.41868000	1.51142500
C	-5.36459000	-3.65824100	1.69708600
O	-6.25955900	-4.26880500	1.14443900
O	-5.36586900	-3.38389000	3.02128200
C	-6.50905200	-3.86523800	3.74418500
H	-6.58163200	-4.95321500	3.66973100
H	-6.35201700	-3.56116400	4.77895800
H	-7.42771600	-3.42424100	3.34919300
C	-2.51022800	2.47840300	-0.86266600
C	-3.94500500	2.29996800	-0.39224700
C	-3.53275700	0.65798200	-1.89710100
C	-2.24914200	1.46202100	-1.77198600
C	-4.11608600	0.77241900	-0.47174700
H	-5.16331900	0.45943500	-0.41899200
H	-3.53810800	0.23405900	0.28109600
C	-4.79501500	2.74209700	-1.63492900
H	-5.85381700	2.76461800	-1.36019800
H	-4.52619600	3.74185200	-1.98424800
C	-4.50165800	1.61795200	-2.67763100
H	-5.41087000	1.07420900	-2.95189800

H	-4.05558500	1.99629800	-3.60228000
H	-4.18794400	2.80201400	0.54116100
H	-3.43603600	-0.33770200	-2.32810300
H	-1.50265800	1.52547400	-2.55440900
O	-0.73594000	3.92329400	-1.48453300
C	-1.88540600	3.83698200	-0.80037900
O	-2.41384500	4.76414400	-0.21939100
C	0.00521200	5.14447200	-1.28690100
H	-0.60020000	6.00925100	-1.56736300
H	0.30088900	5.20929100	-0.23781400
H	0.87873500	5.05965800	-1.93273900
C	-0.87100200	3.19232900	2.13763400
O	0.17782200	3.54476800	1.59213300
O	-1.63199600	2.20588600	1.74261300
C	-1.42565300	3.93595500	3.34695000
H	-0.62263100	4.47237700	3.85572900
H	-2.16247900	4.66469400	2.99213100
H	-1.92973100	3.25540200	4.03711800

TS10

C	-0.86366200	-2.17484500	-1.99592500
C	0.42210000	-2.09163800	-2.50931100
C	1.20273100	-0.94121400	-2.32369500
C	0.58001800	0.14539900	-1.67529500
C	-0.74454600	0.12480900	-1.15208100
C	-1.44575800	-1.11502700	-1.29213400
H	-1.41355700	-3.10260600	-2.10064800
Cl	1.03300700	-3.47221100	-3.39677900
C	2.61430900	-0.87387900	-2.82969300
H	2.75183100	-1.48765900	-3.72251200
H	2.94867400	0.14160700	-3.03612200
S	3.88746200	-1.55765300	-1.70495900
O	5.19393900	-1.39893800	-2.33404100
O	3.47777000	-2.84950700	-1.16221800
O	3.72260200	-0.40129200	-0.49748900
C	4.68270600	-0.32483000	0.50351700
C	5.16527600	0.95588300	0.82180700
C	5.09413600	-1.45635800	1.20399600
C	6.09379300	1.07318600	1.87667900
C	6.03370300	-1.31392900	2.23326000
H	4.67205400	-2.41655100	0.94256000

C	6.53003800	-0.04089200	2.56908200
H	6.46855400	2.05751500	2.13539500
H	7.24948000	0.04113300	3.37575100
C	4.71781700	2.11654700	0.11976100
N	4.36203700	3.08229200	-0.42434300
O	6.51099800	-2.34425400	2.96760800
C	6.05615800	-3.66350700	2.67480300
H	6.58543200	-4.31927300	3.36651600
H	4.97612300	-3.75866000	2.83715000
H	6.29616700	-3.94897500	1.64415800
Cl	1.51041600	1.61702900	-1.55704700
Pd	-1.00559200	1.08394300	0.77427000
C	-4.10730900	-1.98993500	1.27990400
C	-5.20133300	-2.29243300	0.45957700
C	-5.06184600	-2.21213900	-0.93227800
C	-3.85182700	-1.81758800	-1.49222600
C	-2.76337400	-1.46756500	-0.67522400
C	-2.89662700	-1.58580100	0.71855100
H	-4.20345500	-2.07785500	2.35593700
H	-5.91305300	-2.46442200	-1.55557000
H	-3.75092000	-1.76061300	-2.57223100
H	-2.04616700	-1.38132300	1.36041000
C	-6.52361700	-2.71638700	1.00375400
O	-7.48916200	-2.99444900	0.31911300
O	-6.53672300	-2.75752000	2.35426000
C	-7.78519000	-3.15509400	2.94268800
H	-8.06350000	-4.15909400	2.61279500
H	-7.62130600	-3.13653200	4.01993100
H	-8.58034800	-2.45972300	2.66256900
C	-1.87325400	2.65372700	-0.24612700
C	-3.39373200	2.85723500	-0.17693800
C	-3.03525500	1.56687500	-2.00283400
C	-1.63013800	1.79703700	-1.43182300
C	-3.93013500	1.53765900	-0.74292800
H	-4.99460800	1.58270900	-0.99346300
H	-3.75656700	0.68982300	-0.08646100
C	-3.73071000	3.82675100	-1.35287700
H	-4.78747300	4.10780400	-1.30170100
H	-3.14744700	4.74920100	-1.31974400
C	-3.43972100	2.94964000	-2.61058100
H	-4.33207900	2.82357200	-3.23108300

H	-2.65708200	3.36659600	-3.25259100
H	-3.75828300	3.18304700	0.79606400
H	-3.11596600	0.73642900	-2.70471900
H	-0.87055900	2.15024100	-2.12251200
O	0.14325700	3.94687000	-0.38679400
C	-1.09016900	3.87781400	0.14600300
O	-1.54638200	4.72501900	0.88979200
C	0.96721300	5.04076000	0.06067700
H	0.60035700	5.98464700	-0.35156900
H	0.95581000	5.10004400	1.15084100
H	1.96977300	4.81910000	-0.30472100
C	-0.38904100	0.55182000	3.15577900
O	-1.00805000	1.62259200	2.82197300
O	-0.09567600	-0.30437200	2.26356900
C	0.00893300	0.34313700	4.59318400
H	1.01009200	0.76076400	4.74628300
H	-0.68265300	0.86068300	5.26037800
H	0.04533700	-0.72300200	4.82477200

int19

C	0.98154400	2.59095700	0.29524300
C	-0.30697500	2.86391400	-0.14556700
C	-1.07016800	1.91394100	-0.84770100
C	-0.43614800	0.67955800	-1.11074800
C	0.85842300	0.35455600	-0.66981300
C	1.56828000	1.33878200	0.06140500
H	1.52640100	3.34837500	0.84714100
Cl	-0.94807100	4.46657200	0.17679800
C	-2.46366500	2.22216600	-1.30757000
H	-2.58877000	3.28017400	-1.54764600
H	-2.77876900	1.61779400	-2.15799000
S	-3.77146400	1.95539400	-0.05067600
O	-5.04115700	2.42377700	-0.59507300
O	-3.33757700	2.36423500	1.28178600
O	-3.74516800	0.27430300	-0.11093700
C	-4.83508600	-0.41033000	0.41137700
C	-5.56317100	-1.23120600	-0.46354100
C	-5.14081100	-0.32482900	1.76709700
C	-6.62710000	-1.98767500	0.06737400
C	-6.21537600	-1.07185500	2.26695700
H	-4.53849900	0.31661800	2.39578400

C	-6.95342800	-1.90845400	1.40931500
H	-7.19504900	-2.63165400	-0.59515400
H	-7.77437500	-2.48203800	1.82448000
C	-5.22736100	-1.29732900	-1.85048900
N	-4.96129500	-1.36230100	-2.98168000
O	-6.60954400	-1.06080700	3.56152000
C	-5.91788900	-0.21727200	4.47870700
H	-6.41432500	-0.35426300	5.43970000
H	-4.86379800	-0.50521700	4.56960900
H	-5.98302400	0.83548200	4.18041600
Cl	-1.28692800	-0.51094300	-2.09278000
Pd	1.57647100	-1.50298800	-0.94930100
C	4.54262500	-0.18431900	1.87655000
C	5.55911700	0.72590600	1.55660300
C	5.26397300	1.83314500	0.75135400
C	3.97238400	2.02471000	0.27135000
C	2.94996200	1.10881800	0.57374300
C	3.25195500	0.00330200	1.38751600
H	4.76563600	-1.03431400	2.51102700
H	6.06028600	2.53026100	0.51339000
H	3.75332500	2.88351400	-0.35689000
H	2.46658000	-0.69574400	1.65449100
C	6.95962600	0.57317900	2.04355900
O	7.86534600	1.34093800	1.78083500
O	7.12114900	-0.52262300	2.81881100
C	8.45156900	-0.72703600	3.31892400
H	8.76456200	0.11845700	3.93666300
H	8.40542200	-1.63974700	3.91277300
H	9.15934800	-0.84035400	2.49396800
C	2.77831300	-0.18924600	-3.47358600
O	2.64136200	-1.16437900	-2.72389400
C	1.20395200	-3.52697100	0.43676200
O	1.93119300	-3.64855700	-0.59084100
O	0.72823100	-2.36048300	0.72450500
C	0.85263100	-4.69776100	1.30968700
H	-0.13127600	-5.07744700	1.01375000
H	1.58776600	-5.49396500	1.18315500
H	0.79343300	-4.38876300	2.35557000
O	2.23409300	0.98980100	-3.24860800
H	1.72050600	0.94692000	-2.40689800
C	3.59013400	-0.26860800	-4.73126800

H	2.94326300	-0.06929000	-5.59101800
H	4.36487200	0.50307700	-4.71672200
H	4.03900800	-1.25623500	-4.82176800

TS11

C	0.76229100	-2.85325300	-0.09891700
C	-0.51330400	-3.11362600	0.38711800
C	-1.20625600	-2.20218700	1.20875200
C	-0.50462200	-1.03239200	1.55262100
C	0.76431100	-0.68925000	1.03967100
C	1.39975700	-1.64237400	0.19478500
H	1.25143400	-3.59031300	-0.72487700
Cl	-1.22821200	-4.66090000	-0.01968200
C	-2.60580500	-2.47264600	1.66937200
H	-2.79279700	-3.53273400	1.85452600
H	-2.88213800	-1.89721700	2.55257100
S	-3.89095500	-2.06059500	0.42639200
O	-5.19701500	-2.40767900	0.97985700
O	-3.51934900	-2.46947100	-0.92187600
O	-3.71332500	-0.37661200	0.51309700
C	-4.20595900	0.37473300	-0.53976900
C	-3.30697300	1.23217000	-1.20025400
C	-5.55118200	0.32919900	-0.88899600
C	-3.79422300	2.06542900	-2.22956600
C	-6.01096000	1.14741900	-1.93128400
H	-6.20881300	-0.33473300	-0.34426400
C	-5.12491400	2.02029200	-2.59473900
H	-3.10976500	2.73907800	-2.73326900
H	-5.51394300	2.64917900	-3.38708400
C	-1.94362800	1.25810700	-0.80827900
N	-0.83704100	1.26735900	-0.46658600
O	-7.28851400	1.17649100	-2.35980100
C	-8.24421500	0.31207700	-1.74486600
H	-9.18501200	0.49780600	-2.26274300
H	-7.96207000	-0.74004500	-1.86319200
H	-8.36182600	0.54404700	-0.68024700
Cl	-1.21400500	0.06314500	2.72953900
Pd	0.91883200	1.47638200	0.48728800
C	4.45123400	-0.19997000	-1.57748400
C	5.40690800	-1.18886000	-1.31388000
C	5.04500000	-2.31414600	-0.56151500

C	3.74745100	-2.44684100	-0.08178600
C	2.78248300	-1.45249400	-0.32913300
C	3.15305200	-0.33204500	-1.08954200
H	4.72338600	0.66862500	-2.16557000
H	5.79635000	-3.07049100	-0.36163600
H	3.47976800	-3.31459300	0.51361300
H	2.41838100	0.43469500	-1.31454500
C	6.81174600	-1.10091800	-1.80564000
O	7.66589700	-1.94089000	-1.59731300
O	7.04021700	0.02555800	-2.51702100
C	8.37783400	0.17247800	-3.01777900
H	8.62959200	-0.65141200	-3.69034900
H	8.38858200	1.12171100	-3.55315800
H	9.09715400	0.18666300	-2.19514000
C	3.04606900	1.19833900	2.45350900
O	2.64359100	1.91381500	1.47716200
C	0.31086900	4.23912500	0.39256300
O	1.05686900	3.36138900	-0.24088400
O	-0.48014300	3.98470200	1.29538000
C	0.54368400	5.66051000	-0.11075900
H	-0.21186800	6.32649100	0.30809000
H	1.53721800	5.99613800	0.20301800
H	0.51708300	5.69469600	-1.20318000
O	2.51346000	0.10939000	2.81299800
H	1.57728100	-0.17473000	1.90741300
C	4.22669300	1.72707200	3.23549900
H	4.76039900	0.90661000	3.71616700
H	4.88980100	2.29568800	2.58226600
H	3.85023400	2.40187300	4.01162600

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C	-1.98008400	1.27419400	-0.28098000
C	-0.61564900	1.37540900	-0.03061600
C	0.05454400	0.51616400	0.86212400
C	-0.74688600	-0.44830400	1.50405600
C	-2.11185900	-0.56316800	1.26756300
C	-2.74912600	0.29547500	0.36186100
H	-2.43423000	1.94542200	-0.99950300
Cl	0.26408000	2.63980300	-0.86794600
C	1.52516200	0.63274800	1.13193400

H	1.90425500	1.64904800	1.01681800
H	1.78730700	0.25345900	2.11963000
S	2.53304100	-0.37873400	-0.02081000
O	2.75695600	0.30727800	-1.28743100
O	2.09910800	-1.76980600	0.00936800
O	3.95985800	-0.27919900	0.89443400
C	5.15232100	-0.06637100	0.21933900
C	5.67979900	1.23304800	0.16967300
C	5.82664400	-1.15271300	-0.32811000
C	6.93031600	1.42162400	-0.44994600
C	7.06522800	-0.94212400	-0.94788000
H	5.37241700	-2.13176200	-0.25304200
C	7.61390300	0.35256300	-1.00076800
H	7.35212200	2.41958100	-0.49413000
H	8.57582700	0.48762400	-1.48186100
C	4.94565800	2.32215700	0.72978400
N	4.33059700	3.19783600	1.18826700
O	7.80850300	-1.91976000	-1.51603800
C	7.30047800	-3.25160300	-1.51768900
H	8.04799500	-3.85288500	-2.03512000
H	7.17159300	-3.63140800	-0.49737000
H	6.34670400	-3.31413400	-2.05401200
Cl	-0.04714800	-1.53937200	2.68929100
C	-6.18688400	-1.20279500	-0.19885600
C	-6.96551600	-0.05612600	-0.40219100
C	-6.35831500	1.20513700	-0.35542900
C	-4.99566300	1.31907300	-0.10898500
C	-4.20440800	0.17554000	0.09766900
C	-4.82308800	-1.08536200	0.04791200
H	-6.65166900	-2.18061000	-0.24372000
H	-6.97504400	2.08428200	-0.50651800
H	-4.54364100	2.30401500	-0.04813500
H	-4.22509600	-1.98221800	0.17537600
C	-8.43088400	-0.11588700	-0.66881600
O	-9.13454000	0.85759700	-0.85410300
O	-8.90185300	-1.38347800	-0.68195400
C	-10.31090700	-1.50921100	-0.93340600
H	-10.56563500	-1.09103600	-1.91014700
H	-10.51944400	-2.57838000	-0.90741400
H	-10.88597900	-0.98599400	-0.16573600
H	-2.68111600	-1.30531600	1.81343300

TS12

C	0.10456400	1.22024300	1.87751000
C	-1.22521300	1.50286700	2.19309300
C	-2.16922100	1.95515500	1.24548100
C	-1.66128400	2.32182400	-0.02809400
C	-0.34909100	2.06799800	-0.36251000
C	0.47984500	1.34415000	0.52671600
H	0.77218000	0.84008800	2.64095300
H	4.08610500	-0.29506500	0.48421400
Cl	-1.72403400	1.24131100	3.86498400
C	-3.63057100	1.98646100	1.53314900
H	-3.86587700	2.23754300	2.56998600
H	-4.18381700	2.63952100	0.85935700
S	-4.47026800	0.34888200	1.34128200
O	-5.89152200	0.58340100	1.08055400
O	-4.06356400	-0.61193500	2.36020100
O	-3.72236100	-0.10994000	-0.11291400
C	-3.94978100	-1.40191900	-0.55625400
C	-2.85849800	-2.28514000	-0.66564100
C	-5.23202000	-1.78563200	-0.94401800
C	-3.09265900	-3.57338600	-1.19565900
C	-5.44223800	-3.07663900	-1.44446200
H	-6.03464500	-1.06848400	-0.84283800
C	-4.36058500	-3.96781600	-1.57605200
H	-2.25673800	-4.25737800	-1.29417300
H	-4.54687500	-4.95747900	-1.97723100
C	-1.53871000	-1.92156900	-0.27116600
N	-0.43775200	-1.68814400	0.02996700
O	-6.64615900	-3.55056600	-1.83485800
C	-7.78922800	-2.70809300	-1.70211700
H	-8.63641600	-3.30300600	-2.04389900
H	-7.94625900	-2.41122900	-0.65893600
H	-7.69812200	-1.81183400	-2.32677700
Cl	-2.69110800	3.14786000	-1.19961000
Pd	1.38792900	-0.34335900	-0.08816000
C	4.55712500	-3.44398200	1.11602300
H	4.46967000	-4.17197200	0.30601200
H	3.97461400	-3.82040400	1.96262400
N	5.93810500	-3.29798500	1.51550000
C	3.88312800	-2.17070000	0.61517800

O	2.85664700	-2.22115700	-0.05097400
O	4.48010000	-1.04663300	0.99372800
C	6.87270500	-2.92333600	0.58280000
O	6.58238300	-2.82006000	-0.60292800
C	8.26578900	-2.64509200	1.11672700
H	8.99633700	-3.06344600	0.42177900
H	8.42317400	-1.56208000	1.15100500
H	8.43818500	-3.05563800	2.11536300
H	6.14987300	-3.18657300	2.49524800
C	1.88997100	1.91209100	-0.67615700
C	2.67900900	3.10963800	-0.08366800
C	0.96026800	4.08851500	-1.20605600
C	0.63978800	2.57419400	-1.36978500
C	1.57892900	4.15333600	0.20928800
H	2.00296300	5.13734400	0.43476900
H	0.89617100	3.87970800	1.01446500
C	3.38474500	3.80585700	-1.28342800
H	4.04547600	4.59365300	-0.90594000
H	4.00291700	3.12587500	-1.87260700
C	2.19035600	4.41008900	-2.09293500
H	2.30195600	5.49139800	-2.22074900
H	2.10016100	3.96983600	-3.09080800
H	3.34676500	2.84923700	0.73888300
H	0.09476600	4.73000400	-1.38653600
H	0.48737700	2.27762700	-2.41017900
O	3.96594200	0.72922300	-1.05551100
C	2.67894800	0.98342500	-1.55057600
O	2.36889000	0.62744500	-2.68075800
C	4.83491400	0.04037400	-1.98463700
H	5.73873600	-0.20117300	-1.42678700
H	4.36366700	-0.87323200	-2.34852000
H	5.06341400	0.69086700	-2.83224500

TS13

C	-0.38953800	1.39249700	-1.36015900
C	0.75566600	1.91141300	-1.97851200
C	1.84903500	2.42857900	-1.25674900
C	1.66530000	2.59704000	0.13293800
C	0.55343000	2.07227600	0.76632400
C	-0.39967800	1.34213600	0.03763700
H	-1.18483900	0.98717600	-1.97043300

Cl	0.80755800	1.85894400	-3.73398100
C	3.17212900	2.69917800	-1.89702600
H	3.09277200	3.02527300	-2.93620100
H	3.78423300	3.40428100	-1.33578900
S	4.21376500	1.18668300	-2.03150900
O	5.58772400	1.59822400	-2.31229800
O	3.57134600	0.14842600	-2.82606900
O	4.10993900	0.72454700	-0.40506200
C	4.58164600	-0.53496700	-0.06152800
C	3.68457100	-1.45362100	0.51475500
C	5.92808500	-0.84584900	-0.22739300
C	4.18169300	-2.70776100	0.93274200
C	6.39531300	-2.10436200	0.17724600
H	6.57999200	-0.10379400	-0.66717000
C	5.51364600	-3.03167000	0.76522000
H	3.49632700	-3.41936100	1.37999700
H	5.90260500	-3.99450300	1.07583900
C	2.30082800	-1.16070000	0.67318000
N	1.16361900	-0.98154000	0.82079100
O	7.67593600	-2.50986200	0.05295200
C	8.62061100	-1.63367300	-0.56062200
H	9.56372100	-2.17991600	-0.57399700
H	8.32556700	-1.38620600	-1.58647500
H	8.74223300	-0.71118300	0.01878200
Cl	2.84980100	3.45851600	1.10505900
C	-1.26929800	1.33184900	1.93085600
C	-2.45250800	2.30562600	1.96854900
C	-0.64803700	3.62680600	2.37867900
C	-0.00323000	2.22272500	2.13357000
C	-1.85540100	3.61708700	1.41508300
H	-2.52441200	4.46800800	1.57583300
H	-1.59426700	3.57811400	0.35680500
C	-2.61913500	2.71282100	3.47180800
H	-3.53642600	3.30263700	3.56400900
H	-2.72080200	1.85993100	4.14397700
C	-1.35268100	3.58263400	3.75499300
H	-1.62677500	4.59097900	4.07948400
H	-0.71300400	3.15197300	4.53154500
H	-3.36455800	1.93220000	1.50669000
H	0.06789000	4.44282200	2.26115000
H	0.64277500	1.90087600	2.95280100

O	-2.55271600	-0.36407900	3.05257100
C	-1.31054900	0.13517600	2.87468300
O	-0.34473000	-0.23821600	3.51487800
C	-2.64160600	-1.51500100	3.92021600
H	-3.70699100	-1.72255200	4.01307500
H	-2.12599700	-2.36194600	3.46101400
H	-2.20038100	-1.29187400	4.89344500
Pd	-1.00058600	-0.71268700	0.40225900
C	-5.23206200	-0.20923500	-0.39336000
C	-5.29089300	-0.32378300	-1.78772400
C	-4.11983100	-0.62342300	-2.49595600
C	-2.90974200	-0.78555900	-1.82386400
C	-2.84077600	-0.62127400	-0.42962600
C	-4.01883900	-0.36667200	0.28125100
H	-6.13860300	-0.00423100	0.16595300
H	-4.17653500	-0.74280100	-3.57314800
H	-2.02867000	-1.06753500	-2.39183300
H	-3.99987800	-0.30225900	1.36130900
I	-1.31387300	-3.37339000	0.32026500
C	-6.55210800	-0.16093500	-2.55735100
O	-6.64294600	-0.25310300	-3.76699800
O	-7.61598800	0.11014400	-1.76106400
C	-8.86362800	0.27253100	-2.44920800
H	-9.12817800	-0.63939000	-2.99079400
H	-9.60194100	0.48514200	-1.67564100
H	-8.80729000	1.09844000	-3.16316900

TS14

C	0.53881500	0.27014600	1.73121800
C	-0.59550200	0.28636200	2.55368300
C	-1.70321700	1.12401700	2.31747800
C	-1.55327300	2.10645100	1.31365600
C	-0.45669300	2.09051500	0.47426300
C	0.51967200	1.08484400	0.59144900
H	1.34359500	-0.41788500	1.95166500
Cl	-0.61262500	-0.82876500	3.91052600
C	-3.00591600	0.94741800	3.02849000
H	-2.89376000	0.57201800	4.04781400
H	-3.61560900	1.85017100	3.03245200
S	-4.08079900	-0.32932100	2.25134500
O	-5.45090700	-0.11513000	2.71455000

O	-3.47957500	-1.65439300	2.30019600
O	-3.95467900	0.23901700	0.66035700
C	-4.44364000	-0.56483000	-0.35935800
C	-3.57621100	-0.90282200	-1.41492600
C	-5.77729000	-0.96493100	-0.36311400
C	-4.09129200	-1.65989900	-2.48995300
C	-6.25924300	-1.73465200	-1.43052300
H	-6.40917500	-0.66989800	0.46302700
C	-5.40854800	-2.07402800	-2.49969900
H	-3.42979900	-1.92216500	-3.30819900
H	-5.80851400	-2.66335500	-3.31669200
C	-2.20546700	-0.51741300	-1.42504700
N	-1.08219700	-0.23179800	-1.48804200
O	-7.52859700	-2.18376000	-1.52396400
C	-8.43733000	-1.90567700	-0.45946000
H	-9.37483000	-2.38656400	-0.73871800
H	-8.07923100	-2.32290900	0.48836400
H	-8.60046600	-0.82758900	-0.34677200
Cl	-2.75992500	3.36593000	1.09097900
C	1.39709600	2.23992000	-0.82578600
C	2.54092900	3.05422300	-0.20116400
C	0.69750700	4.33292700	0.16565600
C	0.10228200	3.05429400	-0.50830700
C	1.86903400	3.76263300	0.99568800
H	2.50760800	4.54800500	1.41148800
H	1.57256700	3.09472900	1.80523300
C	2.74978200	4.28592700	-1.14303700
H	3.63845700	4.82768200	-0.80435100
H	2.92103200	4.01170200	-2.18459100
C	1.45327200	5.12979200	-0.92513500
H	1.68876000	6.13785600	-0.57076800
H	0.86310400	5.23462600	-1.84077100
H	3.44833600	2.48576700	-0.00428300
H	-0.05398300	4.90902000	0.70918400
H	-0.51749000	3.27405100	-1.37966000
O	2.79290900	1.59391600	-2.67619900
C	1.52398800	1.87230400	-2.29979000
O	0.60233000	1.96784100	-3.09092600
C	2.94586400	1.12863300	-4.03458100
H	4.02029200	1.02398500	-4.18273300
H	2.44727800	0.16295800	-4.14501300

H	2.52496200	1.85230700	-4.73511300
Pd	1.08997600	-0.29627300	-0.95247300
C	5.27544100	-0.61761400	0.11907200
C	5.26371200	-1.72886000	0.97094400
C	4.05451800	-2.39807000	1.20306000
C	2.87328000	-1.95542600	0.60858900
C	2.88369900	-0.81693100	-0.21447400
C	4.09398700	-0.16812300	-0.47642300
H	6.21102600	-0.10751400	-0.08392600
H	4.05663200	-3.27301500	1.84530500
H	1.95409300	-2.51250200	0.75948300
H	4.12875000	0.67127200	-1.15783700
C	6.49022600	-2.24730400	1.63170300
O	6.52409200	-3.20714600	2.37830400
O	7.59603000	-1.52811500	1.31370100
C	8.81264300	-1.98617900	1.91844500
H	9.02785600	-3.01626800	1.62264000
H	9.59243700	-1.31429200	1.55880600
H	8.74334500	-1.94388400	3.00865700
C	0.91809600	-2.86120600	-2.07756500
O	1.48139200	-1.73251600	-2.40868100
O	0.28855300	-3.04637200	-1.03102600
C	1.11691000	-3.97233300	-3.10064500
H	2.17216600	-4.26344800	-3.11680100
H	0.50773900	-4.83804800	-2.83833000
H	0.86028800	-3.61972700	-4.10355700

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C	-0.80028700	-2.86398900	-0.52853600
C	-2.05205700	-2.59405200	-0.00978200
C	-2.21316400	-2.03816700	1.28973100
C	-1.05574900	-1.79272100	2.04248300
C	0.26457100	-2.01692000	1.52719200
C	0.34966000	-2.58002500	0.22745000
H	-0.68553400	-3.32415700	-1.50237900
H	1.28246400	-2.93463800	-0.19111000
Cl	-3.44346200	-3.02332200	-0.97157900
C	-3.57857900	-1.73064100	1.83132500
H	-4.36698000	-2.30055000	1.34030900
H	-3.64125000	-1.87920100	2.91044900
S	-4.08773400	0.02110700	1.63879100

O	-2.99361500	0.93525700	1.95349600
O	-5.40200200	0.19427600	2.24446700
O	-4.25398600	-0.02445300	-0.03232100
C	-4.94816100	1.01256200	-0.64922600
C	-6.09292800	0.67315900	-1.38586800
C	-4.47171100	2.31899700	-0.58417900
C	-6.76176100	1.70118200	-2.08054300
C	-5.16609300	3.32632400	-1.26754200
H	-3.57970800	2.52025900	-0.00691300
C	-6.31114300	3.00759400	-2.02110600
H	-7.64387700	1.45414700	-2.66103700
H	-6.82374500	3.80459100	-2.54771100
C	-6.55647900	-0.67713400	-1.43383500
N	-6.93967900	-1.77490300	-1.48360700
O	-4.80332200	4.62905600	-1.26849500
C	-3.66405600	5.02276300	-0.50710500
H	-3.57914000	6.10174000	-0.63781900
H	-3.79529800	4.79226200	0.55632400
H	-2.75140400	4.53854300	-0.87480500
Cl	-1.23774300	-1.27667400	3.70085000
Pd	0.87441000	-0.26728900	0.19717200
C	2.34008300	2.05699500	-1.02015800
O	1.31295100	1.68161800	-0.37012500
O	3.12333400	1.33340700	-1.68942100
C	2.18234400	-0.46992400	1.79849900
C	3.62551000	-0.85109500	1.46345000
C	2.70723600	-2.78352500	2.23150500
C	1.53886300	-1.76162700	2.35796600
C	3.50863500	-2.31197700	0.99145500
H	4.48778600	-2.80013400	0.94260700
H	3.03657700	-2.44251700	0.01917700
C	4.32255100	-1.06833900	2.85323000
H	5.40143500	-1.15152800	2.69018700
H	4.16743200	-0.23841500	3.54682600
C	3.70795600	-2.41491200	3.35761300
H	4.47555900	-3.18899600	3.44859500
H	3.22377700	-2.31762800	4.33410900
H	4.14325400	-0.14520300	0.81508200
H	2.38078200	-3.82625300	2.23893900
H	1.24479000	-1.62250500	3.39850300
O	2.84835900	1.75818100	2.22300600

C	1.96930300	0.80789200	2.58192200
O	1.12969000	0.94838800	3.44908400
C	2.72309300	3.02719100	2.90451400
H	3.40514900	3.70096200	2.38772200
H	1.69251800	3.38340000	2.84179900
H	2.99599100	2.91327600	3.95691000
O	2.36006500	-2.25205400	-3.75240600
C	2.23944800	-3.38937900	-3.14977500
O	2.21975300	-3.55263500	-1.91687700
C	2.13207800	-4.58553400	-4.08865200
H	1.36492000	-4.40377400	-4.84644200
H	3.08211500	-4.71422800	-4.61725800
H	1.90360200	-5.49443900	-3.53082800
Ag	2.64468400	-0.59809900	-2.49716900
C	2.59250400	3.56634400	-1.01244400
H	1.85363800	4.01738300	-1.68915200
H	2.41128600	3.96414800	-0.01451400
N	3.93709400	3.92743300	-1.39755900
C	4.81383400	4.47873900	-0.50007500
O	4.47778900	4.84012500	0.62394600
C	6.24050800	4.63573800	-0.99698600
H	6.88962700	3.97257000	-0.41714500
H	6.36288600	4.41100500	-2.05976200
H	6.56650300	5.66077400	-0.80573000
H	4.30597200	3.48712600	-2.22799900

TS15

C	-0.57933000	-0.96992900	-1.39058700
C	-1.94249300	-1.23644600	-1.38327700
C	-2.57812300	-1.79209400	-0.25352500
C	-1.76409800	-2.06816900	0.86558600
C	-0.39510200	-1.77838700	0.90070200
C	0.21122400	-1.24358700	-0.26277100
H	-0.12405900	-0.58799100	-2.29882700
H	1.32330000	-1.89416000	-0.74369200
Cl	-2.84127100	-0.91794000	-2.85553400
C	-4.04684100	-2.09561900	-0.24990200
H	-4.45625600	-2.20730200	-1.25405900
H	-4.28186400	-2.98400200	0.33927100
S	-5.10453800	-0.81627600	0.52890200
O	-4.52483400	-0.30803600	1.76811100

O	-6.48786200	-1.27637000	0.49145100
O	-4.88187800	0.34326300	-0.66665600
C	-5.70259500	1.46542800	-0.64959200
C	-6.51148800	1.69173700	-1.77391600
C	-5.65825400	2.35711900	0.41878700
C	-7.29074200	2.86574000	-1.80354600
C	-6.45696900	3.50733500	0.37354300
H	-5.00725000	2.13580600	1.25319200
C	-7.26985800	3.75880900	-0.74719200
H	-7.91600200	3.05837000	-2.66850500
H	-7.87114500	4.66082300	-0.76024000
C	-6.53305000	0.76203300	-2.85837600
N	-6.55605500	0.01739400	-3.75245200
O	-6.50213300	4.43629400	1.35615900
C	-5.71600200	4.22928300	2.52738200
H	-5.92650400	5.07765100	3.17901200
H	-5.99474000	3.29915200	3.03580100
H	-4.64547700	4.20813200	2.29158300
Cl	-2.48876800	-2.83277400	2.27645800
Pd	1.95640900	-0.19225200	0.16772200
C	4.24600800	1.73646000	-0.20394400
O	3.53354100	1.15093500	0.65461400
O	4.28059300	1.50122900	-1.45789000
C	1.63717900	-0.88486800	2.11767300
C	2.83481800	-1.72963100	2.56669900
C	1.13653300	-3.23843800	2.48037100
C	0.43766900	-1.87783800	2.14778900
C	2.54486800	-3.07556300	1.86467100
H	3.22831500	-3.86905100	2.18663400
H	2.55992700	-3.02639900	0.77603100
C	2.60622100	-2.12835900	4.06375400
H	3.53506900	-2.54717900	4.46378400
H	2.34703200	-1.27167500	4.68910100
C	1.47655400	-3.20545800	3.98866600
H	1.84100200	-4.18360500	4.31819900
H	0.60912200	-2.95503300	4.60722000
H	3.80240100	-1.26108000	2.38595700
H	0.56131500	-4.11084500	2.16383000
H	-0.21494300	-1.59787500	2.98159200
O	2.43526800	0.95379700	3.39676900
C	1.34956000	0.43955400	2.78435500

O	0.26042300	0.98496800	2.78562300
C	2.25558700	2.25141500	3.98813900
H	3.21383200	2.50061400	4.44283800
H	1.99230800	2.98412000	3.22135100
H	1.46501200	2.22574200	4.74195000
O	2.60026200	-1.86948400	-3.25910100
C	2.16755600	-2.90273800	-2.65341900
O	1.82042400	-2.96299500	-1.43467600
C	2.01987000	-4.16425900	-3.47860200
H	0.99566400	-4.20477600	-3.86595300
H	2.70953000	-4.15925200	-4.32323500
H	2.17633900	-5.04393900	-2.85225600
Ag	3.37495400	-0.17475000	-2.32294500
C	5.12492200	2.86575700	0.31606100
H	4.44927500	3.64535900	0.69737500
H	5.70286200	2.51481400	1.17563300
N	6.03586100	3.37521800	-0.68216000
C	7.29515100	3.79073100	-0.34355500
O	7.67884300	3.83760100	0.81926300
C	8.18098400	4.20464400	-1.50785600
H	9.09526700	3.60567900	-1.48244400
H	7.70571200	4.09254000	-2.48625100
H	8.47318600	5.24966000	-1.37299200
H	5.77896600	3.23919200	-1.64858800

int21

C	-0.61280400	-0.82467600	-0.88205000
C	-1.88061900	-1.31798600	-0.56470300
C	-2.42996600	-1.18107500	0.72341300
C	-1.61230900	-0.55981000	1.69498600
C	-0.33357400	-0.06988800	1.41347000
C	0.16340700	-0.18386500	0.09346800
H	-0.25467800	-0.93220300	-1.90206400
H	0.60763800	-2.50255300	0.39924200
Cl	-2.75918400	-2.15931000	-1.83182400
C	-3.79824200	-1.69311500	1.05788100
H	-4.13372600	-2.47632800	0.37780600
H	-3.86462000	-2.05289500	2.08650100
S	-5.14117000	-0.44511500	0.99841200
O	-4.72639800	0.83624400	1.56121600
O	-6.38169600	-1.07843400	1.43285400

O	-5.16767000	-0.29410700	-0.67677500
C	-6.24791500	0.35728700	-1.25842600
C	-7.01512100	-0.36723200	-2.18402900
C	-6.50454800	1.69684700	-0.97758900
C	-8.06736300	0.30171000	-2.84108500
C	-7.56921900	2.33333500	-1.62882300
H	-5.87327200	2.20858800	-0.26427700
C	-8.34579200	1.62877100	-2.56730000
H	-8.66463300	-0.24288600	-3.56423400
H	-9.15742400	2.14835400	-3.06389800
C	-6.72863500	-1.74040000	-2.45436500
N	-6.50424000	-2.85812800	-2.68868400
O	-7.91644000	3.62530100	-1.42677500
C	-7.18046400	4.38871800	-0.47378200
H	-7.64502000	5.37497600	-0.46194600
H	-7.24061700	3.94366700	0.52606000
H	-6.12827600	4.48570300	-0.76620900
Cl	-2.21979800	-0.40295400	3.34226200
Pd	1.90837000	0.63417800	-0.34634400
C	4.77953200	0.78082200	-1.48880200
O	3.71516600	1.40876500	-1.23259500
O	4.98535200	-0.46508900	-1.33605600
C	1.78630900	1.25810000	1.64002400
C	2.99610500	0.76257400	2.45331800
C	1.23022600	-0.20732900	3.50366900
C	0.55096800	0.65251100	2.38661700
C	2.54738600	-0.66220000	2.84035100
H	3.23038200	-1.15119500	3.54381100
H	2.40212000	-1.31703600	1.97523400
C	2.96142300	1.46417000	3.84816800
H	3.90720700	1.28206200	4.36883900
H	2.84687800	2.54752800	3.76612200
C	1.76486200	0.77030100	4.57530700
H	2.10431400	0.22285100	5.46050000
H	0.99889600	1.47966800	4.90282800
H	3.95292500	0.86875400	1.94156900
H	0.58579000	-0.99411600	3.89917100
H	-0.03005000	1.46028800	2.84598600
O	2.88651100	3.31600600	1.20155400
C	1.67367200	2.73857600	1.37024300
O	0.62825200	3.35971700	1.31010600

C	2.86491800	4.70875300	0.84603400
H	3.90975000	5.01222100	0.78808700
H	2.37378600	4.84623600	-0.12060300
H	2.33373400	5.29187500	1.60206000
O	2.60996400	-3.74597700	-0.01627900
C	1.55842500	-4.17131800	0.47147900
O	0.49044500	-3.42975500	0.70190000
C	1.37406400	-5.61115200	0.85499100
H	0.59258100	-6.05280000	0.22889600
H	2.30829300	-6.15430700	0.72295200
H	1.03581100	-5.67660000	1.89269800
Ag	3.42967000	-1.75425500	-0.54369800
C	5.92409700	1.61888200	-2.04375300
H	5.56228400	2.13060500	-2.94460800
H	6.15370800	2.41295600	-1.32344900
N	7.09682100	0.82014500	-2.31962700
C	8.28013400	1.40308800	-2.66386000
O	8.39596000	2.61776600	-2.78776300
C	9.44359700	0.44829700	-2.88753400
H	10.25516900	0.71731000	-2.20590100
H	9.18614900	-0.60413100	-2.73863100
H	9.81729800	0.58223200	-3.90635600
H	7.01058100	-0.17451700	-2.16941500

int22

C	0.85431700	-1.64155300	2.28034300
C	2.16237900	-1.16269400	2.26677700
C	3.06838400	-1.48806800	1.24025200
C	2.60821900	-2.39028500	0.25604800
C	1.30609900	-2.89627300	0.24608700
C	0.40592400	-2.47831300	1.25134600
H	0.19113800	-1.33263700	3.08282900
Cl	2.65234300	-0.10591300	3.59003900
C	4.42247200	-0.85433600	1.17058300
H	4.77147600	-0.52145900	2.14747400
H	5.18460900	-1.47537400	0.69891700
S	4.38475000	0.68632600	0.16036700
O	3.20682800	1.48613900	0.49253700
O	4.73802900	0.44442900	-1.23367900
O	5.71369800	1.42599200	0.91805100
C	6.64478100	2.07279700	0.12150300

C	7.79906500	1.38152900	-0.27969200
C	6.44560600	3.41192400	-0.20031800
C	8.77188000	2.07994800	-1.02101400
C	7.42304200	4.08707700	-0.94305300
H	5.53923700	3.89344700	0.14238300
C	8.58908600	3.41185600	-1.34870400
H	9.66954400	1.55909700	-1.33576600
H	9.33161500	3.95811500	-1.91934800
C	7.96180400	0.00431100	0.06081000
N	8.07853400	-1.11844300	0.34508900
O	7.33638900	5.38653600	-1.31294800
C	6.17385500	6.12353800	-0.94803300
H	6.31522900	7.12393700	-1.35786300
H	5.26808400	5.67842500	-1.37663400
H	6.06724000	6.18914700	0.14142600
Cl	3.71174800	-2.88149800	-1.02923300
Pd	-1.51182400	-2.91360400	1.04092600
C	-4.28306300	-1.98320500	0.33283400
O	-3.65865700	-2.85802600	1.01335700
O	-3.78700000	-1.05631200	-0.36269800
C	-0.80546300	-3.96294000	-0.61392300
C	-1.05909500	-5.46185100	-0.34311200
C	1.19906000	-5.34352500	-0.52073700
C	0.75663700	-3.86030600	-0.76267000
C	0.16765100	-5.83766000	0.51549000
H	0.23816600	-6.91506200	0.69879900
H	0.21223400	-5.31029000	1.47171200
C	-0.75005500	-6.26253200	-1.64694900
H	-1.07515700	-7.29914900	-1.50994800
H	-1.28338300	-5.87152900	-2.51451600
C	0.80344900	-6.16741600	-1.76745700
H	1.26670400	-7.15878000	-1.73497600
H	1.12951300	-5.68848500	-2.69673300
H	-2.04777500	-5.67584500	0.06588500
H	2.25141900	-5.43011000	-0.24319900
H	1.03439200	-3.54887600	-1.77491800
O	-1.09662400	-2.25540400	-2.27540400
C	-1.64326300	-3.38285800	-1.72150600
O	-2.69380100	-3.84449100	-2.12108200
C	-1.84419400	-1.69631600	-3.37531500
H	-2.81678500	-1.33990900	-3.02757300

H	-1.23743000	-0.87175000	-3.75005200
H	-1.99303600	-2.44670900	-4.15468600
Ag	-1.62427600	-0.44178700	-0.14358800
C	-5.81409800	-2.09147400	0.41736800
H	-6.10348800	-3.11184000	0.15369600
H	-6.08413600	-1.93252600	1.46475000
N	-6.54517300	-1.14945900	-0.40019500
C	-6.61855000	0.17323300	-0.05561700
O	-6.24316100	0.58636000	1.03911200
C	-7.19725700	1.08994700	-1.12076100
H	-7.64737500	1.95992900	-0.64044700
H	-6.38667700	1.44372500	-1.76809600
H	-7.94013900	0.58760500	-1.74746400
H	-6.68512400	-1.38802100	-1.37098000
C	-3.44915900	5.26877400	-0.34182800
C	-4.65007000	4.66513100	0.05504900
C	-4.65119100	3.33484300	0.48945100
C	-3.46543200	2.60018000	0.51919300
C	-2.28875000	3.21796300	0.10503100
C	-2.25680400	4.54461500	-0.32213300
H	-3.44795700	6.30029900	-0.67493900
H	-5.57212100	2.85344300	0.80169100
H	-3.49737500	1.56652700	0.84429900
H	-1.33132100	5.01085600	-0.64133100
I	-0.42699500	2.10875600	0.11984600
C	-5.95686400	5.38433200	0.00902800
O	-7.03536500	4.86207300	0.21122300
O	-5.81252400	6.69418500	-0.29217000
C	-7.03601900	7.44469100	-0.36138900
H	-7.55911600	7.41377400	0.59739200
H	-6.74131400	8.46511100	-0.60540400
H	-7.69315100	7.03835800	-1.13428400

TS16

C	0.66477800	0.42378200	-1.43272100
C	2.02836700	0.69386900	-1.52258200
C	2.82339500	0.93064100	-0.38843900
C	2.15307900	0.90807800	0.85227500
C	0.78052600	0.65359600	0.97691000
C	0.02579700	0.38987500	-0.18876300
H	0.12263100	0.23686400	-2.35157200

Cl	2.73157300	0.75365200	-3.13816200
C	4.29419500	1.20123400	-0.49948700
H	4.55643100	1.62514900	-1.46904100
H	4.67850500	1.84002800	0.29660800
S	5.30392800	-0.32755300	-0.39975500
O	4.87387300	-1.29586600	-1.40137800
O	5.54358400	-0.73950400	0.97831400
O	6.73037300	0.39451000	-0.98627300
C	7.92481500	0.06987800	-0.36680300
C	8.45869400	0.95414500	0.58415900
C	8.59877900	-1.08640900	-0.74866200
C	9.71257500	0.65057200	1.14940000
C	9.84106500	-1.37431800	-0.16877700
H	8.13967400	-1.72739600	-1.48975200
C	10.39498300	-0.49523100	0.78055700
H	10.13814700	1.32639900	1.88314900
H	11.35985300	-0.73897800	1.21066500
C	7.72935000	2.12283700	0.96023600
N	7.12286700	3.07055800	1.25900200
O	10.58351300	-2.46758900	-0.46226100
C	10.07279700	-3.40588300	-1.40456700
H	10.82095800	-4.19606900	-1.47238000
H	9.12088200	-3.83282000	-1.06770200
H	9.93777100	-2.94765600	-2.39160400
Cl	3.08344800	1.21111400	2.31769600
Pd	-1.91496100	-0.11410200	0.06327400
C	-4.22705300	-2.11212000	0.84801800
O	-3.92011200	-0.90620500	0.60114700
O	-3.60146900	-3.14732500	0.46704100
C	-1.38266100	0.02267700	2.11343100
C	-2.29508500	1.07917800	2.76504400
C	-0.22745000	1.99282300	2.95786100
C	0.06127800	0.60512700	2.29032800
C	-1.58689400	2.38713100	2.34769400
H	-2.02253600	3.27217300	2.82383200
H	-1.55515600	2.54816500	1.26843100
C	-2.04119100	1.09482600	4.30447300
H	-2.79968200	1.72310400	4.78346900
H	-2.11841200	0.10142000	4.74813700
C	-0.61950500	1.72936600	4.42999600
H	-0.65064400	2.66828200	4.99223800

H	0.09641400	1.07281500	4.93532500
H	-3.34716600	0.96969700	2.50045700
H	0.58982600	2.70548100	2.83320400
H	0.63758500	-0.01411100	2.98692600
O	-0.53085000	-2.19455300	2.26884900
C	-1.57442400	-1.38880700	2.59442900
O	-2.53705700	-1.79906700	3.22074400
C	-0.65559100	-3.56368500	2.68904000
H	-1.53506000	-4.02149900	2.22900100
H	0.25890700	-4.05495000	2.35651500
H	-0.74750700	-3.62652800	3.77635000
Ag	-2.23280200	-2.66711500	-1.17274100
C	-5.46776300	-2.30665300	1.72632100
H	-5.16032900	-2.08728900	2.75255700
H	-6.20876100	-1.56486100	1.42274000
N	-6.04930300	-3.62796800	1.66623100
C	-6.62799600	-4.05607000	0.49842300
O	-6.82673000	-3.29657900	-0.44251700
C	-7.00861500	-5.52690600	0.45611000
H	-7.94855400	-5.63061700	-0.08879000
H	-6.23978000	-6.07877200	-0.09544300
H	-7.11187300	-5.97302200	1.44934000
H	-5.69658300	-4.32436300	2.30568300
C	-2.49019800	3.95373100	-1.28106500
C	-3.73778800	4.19483100	-0.68691400
C	-4.57560800	3.11770300	-0.37014700
C	-4.18940700	1.80478400	-0.63865200
C	-2.91958100	1.60231900	-1.18185200
C	-2.07562400	2.65172400	-1.55487000
H	-1.84301000	4.78513200	-1.53603200
H	-5.54232900	3.32047600	0.07900200
H	-4.83146400	0.96868600	-0.39422500
H	-1.11360100	2.46698200	-2.01433800
I	-2.77972100	-0.27098600	-2.73707800
C	-4.22866400	5.57019400	-0.38600600
O	-5.30428400	5.81544200	0.12390300
O	-3.34033600	6.52248600	-0.74453700
C	-3.75057100	7.87419400	-0.47948200
H	-3.92231000	8.01963800	0.58980100
H	-2.93070800	8.50285400	-0.82588400
H	-4.67104500	8.10847200	-1.01971300

int23

C	0.88466000	1.27233600	-0.36521600
C	2.21582700	1.51507300	-0.03543900
C	2.97707500	0.61235500	0.72853400
C	2.31245200	-0.54963200	1.16485800
C	0.96233800	-0.81304600	0.88103200
C	0.26132700	0.11233300	0.08730900
H	0.36219200	1.98469800	-0.99005900
Cl	2.91828800	3.02136600	-0.60364900
C	4.41464300	0.88460400	1.06231400
H	4.63291300	1.95246800	1.05214900
H	4.72905800	0.45701400	2.01520900
S	5.57316300	0.18333100	-0.17615800
O	5.19552900	0.59952400	-1.52089300
O	5.90346600	-1.20793000	0.10913600
O	6.89500700	1.14234800	0.29390500
C	8.14102700	0.54137700	0.37086700
C	8.60238400	0.08662100	1.61640500
C	8.92838800	0.46597600	-0.77373900
C	9.90246000	-0.44995600	1.69125800
C	10.21647500	-0.07745500	-0.67944200
H	8.51842100	0.83659400	-1.70403900
C	10.69872400	-0.53134000	0.56255000
H	10.27356700	-0.80303400	2.64719000
H	11.70045300	-0.94335800	0.60915800
C	7.75446800	0.16686600	2.76247900
N	7.04747700	0.23792300	3.68465900
O	11.06881800	-0.20206600	-1.72284600
C	10.63567700	0.21983900	-3.01310600
H	11.46676700	0.01261200	-3.68759700
H	9.75186400	-0.34005100	-3.34044400
H	10.41402700	1.29358800	-3.02908400
Cl	3.21206100	-1.73538500	2.10165100
Pd	-1.57374100	-0.44709900	-0.52104500
C	-4.66492300	-1.69012500	-1.19678200
O	-3.39819600	-1.64568700	-1.15161500
O	-5.44107600	-0.74654800	-1.51805300
C	-1.14790900	-2.19840600	0.65347900
C	-2.07693500	-2.51533600	1.81976200
C	-0.06603000	-2.22201400	2.83609500

C	0.26702800	-2.07141800	1.31239100
C	-1.47950000	-1.62137000	2.93118600
H	-1.95076000	-1.80095100	3.90252900
H	-1.52141300	-0.55445900	2.71282700
C	-1.71499400	-3.93732800	2.37776700
H	-2.49860000	-4.22037000	3.08735300
H	-1.68297400	-4.69623400	1.59721600
C	-0.34699900	-3.71818800	3.09520900
H	-0.42476400	-3.91205300	4.16952800
H	0.44601600	-4.36439600	2.70526400
H	-3.13878300	-2.41839500	1.59946100
H	0.69488600	-1.78366400	3.48265600
H	0.88638500	-2.92403800	1.00157300
O	-0.67726100	-2.32019700	-1.62347600
C	-1.16891600	-3.07374700	-0.58182200
O	-1.51970900	-4.21901000	-0.70515400
C	-0.77442600	-2.88364600	-2.95382600
H	-1.82273100	-3.06819600	-3.19331400
H	-0.35041600	-2.13233500	-3.61704300
H	-0.20577000	-3.81354300	-2.99494400
Ag	-4.21796500	0.90318000	-2.26900900
C	-5.30836500	-3.05257500	-0.88350600
H	-5.42961600	-3.59496000	-1.82662000
H	-4.62627700	-3.62324900	-0.25274200
N	-6.60204300	-2.94912300	-0.23927800
C	-6.68051100	-2.44574500	1.02851200
O	-5.67284000	-2.21071400	1.69447700
C	-8.07735900	-2.20327300	1.56675100
H	-8.12639800	-2.57082300	2.59382700
H	-8.26423200	-1.12493200	1.59294600
H	-8.85951100	-2.68239600	0.97206900
H	-7.42416700	-2.90741500	-0.82257900
C	-2.76127400	3.02957600	1.75882700
C	-3.98755500	2.62924200	2.30299200
C	-4.43933200	1.32388700	2.07821200
C	-3.68397900	0.42858200	1.31992200
C	-2.46410200	0.84121500	0.77211900
C	-1.99806600	2.14021400	0.99848000
H	-2.39901000	4.03752700	1.92729700
H	-5.38532100	1.00698600	2.50400400
H	-4.07323200	-0.57044700	1.18080000

H	-1.05899200	2.48399200	0.58948700
I	-1.70735300	1.53198400	-2.98009300
C	-4.84188300	3.53805200	3.11795900
O	-5.91851600	3.23018700	3.59188800
O	-4.28788800	4.76217000	3.27761100
C	-5.06556000	5.68880000	4.05026500
H	-5.22819900	5.30636900	5.06113400
H	-4.48352800	6.60991300	4.07801500
H	-6.03695200	5.86219700	3.58019200

int24

C	0.09998600	0.30292300	-1.05855000
C	1.26604900	1.04954500	-1.22516400
C	1.75719900	1.90054600	-0.21536600
C	0.99095700	1.99067400	0.96529700
C	-0.19831400	1.27524100	1.15980200
C	-0.61569700	0.42331500	0.12788100
H	-0.22996100	-0.36460600	-1.84741100
Cl	2.09740500	0.91237900	-2.76343100
C	3.02081100	2.68805800	-0.38719000
H	3.28132500	2.85153700	-1.43309600
H	2.98105900	3.64852000	0.12973300
S	4.52310900	1.92313700	0.34183900
O	4.21974700	1.16082800	1.54977100
O	5.59769200	2.90967200	0.33536800
O	4.79721100	0.82243300	-0.90317800
C	6.06517400	0.26709800	-1.01279800
C	6.75730200	0.47517400	-2.21571200
C	6.58924000	-0.51694400	0.01182800
C	8.01430300	-0.14214400	-2.37373900
C	7.85023000	-1.10242400	-0.16084300
H	6.00704100	-0.65107800	0.91341800
C	8.55693600	-0.91544800	-1.36324200
H	8.55808900	0.00402800	-3.30065400
H	9.52648300	-1.38771800	-1.47386600
C	6.19527100	1.28829600	-3.24705000
N	5.74616300	1.94652800	-4.09530600
O	8.46234900	-1.87247500	0.76860100
C	7.81122200	-2.08071400	2.01887300
H	8.48957700	-2.69904200	2.60726900
H	7.63532200	-1.13265900	2.54020900

H	6.85830100	-2.60775400	1.89025500
Cl	1.54484600	3.04207800	2.26514400
Pd	-2.11893100	-0.82769400	0.49503900
C	-5.81793000	0.56846500	-1.00234900
C	-5.50926800	1.43878200	-2.05539300
C	-4.16790500	1.68542600	-2.36839300
C	-3.14189300	1.08411300	-1.63779300
C	-3.46111100	0.22537100	-0.58236300
C	-4.79916100	-0.04114000	-0.26862800
H	-6.85453500	0.36290100	-0.75932700
H	-3.93841500	2.35746100	-3.18902600
H	-2.11431900	1.29790300	-1.89958000
H	-5.05537400	-0.73205400	0.52585600
C	-6.55468900	2.11975700	-2.86878400
O	-6.32472300	2.87788200	-3.79105700
O	-7.80831900	1.80364100	-2.46825100
C	-8.86326700	2.43047300	-3.21342800
H	-8.80815800	2.15152500	-4.26868900
H	-9.79133200	2.07027200	-2.76955200
H	-8.79669700	3.51853500	-3.13450200
C	-2.14181500	0.18276200	2.35118600
C	-3.41236100	0.94674300	2.74384000
C	-1.83056200	2.57268800	2.74450500
C	-1.01042700	1.27983500	2.42365700
C	-3.17346500	2.30249500	2.04138400
H	-3.93841600	3.04277500	2.29714500
H	-3.09862000	2.23243800	0.95603500
C	-3.32657900	1.38037900	4.24228700
H	-4.30233700	1.77675200	4.54144800
H	-3.08924000	0.54916300	4.90451600
C	-2.24060700	2.50305300	4.23297500
H	-2.65601100	3.46140200	4.56000700
H	-1.39243200	2.27740800	4.88736500
H	-4.33533100	0.41737100	2.50355300
H	-1.30896500	3.48829600	2.46230400
H	-0.33811100	1.06948500	3.26603000
O	-0.96217500	-1.82575700	2.28245300
C	-1.79927900	-1.08994300	3.09750800
O	-2.17498900	-1.47850100	4.17420700
C	-0.62172400	-3.17924800	2.69742600
H	-0.43668600	-3.74395600	1.78520300

H	0.27029200	-3.13064700	3.32528700
H	-1.45312500	-3.60490200	3.25833600
C	-2.90315300	-3.10380900	-0.38520100
O	-2.06418700	-2.43245000	-1.06180200
O	-3.44692800	-2.61601900	0.65622600
C	-3.27633000	-4.51969200	-0.81567900
H	-4.22523700	-4.48120300	-1.35974400
H	-3.43181000	-5.11060600	0.08915100
N	-2.27504800	-5.15180600	-1.64892600
C	-1.04180500	-5.42591600	-1.11784900
O	-0.81913400	-5.31414700	0.08415500
C	0.01707500	-5.88184400	-2.10417300
H	0.59378700	-6.69079800	-1.65172300
H	-0.39788500	-6.21980400	-3.05754500
H	0.70302800	-5.05002800	-2.29555800
H	-2.34515600	-5.02855900	-2.64808800

TS17

C	-0.03539100	0.84714700	-0.83921100
C	1.24862800	1.37843400	-0.75847000
C	1.87586800	1.61989300	0.47902200
C	1.14652800	1.26913000	1.63499200
C	-0.13186400	0.69822400	1.60021500
C	-0.72485300	0.52534000	0.32873700
H	-0.49939300	0.72891000	-1.81066500
Cl	2.03447200	1.81214100	-2.26207700
C	3.24200400	2.22816300	0.57037700
H	3.51466800	2.79775600	-0.31838500
H	3.35288300	2.85930400	1.45360700
S	4.61847400	1.02686100	0.78051300
O	4.20169700	-0.15998900	1.52187300
O	5.82007100	1.76046100	1.16137300
O	4.74288600	0.59463000	-0.84152900
C	5.94659100	0.06287700	-1.28633300
C	6.59624800	0.73387100	-2.33345400
C	6.44315900	-1.12252600	-0.75090000
C	7.78017300	0.17010400	-2.84983600
C	7.63434800	-1.65089200	-1.26559800
H	5.89483700	-1.60318700	0.04807400
C	8.29587600	-1.00076200	-2.32396600
H	8.28981500	0.67343100	-3.66414600

H	9.21016900	-1.43716000	-2.70978000
C	6.06326300	1.95260300	-2.85413600
N	5.63300900	2.94531700	-3.28309800
O	8.21598500	-2.78693600	-0.81664700
C	7.61195000	-3.48001300	0.27196100
H	8.25847900	-4.33395300	0.47533000
H	7.55134500	-2.84651500	1.16447000
H	6.60904100	-3.83806100	0.01026300
Cl	1.87533700	1.55225800	3.21300400
Pd	-2.33775600	-0.74438300	0.39287200
C	-3.93589100	2.42758600	-1.69608600
C	-4.04163400	3.55940600	-0.87978400
C	-3.40767500	3.56246000	0.36784700
C	-2.69317100	2.45138100	0.80801900
C	-2.63203500	1.30351500	0.00856200
C	-3.21916300	1.30984200	-1.26720800
H	-4.41034800	2.41735400	-2.67074000
H	-3.46858700	4.45520300	0.98143100
H	-2.16885700	2.50591300	1.75132100
H	-3.15284000	0.44278900	-1.91599900
C	-4.78594300	4.78459200	-1.28923400
O	-4.88458900	5.78453900	-0.60518800
O	-5.34404100	4.66243300	-2.51294500
C	-6.07696200	5.81113700	-2.96992600
H	-5.42209600	6.68365400	-3.03287700
H	-6.45641200	5.54387800	-3.95584700
H	-6.90061900	6.03667700	-2.28822700
C	-1.75417200	-1.06695100	2.38169900
C	-2.90998800	-0.95987700	3.37992800
C	-1.62425400	0.85192300	3.86162800
C	-0.77037000	0.05381500	2.80695900
C	-3.09737400	0.56381200	3.47381600
H	-3.78598800	0.85115900	4.27516900
H	-3.44675200	1.01334500	2.54867300
C	-2.34952100	-1.26146600	4.81316400
H	-3.19425000	-1.40290100	5.49405900
H	-1.75496500	-2.17446400	4.84454200
C	-1.53805500	0.02752400	5.16945300
H	-2.00419400	0.57493700	5.99455600
H	-0.50535300	-0.18574100	5.46214700
H	-3.77655000	-1.56533600	3.11378200

H	-1.32984900	1.89833800	3.97023300
H	0.06204300	-0.40645400	3.35309900
O	-0.03554100	-2.45343500	1.47528900
C	-1.15483200	-2.45706300	2.23697100
O	-1.59972800	-3.45579600	2.75962100
C	0.60291500	-3.73292800	1.30692700
H	1.48119800	-3.53990400	0.69245300
H	0.89235300	-4.14590700	2.27597600
H	-0.07373700	-4.43170100	0.80936100
C	-3.61494100	-2.64415800	-0.89124400
O	-3.15157200	-1.78765100	-1.68588500
O	-3.44317400	-2.54445900	0.38109400
C	-4.39865600	-3.84059300	-1.38903100
H	-5.39170400	-3.83144700	-0.92210400
H	-3.91002600	-4.75448900	-1.02798400
N	-4.49254600	-3.81987800	-2.83077800
C	-5.18312400	-4.78048200	-3.50853100
O	-5.74830100	-5.70364900	-2.93276700
C	-5.20177700	-4.63136400	-5.02267500
H	-6.24139700	-4.58760900	-5.35822700
H	-4.67146300	-3.74661400	-5.38569400
H	-4.75337800	-5.52306400	-5.46948900
H	-4.03187700	-3.05256400	-3.29954500

int25

C	-1.04401500	-1.43646500	-1.35594200
C	0.18702700	-1.17545900	-1.91153600
C	0.56890100	0.14203500	-2.26197100
C	-0.34088800	1.16318900	-1.95852800
C	-1.58505500	0.96874600	-1.25351100
C	-1.96523500	-0.40531500	-1.04114200
H	-1.34197900	-2.46354600	-1.18775000
Cl	1.21264000	-2.53941800	-2.28012900
C	1.87588200	0.40940300	-2.95057500
H	2.28083900	-0.46771200	-3.45636900
H	1.80784100	1.23269400	-3.66246700
S	3.22761700	0.96393000	-1.83611000
O	2.72022500	1.84227100	-0.78867400
O	4.36707000	1.35538000	-2.65696900
O	3.55750600	-0.52374100	-1.12040000
C	4.88897500	-0.83916600	-0.85894600

C	5.62241500	-1.53997500	-1.83057400
C	5.42644300	-0.51076600	0.38049600
C	6.94636000	-1.90930600	-1.52278300
C	6.75221000	-0.88038400	0.66254800
H	4.80063200	-0.00602500	1.10561600
C	7.50415100	-1.58289400	-0.29987100
H	7.52772700	-2.45104300	-2.26094800
H	8.52430300	-1.85776300	-0.05635700
C	5.02642300	-1.86628600	-3.08577200
N	4.52263600	-2.13453200	-4.10075800
O	7.38788300	-0.61017000	1.81923700
C	6.70781400	0.16585500	2.81570400
H	7.41553200	0.26029500	3.63987200
H	6.46629200	1.16310900	2.42913100
H	5.79252200	-0.32758200	3.15661900
Cl	0.02370400	2.75265000	-2.61332900
Pd	-1.15138000	0.59124200	1.01013200
C	-4.87545900	-2.39146800	0.40351800
C	-5.85751300	-2.19657800	-0.57732300
C	-5.56918000	-1.39923100	-1.69125900
C	-4.32455000	-0.78913100	-1.81575900
C	-3.34980300	-0.94875400	-0.81928800
C	-3.63093700	-1.78095000	0.27690900
H	-5.09061500	-3.01944200	1.26028400
H	-6.33070000	-1.27718200	-2.45404800
H	-4.09981400	-0.19805300	-2.69775800
H	-2.87311600	-1.92994200	1.04040200
C	-7.21095700	-2.81846300	-0.49622500
O	-8.08059300	-2.67639800	-1.33343100
O	-7.36973200	-3.56315900	0.61983000
C	-8.65597800	-4.18791900	0.76119100
H	-8.84546200	-4.86946700	-0.07172100
H	-8.61496900	-4.73463000	1.70299700
H	-9.44740900	-3.43491700	0.78713500
C	-2.07380900	2.40823300	0.72345700
C	-3.43886300	2.63413200	1.38619900
C	-3.94216300	2.28492800	-0.79904900
C	-2.38514900	2.22606700	-0.79472300
C	-4.36075300	1.71273200	0.57600100
H	-5.42141600	1.88894200	0.78463600
H	-4.15204800	0.65726500	0.72303000

C	-3.94813300	4.03168600	0.91206800
H	-4.83590600	4.30720900	1.49064700
H	-3.20884800	4.81947900	1.06164200
C	-4.30361200	3.78216000	-0.58947100
H	-5.37095700	3.93514100	-0.77665200
H	-3.75857700	4.44240600	-1.27206600
H	-3.42572400	2.51183700	2.46930000
H	-4.40907500	1.84751300	-1.68158900
H	-2.00520500	3.06044300	-1.38132700
O	0.08106100	3.38355200	0.41806700
C	-1.01063800	3.35990200	1.20959700
O	-1.10735100	4.01456700	2.23009200
C	1.17454400	4.19852300	0.87999400
H	1.98696600	4.00927800	0.18227900
H	0.88676200	5.25327800	0.88087300
H	1.45867200	3.90639000	1.89328400
C	0.08498700	-0.44432100	2.95687600
O	0.05426000	-1.14067600	1.90486300
O	-0.56672900	0.65546800	3.04298600
C	0.90202100	-0.88170800	4.16585800
H	0.22054900	-1.05787700	5.00556300
H	1.57050400	-0.06472200	4.44470900
N	1.71172000	-2.05254300	3.90441700
C	3.01780900	-1.92558600	3.51303100
O	3.62287500	-0.85711500	3.57708300
C	3.68393600	-3.19802500	3.02314500
H	4.60948400	-3.35049200	3.58406900
H	3.05618700	-4.08728200	3.12088400
H	3.95383200	-3.06671700	1.97121400
H	1.22137800	-2.88277600	3.60419600

TS18

C	-0.67033400	-3.57489200	-0.28186500
C	0.57095800	-3.81874900	-0.84736000
C	1.28527000	-2.79554400	-1.49085600
C	0.60671000	-1.57428600	-1.67077100
C	-0.67324500	-1.27450400	-1.13266900
C	-1.27000600	-2.31047900	-0.34781200
H	-1.15409600	-4.36140400	0.28518200
Cl	1.22695900	-5.43758400	-0.71526200
C	2.71062100	-2.99693600	-1.90721500

H	2.91223500	-4.02100700	-2.22886600
H	3.04260500	-2.30341300	-2.67788000
S	3.91290900	-2.78136100	-0.53637300
O	5.25690100	-2.97016300	-1.07727700
O	3.49737900	-3.46546300	0.68104700
O	3.65882300	-1.12461700	-0.30377100
C	4.15398900	-0.54839400	0.85650300
C	3.25543100	0.18944100	1.64935600
C	5.50297600	-0.63815500	1.18477300
C	3.75001100	0.85555500	2.79117000
C	5.96747900	0.00939600	2.33891600
H	6.16135400	-1.20148900	0.53774800
C	5.08358700	0.76303500	3.13640200
H	3.06653900	1.43924100	3.39803200
H	5.47506200	1.26413400	4.01409000
C	1.88363700	0.27373600	1.29052600
N	0.76431300	0.34326100	0.98850700
O	7.24919300	-0.02153100	2.75619100
C	8.20196900	-0.77536300	2.00674500
H	9.14621500	-0.67050700	2.54083900
H	7.92266200	-1.83384200	1.95973200
H	8.31156800	-0.37888200	0.99087600
Cl	1.42060500	-0.35128000	-2.62831300
Pd	-0.85140600	0.75844600	-0.37580500
C	-3.58030300	-1.21664800	2.46960100
C	-4.67839300	-2.06334700	2.27484800
C	-4.66053300	-2.98332100	1.21803600
C	-3.56598400	-3.04665100	0.36366600
C	-2.47382600	-2.17676600	0.52846600
C	-2.48680300	-1.27600900	1.60714800
H	-3.58148200	-0.51477300	3.29539400
H	-5.51514600	-3.63805600	1.08543900
H	-3.56259900	-3.76134400	-0.45428200
H	-1.63491000	-0.62800200	1.77834300
C	-5.88055300	-2.04046900	3.15811500
O	-6.84788800	-2.76315600	3.01519900
O	-5.77889700	-1.12212200	4.14249500
C	-6.90776300	-1.04302300	5.02761100
H	-7.06610600	-1.99837900	5.53408300
H	-6.66217300	-0.26244200	5.74718400
H	-7.81287700	-0.78390600	4.47284100

C	-2.04473400	1.16641700	-2.02722300
C	-3.56880400	1.30067300	-1.89755300
C	-3.18529400	-0.86793500	-2.42846900
C	-1.78577300	-0.24855000	-2.36285900
C	-3.97554700	-0.07553700	-1.36200900
H	-5.05246700	-0.25893100	-1.42967400
H	-3.65097200	-0.24364200	-0.34025900
C	-4.11386200	1.20611800	-3.35646300
H	-5.19167700	1.39739400	-3.35693300
H	-3.65463700	1.93454500	-4.02782700
C	-3.80417200	-0.27530000	-3.73946200
H	-4.71484300	-0.82890800	-3.98783200
H	-3.12859000	-0.36521400	-4.59625900
H	-3.89263900	2.18063500	-1.34464000
H	-3.21363700	-1.95715400	-2.38218400
H	-1.11322100	-0.43504800	-3.19457500
O	-0.27469300	2.05082400	-3.38169700
C	-1.39744800	2.34551600	-2.69949500
O	-1.87228400	3.46326200	-2.64340700
C	0.46469100	3.19334400	-3.85366600
H	-0.15237000	3.80479300	-4.51590300
H	0.79256000	3.78494900	-2.99640800
H	1.31889400	2.78459300	-4.39399100
C	-0.31468000	3.52338100	0.24688400
O	0.68716600	3.41384400	-0.47266600
O	-1.19169600	2.60416900	0.49324800
C	-0.62628800	4.85149400	0.94459900
H	-1.57883600	5.22894000	0.55032500
H	-0.77583400	4.69019400	2.01687300
N	0.45717300	5.78294700	0.71904300
C	0.65859800	6.87446100	1.50297100
O	-0.10113600	7.19080500	2.41468000
C	1.89573200	7.69869800	1.16620200
H	2.51190400	7.79218000	2.06471400
H	2.49987800	7.27630300	0.35832500
H	1.58060600	8.70702700	0.88266900
H	1.13934300	5.47263400	0.03868400

int26

C	0.27922800	-3.72568600	-0.46082500
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C	1.50933900	-3.67989500	-1.09998100
C	1.98944200	-2.49144300	-1.67238500
C	1.10372100	-1.39316000	-1.66434500
C	-0.10489800	-1.36786600	-0.95985300
C	-0.50129800	-2.56557000	-0.32139200
H	-0.04223600	-4.65043500	0.00440000
Cl	2.46294200	-5.15592600	-1.15924300
C	3.40700400	-2.35475200	-2.12914800
H	3.83210100	-3.28917300	-2.50178800
H	3.55687200	-1.56302600	-2.86188000
S	4.54962000	-1.93353100	-0.74804200
O	5.87925200	-1.68630400	-1.30131500
O	4.37474400	-2.80911700	0.40324900
O	3.85220300	-0.43281400	-0.35751700
C	4.17562000	0.17474200	0.83976400
C	3.12153200	0.76740500	1.56646900
C	5.49166500	0.26814800	1.28352200
C	3.42481700	1.46733600	2.75512400
C	5.76468700	0.94209500	2.48236500
H	6.27807300	-0.17252400	0.68627500
C	4.72369900	1.54891300	3.21320600
H	2.61905200	1.93703600	3.30871000
H	4.96838500	2.07557900	4.12819400
C	1.78040000	0.67278300	1.10939800
N	0.68352400	0.59249000	0.73917700
O	6.99948900	1.07466700	3.00563000
C	8.10520900	0.47109200	2.33315400
H	8.97756400	0.68651800	2.94991500
H	7.97387200	-0.61334300	2.24870200
H	8.24764200	0.90310200	1.33612700
Cl	1.56897300	0.04929100	-2.56922700
Pd	-0.95678500	0.45086900	-0.54162400
C	-2.97330300	-1.98157600	2.51210700
C	-3.91412100	-2.99262500	2.27664100
C	-3.73855800	-3.85492400	1.18649600
C	-2.64268900	-3.70450600	0.34323100
C	-1.70298300	-2.68082100	0.55735300
C	-1.88108800	-1.82880100	1.66068700
H	-3.09717500	-1.32087500	3.36233800
H	-4.47222100	-4.63625900	1.01873900
H	-2.51570300	-4.37727300	-0.50033900

H	-1.15087100	-1.05378000	1.86382600
C	-5.10609600	-3.20171800	3.14696800
O	-5.93884600	-4.07068300	2.97295200
O	-5.16587400	-2.31162700	4.16209700
C	-6.29438900	-2.45626800	5.03858600
H	-6.28442800	-3.43774100	5.51932800
H	-6.19348900	-1.66447100	5.78054000
H	-7.22902400	-2.34629400	4.48311300
C	-2.56469800	1.08814200	-2.10784000
C	-3.99718000	1.08356800	-1.59905800
C	-3.46197900	-1.06199000	-2.09019100
C	-2.22738200	-0.22857100	-2.39159800
C	-4.08348900	-0.28869700	-0.90675800
H	-5.11345400	-0.59402100	-0.69919100
H	-3.49683000	-0.34783300	0.01145500
C	-4.84248000	0.79853100	-2.88990600
H	-5.90618000	0.89038700	-2.65150500
H	-4.62451000	1.50758900	-3.69203400
C	-4.46292000	-0.67450000	-3.23895900
H	-5.33363600	-1.33608700	-3.20094300
H	-4.01606500	-0.77851000	-4.23217700
H	-4.28872300	1.96813000	-1.03799200
H	-3.30232600	-2.13263000	-1.97074300
H	-1.46654600	-0.51960200	-3.10550600
O	-0.85743100	2.13816100	-3.37837700
C	-2.01869000	2.33270900	-2.73595900
O	-2.61375900	3.39044100	-2.69341900
C	-0.20771100	3.33746800	-3.84424400
H	-0.86238900	3.88931200	-4.52226600
H	0.05177400	3.95586700	-2.98266600
H	0.68803100	2.99838900	-4.36375700
C	-1.09833200	3.30737200	0.18772200
O	-0.08483200	3.49587000	-0.49533900
O	-1.75407600	2.19557500	0.30453300
C	-1.71866500	4.45360500	0.99367300
H	-2.72770400	4.63866100	0.60235000
H	-1.84131900	4.15781000	2.04056900
N	-0.87930700	5.62658400	0.89462400
C	-0.94883300	6.65018500	1.78651000
O	-1.77223100	6.68508900	2.69696300
C	0.06376700	7.76907400	1.57466400

H	0.64218800	7.89971000	2.49347900
H	0.74879900	7.59114700	0.74098800
H	-0.47655500	8.70308700	1.39616100
H	-0.13602800	5.55450000	0.21152100

int27

C	-0.46652100	-3.47007700	0.83785000
C	-1.70462500	-3.22789000	1.41751300
C	-2.08108600	-1.94105800	1.83642600
C	-1.10535700	-0.93256100	1.69643200
C	0.08778500	-1.10458200	0.99171800
C	0.41575900	-2.41078400	0.56907000
H	-0.21292500	-4.47688300	0.52608300
Cl	-2.80089500	-4.58898300	1.61747300
C	-3.47710800	-1.62328300	2.26650000
H	-3.99333200	-2.47080400	2.72224800
H	-3.54774100	-0.75372100	2.91907800
S	-4.57093800	-1.22359500	0.83956700
O	-5.88495400	-0.83568700	1.34712900
O	-4.44741900	-2.19012900	-0.24342300
O	-3.75724500	0.19333900	0.35428100
C	-4.01024800	0.73331900	-0.88913200
C	-2.90236700	1.21989400	-1.61747300
C	-5.30397700	0.86348400	-1.38631000
C	-3.12905000	1.84661800	-2.86303000
C	-5.50146100	1.46493900	-2.63739200
H	-6.13251900	0.50738200	-0.78970800
C	-4.40609100	1.96330500	-3.37142800
H	-2.28157200	2.23076300	-3.42041500
H	-4.59254700	2.43450600	-4.32934200
C	-1.58519100	1.08330700	-1.10581300
N	-0.51483500	0.96554600	-0.67393200
O	-6.70945800	1.62506500	-3.21160800
C	-7.86810400	1.13009000	-2.53869600
H	-8.70686000	1.34684500	-3.19990700
H	-7.79951500	0.04909400	-2.37447600
H	-8.01804700	1.63926400	-1.57998000
Cl	-1.40699800	0.63532900	2.46235900
Pd	1.13078600	0.51036200	0.40975200
C	3.22631000	-2.36786000	-1.99851000
C	4.05324000	-3.39254700	-1.51939000

C	3.68335900	-4.09001400	-0.36216200
C	2.50821800	-3.76513700	0.30652300
C	1.67901600	-2.72967800	-0.15686800
C	2.05287500	-2.04207300	-1.32316200
H	3.50213900	-1.83275200	-2.89975300
H	4.33284600	-4.88085900	-0.00226200
H	2.23597600	-4.30220900	1.21047500
H	1.41263700	-1.25843100	-1.71471400
C	5.32258100	-3.78375100	-2.19344500
O	6.06511200	-4.66513400	-1.80458800
O	5.56875600	-3.04696000	-3.30091400
C	6.78127800	-3.37412400	-3.99589000
H	6.76330700	-4.41338000	-4.33392400
H	6.82495500	-2.69477800	-4.84711300
H	7.64833600	-3.23165800	-3.34596700
C	3.14362300	0.40899100	2.64166300
O	2.69392300	-0.13135200	1.60209500
C	2.27330300	3.27031500	0.25984500
O	2.18130500	3.38246600	1.51598000
O	2.13744000	2.20177800	-0.40839900
C	2.57314800	4.52311600	-0.55452000
H	1.73661600	4.70351000	-1.24130700
H	3.44375700	4.32358800	-1.19101400
O	2.89375000	1.60692800	3.04461900
H	2.46098200	2.28185400	2.33128800
C	4.06509000	-0.38927300	3.52744200
H	3.63215700	-0.45036400	4.53038700
H	4.21404700	-1.38888200	3.12187200
H	5.02331400	0.12996200	3.61794400
N	2.79382900	5.66245400	0.30692300
C	2.96772400	6.91410600	-0.19967200
C	3.14719900	8.02020100	0.83063500
H	4.11695500	8.49871600	0.66762100
H	2.37855000	8.78071700	0.66804300
H	3.09233300	7.67190000	1.86571500
O	2.98545700	7.13548900	-1.40666200
H	2.71698700	5.48521800	1.29897200

TS19

C	-0.89721000	-3.42629500	-0.03171500
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C	0.36958800	-3.70589100	-0.53038800
C	1.09681900	-2.77805500	-1.30380800
C	0.43717600	-1.56955500	-1.58862300
C	-0.82282900	-1.21064500	-1.06106600
C	-1.49317400	-2.18145400	-0.26326400
H	-1.41236900	-4.17684600	0.55611200
Cl	1.02816500	-5.29505900	-0.20376200
C	2.48770700	-3.07337700	-1.77579800
H	2.63705600	-4.12841400	-2.01598500
H	2.78778800	-2.46336900	-2.62740100
S	3.78268100	-2.77360900	-0.51104900
O	5.07669600	-3.13684500	-1.08120500
O	3.39141300	-3.23905100	0.81287000
O	3.66601600	-1.08089700	-0.50732200
C	4.17956900	-0.40807300	0.58820500
C	3.30787900	0.44424400	1.29138400
C	5.51917100	-0.52285900	0.94170700
C	3.81646000	1.20022200	2.36939500
C	6.00045900	0.21902100	2.03105100
H	6.15655500	-1.17946100	0.36500400
C	5.14169400	1.08557000	2.73809900
H	3.15335100	1.86915600	2.90693300
H	5.54749500	1.65436000	3.56659400
C	1.95094100	0.54194700	0.89083300
N	0.85043900	0.61023600	0.53546200
O	7.27413300	0.17796500	2.46697600
C	8.20395100	-0.68568600	1.81169300
H	9.14669100	-0.56043100	2.34381900
H	7.88438300	-1.73187700	1.87281000
H	8.33692200	-0.40148300	0.76172800
Cl	1.18556800	-0.44084200	-2.70807100
Pd	-0.90089000	0.92067700	-0.39887800
C	-4.49868800	-0.72925400	1.57847600
C	-5.48453900	-1.67362100	1.26782600
C	-5.15772300	-2.77202800	0.46171200
C	-3.86471500	-2.92249500	-0.02476500
C	-2.86921000	-1.97186400	0.26957100
C	-3.20490900	-0.87849500	1.08370400
H	-4.74368000	0.11772200	2.20852900
H	-5.93246200	-3.49369700	0.22620500
H	-3.62467200	-3.76834100	-0.66195000

H	-2.44697800	-0.14737300	1.34661200
C	-6.88697700	-1.56622500	1.76451300
O	-7.76499000	-2.36975400	1.51612700
O	-7.08104500	-0.46891400	2.52819600
C	-8.41409900	-0.30407300	3.03696700
H	-8.69143600	-1.15106400	3.66947500
H	-8.39505300	0.61832000	3.61697000
H	-9.13169900	-0.22814100	2.21629200
C	-3.03910700	0.82065300	-2.36623500
O	-2.61439700	1.45934700	-1.34391100
C	-0.38686600	3.70727900	-0.28659200
O	0.21489000	3.55096400	-1.34873500
O	-0.95307700	2.77839300	0.43027100
C	-0.54764600	5.09935700	0.33412800
H	-0.18689900	5.09738700	1.36797200
H	-1.61896900	5.33439100	0.38295100
O	-2.54131200	-0.25645800	-2.79652100
H	-1.60510900	-0.63304200	-1.89675800
C	-4.20374200	1.43994600	-3.10461900
H	-4.75970700	0.67310100	-3.64470800
H	-4.85124300	1.97675700	-2.41011300
H	-3.80695600	2.16053400	-3.82760900
N	0.18282100	6.06263200	-0.45814700
C	0.51955000	7.28907500	0.02430700
C	1.35522900	8.15197400	-0.91231000
H	0.78155000	9.04578200	-1.17448400
H	2.24918400	8.48509900	-0.37842800
H	1.65421100	7.64166400	-1.83206700
O	0.16653800	7.68524100	1.13159300
H	0.55636000	5.70009900	-1.32641400

TS1^p

C	-1.35563700	-1.98527300	0.91946700
C	-0.07943500	-2.53705900	0.95870500
C	0.75642800	-2.55096400	-0.17708100
C	0.18243900	-2.11440400	-1.38962300
C	-1.10067100	-1.58508000	-1.44650300
C	-1.86853200	-1.44638000	-0.27503200
H	-1.48624700	-1.23771400	-2.39923100
H	-3.18008000	-1.50325700	-0.40541700
Cl	0.47828300	-3.22118100	2.47808200

C	2.19878600	-2.94219100	-0.09480000
H	2.38624700	-3.72935700	0.63913100
H	2.61630900	-3.23025000	-1.05865300
S	3.29466100	-1.58650000	0.49272500
O	4.67122100	-1.92234600	0.13864000
O	2.95914400	-1.14952000	1.84113900
O	2.74141600	-0.39231900	-0.57648900
C	3.06976000	0.92085100	-0.27954400
C	2.02587600	1.82740800	-0.01729800
C	4.39721300	1.33483600	-0.30483300
C	2.34834300	3.18380700	0.21140100
C	4.69797700	2.68208200	-0.05556600
H	5.16354800	0.60206900	-0.51789000
C	3.66301700	3.60488000	0.19639500
H	1.54801200	3.88978200	0.40495400
H	3.92398700	4.64144100	0.37583300
C	0.66947000	1.40641800	0.01290100
N	-0.45066200	1.11028300	0.03856500
O	5.94709000	3.18750100	-0.04810500
C	7.04965800	2.30995200	-0.27816800
H	7.94126000	2.93255000	-0.20648800
H	7.09236500	1.51936700	0.47920200
H	6.99746300	1.86081300	-1.27651700
Pd	-2.45592600	0.67500000	0.00400500
C	-5.15286000	1.74444200	0.22336700
H	-5.83803200	1.99519700	-0.59536400
H	-5.74887500	1.69237200	1.14364600
N	-4.44568900	0.48992300	-0.02842400
C	-4.17204900	2.91840600	0.37823400
O	-2.88907400	2.61579400	0.29909800
O	-4.58657800	4.04602300	0.56437900
C	-5.07510000	-0.64208700	-0.28669200
O	-4.45326300	-1.73420400	-0.51526600
C	-6.58867400	-0.68720600	-0.32411400
H	-6.97380600	-0.03880300	-1.11787200
H	-6.90806100	-1.71186000	-0.50898700
H	-7.01380700	-0.33622400	0.62131600
H	-1.94437100	-1.95738000	1.83042200
Cl	1.10059000	-2.19754000	-2.88993000
int3 ^p			
C	1.12817400	-1.74136400	-0.98960400

C	-0.05982100	-2.46855700	-0.98100200
C	-0.86014000	-2.57044800	0.17323200
C	-0.28721500	-2.09220700	1.36758100
C	0.90870300	-1.38422700	1.38191100
C	1.57503400	-1.10106200	0.17760900
H	1.25290200	-0.96293800	2.32065200
H	3.37871400	-1.72233800	0.43723000
Cl	-0.58353500	-3.21393900	-2.48597800
C	-2.29880200	-2.96281500	0.11003200
H	-2.51560800	-3.72165400	-0.64505700
H	-2.70808600	-3.26428700	1.07280900
S	-3.38427800	-1.56282200	-0.42984200
O	-4.72687100	-1.78425500	0.10530400
O	-3.19513200	-1.23645700	-1.83745000
O	-2.63849100	-0.32782700	0.47604600
C	-3.00001600	0.98327700	0.22070000
C	-1.97468400	1.93155500	0.01665400
C	-4.33746500	1.37083200	0.23686200
C	-2.33337000	3.28715500	-0.16653800
C	-4.66915900	2.71684900	0.02845500
H	-5.09271100	0.61831300	0.41559800
C	-3.65678800	3.67657900	-0.16729500
H	-1.54745000	4.02001500	-0.31399400
H	-3.94052700	4.71211500	-0.31467300
C	-0.59779900	1.57939000	0.00021600
N	0.54086100	1.35925800	-0.01590800
O	-5.93217900	3.18662900	0.01409000
C	-7.01352900	2.26993500	0.18630900
H	-7.92114600	2.86887000	0.11340000
H	-7.01408300	1.50511800	-0.59809000
H	-6.97234700	1.78770000	1.16955200
Pd	2.49039100	0.73033500	0.00630900
C	5.31264900	1.47154500	-0.25312600
H	6.07814600	1.59469200	0.52012100
H	5.82768400	1.36658600	-1.21574300
N	4.48247000	0.28292900	0.01170500
C	4.48937600	2.77642500	-0.30825400
O	3.19460200	2.64238200	-0.20287000
O	5.08903800	3.82804800	-0.45264400
C	5.04747900	-0.85901000	0.23656300
O	4.34306700	-1.95222500	0.48269900

C	6.53382900	-1.08219900	0.25001000
H	6.99775400	-0.51128500	1.06073100
H	6.74271900	-2.14176900	0.39274000
H	6.98389400	-0.74336100	-0.68756700
H	1.64848200	-1.60932300	-1.93263700
Cl	-1.13894900	-2.28854900	2.89882000

int28

C	0.64257700	-1.66953300	-0.99407400
C	-0.51122800	-2.44729700	-0.92644800
C	-1.27544500	-2.54713900	0.25234500
C	-0.68855500	-2.01794100	1.41816800
C	0.47168300	-1.25400300	1.38307000
C	1.06593800	-0.98213600	0.14675800
H	0.82744700	-0.78791900	2.29477800
Cl	-1.05065600	-3.24828800	-2.39588400
C	-2.71411300	-2.93467500	0.22867000
H	-2.95652900	-3.70086700	-0.51089500
H	-3.10751700	-3.21301700	1.20475700
S	-3.80504300	-1.52957300	-0.31289800
O	-5.10539300	-1.66942000	0.34178100
O	-3.72399800	-1.29825100	-1.74970400
O	-2.95471000	-0.24981300	0.44348300
C	-3.32973900	1.05088700	0.17048300
C	-2.31147700	2.00481200	-0.06238900
C	-4.66846800	1.43688100	0.19204700
C	-2.68253100	3.35422700	-0.27235700
C	-5.01028000	2.77557500	-0.04322100
H	-5.42053400	0.68876300	0.39893900
C	-4.00665100	3.73766000	-0.27104400
H	-1.90293800	4.08897200	-0.44238500
H	-4.29777400	4.76788400	-0.43924900
C	-0.93016700	1.67362900	-0.08026100
N	0.21490300	1.47665200	-0.09869700
O	-6.27550100	3.23668400	-0.05444600
C	-7.35060100	2.31875300	0.15285600
H	-8.26165000	2.91194000	0.07687500
H	-7.35659800	1.53585200	-0.61329700
H	-7.29452700	1.86051900	1.14660100
Pd	2.09564600	0.69675300	-0.05846600
C	6.01538600	1.48843500	-0.26263300

H	6.30524000	2.20959000	0.51060500
H	6.23584500	1.97515200	-1.22237100
N	6.74411500	0.24893300	-0.10631800
C	4.52332500	1.26459700	-0.18752100
O	3.71811300	2.22998900	-0.27628500
O	4.07046000	0.06544800	-0.03993600
C	8.09274600	0.25123900	0.10195600
O	8.74490400	1.28910800	0.12119900
C	8.72833900	-1.11538000	0.30682800
H	9.52203400	-1.24767800	-0.43319400
H	9.19704900	-1.14043100	1.29461600
H	8.02275300	-1.94678500	0.22627900
H	1.13616300	-1.53671600	-1.95017200
Cl	-1.49266700	-2.20359800	2.97527900
H	6.20042800	-0.60124200	-0.06883600

int29

C	-0.55814700	-2.06888300	-1.29611900
C	-1.90521000	-2.38441900	-1.45977400
C	-2.77915200	-2.52109100	-0.36447700
C	-2.17694800	-2.53453000	0.90926300
C	-0.82884900	-2.25216700	1.09804100
C	-0.04641800	-1.90063000	-0.00697100
H	-0.43358700	-2.19463100	2.10664500
Cl	-2.51496500	-2.55036100	-3.10110600
C	-4.26049000	-2.43730700	-0.51741900
H	-4.63478900	-2.89528000	-1.43567200
H	-4.80671300	-2.82043600	0.34284300
S	-4.85688200	-0.69018700	-0.69160300
O	-6.21887200	-0.60891500	-0.16533300
O	-4.53784300	-0.13255700	-1.99990900
O	-3.80035300	0.03565800	0.43324300
C	-3.73386200	1.41665500	0.47296700
C	-2.45979500	2.02490200	0.48032800
C	-4.89086000	2.18586500	0.57339700
C	-2.38354900	3.43242500	0.59403300
C	-4.78933000	3.58107000	0.65897500
H	-5.84781100	1.68313800	0.58767600
C	-3.52524900	4.20214500	0.67516600
H	-1.40637500	3.90283200	0.60932100
H	-3.47431200	5.28185800	0.75362900

C	-1.25004000	1.28231300	0.39397400
N	-0.22507000	0.74067600	0.33759700
O	-5.84941700	4.40869200	0.74422800
C	-7.16499200	3.85391700	0.71462000
H	-7.84402900	4.70482300	0.76651300
H	-7.34100600	3.29933400	-0.21367100
H	-7.33780700	3.19614300	1.57393500
Pd	1.43708900	-0.56163600	0.30528100
C	3.86694800	3.01951300	0.08284000
H	4.73459500	2.72978600	0.68851200
H	3.25258400	3.66406800	0.72279400
N	4.26871700	3.70520700	-1.12412900
C	3.07305400	1.76105900	-0.28485400
O	2.88557900	1.46480300	-1.47179300
O	2.66130700	1.09591400	0.74568400
C	4.94564600	4.88267700	-1.10030000
O	5.27400000	5.43586300	-0.05376300
C	5.27605700	5.47608200	-2.46399000
H	6.36077100	5.58950100	-2.54540700
H	4.91625900	4.87612300	-3.30445500
H	4.84003300	6.47699900	-2.52746700
H	0.04543900	-1.86784800	-2.17425400
Cl	-3.15603600	-2.81965300	2.34624600
H	3.97993300	3.25178100	-1.98212500
C	3.38155900	-1.64981600	0.47824300
C	4.28656400	-1.56155900	-0.75036700
C	2.75238700	-3.17541600	-1.18046500
C	2.44801100	-2.65192700	0.20945200
C	3.30043900	-1.91350300	-1.88287100
H	3.80795400	-2.14304000	-2.82491700
H	2.56091100	-1.12691000	-2.05129700
C	5.13768700	-2.87539300	-0.69629500
H	5.90345500	-2.84599000	-1.47702200
H	5.65083200	-2.99963700	0.26071800
C	4.08110900	-3.98978600	-0.97931900
H	4.31102800	-4.54060600	-1.89629900
H	4.00227800	-4.72194500	-0.17014700
H	4.85641500	-0.64131600	-0.85294700
H	1.95042000	-3.73076200	-1.66764500
H	1.97174100	-3.24501200	0.98076600
O	4.99759800	-0.70608500	1.89430600

C	3.80081000	-1.31504100	1.87694900
O	3.15729900	-1.58718200	2.87221000
C	5.46452700	-0.30232600	3.19547600
H	6.43979200	0.15267500	3.02663100
H	4.77216200	0.42020100	3.63262200
H	5.54951000	-1.16705200	3.85776000

TS20

C	-0.40568800	-2.42665000	-0.95183200
C	-1.76170500	-2.73605000	-0.88035100
C	-2.50829100	-2.56434500	0.30134300
C	-1.77219700	-2.23407000	1.45841100
C	-0.41175400	-1.95771300	1.42150500
C	0.25073700	-1.94751700	0.18596900
H	0.10294500	-1.66506600	2.33047000
Cl	-2.53972900	-3.32718500	-2.34056100
C	-4.00112100	-2.59065600	0.31106400
H	-4.42656200	-3.30890900	-0.39347900
H	-4.42035400	-2.75029200	1.30326200
S	-4.75779000	-1.00235700	-0.25356100
O	-6.09394800	-0.89387700	0.32923800
O	-4.55214500	-0.77450700	-1.67803400
O	-3.71840900	0.05234600	0.58095500
C	-3.75210800	1.39311300	0.23489100
C	-2.54065700	2.02386200	-0.11220400
C	-4.94423100	2.10987700	0.29336800
C	-2.55869400	3.40771100	-0.39870500
C	-4.94107200	3.47681600	-0.01727100
H	-5.84803500	1.59031900	0.58028900
C	-3.73749500	4.12416500	-0.35881900
H	-1.62850400	3.90073100	-0.65954200
H	-3.76167400	5.18381500	-0.58513800
C	-1.30632100	1.31856000	-0.16633300
N	-0.26878800	0.80064900	-0.21490100
O	-6.04120400	4.25547800	-0.00267700
C	-7.30210500	3.66483500	0.31367300
H	-8.03193400	4.47064800	0.23731000
H	-7.55725600	2.86982300	-0.39572300
H	-7.30756900	3.26300600	1.33331500
Pd	1.53620600	-0.34254800	-0.04614000
C	3.83340800	3.01206500	-1.51687700

H	3.37571200	3.57909200	-2.33535500
H	4.86018500	2.79650400	-1.83729200
N	3.82229900	3.77855700	-0.28646000
C	3.08804800	1.68029700	-1.37730500
O	2.63709100	1.43091300	-0.18140800
O	2.96974100	0.95038100	-2.36235300
C	4.39433700	5.00805200	-0.19568200
O	4.95812000	5.54806900	-1.14334500
C	4.29247300	5.67983300	1.16879900
H	3.74281200	5.09325300	1.91069800
H	5.30181200	5.87218800	1.54373800
H	3.80260700	6.64991000	1.04744700
H	0.09978200	-2.49223700	-1.90772600
Cl	-2.58252400	-2.10478900	3.01595300
H	3.36038600	3.33798900	0.49656900
C	3.28663100	-1.48341100	0.28613300
C	4.14791300	-1.76458600	-0.95211900
C	2.62984500	-3.44932200	-0.83271000
C	2.34026100	-2.55699400	0.36054600
C	3.12110300	-2.43359000	-1.88855600
H	3.59210200	-2.91956700	-2.74841300
H	2.36296600	-1.73230500	-2.24414700
C	5.02870500	-2.99372800	-0.56711000
H	5.74998300	-3.19493800	-1.36511300
H	5.59682800	-2.83028700	0.35213000
C	3.98266200	-4.14616100	-0.44737400
H	4.18347800	-4.95247300	-1.15903700
H	3.94963200	-4.59571800	0.54996200
H	4.68282700	-0.90624800	-1.35025400
H	1.83538000	-4.14311100	-1.10919300
H	2.05816100	-2.96777600	1.32253200
O	5.01184500	-0.29844700	1.36242200
C	3.82917900	-0.90831500	1.55710200
O	3.27769300	-0.98686900	2.64121100
C	5.58435700	0.32856500	2.52390900
H	6.53226100	0.74933400	2.19050200
H	4.92318900	1.11578500	2.89308900
H	5.74409800	-0.40522300	3.31754100

int30

C	1.26207800	-2.78451100	-0.91113500
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C	-0.05811600	-3.16565100	-0.76964000
C	-0.82124800	-2.88845600	0.39910800
C	-0.14618600	-2.23099800	1.42869000
C	1.20523500	-1.83300600	1.32397400
C	1.93174700	-2.11917300	0.14172500
H	1.73059700	-1.48246400	2.20753700
Cl	-0.77911100	-4.07858600	-2.08114700
C	-2.24409200	-3.34353400	0.53149400
H	-2.41102800	-4.30760600	0.04612900
H	-2.56598000	-3.40677500	1.57101300
S	-3.51067900	-2.28603600	-0.27020600
O	-4.80111800	-2.95080800	-0.11190800
O	-3.08310000	-1.77622600	-1.56530300
O	-3.43690600	-1.01376600	0.83704300
C	-3.94703200	0.21146300	0.41888700
C	-3.04232300	1.22378400	0.05958900
C	-5.31895700	0.42828400	0.42195800
C	-3.53729800	2.49949900	-0.28323000
C	-5.80036000	1.69650400	0.06110600
H	-5.97327100	-0.38550500	0.70406000
C	-4.90222400	2.72603200	-0.28007200
H	-2.83420800	3.28691700	-0.54325900
H	-5.30758400	3.69634900	-0.54406900
C	-1.65307500	0.92758500	0.04216200
N	-0.53108700	0.63872900	0.04322200
O	-7.11117000	2.02306000	0.02296700
C	-8.07788700	1.02041900	0.32637300
H	-9.04961000	1.49957700	0.20570000
H	-8.00081300	0.17135000	-0.36243600
H	-7.97369000	0.66478400	1.35833200
Pd	1.56095600	0.20869800	0.12147500
C	1.50597200	3.87160500	-2.05198900
H	0.67448000	3.94210600	-2.75346900
H	2.41500000	4.19367000	-2.57004900
N	1.24799600	4.76777900	-0.93874900
C	1.65515300	2.38263200	-1.67258000
O	1.90618900	2.17707100	-0.41186700
O	1.54442700	1.53065200	-2.55140300
C	-0.00037300	4.84058600	-0.39044000
O	-0.99254400	4.36474900	-0.94143600
C	-0.09119500	5.56211100	0.94390900

H	0.77667300	6.19360400	1.15256300
H	-0.99536600	6.17406000	0.95493800
H	-0.17999600	4.81765400	1.74240700
H	1.78639600	-3.02730000	-1.82593100
Cl	-0.93807100	-1.90453000	2.95735600
H	2.02487700	4.94839600	-0.31911400
C	3.56626200	-0.27143300	0.25700200
C	4.41972300	0.13785400	-0.95401400
C	4.21114200	-2.11138700	-1.17198000
C	3.43738600	-1.81964700	0.13513400
C	3.92926000	-0.85573300	-2.03018300
H	4.54092200	-0.82529400	-2.93830900
H	2.88507800	-0.69455400	-2.30603400
C	5.86763300	-0.37941100	-0.71375800
H	6.53612500	0.02485800	-1.48123600
H	6.26956800	-0.07237300	0.25511100
C	5.71760300	-1.92890100	-0.85391300
H	6.32657400	-2.31445700	-1.67752800
H	6.01709400	-2.46864000	0.05073800
H	4.35540800	1.19629000	-1.19955800
H	3.98270100	-3.08293800	-1.61934300
H	3.88404700	-2.33927600	0.99073400
O	4.53555600	1.44056700	1.58011400
C	3.92341400	0.23601900	1.61526400
O	3.68682400	-0.34660100	2.66650000
C	4.82863400	2.02142300	2.86001300
H	5.34213900	2.95866600	2.64536800
H	3.90640000	2.20974600	3.41592300
H	5.46755500	1.35970400	3.45000800

int31

C	-0.35748600	3.56195700	-0.72833300
C	1.01249700	3.42421800	-0.61498600
C	1.61769100	2.54075600	0.31860200
C	0.75321100	1.86149500	1.18357600
C	-0.65904500	1.96925700	1.09507200
C	-1.22395600	2.81982900	0.10665200
H	-1.26139100	1.52268400	1.88869500
Cl	2.00953500	4.41110000	-1.66454900
C	3.10353000	2.33421100	0.36317100
H	3.65927200	3.19868900	-0.00022200

H	3.46322200	2.04929600	1.35235900
S	3.58519600	0.95553700	-0.74633900
O	3.35366200	1.32474400	-2.13720100
O	3.11338100	-0.32244100	-0.22603400
O	5.25050800	1.06689200	-0.47715300
C	5.95169200	-0.09672900	-0.18661000
C	6.28092400	-0.37326500	1.14921100
C	6.36670400	-0.91744700	-1.22972700
C	7.05827900	-1.51624700	1.42136500
C	7.13146500	-2.05472300	-0.93697400
H	6.08840500	-0.64856900	-2.24019800
C	7.47715800	-2.34532200	0.39623000
H	7.32186800	-1.74252200	2.44866100
H	8.07269000	-3.22908600	0.59519600
C	5.82023000	0.48790600	2.19045700
N	5.42764700	1.20044000	3.02333900
O	7.58661100	-2.92556800	-1.86603600
C	7.25000500	-2.70594700	-3.23322000
H	7.70205700	-3.52970800	-3.78595900
H	6.16415500	-2.71806300	-3.38328900
H	7.65908300	-1.75619900	-3.59786500
Pd	-1.47768500	0.58603700	-0.56815500
H	-0.75660100	4.24975800	-1.46130000
Cl	1.39346200	0.87143600	2.46527300
C	-3.27752500	1.55029700	-0.31926200
C	-4.01418600	1.74030300	-1.65696800
C	-3.31941800	3.82945400	-1.10142500
C	-2.75379000	2.96158300	0.04973400
C	-3.21283700	2.88163700	-2.31985300
H	-3.71388300	3.27751500	-3.20903800
H	-2.19329900	2.59542500	-2.59020400
C	-5.34511800	2.48870600	-1.32945000
H	-5.95573300	2.52542700	-2.23714500
H	-5.93844200	1.99919400	-0.55480800
C	-4.85579900	3.90989600	-0.90825600
H	-5.27957900	4.68515400	-1.55354000
H	-5.12695900	4.15277100	0.12294100
H	-4.14055600	0.81741900	-2.22096600
H	-2.84417200	4.80975200	-1.19172900
H	-3.12513800	3.27684200	1.02980600
O	-4.24164200	-0.46683200	0.46285400

C	-4.07387500	0.82621300	0.75194800
O	-4.57820200	1.40769700	1.69064100
C	-5.00953400	-1.24467900	1.40963000
H	-5.12613400	-2.21979400	0.93908800
H	-4.45468500	-1.30472400	2.34829900
H	-5.97917400	-0.77305100	1.58361600
C	-1.41881300	-0.85666000	3.67183600
O	-2.06884200	-0.03373400	2.99515700
O	-0.85037600	-1.91192600	3.19595600
O	-1.67110100	-2.68418900	-0.86728900
C	-2.19294200	-2.03627600	-1.80701500
O	-2.19374100	-0.77509100	-1.97862200
C	-2.89936100	-2.82866700	-2.92010900
H	-2.28038400	-2.79264300	-3.82178600
H	-3.83813700	-2.31739200	-3.13897100
Ag	-1.22224900	-2.06962300	1.12705000
N	-3.17593400	-4.20506200	-2.57707000
C	-4.12447400	-4.48175400	-1.62142200
O	-4.89717900	-3.62505400	-1.20740500
C	-4.15175300	-5.91641800	-1.12496700
H	-3.69551800	-6.62129800	-1.82567200
H	-3.61148400	-5.97231700	-0.17361100
H	-5.18756400	-6.20536400	-0.93907300
H	-2.42198900	-4.86809700	-2.68475100
C	-1.22071100	-0.63387000	5.16536200
H	-1.23460200	-1.58367900	5.70458000
H	-0.23809100	-0.17605600	5.32574300
H	-1.98529300	0.03960100	5.55560700

TS21

C	-0.76854300	-3.46596100	0.39267400
C	-2.02007800	-2.94074200	0.70816500
C	-2.24368000	-1.55952000	0.90861700
C	-1.10332600	-0.74803900	0.83673300
C	0.19136000	-1.24161300	0.58029900
C	0.33767100	-2.62284300	0.29956400
H	1.01386300	-0.78716700	1.47371400
Cl	-3.34417700	-4.07677500	0.86248900
C	-3.60955800	-1.00419500	1.18759700
H	-4.26469100	-1.74080600	1.65316900
H	-3.58727300	-0.09790000	1.79478100

S	-4.47824300	-0.52535200	-0.35343100
O	-4.61395300	-1.67565200	-1.23817800
O	-4.00294000	0.75597600	-0.86148000
O	-5.98876000	-0.27883900	0.37893900
C	-6.71829100	0.84222800	0.01257900
C	-6.64969400	1.99171300	0.81528100
C	-7.54988600	0.77450900	-1.10041500
C	-7.45774300	3.09358300	0.47336500
C	-8.34040500	1.88423300	-1.42806600
H	-7.56283900	-0.14060200	-1.67768500
C	-8.29090900	3.04271400	-0.63017700
H	-7.41706700	3.98790000	1.08549400
H	-8.91563600	3.88573700	-0.90288800
C	-5.76793500	2.02367900	1.93778500
N	-5.03864900	2.02887800	2.84525200
O	-9.18234700	1.93310600	-2.48584000
C	-9.26338100	0.80110700	-3.34757100
H	-9.97865300	1.07051600	-4.12494500
H	-8.29284300	0.57841200	-3.80598200
H	-9.62579200	-0.08405300	-2.81143600
Pd	1.57158600	-0.11625900	-0.48695000
H	-0.67953400	-4.53165300	0.21835100
Cl	-1.23233100	0.98055500	1.10791800
C	2.59996500	-1.91362700	-0.62735100
C	2.86961900	-2.22196200	-2.11569100
C	1.64609200	-3.99720300	-1.41826900
C	1.70194300	-3.10211500	-0.13790500
C	1.57207500	-2.94161800	-2.54086700
H	1.64246500	-3.37748400	-3.54284000
H	0.68220300	-2.30706300	-2.49329400
C	3.88241500	-3.40694400	-2.17107900
H	4.19467200	-3.55627400	-3.20990500
H	4.78808400	-3.22164900	-1.58950300
C	3.04590200	-4.61491300	-1.64869400
H	2.99205200	-5.41413500	-2.39452700
H	3.45895000	-5.04961400	-0.73304800
H	3.17896600	-1.35254600	-2.69374000
H	0.84128500	-4.73505400	-1.39453100
H	2.18935700	-3.62388400	0.69418800
O	4.71040400	-0.85822500	-0.37743400
C	3.82297800	-1.67095600	0.23182800

O	4.00808500	-2.16949600	1.32591600
C	5.92403200	-0.57130100	0.34793700
H	6.47725200	0.12180200	-0.28447500
H	5.68765300	-0.11698000	1.31395100
H	6.48738900	-1.49229700	0.51922000
C	1.77439800	0.12634900	3.63107100
O	1.34283600	-0.77337000	2.85593800
O	2.31533500	1.23134500	3.30326400
O	3.71631800	2.45598300	-0.46732200
C	3.54102100	1.90189200	-1.58779800
O	2.72335800	0.97667000	-1.87587700
C	4.39824600	2.38843000	-2.76489300
H	3.72999500	2.74787400	-3.55326500
H	4.93282200	1.51838300	-3.15204100
Ag	2.88821400	1.77256000	1.36240700
N	5.36981400	3.40237600	-2.42942300
C	6.57181500	3.04945500	-1.86803100
O	6.95700900	1.88627300	-1.81892300
C	7.39919200	4.20134600	-1.32455600
H	7.11545900	5.17095800	-1.74311000
H	7.27767200	4.24269200	-0.23677500
H	8.45237700	4.00755600	-1.53525200
H	5.02417900	4.33216600	-2.24150800
C	1.61805000	-0.13389200	5.12002500
H	2.15918200	0.60829300	5.70704800
H	0.55447500	-0.09636200	5.37654600
H	1.97651300	-1.13955200	5.35309100

int32

C	0.50737300	3.14508200	1.24181200
C	1.74065500	2.52959300	1.44861100
C	2.03401500	1.24453800	0.94926000
C	0.99413000	0.62784100	0.22700100
C	-0.24821900	1.20297300	-0.01481700
C	-0.48461800	2.48787300	0.51136200
H	0.54188500	-1.75528800	1.83882300
Cl	2.93005700	3.40022400	2.41183000
C	3.34210800	0.56068800	1.21549800
H	3.82282300	0.93259000	2.12097200
H	3.24645500	-0.52441900	1.27042400
S	4.58062000	0.84324800	-0.10448700

O	5.03363500	2.22789500	-0.10868700
O	4.20609000	0.17365200	-1.34440900
O	5.80753000	-0.07629000	0.63969000
C	6.54268700	-0.94284000	-0.15061900
C	6.19978800	-2.30478000	-0.17312400
C	7.64360100	-0.45658400	-0.84926900
C	7.00684700	-3.18587800	-0.91964700
C	8.42806300	-1.34756900	-1.59342900
H	7.86227600	0.60155900	-0.79122200
C	8.10420000	-2.71720700	-1.61947200
H	6.75478100	-4.24046500	-0.94337500
H	8.73016800	-3.38619800	-2.19907200
C	5.05139900	-2.76637100	0.53881300
N	4.10925400	-3.13043900	1.11834900
O	9.51598400	-0.98694900	-2.31194700
C	9.88444700	0.38921000	-2.35060600
H	10.76437400	0.44277100	-2.99201500
H	9.08385900	1.00469300	-2.77701100
H	10.13954900	0.76271100	-1.35175900
Pd	-1.69221800	0.30839300	-1.02110700
H	0.33153700	4.12991400	1.66238600
Cl	1.20946200	-1.03574600	-0.39135100
C	-2.76860300	2.01181500	-0.47496600
C	-3.22091500	2.73271900	-1.76156700
C	-1.84548500	4.24776100	-0.78152800
C	-1.84452200	3.06474900	0.24063300
C	-1.94424500	3.51791900	-2.13791400
H	-2.10066600	4.20426700	-2.97703300
H	-1.08702800	2.87592700	-2.35832700
C	-4.17609400	3.90482300	-1.37431000
H	-4.63359900	4.30962200	-2.28314600
H	-4.99075300	3.58395400	-0.72298800
C	-3.22211500	4.94538700	-0.70732100
H	-3.20645500	5.88631600	-1.26705100
H	-3.50904500	5.18461200	0.32226800
H	-3.63722200	2.06552000	-2.51678100
H	-0.99351500	4.92045300	-0.65171900
H	-2.29629200	3.38464000	1.18802900
O	-4.96679600	1.14066100	-0.23728000
C	-3.82031200	1.40239100	0.41366500
O	-3.66229400	1.14631700	1.60555600

C	-6.02836200	0.52471900	0.52380900
H	-6.75033800	0.16914000	-0.20930000
H	-5.64295700	-0.31226400	1.10746100
H	-6.47333400	1.26186400	1.19804300
C	-0.32466900	-1.69735400	3.54958200
O	0.76080700	-1.76564900	2.79236800
O	-1.47344400	-1.63859900	3.11334500
O	-3.88894300	-2.09388400	-0.39581500
C	-3.91696100	-1.66579000	-1.58415300
O	-3.13701900	-0.82203500	-2.11908100
C	-5.00861300	-2.20763000	-2.51789500
H	-4.52378900	-2.58859800	-3.42252900
H	-5.63997000	-1.36554500	-2.81072600
Ag	-2.52345400	-1.31350900	1.16206300
N	-5.86652600	-3.21312800	-1.93437300
C	-7.05133900	-2.87240500	-1.33570300
O	-7.54386200	-1.75206800	-1.42548200
C	-7.72819000	-3.98863900	-0.55713100
H	-7.37512400	-4.98540500	-0.83596600
H	-7.54205100	-3.83983100	0.51192100
H	-8.80580100	-3.92576900	-0.71882400
H	-5.43312600	-4.07837400	-1.64709500
C	-0.01244200	-1.69250900	5.01917000
H	-0.93408600	-1.77397600	5.59309500
H	0.66824000	-2.51295500	5.25984600
H	0.49757300	-0.75735900	5.27192200

int33

C	1.83231400	-3.74266100	-0.19434900
C	2.63478700	-2.99664500	-1.05490200
C	2.17610100	-1.80530600	-1.65076100
C	0.86108800	-1.43252400	-1.30785700
C	0.04057000	-2.08976800	-0.40048000
C	0.55424900	-3.29470300	0.13749100
Cl	4.23756600	-3.61797300	-1.41704700
C	3.03022200	-1.01591300	-2.59597400
H	3.85443600	-1.60328100	-3.00139600
H	2.46114800	-0.58454800	-3.42308000
S	3.84855200	0.46148100	-1.88114800
O	2.92230600	1.26338300	-1.07858600
O	4.65407600	1.10202300	-2.91476100

O	4.85660100	-0.36990600	-0.83014800
C	5.87338000	0.33791400	-0.19743400
C	7.19020200	-0.10236200	-0.39996800
C	5.57452800	1.39556200	0.65790200
C	8.22236900	0.55328900	0.30137300
C	6.62033900	2.04547800	1.32510900
C	7.94699700	1.61245300	1.14785100
H	9.24454200	0.21918900	0.16100800
H	8.73754400	2.12604500	1.68318200
C	7.47557800	-1.18597000	-1.28625100
N	7.72929900	-2.06808700	-2.00143900
O	6.44560100	3.08972100	2.16873400
C	5.13611000	3.63024900	2.32554600
H	5.24326000	4.47311500	3.00888400
H	4.73602200	3.98604300	1.36879500
H	4.44289500	2.89887200	2.75760300
Pd	-1.70843500	-1.47252800	0.31249900
H	2.21717100	-4.67334900	0.20979200
Cl	0.18269400	0.01459900	-2.16297200
C	-1.78228300	-3.39525500	1.09289800
C	-2.05847400	-3.23746800	2.59708900
C	0.02015100	-4.14744900	2.53981600
C	-0.37359400	-4.07380000	1.02858300
C	-0.65055200	-2.88958700	3.13086700
H	-0.60672000	-2.86216100	4.22495000
H	-0.25720600	-1.94889100	2.73432500
C	-2.26295500	-4.66108700	3.20255100
H	-2.64589100	-4.56821500	4.22411800
H	-2.99219900	-5.24790200	2.63945200
C	-0.82435600	-5.27089900	3.18650100
H	-0.47102000	-5.47915200	4.20166500
H	-0.76644000	-6.20848000	2.62340000
H	-2.86891500	-2.54532700	2.82421300
H	1.09746600	-4.24754200	2.69770100
H	-0.46063900	-5.09145800	0.62730100
O	-2.43647500	-4.61757800	-0.84085800
C	-2.89210900	-3.98393200	0.27214100
O	-4.07711600	-3.92262400	0.55010900
C	-3.45303300	-5.14717700	-1.70308200
H	-4.08949300	-5.85444800	-1.16531700
H	-4.07880700	-4.34227700	-2.09898200

H	-2.92142500	-5.64810200	-2.51230200
H	4.54109200	1.68429100	0.78559600
C	-4.40929800	-0.07840800	0.42609800
O	-3.52522700	-0.65003100	1.11917600
O	-4.33386400	0.25344400	-0.79807100
Ag	-2.38894300	0.31911400	-1.75361400
C	-5.71870000	0.23642600	1.16416100
H	-6.24727700	-0.70619900	1.33384500
H	-5.44905300	0.64569500	2.13947900
N	-6.59294000	1.16307600	0.47857000
C	-6.23616700	2.47796900	0.35503900
O	-5.28399500	2.95531600	0.96679000
C	-7.09867900	3.30885900	-0.57864400
H	-8.07765700	2.86202100	-0.77299700
H	-7.23189100	4.30138600	-0.14450000
H	-6.57404500	3.42847200	-1.53260700
H	-7.23561000	0.78488000	-0.20136900
C	0.73286000	2.89172100	1.33053800
C	-0.10813500	2.97909000	2.44711200
C	-1.48220100	3.18532800	2.26877900
C	-2.02785100	3.31075800	0.99013700
C	-1.15855300	3.22866400	-0.09617300
C	0.21238800	3.01891200	0.04224100
H	1.79325600	2.71226600	1.45838200
H	-2.12356700	3.23849600	3.14177200
H	-3.09805600	3.43865600	0.86569300
H	0.86961800	2.92739100	-0.81384500
I	-1.97757200	3.40116100	-2.09758500
C	0.39624000	2.84607500	3.84438200
O	-0.30438300	2.90895400	4.83438700
O	1.73580700	2.64415700	3.90316900
C	2.26145300	2.48770700	5.23229200
H	1.79692300	1.63350500	5.73042200
H	3.33191800	2.32271400	5.11005300
H	2.07592200	3.38531400	5.82722100

TS22

C	1.38495800	-1.10099200	3.03428800
C	2.36225400	-1.73207300	2.27581100
C	2.14915100	-2.03613300	0.92064800
C	0.90749600	-1.63704900	0.37409500

C	-0.05435100	-0.88878100	1.05967400
C	0.19185800	-0.68748600	2.43957300
Cl	3.84774200	-2.20572800	3.08426100
C	3.18051200	-2.74305500	0.09817900
H	3.91792400	-3.27738800	0.69743700
H	2.74063900	-3.42438100	-0.63151500
S	4.17949000	-1.62603000	-0.97052300
O	3.43996400	-0.42323700	-1.35143500
O	4.87087800	-2.42105400	-1.97960100
O	5.29922300	-1.16741900	0.20701600
C	6.57291900	-0.81555500	-0.21527900
C	7.64105400	-1.63755100	0.17498200
C	6.77276200	0.35092400	-0.94842200
C	8.94647100	-1.24626600	-0.18323100
C	8.07763400	0.70913500	-1.31086500
C	9.16422700	-0.09347300	-0.91640300
H	9.78288100	-1.86770600	0.11749400
H	10.16445200	0.21176100	-1.20222900
C	7.39838400	-2.83858900	0.90931100
N	7.20616200	-3.81997400	1.50476700
O	8.39111800	1.81290400	-2.02906000
C	7.33470400	2.65088600	-2.48832100
H	7.81410500	3.44937600	-3.05518500
H	6.64503600	2.10310300	-3.14099100
H	6.77601500	3.08524000	-1.65053900
Pd	-1.77358300	-0.05354200	0.33359600
H	1.55267800	-0.94577900	4.09490700
Cl	0.54526200	-2.20265600	-1.26899500
C	-2.19326300	0.14395800	2.41313100
C	-2.53508800	1.61573500	2.70630900
C	-0.66045200	1.26849000	3.93596100
C	-0.91841600	-0.12082900	3.27443700
C	-1.12641400	2.24120400	2.83748400
H	-1.16007000	3.28231500	3.17475500
H	-0.52590300	2.18416100	1.92961800
C	-3.03238300	1.73125400	4.18208600
H	-3.42285300	2.74159700	4.34310700
H	-3.83937900	1.03284000	4.40562500
C	-1.73892700	1.48554400	5.02215100
H	-1.49338300	2.35565100	5.63949600
H	-1.82790900	0.62590100	5.69515600

H	-3.22050000	2.05768300	1.98383000
H	0.36704300	1.38788000	4.29002300
H	-1.14420300	-0.85612200	4.05773700
O	-2.87822100	-2.11986900	2.67376900
C	-3.31937100	-0.84044000	2.58389300
O	-4.50295300	-0.55605700	2.65126900
C	-3.90693800	-3.11810100	2.78484300
H	-4.50211500	-2.95998200	3.68785600
H	-4.56276500	-3.08048500	1.91157800
H	-3.38290900	-4.07241000	2.83606100
H	5.91132900	0.94751900	-1.21732200
C	-4.80302100	-0.15319900	-0.22051700
O	-3.81994400	0.63995800	-0.08940300
O	-4.74515600	-1.39444100	-0.47057400
Ag	-2.92560600	-1.90046200	-1.60409900
C	-6.18272900	0.48441100	-0.02319700
H	-6.30024300	0.66077000	1.04931800
H	-6.17342000	1.45098700	-0.53134600
N	-7.28917400	-0.30883200	-0.50723500
C	-7.41956400	-0.53913600	-1.85278600
O	-6.73029700	0.04506100	-2.68092600
C	-8.47766100	-1.55733700	-2.24534900
H	-9.21398900	-1.74131400	-1.45784000
H	-8.98764100	-1.20448100	-3.14366400
H	-7.98614000	-2.50455500	-2.49196200
H	-7.70707100	-0.96921200	0.13097700
C	1.03746500	3.13899000	-0.38587000
C	0.19375700	4.24287000	-0.18521300
C	-1.19413300	4.08515200	-0.30205000
C	-1.74902100	2.84488300	-0.61271700
C	-0.87995300	1.75976100	-0.75444400
C	0.51161400	1.88670600	-0.70007900
H	2.11209900	3.25853100	-0.30939300
H	-1.83356600	4.95027300	-0.15994100
H	-2.81896800	2.71345300	-0.71541500
H	1.17106300	1.04627100	-0.87935100
I	-1.55015600	0.33943400	-2.69529800
C	0.71376600	5.60145400	0.13148900
O	0.01402500	6.57882400	0.31491200
O	2.06474300	5.63607400	0.19546300
C	2.62780900	6.92194100	0.49883000

H	2.27213400	7.27890700	1.46853400
H	3.70737800	6.77328400	0.51784300
H	2.35333900	7.65213700	-0.26656000

int34

C	1.30019700	-3.12178300	-1.69655200
C	2.19732900	-2.18060500	-2.19505500
C	1.97487300	-0.79540200	-2.05922000
C	0.79315200	-0.41015700	-1.39335600
C	-0.07855600	-1.33305600	-0.82131400
C	0.16376000	-2.70248400	-1.00055000
Cl	3.59595100	-2.77885100	-3.06388300
C	2.93229500	0.22920200	-2.58728800
H	3.57792300	-0.15139300	-3.37893800
H	2.42276800	1.13114600	-2.93326800
S	4.08664700	0.89074600	-1.32133900
O	3.45414200	0.96443900	-0.00521900
O	4.79655200	2.03701000	-1.87333300
O	5.13088300	-0.43168500	-1.30164300
C	6.42963400	-0.23297500	-0.85198300
C	7.47099100	-0.60109400	-1.71780100
C	6.67616300	0.25306600	0.42948800
C	8.79608000	-0.47567200	-1.25419300
C	8.00271100	0.39257700	0.85762400
C	9.06173400	0.01686000	0.01056100
H	9.61058600	-0.76270200	-1.91022100
H	10.07821400	0.12625400	0.37110500
C	7.18928200	-1.08995000	-3.03004400
N	6.97147000	-1.49224900	-4.10025400
O	8.36105400	0.86767100	2.07278500
C	7.33930600	1.31092200	2.96170400
H	7.85692200	1.67937100	3.84774300
H	6.74947600	2.12182900	2.51914300
H	6.67243200	0.48818700	3.24642200
Pd	-1.74655800	-0.79804100	0.15666900
H	1.48958800	-4.17637800	-1.86703100
Cl	0.33768700	1.28427900	-1.29468000
C	-2.14490800	-2.87903400	0.00340300
C	-2.45704500	-3.55325600	1.33628500
C	-0.60256700	-4.65511100	0.61454800
C	-0.90734000	-3.65948300	-0.54863200

C	-1.03043600	-3.85779800	1.86018200
H	-1.05152400	-4.46961200	2.76732500
H	-0.42735500	-2.97053000	2.04763800
C	-2.96563300	-5.00885900	1.05356500
H	-3.33616000	-5.41705900	1.99888400
H	-3.78453700	-5.04415500	0.33622900
C	-1.68382000	-5.75999900	0.57145300
H	-1.42485600	-6.57737800	1.25093600
H	-1.80105200	-6.19209600	-0.42751800
H	-3.12594500	-2.97560000	1.97296000
H	0.42698900	-5.02005300	0.59869700
H	-1.22771300	-4.23422400	-1.42987100
O	-3.97834400	-3.51918000	-1.44537400
C	-3.16131500	-2.56609600	-1.06626700
O	-3.11156800	-1.43939600	-1.57690700
C	-4.92693400	-3.20037600	-2.51407300
H	-5.68152400	-2.51540100	-2.12455800
H	-4.39083800	-2.76153500	-3.35661200
H	-5.36294800	-4.16035300	-2.78456700
H	5.83616800	0.51053500	1.06045200
C	-4.58356300	0.31209300	0.79067800
O	-3.63705700	-0.46673400	1.13615900
O	-4.52374500	1.31143000	0.03850400
Ag	-3.01876400	2.70546000	-0.62261500
C	-5.95094600	-0.01271900	1.42038200
H	-6.01962800	-1.08869600	1.57841100
H	-5.99800400	0.48232000	2.39614100
N	-7.07325100	0.41905700	0.61478200
C	-7.39519200	-0.28172600	-0.51444400
O	-6.89030900	-1.37646100	-0.75977000
C	-8.41318400	0.36685800	-1.43215700
H	-8.99350500	1.15367300	-0.94342100
H	-7.88884200	0.80179700	-2.28967400
H	-9.08946300	-0.40247200	-1.80973600
H	-7.32577900	1.39598700	0.65139800
C	1.19222500	0.24854800	3.16419900
C	0.44847800	0.16396000	4.34517000
C	-0.88579000	-0.25793200	4.28530100
C	-1.47003900	-0.58790900	3.06477700
C	-0.71907200	-0.49774100	1.88313600
C	0.61961800	-0.09356500	1.93548500

H	2.22400700	0.57936200	3.19260200
H	-1.45697400	-0.31699700	5.20612800
H	-2.50851900	-0.89160900	3.03660600
H	1.23824900	-0.01961400	1.05321600
I	-1.44992500	4.68096700	-1.38672000
C	1.01275600	0.50234500	5.68259100
O	0.39600500	0.42236400	6.72741800
O	2.29983500	0.91160000	5.61425900
C	2.89334500	1.26633200	6.87267500
H	2.90416700	0.40815600	7.54954600
H	3.90975800	1.58364400	6.63975700
H	2.33669300	2.07939100	7.34499500

int35

C	-0.66864400	-1.58819500	0.43521600
C	-1.72520700	-2.45870800	0.08124400
C	-1.44954500	-3.42315900	-0.90608500
C	-0.20621700	-3.50980200	-1.51949400
C	0.80014200	-2.59952900	-1.18824200
C	0.57250600	-1.61764600	-0.21043500
C	-3.08250100	-2.34259500	0.71267400
H	-3.63199400	-3.28409600	0.69940500
H	-3.04812700	-1.94768900	1.72832800
S	-4.13374000	-1.17116700	-0.22868200
O	-4.50955100	-1.74227100	-1.51525300
O	-3.61153600	0.18879800	-0.14204100
O	-5.49524200	-1.28880100	0.77169200
C	-6.10055600	-0.12063500	1.21042500
C	-5.91266500	0.27195700	2.54487900
C	-6.92922400	0.58974500	0.34786000
C	-6.59609500	1.41398600	3.00727200
C	-7.58830400	1.73102700	0.82333900
H	-7.04366500	0.23543500	-0.66807700
C	-7.42045600	2.13413900	2.16156800
H	-6.46315400	1.72700500	4.03705900
H	-7.94681100	3.01717700	2.50577500
C	-5.03711600	-0.47227400	3.39232400
N	-4.31232100	-1.08438500	4.06727000
O	-8.41033700	2.50217600	0.07554800
C	-8.59562300	2.17217700	-1.29835900
H	-9.26571900	2.93336000	-1.69847800

H	-7.64623000	2.19744400	-1.84569900
H	-9.05808300	1.18458700	-1.41325100
Pd	2.14729700	-0.45679500	0.27714600
C	2.10080800	3.21937900	-1.82672700
C	0.75807200	3.47453800	-2.13049600
C	-0.21640700	2.54319300	-1.75649200
C	0.13376500	1.36518800	-1.09344700
C	1.47755700	1.12268200	-0.79962900
C	2.46334800	2.04730100	-1.16119000
H	2.86334100	3.93865200	-2.10410700
H	-1.25654900	2.74715500	-1.98823700
H	-0.65129900	0.67622500	-0.81842500
H	3.50313900	1.87725500	-0.91149600
C	0.31551100	4.70931300	-2.83670900
O	-0.83719100	4.96154900	-3.12832400
O	1.34772400	5.53680300	-3.12491200
C	0.98550900	6.75109000	-3.79940500
H	0.29186200	7.33705900	-3.19120700
H	1.91838900	7.29499600	-3.94789200
H	0.51125000	6.53224100	-4.75950300
C	3.12755500	-1.60456400	-1.20141500
C	3.68135000	-0.88163700	-2.43423100
C	2.25297700	-2.39533400	-3.33447900
C	2.16805800	-2.68809100	-1.80400900
C	2.44414000	-0.86665000	-3.36178600
H	2.68028100	-0.48711600	-4.36088700
H	1.59649700	-0.30895700	-2.96267800
C	4.61682200	-1.85383800	-3.22453000
H	5.12102000	-1.27877900	-4.00787100
H	5.38552900	-2.29992700	-2.59548900
C	3.62650400	-2.89348600	-3.83773700
H	3.66233200	-2.88242300	-4.93145100
H	3.83899100	-3.91875400	-3.51672400
H	4.15172100	0.07621100	-2.21279700
H	1.39621500	-2.78851200	-3.88735600
H	2.56477900	-3.69375500	-1.60606900
O	3.40084800	-2.37740200	0.98438900
C	4.10778600	-2.13430100	-0.17697200
O	5.29880900	-2.29808100	-0.25800100
C	4.17728300	-2.71403900	2.15913100
H	3.44852500	-2.86661700	2.95323500

H	4.74743900	-3.62485200	1.97094500
H	4.85457200	-1.89279300	2.39950200
C	3.22606700	1.04121300	2.10472200
O	2.01113000	0.73835100	2.24116300
O	3.88861200	0.63864200	1.08121500
C	3.90966200	1.91069300	3.14066200
H	3.42337300	2.89671000	3.11012600
H	3.72533100	1.51199200	4.14251700
H	-0.02717400	-4.28664400	-2.25513900
Cl	-2.66313300	-4.60324500	-1.37353300
Cl	-0.90386500	-0.45949200	1.75468100
N	5.33616500	1.99615400	2.91481600
C	6.21531300	2.13444200	3.95264600
O	5.84514700	2.26824400	5.11316900
C	7.68668400	2.13079700	3.56603600
H	7.86582200	1.90996700	2.51013200
H	8.11425600	3.11020500	3.79955100
H	8.20826100	1.39362300	4.18165500
H	5.66169600	1.78465700	1.98272100

TS23

C	-0.43147500	-1.09096700	0.16700800
C	-1.42807300	-2.00299900	-0.24394500
C	-1.13250200	-2.80116700	-1.36369100
C	0.10266300	-2.74108900	-2.00317000
C	1.06251200	-1.81429600	-1.60481600
C	0.77177300	-0.92572300	-0.53913000
C	-2.73520900	-2.12732300	0.48453900
H	-3.18651900	-3.10991500	0.34534100
H	-2.65673700	-1.90859200	1.55000400
S	-3.99161100	-0.95586000	-0.15538500
O	-4.21338600	-1.18032900	-1.57807600
O	-3.79027600	0.39020600	0.36704900
O	-5.30046000	-1.65543800	0.66733000
C	-6.19902200	-0.81431800	1.30586300
C	-6.06487200	-0.59887400	2.68641900
C	-7.24779500	-0.26327600	0.57688700
C	-7.03211000	0.19330200	3.33535700
C	-8.19514200	0.52854600	1.23955500
H	-7.30106500	-0.46902900	-0.48409100
C	-8.08141600	0.74904100	2.62512700

H	-6.94309800	0.36650300	4.40223600
H	-8.83011100	1.36158300	3.11460000
C	-4.96245000	-1.17008200	3.39128300
N	-4.05337500	-1.64201300	3.94469600
O	-9.25290900	1.11633200	0.63486700
C	-9.41619600	0.94963200	-0.77097000
H	-10.31127200	1.51335800	-1.03470400
H	-8.55734400	1.34939800	-1.32263300
H	-9.56022300	-0.10506800	-1.03397700
Pd	2.46417300	0.03737000	0.12834100
C	0.10110500	3.32056900	-0.65839900
C	-0.21732700	3.40465000	-2.01657600
C	0.04854500	2.31041300	-2.84798000
C	0.63651200	1.15645000	-2.34031300
C	0.99085900	1.09272400	-0.98495200
C	0.68590800	2.16555800	-0.13392600
H	-0.10895000	4.15473900	0.00099800
H	-0.22979500	2.36879700	-3.89491200
H	0.78051200	0.31316200	-2.99996200
H	0.92611100	2.13096100	0.92116500
C	-0.85100400	4.60879600	-2.62524700
O	-1.14419000	4.70751000	-3.80104900
O	-1.06397200	5.59001500	-1.72186900
C	-1.67600200	6.78050100	-2.24227300
H	-2.65819400	6.55399300	-2.66452500
H	-1.77023200	7.45723800	-1.39330100
H	-1.05152700	7.22476000	-3.02136700
C	3.48555900	-1.27483300	-1.14485900
C	4.50961400	-0.56653000	-2.04090900
C	2.92443500	-1.27780500	-3.50407700
C	2.47590800	-1.90732500	-2.13473400
C	3.60548700	0.05844700	-3.11738400
H	4.17787400	0.47408800	-3.95324100
H	2.94602400	0.83278200	-2.73610200
C	5.24638300	-1.65603200	-2.89093500
H	6.11591700	-1.19901800	-3.37314700
H	5.61537900	-2.48249900	-2.28246600
C	4.17155000	-2.08580700	-3.94385100
H	4.47111100	-1.79885700	-4.95658300
H	3.99158100	-3.16575600	-3.95174300
H	5.18485100	0.09467200	-1.49796300

H	2.13039500	-1.23565200	-4.25444100
H	2.67214500	-2.98545800	-2.19880300
O	3.15716100	-3.01621600	0.45527600
C	4.08581000	-2.20615800	-0.10762200
O	5.26316500	-2.24727700	0.18381700
C	3.65213600	-3.92052300	1.46010100
H	2.78575000	-4.49263100	1.78968700
H	4.41480800	-4.58056000	1.04010800
H	4.08437900	-3.36250600	2.29404100
C	3.72719500	1.10178400	2.15877400
O	2.49009500	1.27684700	2.22569600
O	4.25588300	0.46524400	1.16454400
C	4.64339400	1.62075500	3.24721700
H	4.54831900	2.71207700	3.30054800
H	4.27243400	1.24240200	4.20880100
H	0.32329000	-3.44898800	-2.79501500
Cl	-2.28160200	-3.98792900	-1.95042000
Cl	-0.68103000	-0.16923500	1.62947200
N	6.01979800	1.24238300	3.01167300
C	7.03624000	1.82479800	3.70991800
O	6.83034400	2.65072900	4.59287600
C	8.43844300	1.37774100	3.32436700
H	8.45949200	0.63292500	2.52416000
H	9.01319300	2.25437300	3.01293900
H	8.93059900	0.96416300	4.20884800
H	6.19425000	0.61402400	2.23992200

int36

C	-0.72271500	0.86039500	0.12210000
C	-1.38599600	-0.35505500	-0.21723800
C	-0.75805200	-1.15337900	-1.16200600
C	0.49233600	-0.80314700	-1.71956000
C	1.15873800	0.40263900	-1.35009700
C	0.50361500	1.27054700	-0.41239500
C	-2.69197300	-0.75570100	0.40595800
H	-2.82127800	-1.83781600	0.38626800
H	-2.81404200	-0.39438100	1.42749300
S	-4.14448100	-0.11409200	-0.51625500
O	-3.99791200	-0.40504600	-1.93736900
O	-4.54385900	1.21211600	-0.06290200
O	-5.24214800	-1.23907200	0.11654400

C	-6.49165300	-0.78350400	0.51340400
C	-6.69579800	-0.42724200	1.85558200
C	-7.52533700	-0.76060900	-0.41698000
C	-7.99156900	-0.04525800	2.25399500
C	-8.80643600	-0.37317500	-0.00136300
H	-7.30641400	-1.05057900	-1.43615800
C	-9.03182800	-0.01879900	1.34193800
H	-8.16554400	0.23141600	3.28804900
H	-10.03265100	0.27389700	1.63865600
C	-5.60141400	-0.44811800	2.77225900
N	-4.69315200	-0.46813300	3.50010800
O	-9.88558500	-0.31385400	-0.81488300
C	-9.72320500	-0.64256700	-2.19168300
H	-10.70618400	-0.51437500	-2.64535400
H	-9.00604600	0.02745600	-2.68016600
H	-9.39724900	-1.68180700	-2.31859600
Pd	2.17566500	-1.44517400	-0.36341000
C	2.16963300	4.10399400	1.50425100
C	1.92051500	5.19132400	0.65685600
C	1.20686600	4.99331400	-0.53207800
C	0.75870600	3.72175800	-0.87523300
C	1.02340900	2.62507600	-0.04024500
C	1.71837100	2.83253000	1.15884900
H	2.70983100	4.25915700	2.43088000
H	1.01216700	5.84846500	-1.17024200
H	0.20010000	3.57377800	-1.79482100
H	1.89746900	1.99554800	1.82655300
C	2.37858000	6.57595400	0.97141600
O	2.18938400	7.53919200	0.25453800
O	3.03399300	6.64671600	2.15080000
C	3.49770600	7.95645900	2.51626800
H	2.65903200	8.65257500	2.59414400
H	3.98755200	7.83564200	3.48221300
H	4.20234600	8.33602900	1.77211500
C	3.32599800	-0.64035700	-1.86215700
C	4.65712400	-0.12337500	-1.29261000
C	3.46900800	1.75899200	-1.74219100
C	2.47284100	0.64209500	-2.15133500
C	4.21081800	1.14192000	-0.53609900
H	5.05404100	1.75462500	-0.20127700
H	3.57008200	0.93203600	0.32352800

C	5.44627300	0.50912600	-2.47331000
H	6.45047100	0.78534500	-2.13503200
H	5.56929300	-0.17744000	-3.31378300
C	4.59411500	1.77206400	-2.81441800
H	5.18459700	2.68855400	-2.72344200
H	4.19133700	1.74913500	-3.83257000
H	5.21126500	-0.87658900	-0.73238700
H	3.01957900	2.73653800	-1.59152200
H	2.19878400	0.74100100	-3.20730300
O	2.53535100	-1.70020600	-3.86350100
C	3.48676700	-1.72334600	-2.88703700
O	4.37516400	-2.55283400	-2.86900100
C	2.63464800	-2.75303800	-4.84081700
H	1.82370400	-2.57519300	-5.54678400
H	3.60200000	-2.71411900	-5.34621200
H	2.52380900	-3.72986500	-4.36384100
C	2.58835900	-2.88227700	1.67110200
O	1.41768800	-2.43641000	1.50517100
O	3.51748100	-2.58674600	0.83431500
C	2.90235200	-3.78303200	2.84480300
H	2.66304200	-3.26020800	3.77764500
H	2.21912100	-4.64218700	2.79833500
H	0.82035600	-1.34290700	-2.60020200
Cl	-1.46557500	-2.65053300	-1.71518800
Cl	-1.52155200	1.90593600	1.27622800
N	4.29072800	-4.18854400	2.84509400
C	4.89565800	-4.62874500	3.98675600
O	4.28269800	-4.76323500	5.03999400
C	6.37737200	-4.94990000	3.86106000
H	6.78592800	-4.76483000	2.86390100
H	6.92900300	-4.35154600	4.59123700
H	6.53216600	-6.00121500	4.11893600
H	4.82053300	-3.99808400	2.00647000

TS24

C	0.57543300	0.00006800	2.59805500
C	1.89820900	-0.31045400	2.88498400
C	2.59775100	-1.28684700	2.15734900
C	1.83603300	-2.05818600	1.25402000
C	0.48688800	-1.80177300	0.96331100
C	-0.10746800	-0.67289800	1.57829200

Cl	2.68739100	0.58254100	4.17524000
C	4.08314100	-1.42333800	2.24862000
H	4.46978800	-1.22141500	3.25023800
H	4.44952100	-2.38535900	1.89601600
S	5.00096400	-0.18730300	1.22906300
O	6.31039100	-0.74562500	0.89726500
O	4.88900800	1.16082000	1.77081600
O	4.01979900	-0.25671100	-0.15616100
C	4.18574600	0.73783600	-1.10617600
C	3.05197100	1.47125400	-1.50800700
C	5.42920900	0.95869400	-1.69141300
C	3.20018200	2.43906800	-2.52718200
C	5.55718300	1.94064400	-2.68392000
H	6.26949500	0.36259800	-1.36310500
C	4.43144000	2.67635200	-3.10367700
H	2.32949100	3.00103400	-2.84726400
H	4.55629500	3.42188900	-3.88036800
C	1.77020300	1.25495000	-0.93077900
N	0.69972100	1.11093300	-0.50548400
O	6.71687200	2.24052000	-3.30161400
C	7.90536900	1.55140100	-2.91238800
H	8.70418000	1.97600800	-3.52016500
H	8.12676500	1.71063900	-1.85126100
H	7.82509100	0.47713000	-3.11387600
Pd	-1.21071300	0.61858900	0.35345500
C	-2.38165600	3.08998100	-0.53885800
O	-2.11373300	1.91406800	-1.00578100
O	-2.18136700	3.48497700	0.61740200
H	0.11036800	0.81698300	3.13331100
Cl	2.63918800	-3.37099700	0.39441400
C	-3.05837100	0.03542400	1.17367300
C	-3.72049500	1.00146900	2.16785200
C	-2.38730400	-0.36293400	3.39737700
C	-2.21213200	-0.82984700	1.95903600
C	-2.61680700	1.15727500	3.22946500
H	-2.97805100	1.62733700	4.14940500
H	-1.76268800	1.72197800	2.85132100
C	-4.75119700	0.13180600	2.95137900
H	-5.34412500	0.76945200	3.61441300
H	-5.44957000	-0.39027300	2.29231900
C	-3.83664000	-0.83526100	3.76606700

H	-3.98592700	-0.72291200	4.84421000
H	-4.00287000	-1.88951700	3.52413400
H	-4.11060200	1.91700600	1.73053600
H	-1.62168700	-0.69549400	4.09897000
H	-2.15177400	-1.88297100	1.70670200
O	-4.80785600	0.31813800	-0.36960200
C	-3.83519700	-0.52783100	0.02139600
O	-3.63852600	-1.61292900	-0.49101500
C	-5.57195600	-0.10727300	-1.51178900
H	-6.32300900	0.66696400	-1.66524700
H	-4.92502400	-0.19252900	-2.38775400
H	-6.04535600	-1.07330300	-1.32053000
C	-3.01143300	4.02393500	-1.57772000
H	-2.35084700	4.09772700	-2.44960900
H	-3.94465000	3.57597900	-1.94076600
C	-1.39594400	-4.76742600	-0.45953300
C	-1.63105800	-4.35673100	-1.77807500
C	-1.17623400	-3.10383600	-2.20281000
C	-0.49764200	-2.26584600	-1.32328700
C	-0.25558500	-2.67074300	-0.00360300
C	-0.70711000	-3.93239600	0.41528400
H	-1.74650500	-5.73811900	-0.12876600
H	-1.36969800	-2.79929700	-3.22550000
H	-0.15236200	-1.29512500	-1.66145400
H	-0.50855500	-4.26158200	1.43157700
C	-2.35479400	-5.20768900	-2.76432100
O	-2.56115800	-4.89824500	-3.92157400
O	-2.76321000	-6.38345100	-2.23160400
C	-3.46934000	-7.24816400	-3.13330400
H	-2.83854500	-7.51558600	-3.98497000
H	-3.72452500	-8.13458000	-2.55242600
H	-4.37320400	-6.76000800	-3.50641400
N	-3.24381300	5.32082100	-0.98316400
C	-3.74984300	6.36455000	-1.68951900
O	-4.05466400	6.27546900	-2.87625800
C	-3.91855800	7.66274500	-0.90994100
H	-3.59937900	7.59486000	0.13382200
H	-3.34497600	8.44945700	-1.40800900
H	-4.97089400	7.95885900	-0.94242900
H	-2.97842600	5.39125500	-0.00871600

int37

C	-0.76966600	0.05323400	2.52899500
C	-2.07033300	0.41895300	2.85793200
C	-2.75789400	1.40565000	2.13243100
C	-1.99092400	2.16075900	1.22100400
C	-0.66078500	1.85320800	0.89722000
C	-0.10765500	0.69320900	1.47938400
Cl	-2.86251200	-0.44041000	4.17080300
C	-4.24507000	1.51769900	2.17979500
H	-4.66515200	1.30575500	3.16556500
H	-4.62252200	2.46713300	1.80568000
S	-5.09438900	0.24833500	1.12843100
O	-6.35201100	0.81320500	0.64118100
O	-5.07008200	-1.07265000	1.74402700
O	-3.98315900	0.21627200	-0.16659100
C	-4.09824100	-0.80105200	-1.09602900
C	-2.93066300	-1.50292200	-1.46705100
C	-5.32051200	-1.08293100	-1.70146100
C	-3.02852700	-2.49888600	-2.46651700
C	-5.39639200	-2.09200300	-2.67137000
H	-6.18849400	-0.50865900	-1.40888700
C	-4.23912400	-2.79706600	-3.05615900
H	-2.13210600	-3.03426000	-2.76016100
H	-4.32344000	-3.56491600	-3.81628500
C	-1.65798900	-1.23605700	-0.89251500
N	-0.58801800	-1.05737200	-0.47860100
O	-6.53398100	-2.44609300	-3.30042200
C	-7.75239800	-1.78889100	-2.94897100
H	-8.52485500	-2.25526800	-3.56016100
H	-7.98741000	-1.93019900	-1.88831500
H	-7.70467000	-0.71772300	-3.17519800
Pd	1.21461900	-0.45874400	0.45609000
C	2.33640600	-2.98840700	-0.41427100
O	2.22363800	-1.77298300	-0.84413300
O	1.99012800	-3.40824400	0.69744900
H	-0.32150900	-0.79183800	3.03835200
Cl	-2.77216500	3.49627200	0.37256500
C	3.31913400	-0.07383500	1.16441500
C	3.85737900	-1.07085200	2.19031000
C	2.55417800	0.40005200	3.32141100
C	2.52222100	0.83082900	1.86638300

C	2.69436300	-1.13414700	3.19923100
H	2.98299300	-1.60568400	4.14382000
H	1.82014300	-1.64678400	2.79173000
C	4.90091800	-0.24123900	3.01317400
H	5.43200800	-0.90497300	3.70190000
H	5.64996200	0.23551500	2.37573900
C	4.00670500	0.78036100	3.78404700
H	4.08853400	0.65112500	4.86745500
H	4.25456400	1.82205400	3.55957500
H	4.22087700	-2.01283200	1.78795200
H	1.75953100	0.79554400	3.95434000
H	2.34927300	1.85014300	1.54071600
O	5.04338000	-0.55775500	-0.35203800
C	4.03804500	0.29871000	-0.09732600
O	3.77908600	1.26850200	-0.78023400
C	5.77831800	-0.29714300	-1.56254600
H	6.55375900	-1.06131000	-1.60307900
H	5.11559900	-0.37364400	-2.42713300
H	6.21966500	0.70193200	-1.53552300
C	2.97628300	-3.93537300	-1.43501100
H	2.39399700	-3.91661800	-2.36406500
H	3.97331300	-3.55879400	-1.69475100
C	1.33622500	4.75402700	-0.50564700
C	1.61359800	4.31706500	-1.80779200
C	1.14035300	3.07057400	-2.23188100
C	0.40091300	2.26688700	-1.36900500
C	0.11734300	2.69654100	-0.06493500
C	0.59120100	3.95076700	0.35320900
H	1.70078300	5.71946500	-0.17433600
H	1.36710600	2.74356000	-3.24061100
H	0.04275500	1.30220700	-1.70991400
H	0.36684800	4.29776100	1.35790600
C	2.39891000	5.13271900	-2.77604800
O	2.63234800	4.80661800	-3.92349900
O	2.83115400	6.29856500	-2.23903900
C	3.59468200	7.13035400	-3.12452100
H	3.00074100	7.41184600	-3.99790900
H	3.86210100	8.01269400	-2.54286600
H	4.49240600	6.60823000	-3.46514800
N	3.04268800	-5.26834700	-0.88078700
C	3.54652000	-6.32018900	-1.57730000

O	3.98196700	-6.20845400	-2.72046600
C	3.53715300	-7.65616800	-0.84529400
H	3.12459200	-7.60210600	0.16603200
H	2.95476200	-8.37385300	-1.42995800
H	4.56129000	-8.03614900	-0.79303600
H	2.67935600	-5.35258100	0.06038700

int38

Pd	1.14729400	0.22667700	-1.79987000
C	2.78097000	-3.35191800	1.92692100
C	3.41006900	-2.17761600	2.36417700
C	2.88971100	-0.93608300	1.98084200
C	1.75598700	-0.85944500	1.17369700
C	1.11989500	-2.03191800	0.73394900
C	1.64842400	-3.27531400	1.12294000
H	3.18118000	-4.31630600	2.21759200
H	3.38265600	-0.03115000	2.31893500
H	1.38922000	0.12168800	0.89092100
H	1.16692500	-4.18900500	0.78725200
C	4.62346100	-2.19519800	3.22915800
O	5.19800600	-1.20345100	3.63331600
O	5.02867700	-3.45352000	3.52532200
C	6.19181800	-3.53722100	4.36212300
H	6.01098300	-3.04967900	5.32346600
H	6.37838500	-4.60208300	4.50181500
H	7.04808700	-3.05675100	3.88189900
C	2.33956700	2.73826500	-1.01829300
O	2.07158700	2.41995900	0.14789700
O	2.07538500	2.05433700	-2.08577800
C	3.05674300	4.05970000	-1.31482900
H	3.98829900	3.84754800	-1.85386900
H	2.44385600	4.66229100	-1.99553400
C	-1.31594400	-2.50764500	0.22282100
C	-2.43524200	-2.55634500	-0.63566900
C	-2.20562200	-2.25972000	-1.98958900
C	-1.00299300	-1.69658600	-2.40434300
C	0.03277000	-1.47129900	-1.48835600
C	-0.06686700	-2.00967400	-0.17992100
C	-3.81917000	-2.73815700	-0.10265900
H	-4.48801300	-3.24923600	-0.79869300
H	-3.84920100	-3.22251100	0.87115800

S	-4.69402500	-1.12846200	0.16054200
O	-5.67624600	-1.30545400	1.22847000
O	-5.07707600	-0.50311800	-1.09884600
O	-3.37653500	-0.24665300	0.77729300
C	-3.51509700	1.12420600	0.91299600
C	-2.51397000	1.95348200	0.36467600
C	-4.57574900	1.66526400	1.63419600
C	-2.60414100	3.34967200	0.57005900
C	-4.65918200	3.05510300	1.79959800
H	-5.31133200	0.99478800	2.05637100
C	-3.66100300	3.89557600	1.26845800
H	-1.82787400	3.98907500	0.16421600
H	-3.74263000	4.96504300	1.42374100
C	-1.41159700	1.43673700	-0.36715800
N	-0.48302800	1.08271800	-0.96444700
O	-5.65213600	3.67500400	2.46636000
C	-6.71143100	2.89135000	3.01726000
H	-7.39837900	3.60445300	3.47259400
H	-7.23289900	2.32518600	2.23764200
H	-6.33846100	2.20325400	3.78429700
H	-0.91505900	-1.35735700	-3.43145600
Cl	-3.46311400	-2.51345300	-3.18965400
Cl	-1.53468800	-2.98762500	1.90688900
C	3.16455000	-1.75057400	-2.89181900
C	4.49306700	-2.11292600	-3.48445400
H	5.07879800	-2.65677300	-2.73651300
H	4.34896000	-2.77900600	-4.33897300
H	5.02378500	-1.21080300	-3.78404300
O	2.86184200	-0.56816700	-2.66822100
O	2.37794500	-2.76965500	-2.63089300
H	1.53616800	-2.41980300	-2.22754000
N	3.30666000	4.75963100	-0.07504100
C	3.88016100	5.99047000	-0.03670200
O	4.22024500	6.59475300	-1.05040200
C	4.07712300	6.57782600	1.35546800
H	3.57383400	7.54749600	1.40273700
H	3.70231700	5.93982600	2.16072300
H	5.14423400	6.75835100	1.51343900
H	3.02083800	4.25922800	0.75714100
TS25			
Pd	1.06989400	0.45426300	-1.84837100

C	3.33349500	-3.14331300	1.89641700
C	3.86017700	-1.90807500	2.30005600
C	3.24229000	-0.72562900	1.87809300
C	2.11331700	-0.76759300	1.06208400
C	1.58179400	-2.00148800	0.65618300
C	2.20347000	-3.18592600	1.08718000
H	3.81188600	-4.06185800	2.21571100
H	3.65585900	0.22570800	2.19462200
H	1.65923900	0.16846300	0.75228800
H	1.80334300	-4.14539300	0.77390700
C	5.06586500	-1.79826500	3.16945300
O	5.55281100	-0.74968500	3.54460700
O	5.57262100	-3.00816600	3.50525400
C	6.73686500	-2.96964100	4.34386800
H	6.51402500	-2.46970200	5.28988700
H	7.01070400	-4.01063200	4.51571200
H	7.55122300	-2.43484000	3.84849300
C	1.72628800	3.08379900	-0.98857700
O	1.81456100	2.59939700	0.14309200
O	1.39014200	2.45647300	-2.07643800
C	2.03332800	4.56424900	-1.23663800
H	2.87065900	4.62731700	-1.94398100
H	1.18316100	5.05224300	-1.72412400
C	-0.81667900	-2.64313900	0.15217800
C	-1.91674800	-2.80455200	-0.72104100
C	-1.70417000	-2.52491100	-2.08350800
C	-0.51933900	-1.94291000	-2.51544000
C	0.51815100	-1.65784400	-1.61084300
C	0.40609600	-2.09712700	-0.26345500
C	-3.27066200	-3.18970400	-0.20916500
H	-3.83527500	-3.79564100	-0.92145900
H	-3.23750400	-3.68950900	0.75710600
S	-4.38392100	-1.74910100	0.05586100
O	-5.45760900	-2.15587400	0.95820200
O	-4.68137900	-1.04630300	-1.18509300
O	-3.28377700	-0.79391300	0.92287200
C	-3.59521000	0.54800600	1.07137500
C	-2.72966000	1.50209900	0.50416900
C	-4.70421200	0.93141000	1.81737200
C	-2.99962600	2.87266300	0.71838100
C	-4.96695900	2.29737700	1.99962600

H	-5.33532700	0.16094800	2.23879800
C	-4.10197400	3.26519500	1.45022500
H	-2.33100100	3.61441400	0.29557100
H	-4.32269300	4.31323000	1.61642800
C	-1.59864900	1.11703100	-0.26326900
N	-0.66034300	0.85916100	-0.89226700
O	-6.01590800	2.77761200	2.69432800
C	-6.94631000	1.85818800	3.26778100
H	-7.70521100	2.47186200	3.75261400
H	-7.41463800	1.23577100	2.49729000
H	-6.46215200	1.21855100	4.01436700
H	-0.41161900	-1.68641000	-3.56430400
Cl	-2.93761500	-2.88599300	-3.27924300
Cl	-1.01656800	-3.08784500	1.84589200
C	3.39524800	-0.90967000	-2.98322200
C	4.76605100	-0.91430200	-3.61564500
H	5.51312500	-0.92213600	-2.81477100
H	4.89969800	-1.81517300	-4.21609000
H	4.91093000	-0.01674200	-4.21704300
O	2.85023400	0.22443300	-2.79514000
O	2.87823700	-2.02190800	-2.65624600
H	1.75185900	-1.77844300	-2.13555500
N	2.33217200	5.21414400	0.01974200
C	2.18189000	6.55644800	0.19263900
O	1.86829600	7.31186100	-0.72259100
C	2.44898900	7.06569100	1.60298600
H	1.57964800	7.63559500	1.94191400
H	2.66439400	6.27297800	2.32471900
H	3.29723100	7.75563400	1.57280200
H	2.45981400	4.58558800	0.80267000

p^m

C	5.39951700	-0.77550700	-0.74826100
C	6.05443600	-0.74902300	0.49041600
C	5.50031600	-0.01815600	1.54769000
C	4.30973700	0.67801000	1.36828900
C	3.64353200	0.65164000	0.13267900
C	4.20603200	-0.08285700	-0.92298300
H	5.83080800	-1.33510700	-1.56979500
H	6.01604200	-0.01012000	2.50167100
H	3.87956300	1.23541000	2.19485700

H	3.71109200	-0.10178000	-1.88793700
C	7.33469100	-1.47157400	0.73701200
O	7.93330200	-1.46784000	1.79490800
O	7.76859200	-2.14059500	-0.35560500
C	8.99984600	-2.85981600	-0.18292000
H	8.89815600	-3.61326500	0.60186800
H	9.20136900	-3.33207100	-1.14405100
H	9.80908200	-2.17728200	0.08769900
C	1.16719400	0.92480300	-0.45679500
C	0.01607400	1.72368900	-0.63096800
C	0.15028500	3.10369300	-0.39012900
C	1.35510500	3.65893700	0.02908900
C	2.45958800	2.83608800	0.20110100
C	2.40353800	1.45773700	-0.05083700
C	-1.29424400	1.13753600	-1.07411600
H	-1.90974100	1.87439400	-1.58992200
H	-1.18174100	0.25240500	-1.70072700
S	-2.34241400	0.59293900	0.33040200
O	-2.53777000	1.68840700	1.27151500
O	-1.98173500	-0.73953900	0.79849300
O	-3.76781700	0.46071500	-0.58562300
C	-4.57495900	-0.64668100	-0.37447500
C	-4.47660300	-1.73626100	-1.25355100
C	-5.50596100	-0.62066000	0.65852700
C	-5.35717400	-2.82038400	-1.07325500
C	-6.36684700	-1.71310500	0.82615500
H	-5.53797700	0.24937400	1.30071200
C	-6.28852800	-2.81099000	-0.05053500
H	-5.29463700	-3.66843900	-1.74607400
H	-6.96923100	-3.64140400	0.09792100
C	-3.49382000	-1.72977800	-2.28929000
N	-2.68338700	-1.70805900	-3.12483200
O	-7.30718900	-1.80033200	1.79523400
C	-7.42429300	-0.73288800	2.73264400
H	-8.22005200	-1.02611600	3.41736400
H	-6.49358700	-0.59102500	3.29384400
H	-7.69886900	0.20556400	2.23683900
H	1.42316600	4.72530200	0.20791200
Cl	-1.19892000	4.19836400	-0.63870300
Cl	1.03602400	-0.80295100	-0.73384900
H	3.40430500	3.26828600	0.51430600

TS1^o

C	-1.57419700	1.78087000	-2.02983400
C	-1.17401100	1.43886900	-0.71490100
C	0.02094900	2.02037400	-0.18414400
C	0.75401500	2.88999600	-1.00532300
C	0.38887600	3.13430300	-2.33133900
C	-0.77474600	2.56480000	-2.85188700
H	0.99687700	3.80155100	-2.93245500
H	-1.06763000	2.77654500	-3.87579500
Cl	-2.82758600	1.87419600	0.60229200
C	0.39801400	1.81532100	1.25863000
H	0.60649700	2.76583000	1.75479600
H	-0.39311000	1.28483900	1.79023100
S	1.90216500	0.81656300	1.69817900
O	1.50476300	-0.50876700	2.16098100
O	2.80809100	1.64003000	2.48860700
O	2.62604300	0.61863000	0.16662900
C	3.27423400	-0.57464000	-0.09125700
C	2.53993500	-1.65381700	-0.62048100
C	4.64530000	-0.66639700	0.11024800
C	3.21272900	-2.84461100	-0.95440800
C	5.30314300	-1.85971500	-0.22826700
H	5.16353900	0.18990700	0.52077600
C	4.57816600	-2.94378400	-0.76417200
H	2.65085300	-3.68102700	-1.35520100
H	5.11633400	-3.85090900	-1.01383600
C	1.14016100	-1.47567400	-0.74000400
N	0.01991600	-1.18393000	-0.75796800
O	6.62764900	-2.06180800	-0.07730600
C	7.42532800	-1.02039700	0.48501300
H	8.44080700	-1.41428900	0.52239200
H	7.40514600	-0.12208100	-0.14264500
H	7.09265400	-0.76904300	1.49835500
H	-2.53154200	1.41882600	-2.39169800
Cl	2.14743000	3.76045800	-0.37981800
Pd	-1.85123800	-0.65399500	-0.34346800
C	-4.50239900	-1.88027800	-0.44507000
H	-5.45220900	-2.21564600	-0.02941400
H	-4.64756000	-1.76747100	-1.52902500
N	-4.01897900	-0.60651100	0.10374900

C	-3.48649800	-3.00978100	-0.24338000
O	-2.23652000	-2.62585700	-0.10161800
O	-3.83396400	-4.17815000	-0.24878800
C	-4.80749900	0.06381500	0.91390400
O	-4.57750900	1.23705400	1.44508100
C	-6.17748200	-0.43962700	1.35777000
H	-6.85529900	-0.53927400	0.50452900
H	-6.10264700	-1.40971000	1.85688600
H	-6.59688400	0.28787400	2.05297600

cat1

Pd	-0.00000100	-0.00051000	-0.01002900
C	-2.43612600	0.00000700	-0.00510000
O	-1.76169300	1.08782600	-0.01049400
O	-1.76250100	-1.08823200	-0.01108200
C	2.43610900	0.00107700	-0.00422600
O	1.76293300	-1.08754900	-0.01053300
O	1.76125100	1.08851300	-0.01118200
C	3.93091500	0.00132200	0.03883400
C	-3.93090300	0.00079700	0.03896700
H	4.31919100	0.93022300	-0.38211200
H	4.25614600	-0.07275300	1.08222500
H	4.32082200	-0.86272900	-0.50275600
H	-4.32069900	-0.90468100	-0.42940900
H	-4.25519900	0.01748000	1.08517500
H	-4.32009500	0.89226100	-0.45629000

cat3

Pd	0.35093100	-0.38527000	-0.10351900
C	-2.52319000	-0.04331000	0.10140200
H	-2.62514300	0.23868800	1.15130100
H	-3.46069300	0.18361700	-0.41217800
N	-1.39168900	0.73533400	-0.49380600
C	-2.23814400	-1.55692700	0.05319500
O	-0.96501300	-1.87769600	-0.03091000
O	-3.15378700	-2.34971100	0.13167900
C	-1.21538500	2.13877700	-0.13089500
O	-0.95702700	2.92488600	-1.00844100
C	-1.34801100	2.48763900	1.33017800
H	-2.40539500	2.60726500	1.59208900
H	-0.91838300	1.71848600	1.97652900

H	-0.84397600	3.43983400	1.49533100
C	2.77417500	-0.14196100	0.10244300
O	2.20309600	-1.27904600	0.22298900
O	2.01536100	0.87035400	-0.10867400
C	4.26237300	-0.00401500	0.17089200
H	4.68183600	-0.20012600	-0.82187900
H	4.53446100	1.00965900	0.46955900
H	4.67510500	-0.73795500	0.86578300
H	-1.45077700	0.72412900	-1.51442900

cat4

Pd	1.16164900	-0.37030500	-0.22449300
H	0.56217300	2.14325000	1.10573200
C	1.98654700	2.50391100	-0.24025800
O	1.37859300	2.77924700	0.86126500
C	2.91026100	3.57223700	-0.75917600
H	3.37321500	3.25794800	-1.69325700
H	2.34908700	4.49955000	-0.90342800
H	3.68025800	3.77022300	-0.00745300
O	1.87005300	1.43650700	-0.89467700
C	-2.84382000	0.88039900	0.67773600
C	-1.32538400	0.87261100	0.61056600
O	-0.80258100	0.12512300	-0.29474500
O	-0.70349600	1.59349900	1.42135700
H	-3.18069900	1.90363000	0.46391100
H	-3.13960900	0.68172800	1.71412900
N	-3.44429500	-0.07674900	-0.22369800
H	-2.82387500	-0.58002900	-0.84057500
C	-4.78675400	-0.31681700	-0.19255900
O	-5.53452800	0.27892100	0.57518500
C	-5.29003400	-1.36941100	-1.16854300
H	-6.06517200	-0.92323600	-1.79718700
H	-4.50796000	-1.78794800	-1.80795400
H	-5.75721700	-2.17942200	-0.60146400
C	2.28895500	-2.46370400	0.28693300
O	2.94524400	-1.41835100	-0.05298000
C	2.96858200	-3.76672700	0.56056600
H	2.42146300	-4.32063500	1.32595000
H	2.97394400	-4.36458400	-0.35733000
H	4.00066400	-3.59411800	0.87012600
O	1.01394000	-2.34620900	0.35581900

cat5

Pd	-1.32504400	0.11368600	-0.00570300
C	2.55944700	0.80822400	0.00741900
H	2.76042400	1.42995100	0.89198700
H	2.76467500	1.44194700	-0.86742300
N	3.31614200	-0.42078900	0.00074100
C	1.07763000	0.53015100	0.00225500
O	0.61595800	-0.65948300	0.00017400
O	0.23668800	1.48961500	0.00044300
C	4.68560400	-0.54817200	0.00203300
O	5.21523300	-1.64908600	-0.00246800
C	5.48146700	0.74773000	0.00915000
H	5.25783100	1.36064900	-0.87123600
H	5.25797800	1.35055200	0.89655100
H	6.54056200	0.49313600	0.00769500
H	2.79557400	-1.28935000	-0.00274600
O	-2.87024900	-1.25141800	-0.01257400
C	-3.72155200	-0.29471000	-0.00866200
O	-3.23594100	0.89065200	-0.01284200
C	-5.19337500	-0.54527300	0.02984700
H	-5.42447800	-1.49579400	-0.45436500
H	-5.51632700	-0.60135000	1.07514200
H	-5.72605100	0.27627000	-0.45256900

cat6

Pd	0.00328200	-0.00337400	-1.30758900
C	-1.84981200	-1.84778700	0.00114400
O	-1.45020000	-1.45290500	-1.14362400
O	-1.45005700	-1.45312500	1.14569300
C	-2.95012200	-2.88669500	-0.00197100
H	-2.82689300	-3.56146900	-0.85065200
H	-2.95441700	-3.43990600	0.93764500
H	-3.91230400	-2.37528100	-0.11202900
Pd	0.00389800	-0.00395300	1.30797700
C	-1.84473300	1.84608200	0.00193200
O	-1.44480900	1.45201600	-1.14294300
O	-1.44444500	1.45137000	1.14632900
C	-2.94619900	2.88379100	0.00048600
H	-2.92662100	3.46038300	0.92591400
H	-2.84752000	3.53680300	-0.86798800

H	-3.91013100	2.36835700	-0.06817700
C	1.85213400	1.84528500	0.00027300
O	1.45831600	1.44458500	-1.14443300
O	1.45868900	1.44437700	1.14490100
C	2.88775700	2.94861200	-0.00150900
H	2.36975700	3.91179500	-0.06085800
H	3.47000800	2.92486200	0.92031000
H	3.53559200	2.85628600	-0.87449800
C	1.85161200	-1.85256300	-0.00167000
O	1.45132100	-1.45799800	-1.14610200
O	1.45151900	-1.45872300	1.14328600
C	2.95338900	-2.88977800	0.00021500
H	3.91648700	-2.37432900	0.07949600
H	2.84871900	-3.54849800	0.86370200
H	2.94019800	-3.46043600	-0.92894500

cat7

Pd	1.53207400	-0.13026600	-0.04886300
C	2.47745200	2.11356500	-0.01560900
O	2.18135500	1.52901900	-1.11544400
O	2.23494400	1.47102900	1.06553900
C	3.10823200	3.47013900	0.00704100
H	2.84493200	4.02286500	-0.89641000
H	2.79449200	4.01378500	0.90038500
H	4.19709000	3.35503400	0.04054200
Pd	-1.53032000	-0.14475900	0.04122500
C	-2.50095700	2.08809400	0.00184600
O	-2.19783500	1.50989000	1.10325500
O	-2.25190500	1.44524400	-1.07748500
C	-3.14634300	3.43771000	-0.02457400
H	-2.82702400	3.98742800	-0.91228400
H	-4.23330400	3.31087700	-0.07337700
H	-2.90070400	3.99062900	0.88366800
C	0.06475000	-1.87532600	1.87261800
O	1.18539100	-1.53922500	1.37972700
O	-1.08617500	-1.47823600	1.51507000
C	0.10744300	-2.83748600	3.04054600
H	0.14737500	-2.25381900	3.96636400
H	-0.79509400	-3.44980900	3.05950100
H	1.00069400	-3.46084500	2.98642200
C	-0.04278100	-1.89123400	-1.86613600

O	1.10352800	-1.47354500	-1.51785300
O	-1.16746400	-1.55348500	-1.38352400
C	-0.07596700	-2.93192100	-2.96535100
H	-0.20242400	-3.91886400	-2.50819300
H	-0.92899400	-2.75267700	-3.62214500
H	0.85658600	-2.92025500	-3.52966800

cat8

Pd	-1.55601600	0.05027700	1.29783200
Pd	-0.65000300	0.04524400	-1.16303600
C	0.27159500	-2.11088200	0.56799000
O	-0.45159000	-1.69130300	1.52321400
O	0.31286900	-1.70665900	-0.63482700
C	1.20991400	-3.27019700	0.93657700
H	0.62616900	-4.19426100	0.97755400
H	1.58896700	-3.06779100	1.93981400
C	1.04335800	1.28814700	0.86256500
O	0.16075500	1.07967600	1.75970200
O	0.96260600	1.05117800	-0.38414900
C	2.35120800	1.90376500	1.36443900
H	2.43176600	1.68069400	2.43196000
H	2.29213500	2.99058000	1.23542900
C	-3.20656900	-1.29183900	-0.71649200
O	-2.35802100	-1.00456900	-1.62479300
O	-3.14394800	-1.01410600	0.52568400
C	-2.33937500	2.29919400	-0.39224200
O	-1.68155100	1.80900200	-1.36859700
O	-2.48280000	1.80794600	0.77563300
N	3.50646300	1.45518000	0.63174400
H	3.68191300	0.45468300	0.60142600
C	4.16182400	2.29690100	-0.22596800
O	3.89287400	3.48849500	-0.33004000
C	5.27271100	1.64951300	-1.03805200
H	4.99347400	1.67682100	-2.09580800
H	6.18362400	2.24257600	-0.92549500
H	5.47503300	0.61501200	-0.74848700
N	2.31391500	-3.44224000	0.01839900
C	3.27489300	-2.47611400	-0.08296200
O	3.32522500	-1.53507300	0.70932800
C	4.26897800	-2.64144500	-1.21467900
H	5.27517800	-2.45956500	-0.83068300

H	4.23500800	-3.62960800	-1.68041500
H	4.06039400	-1.88539300	-1.97845400
H	2.18897300	-4.06886100	-0.76247000
C	-3.00417100	3.63398100	-0.64456600
H	-3.82911200	3.78687900	0.05178600
H	-2.26198600	4.42427500	-0.48973500
H	-3.34956900	3.69220100	-1.67803300
C	-4.44892200	-2.02494300	-1.17370600
H	-4.85525000	-2.62580800	-0.35912100
H	-5.20153900	-1.28457800	-1.46520000
H	-4.22494100	-2.64558200	-2.04239200

cat9

Pd	1.25845200	0.57363200	0.84030500
Pd	-1.03241300	0.30122400	-0.84760700
C	1.38247200	1.90629100	-1.73445600
O	2.10946200	1.56590200	-0.74171800
O	0.16819100	1.60153200	-1.92386200
C	2.04285000	2.74326700	-2.80772200
H	2.21718000	2.11485200	-3.68705800
H	1.37059100	3.54976500	-3.10819400
H	2.99136700	3.14866500	-2.45550500
C	-0.95035000	2.55274100	1.05571700
O	0.25625300	2.29323800	1.35623900
O	-1.71126700	1.90567000	0.26245400
C	-1.55899600	3.75669300	1.74185500
H	-0.80517900	4.53558100	1.86813200
H	-2.41284600	4.13219800	1.17732800
H	-1.89554000	3.45294800	2.73911000
C	-2.20784700	-2.35177300	-0.98228700
H	-2.45388000	-3.27306100	-0.45078200
H	-2.91898900	-2.20981300	-1.79974300
N	-2.34583900	-1.17947000	-0.06373500
C	-0.79434000	-2.44749200	-1.55466300
O	-0.27885900	-3.51355500	-1.83134900
O	-0.18378800	-1.28310800	-1.73302200
C	-3.71457400	-0.68200200	0.07205400
O	-4.49958300	-0.81375000	-0.83568800
C	-4.01059800	-0.01708500	1.38965400
H	-3.60779200	-0.59366900	2.22807400
H	-3.53196300	0.96703500	1.39823300

H	-5.08957700	0.10063300	1.48960200
N	2.04797900	-1.33976000	0.33825900
C	3.50893800	-1.36680500	0.29819200
O	4.13171400	-1.71817000	1.27050100
C	4.11157200	-0.93154200	-1.01114500
H	3.72277400	-1.54264600	-1.83346700
H	3.84653700	0.11022900	-1.21452600
H	5.19423100	-1.03898400	-0.95105900
H	1.63444000	-1.44870500	-0.59732000
H	-1.96292900	-1.43034000	0.86144400
C	1.42524900	-2.31473800	1.28736400
H	2.16679800	-2.53172700	2.06016500
H	1.16820900	-3.23161400	0.75398900
C	0.18271400	-1.70684800	1.94285900
O	0.28204700	-0.44170800	2.26449600
O	-0.83026000	-2.37909200	2.13086000

cat10

Pd	-2.26193100	0.46275800	0.33223900
Pd	2.37756200	0.24994900	-0.09734200
C	4.26544200	1.72952000	-0.55033600
O	3.24150900	1.72682800	-1.30907700
O	4.27120100	0.89587400	0.43060500
C	5.39921100	2.68158200	-0.76413900
H	5.19620400	3.60270600	-0.20703200
H	6.32997400	2.25014700	-0.39105700
H	5.48450800	2.93080700	-1.82333000
C	-3.53028700	2.49696300	-0.12892200
O	-2.94773400	2.33253000	0.99312400
O	-3.44847100	1.53426200	-0.97634600
C	-4.25039400	3.76498200	-0.46544000
H	-3.54587500	4.45575800	-0.94128900
H	-5.06197700	3.56222600	-1.16679600
H	-4.63105400	4.23283300	0.44423700
C	-1.16099400	-1.20496200	-1.99860500
H	-1.26387500	-2.11904800	-2.58667800
H	-1.63771300	-0.38945900	-2.54757900
N	-1.84955100	-1.36953300	-0.68540800
C	0.33377400	-0.91811600	-1.78658900
O	1.18549900	-1.47210600	-2.47056400
O	0.53015300	-0.07754100	-0.80703700

C	-3.11923600	-2.06464300	-0.74302900
O	-3.75278700	-2.09506100	-1.77162200
C	-3.52731300	-2.74180600	0.54652100
H	-3.14105700	-2.22740900	1.42880900
H	-4.61557000	-2.80308200	0.58414600
H	-3.12627500	-3.76274000	0.54217500
C	1.05885000	-0.87815400	2.53232700
H	0.58465600	-1.77968600	2.92311800
H	1.65515500	-0.38798300	3.30291100
N	2.01073300	-1.27236600	1.43916500
C	0.00749200	0.13321700	2.02242000
O	0.33704900	1.29964400	1.85637500
O	-1.15081300	-0.41644200	1.78288000
C	1.68364300	-2.47814500	0.71098500
O	0.54468100	-2.89336700	0.69494500
C	2.81898800	-3.11616500	-0.05033800
H	2.68194200	-2.85886400	-1.10671000
H	3.80647300	-2.77589700	0.26991700
H	2.74081500	-4.20079200	0.05332800
H	-1.22409000	-1.79649900	0.00805500
H	2.96309400	-1.32684500	1.79680500

cat11

Pd	-0.86479200	-0.00327100	0.55870700
Ag	1.54154800	0.00463400	-1.08421200
O	1.51418300	2.08822300	-0.52429500
C	1.02105800	2.31416800	0.61656700
O	0.27606900	1.52751400	1.30029400
C	1.30489100	3.65527600	1.26277200
H	0.48491100	4.33758600	1.01391900
H	1.34279300	3.55637500	2.34868000
H	2.23569700	4.07279200	0.87733000
C	-3.04611600	-0.01136000	-0.52884600
O	-2.44145000	-1.10088500	-0.23416300
O	0.28786700	-1.52584500	1.30003300
C	1.03634700	-2.30842400	0.61544900
O	1.52690800	-2.07956100	-0.52595100
C	1.32820000	-3.64806000	1.26109400
H	1.36862100	-3.54870800	2.34688000
H	0.51063100	-4.33417700	1.01477400
H	2.25984400	-4.06140900	0.87321000

C	-4.38626300	-0.00930100	-1.19396400
H	-5.09288600	0.56594600	-0.58893400
H	-4.30661700	0.48332900	-2.16778600
H	-4.74682300	-1.03039100	-1.32294600
O	-2.44823000	1.08274300	-0.23293300

cat12

Pd	-0.59570200	0.89129800	0.39372800
Ag	-1.23232200	-1.58109300	-1.04083300
O	0.91315100	-1.59443000	-1.29242300
C	1.55559700	-1.05429000	-0.35231600
O	1.10180000	-0.26337400	0.54437000
C	3.02932500	-1.42701300	-0.23871900
H	3.06548000	-2.49748600	0.01028400
H	3.50587800	-1.31912800	-1.21693900
C	-0.99773900	3.03061100	-0.69655900
O	-1.90192100	2.45279900	0.00385100
O	-1.73645600	-0.20639400	1.68971000
C	-2.73866900	-0.93966600	1.36977100
O	-2.96266600	-1.45954000	0.24111900
C	-3.74680600	-1.16982300	2.47689400
H	-3.24734500	-1.20971400	3.44623600
H	-4.44187100	-0.32336900	2.49066000
H	-4.31148600	-2.08416400	2.29230900
C	-1.23875200	4.34668300	-1.36372100
H	-0.47538000	5.06214200	-1.04494600
H	-1.14668300	4.22552600	-2.44734400
H	-2.23239700	4.72097800	-1.11503600
O	0.12616400	2.42358600	-0.80110700
N	3.75352300	-0.62025300	0.71532000
H	3.22334900	-0.23346800	1.48225900
C	5.00124800	-0.13355600	0.42564400
O	5.61310100	-0.45346900	-0.58619900
C	5.57760000	0.82880100	1.45186800
H	6.57857900	0.48868300	1.72811900
H	5.68367100	1.81408000	0.98815200
H	4.96873100	0.92542600	2.35490800

cat13

Pd	-0.12588900	-0.26967000	0.66107500
Ag	-2.28532000	0.42601600	-1.16851000

O	-2.86791700	-1.60028300	-0.71778100
C	-2.55334400	-1.99391800	0.44000900
O	-1.68472000	-1.46609300	1.22121600
C	-3.24043800	-3.22936600	0.98501900
H	-2.62799700	-4.10188800	0.73307600
H	-3.32154600	-3.17581000	2.07155500
H	-4.22254100	-3.34914300	0.52619300
C	3.42411300	-1.17219800	-0.80610900
H	3.25539700	-1.63461400	-1.78847600
H	3.89949700	-1.92870600	-0.17287400
N	4.31657100	-0.04053500	-0.87477800
C	2.07427200	-0.81742700	-0.23472300
O	1.18435600	-1.71701500	-0.05702300
O	1.76682000	0.38927900	0.06032800
C	5.51957300	-0.05428200	-0.20584500
O	5.94875700	-1.05795300	0.34588700
C	6.27845200	1.26098100	-0.21070200
H	7.31649400	1.06495500	-0.48806600
H	5.85769800	2.00781300	-0.88923400
H	6.28114700	1.66810700	0.80505000
O	-0.90417900	1.47342200	1.39503000
C	-1.33953600	2.45439700	0.69400400
O	-1.74523900	2.40691400	-0.50113500
C	-1.33502400	3.79703900	1.39641900
H	-1.54871500	3.67186100	2.45915300
H	-0.33416000	4.23237400	1.30403100
H	-2.05534100	4.47093400	0.93172700
H	3.93355900	0.84239300	-1.17880800

A-TS1^m

C	-1.89883300	2.51316500	-0.87768800
H	-2.34407900	3.51004400	-0.87913800
H	-1.82056000	2.15401600	-1.90337800
S	-3.24452400	1.50769200	-0.13927100
O	-4.50383800	1.99193300	-0.70525200
O	-3.09758200	1.32016700	1.29646400
O	-2.84581800	0.05897100	-0.90870300
C	-3.56847000	-1.07733600	-0.55898200
C	-2.84461700	-2.20532400	-0.14168800
C	-4.95576200	-1.10827900	-0.68956600
C	-3.55843700	-3.38720800	0.14565900

C	-5.64329100	-2.28811200	-0.37742600
H	-5.46703200	-0.21771500	-1.02649000
C	-4.93569300	-3.43137400	0.03639400
H	-3.00768200	-4.26550100	0.46400600
H	-5.49138700	-4.33389100	0.26394100
C	-1.42323300	-2.17850700	-0.01751100
N	-0.26551400	-2.20822300	0.08808200
O	-6.98692800	-2.42354700	-0.45692800
C	-7.76654300	-1.29454200	-0.84329300
H	-8.80457700	-1.62633500	-0.81084700
H	-7.62784600	-0.45725700	-0.14976300
H	-7.52068000	-0.96871800	-1.86096500
Pd	2.80715600	-0.12975600	0.29267700
C	1.91367800	2.60045800	1.15821600
H	2.87178900	2.64875100	1.66578600
O	3.60723700	2.05729400	-1.82322700
O	3.86380200	-0.14727200	-1.48745700
C	1.77900900	1.75800400	0.03284300
C	0.51336700	1.73172700	-0.59487800
C	-0.58484200	2.49312100	-0.15630700
C	-0.36412000	3.31346100	0.97075500
C	0.86382000	3.37281500	1.62850800
H	2.75451200	1.84755800	-0.81988000
C	4.07315300	0.92787000	-2.14382000
C	4.95209700	0.81945100	-3.37010400
H	4.64039500	-0.03709000	-3.97237100
H	4.90368900	1.73632100	-3.95671000
H	5.98646000	0.64699100	-3.05523600
C	2.51972300	-2.52929400	1.90111800
C	1.87937600	-1.37292100	2.67593500
O	1.92302900	-0.19356600	2.08311900
O	1.35523700	-1.56771900	3.75517300
H	1.75567800	-2.98424200	1.26835500
H	2.91067100	-3.27662700	2.59627100
N	3.59763200	-2.03566000	0.99451400
H	4.40398100	-1.71317800	1.52872700
C	4.02098700	-2.95931700	-0.04235700
O	3.27116900	-3.81491100	-0.44320500
C	5.42483300	-2.73459600	-0.54968800
H	6.14577700	-2.67574000	0.27330600
H	5.69265300	-3.55747100	-1.21208500

H	5.45183200	-1.79085300	-1.10175000
H	0.98046700	4.01904400	2.49032600
Cl	0.34743000	0.75951400	-2.04712400
Cl	-1.64292000	4.35015700	1.56408300
A-TS1^P			
C	-2.18597900	-3.02740300	0.05994500
H	-2.40674200	-3.81454600	-0.66442700
H	-2.50163600	-3.34613400	1.05290000
S	-3.38760600	-1.72352200	-0.40756900
O	-4.72711200	-2.26229000	-0.17685900
O	-3.05245600	-1.08368500	-1.67089300
O	-3.02092100	-0.64867800	0.84066900
C	-3.50775800	0.65030800	0.74921100
C	-2.62553100	1.69810100	1.06294400
C	-4.83892900	0.89743900	0.41825100
C	-3.11922000	3.01983200	1.02195700
C	-5.29709100	2.21971200	0.36369200
H	-5.49230200	0.06113700	0.21204500
C	-4.42924000	3.28298900	0.67155900
H	-2.44437900	3.83418400	1.26170600
H	-4.80958100	4.29697300	0.62655300
C	-1.26691400	1.47196200	1.43955300
N	-0.15861700	1.36084600	1.77749500
O	-6.56213800	2.56770600	0.03752500
C	-7.48447800	1.54243900	-0.32399200
H	-8.41352800	2.05513100	-0.57415400
H	-7.13191900	0.97801300	-1.19475900
H	-7.66294300	0.85318100	0.50982800
Pd	2.91803700	0.31904200	-0.28685300
C	1.27198200	-2.05945800	-1.25502600
H	1.77340400	-2.01696900	-2.21413300
O	4.33299100	-2.18954800	0.63914700
O	4.24545000	-0.03710200	1.26934000
C	1.89205500	-1.55452400	-0.09869800
C	1.20227600	-1.63899600	1.12552500
C	-0.08644900	-2.15353700	1.17650700
C	-0.75498800	-2.59141900	0.01681800
C	-0.01616200	-2.57670400	-1.18609100
H	3.20283000	-1.80989600	0.09751600
C	4.74715800	-1.21032600	1.32987500
C	5.90127800	-1.43958000	2.27616700

H	5.68773300	-2.30660200	2.90604100
H	6.79671400	-1.67340100	1.69199300
H	6.08410500	-0.55892200	2.89129200
C	3.38253100	2.61723200	-2.00169600
C	2.24052300	1.78190100	-2.61734000
O	1.84173900	0.73517500	-1.91702300
O	1.79417200	2.08276600	-3.70493500
H	3.18298500	3.67387800	-2.18256500
H	4.31694000	2.33119700	-2.49198700
N	3.53970500	2.35678000	-0.54465000
H	4.50890900	2.36842700	-0.23074300
C	2.70347600	3.18728600	0.31911900
O	1.85435300	3.88950800	-0.17089000
C	2.96117300	3.05234100	1.79833600
H	2.95654800	4.04791900	2.24832100
H	2.12322100	2.48475500	2.21834000
H	3.88916300	2.52746700	2.03159500
H	1.66405400	-1.29162000	2.04250400
Cl	-0.86133800	-2.25430200	2.75126700
Cl	-0.71549300	-3.23190400	-2.65713800

B-TS1^m

C	-0.43682300	-3.38751500	2.02549000
C	0.76523800	-3.48940000	1.32792700
C	0.93324000	-2.95805500	0.03088700
C	-0.20147000	-2.36257600	-0.55205700
C	-1.42377100	-2.18952300	0.12856600
C	-1.50435800	-2.72695600	1.42974100
H	-0.51948900	-3.81710400	3.01706100
H	-2.52831600	-2.34818000	-0.58737000
H	-2.43849400	-2.63540500	1.97740200
Cl	2.07604600	-4.35446300	2.10439800
C	2.26096800	-3.00822000	-0.66390500
H	2.82818400	-3.91072000	-0.42692300
H	2.17794400	-2.90687400	-1.74566700
S	3.41692300	-1.67324200	-0.16099700
O	4.68372800	-1.88217600	-0.85741400
O	3.38771800	-1.41898800	1.27361600
O	2.59374500	-0.41183800	-0.92435400
C	2.89033400	0.88984600	-0.54301200
C	1.82799900	1.68478700	-0.07638300

C	4.17146800	1.40722000	-0.68864000
C	2.06341900	3.04335100	0.22886400
C	4.39789500	2.75088700	-0.35171600
H	4.95615700	0.76406300	-1.06316600
C	3.33740100	3.56276600	0.09674300
H	1.23112700	3.66194400	0.55507800
H	3.54480100	4.60145500	0.32758900
C	0.54099700	1.10706700	0.06784300
N	-0.49254800	0.59776800	0.18089600
O	5.60115400	3.35568400	-0.44320700
C	6.72365300	2.59477300	-0.88562000
H	7.57239000	3.27829500	-0.86017800
H	6.91693600	1.74607500	-0.21971900
H	6.57932100	2.23144200	-1.90969900
Cl	-0.12701000	-1.82138000	-2.22103500
Pd	-2.33212800	-0.18379000	0.08148000
C	-3.26653500	3.91727800	-0.58374200
H	-4.28264700	4.15913900	-0.90919300
H	-2.56906300	4.44237700	-1.23746900
N	-3.07897200	4.38769000	0.77707700
C	-3.02696600	2.40649700	-0.80027600
O	-3.02470100	1.71626400	0.30801600
O	-2.86593500	1.97938000	-1.93713000
C	-1.82327900	4.47839900	1.30480300
O	-0.81049900	4.40530200	0.60911300
C	-1.75367200	4.68755100	2.80779800
H	-0.95715800	5.40055000	3.02981500
H	-2.69253200	5.04721200	3.23747200
H	-1.49504500	3.73601300	3.28459400
H	-3.83241000	4.21137800	1.42592900
O	-3.65791500	-2.70852500	-1.12636500
C	-4.52763000	-1.87664700	-0.72931400
O	-4.26251200	-0.81358900	-0.07652400
C	-5.97913600	-2.12915000	-1.06032000
H	-6.16246200	-3.19775900	-1.17695000
H	-6.62440200	-1.70154700	-0.29186100
H	-6.20282900	-1.63141000	-2.00994700

B-TS1^p

C	-0.02705800	-2.86373300	0.67005900
C	1.32314100	-3.00166500	0.36392700

C	1.86895900	-2.47279900	-0.82393600
C	0.95602000	-1.94136100	-1.75934800
C	-0.39886500	-1.82465500	-1.47673100
C	-0.90386800	-2.21903900	-0.22284600
H	-1.05419500	-1.37868400	-2.21764200
H	-2.16538300	-2.70488400	-0.21236100
Cl	2.34718000	-3.84740900	1.51112600
C	3.34594500	-2.40503700	-1.05576500
H	3.88412000	-3.25309800	-0.62611600
H	3.60648400	-2.29701200	-2.10769300
S	4.14867600	-0.96828400	-0.23096200
O	5.43165600	-0.72244500	-0.88274000
O	4.05167000	-1.04492600	1.22019300
O	3.04780900	0.21584500	-0.74759000
C	3.07411000	1.43355900	-0.08626700
C	1.90175000	1.86202800	0.56567600
C	4.21192300	2.23161700	-0.12103200
C	1.89443800	3.13289100	1.18524500
C	4.19110900	3.48109700	0.51770000
H	5.08615500	1.86642700	-0.64253600
C	3.02167700	3.92831900	1.16594100
H	0.99210900	3.47195500	1.68263600
H	3.03168800	4.90185700	1.64210400
C	0.73581400	1.05429700	0.60517900
N	-0.24558100	0.43992500	0.65709600
O	5.23774000	4.32606300	0.55281400
C	6.46390200	3.93964300	-0.07038000
H	7.15509400	4.76340400	0.10590600
H	6.86377500	3.02272300	0.37634100
H	6.33185000	3.79802700	-1.14893300
Pd	-1.98792100	-0.57397600	0.75506500
C	-3.98488200	1.79352200	-0.10631600
H	-4.52419100	0.84133100	-0.20075100
H	-3.09666600	1.72238100	-0.75200500
N	-4.80921500	2.93168600	-0.43792600
C	-3.51052500	1.92352200	1.35213600
O	-3.86968300	2.87003400	2.03806700
O	-2.71618100	0.98860900	1.81686600
C	-5.43366200	3.19943700	-1.62260400
O	-6.12035500	4.20206200	-1.78179500
C	-5.22372400	2.17977600	-2.73611900

H	-5.76975100	2.52031600	-3.61544900
H	-4.16213400	2.07521800	-2.98828200
H	-5.59068400	1.18896700	-2.44447600
H	-0.38884100	-3.23989100	1.62150200
Cl	1.51930300	-1.35952300	-3.32069100
H	-4.94528500	3.59025300	0.32274500
O	-3.27949900	-3.29402900	-0.22278200
C	-4.10665500	-2.56537600	0.40683300
O	-3.82922900	-1.42499900	0.90089800
C	-5.50726600	-3.08615600	0.61595500
H	-6.19188500	-2.26762100	0.83706400
H	-5.83307000	-3.64363100	-0.26377400
H	-5.49538500	-3.77506700	1.46724400

C-TS1^m

C	-0.15963100	-3.23136100	-1.68637500
C	-1.33142300	-3.26270300	-0.93281700
C	-1.47650100	-2.53720600	0.27061400
C	-0.35157900	-1.80931800	0.69900900
C	0.83944600	-1.70677000	-0.04804700
C	0.90023900	-2.44673600	-1.24763000
H	-0.09301500	-3.81224900	-2.59888800
H	1.95534800	-1.70223900	0.65957300
H	1.81275900	-2.41366100	-1.83674000
Cl	-2.63172700	-4.28474800	-1.50743800
C	-2.77082700	-2.53486900	1.02654800
H	-3.30381500	-3.48541700	0.95634700
H	-2.65040300	-2.26415300	2.07526400
S	-4.00439700	-1.34092400	0.37922500
O	-5.23181400	-1.47631500	1.15823600
O	-4.04189500	-1.30579700	-1.07662500
O	-3.20184500	0.06068800	0.90021800
C	-3.57002000	1.26496300	0.32639400
C	-2.56130000	2.02016400	-0.30083800
C	-4.87338000	1.73959700	0.42385800
C	-2.88977000	3.28675700	-0.83043900
C	-5.18480700	2.99098200	-0.12884000
H	-5.61304200	1.13132300	0.92673300
C	-4.18265400	3.76386500	-0.75052000
H	-2.11515100	3.87804800	-1.30634600
H	-4.45268300	4.73137000	-1.15753100

C	-1.24164800	1.50568900	-0.38440300
N	-0.16845800	1.07330800	-0.43840500
O	-6.41332300	3.54236600	-0.10124300
C	-7.48616200	2.81488300	0.49877700
H	-8.36850700	3.44399300	0.38362700
H	-7.64896300	1.85780400	-0.00894000
H	-7.29910100	2.63995100	1.56426400
Cl	-0.38857500	-1.00969200	2.26373500
Pd	1.68172800	0.30217800	-0.39886500
C	3.32668500	2.67657000	-0.17899000
O	2.38926000	2.13912800	-0.91540400
O	3.77401800	2.22843000	0.87975600
O	3.10648200	-1.84333800	1.27395000
C	3.91834400	-1.12029500	0.62469500
O	3.59039000	-0.37619100	-0.35717100
C	5.37848100	-1.10587800	1.05141400
H	5.94788400	-1.84159200	0.47016500
H	5.41147000	-1.41158100	2.10273900
N	5.98306500	0.18456200	0.82662800
H	5.39404700	1.00324000	0.96516600
C	7.13281000	0.29195800	0.09336400
C	7.58410700	1.71715900	-0.18239800
H	7.77541200	1.82110100	-1.25357400
H	6.85610300	2.46803100	0.13448100
H	8.53043900	1.89631300	0.33675200
O	7.77263700	-0.68250700	-0.28994400
C	3.86992100	3.96693900	-0.78537100
H	3.07599300	4.54468900	-1.26321800
H	4.35967600	4.55924400	-0.01072300
H	4.60601200	3.71275600	-1.55579400

C-TS1^p

C	0.43725600	-2.16103300	-1.13219000
C	-0.83407000	-2.69487000	-0.94563300
C	-1.49438300	-2.61406100	0.29734500
C	-0.73892500	-2.11995800	1.38117800
C	0.54553400	-1.61794700	1.21376800
C	1.12995700	-1.55771700	-0.06572000
H	1.06718000	-1.21733300	2.07692300
H	2.51747700	-1.75960200	-0.13659100
Cl	-1.61617300	-3.46506400	-2.31682800

C	-2.94355000	-2.95314900	0.45029400
H	-3.25938900	-3.77914400	-0.19115100
H	-3.22518400	-3.15777400	1.48216000
S	-4.07292900	-1.59590200	-0.07349000
O	-5.36940100	-1.80534500	0.56532000
O	-3.98262700	-1.32740800	-1.50222000
O	-3.27728700	-0.32905400	0.72877300
C	-3.59751700	0.96328400	0.34456300
C	-2.55990500	1.79715900	-0.11482500
C	-4.89945600	1.43602500	0.46868900
C	-2.86204600	3.13838300	-0.44436500
C	-5.18274300	2.76376000	0.11488500
H	-5.66268900	0.76401700	0.83663900
C	-4.15293500	3.61390400	-0.33636600
H	-2.06503400	3.78730600	-0.79122900
H	-4.39889700	4.63775400	-0.59301500
C	-1.22690400	1.32683700	-0.24478200
N	-0.12105600	1.00003100	-0.36004500
O	-6.40843800	3.31671200	0.18577400
C	-7.50846400	2.51175400	0.61282800
H	-8.38305200	3.16011800	0.56517400
H	-7.65162200	1.65225900	-0.05123900
H	-7.36797300	2.16297600	1.64216600
Pd	1.82049600	0.47921900	-0.52910900
C	2.68223300	3.32982200	-0.37109700
O	2.79129800	4.46143800	-0.81386400
O	2.16949400	2.36718800	-1.12848100
H	0.87442900	-2.19224800	-2.12521100
Cl	-1.42929300	-2.07936200	3.00031000
O	3.69041100	-2.06254600	-0.20189100
C	4.34305400	-1.00967000	-0.50017700
O	3.83676900	0.13046700	-0.68644500
C	5.85588300	-1.15735400	-0.69034900
H	6.00671100	-1.43692300	-1.74137600
H	6.19252400	-2.00344200	-0.09138900
N	6.61731200	0.02659300	-0.38412700
H	6.48208400	0.82980100	-0.98643200
C	7.14782500	0.36373300	0.84848400
O	7.55645900	1.49410100	1.05893600
C	7.23579500	-0.74006100	1.89254200
H	6.24509500	-1.10719900	2.18235900

H	7.81533200	-1.59477300	1.52765400
H	7.72864900	-0.32312300	2.76997300
C	3.12838100	2.97026400	1.04073400
H	2.30261600	2.53200100	1.61239800
H	3.93898700	2.23600900	1.00434900
H	3.48240800	3.86951000	1.54668100

E-TS1^m

C	-1.89883300	2.51316500	-0.87768800
H	-2.34407900	3.51004400	-0.87913800
H	-1.82056000	2.15401600	-1.90337800
S	-3.24452400	1.50769200	-0.13927100
O	-4.50383800	1.99193300	-0.70525200
O	-3.09758200	1.32016700	1.29646400
O	-2.84581800	0.05897100	-0.90870300
C	-3.56847000	-1.07733600	-0.55898200
C	-2.84461700	-2.20532400	-0.14168800
C	-4.95576200	-1.10827900	-0.68956600
C	-3.55843700	-3.38720800	0.14565900
C	-5.64329100	-2.28811200	-0.37742600
H	-5.46703200	-0.21771500	-1.02649000
C	-4.93569300	-3.43137400	0.03639400
H	-3.00768200	-4.26550100	0.46400600
H	-5.49138700	-4.33389100	0.26394100
C	-1.42323300	-2.17850700	-0.01751100
N	-0.26551400	-2.20822300	0.08808200
O	-6.98692800	-2.42354700	-0.45692800
C	-7.76654300	-1.29454200	-0.84329300
H	-8.80457700	-1.62633500	-0.81084700
H	-7.62784600	-0.45725700	-0.14976300
H	-7.52068000	-0.96871800	-1.86096500
Pd	2.80715600	-0.12975600	0.29267700
C	1.91367800	2.60045800	1.15821600
H	2.87178900	2.64875100	1.66578600
O	3.60723700	2.05729400	-1.82322700
O	3.86380200	-0.14727200	-1.48745700
C	1.77900900	1.75800400	0.03284300
C	0.51336700	1.73172700	-0.59487800
C	-0.58484200	2.49312100	-0.15630700
C	-0.36412000	3.31346100	0.97075500
C	0.86382000	3.37281500	1.62850800

H	2.75451200	1.84755800	-0.81988000
C	4.07315300	0.92787000	-2.14382000
C	4.95209700	0.81945100	-3.37010400
H	4.64039500	-0.03709000	-3.97237100
H	4.90368900	1.73632100	-3.95671000
H	5.98646000	0.64699100	-3.05523600
C	2.51972300	-2.52929400	1.90111800
C	1.87937600	-1.37292100	2.67593500
O	1.92302900	-0.19356600	2.08311900
O	1.35523700	-1.56771900	3.75517300
H	1.75567800	-2.98424200	1.26835500
H	2.91067100	-3.27662700	2.59627100
N	3.59763200	-2.03566000	0.99451400
H	4.40398100	-1.71317800	1.52872700
C	4.02098700	-2.95931700	-0.04235700
O	3.27116900	-3.81491100	-0.44320500
C	5.42483300	-2.73459600	-0.54968800
H	6.14577700	-2.67574000	0.27330600
H	5.69265300	-3.55747100	-1.21208500
H	5.45183200	-1.79085300	-1.10175000
H	0.98046700	4.01904400	2.49032600
Cl	0.34743000	0.75951400	-2.04712400
Cl	-1.64292000	4.35015700	1.56408300

E-TS1^P

C	-2.18597900	-3.02740300	0.05994500
H	-2.40674200	-3.81454600	-0.66442700
H	-2.50163600	-3.34613400	1.05290000
S	-3.38760600	-1.72352200	-0.40756900
O	-4.72711200	-2.26229000	-0.17685900
O	-3.05245600	-1.08368500	-1.67089300
O	-3.02092100	-0.64867800	0.84066900
C	-3.50775800	0.65030800	0.74921100
C	-2.62553100	1.69810100	1.06294400
C	-4.83892900	0.89743900	0.41825100
C	-3.11922000	3.01983200	1.02195700
C	-5.29709100	2.21971200	0.36369200
H	-5.49230200	0.06113700	0.21204500
C	-4.42924000	3.28298900	0.67155900
H	-2.44437900	3.83418400	1.26170600
H	-4.80958100	4.29697300	0.62655300

C	-1.26691400	1.47196200	1.43955300
N	-0.15861700	1.36084600	1.77749500
O	-6.56213800	2.56770600	0.03752500
C	-7.48447800	1.54243900	-0.32399200
H	-8.41352800	2.05513100	-0.57415400
H	-7.13191900	0.97801300	-1.19475900
H	-7.66294300	0.85318100	0.50982800
Pd	2.91803700	0.31904200	-0.28685300
C	1.27198200	-2.05945800	-1.25502600
H	1.77340400	-2.01696900	-2.21413300
O	4.33299100	-2.18954800	0.63914700
O	4.24545000	-0.03710200	1.26934000
C	1.89205500	-1.55452400	-0.09869800
C	1.20227600	-1.63899600	1.12552500
C	-0.08644900	-2.15353700	1.17650700
C	-0.75498800	-2.59141900	0.01681800
C	-0.01616200	-2.57670400	-1.18609100
H	3.20283000	-1.80989600	0.09751600
C	4.74715800	-1.21032600	1.32987500
C	5.90127800	-1.43958000	2.27616700
H	5.68773300	-2.30660200	2.90604100
H	6.79671400	-1.67340100	1.69199300
H	6.08410500	-0.55892200	2.89129200
C	3.38253100	2.61723200	-2.00169600
C	2.24052300	1.78190100	-2.61734000
O	1.84173900	0.73517500	-1.91702300
O	1.79417200	2.08276600	-3.70493500
H	3.18298500	3.67387800	-2.18256500
H	4.31694000	2.33119700	-2.49198700
N	3.53970500	2.35678000	-0.54465000
H	4.50890900	2.36842700	-0.23074300
C	2.70347600	3.18728600	0.31911900
O	1.85435300	3.88950800	-0.17089000
C	2.96117300	3.05234100	1.79833600
H	2.95654800	4.04791900	2.24832100
H	2.12322100	2.48475500	2.21834000
H	3.88916300	2.52746700	2.03159500
H	1.66405400	-1.29162000	2.04250400
Cl	-0.86133800	-2.25430200	2.75126700
Cl	-0.71549300	-3.23190400	-2.65713800

F-TS1^m

Pd	-2.70564400	0.82489400	-0.37134200
C	-1.52500600	2.41242400	0.56243800
C	-0.59466800	4.42427200	-0.47815300
H	-0.71721500	5.33569400	-1.05145400
C	0.67324100	4.04979900	-0.03510800
C	0.89879900	2.89133500	0.73444500
C	-0.22586300	2.09138600	1.01104900
O	-1.47199100	1.11222500	-1.97342900
C	-0.85656200	0.20663000	-2.62120400
C	-1.67544400	3.61122000	-0.16770700
O	-0.78237600	-1.02847600	-2.35098200
H	-2.43320600	2.20670200	1.43948200
H	-2.66812300	3.90399900	-0.49797200
C	-0.09052500	0.67784700	-3.84015800
H	0.90710200	0.98758600	-3.50949800
H	-0.58538100	1.53617200	-4.29700900
H	0.01727600	-0.13596500	-4.55845800
C	-4.01734800	-1.59805700	-1.62348200
O	-3.97351900	-0.33558300	-1.52409700
O	-3.14200100	-2.43368600	-1.25002100
C	-5.27653400	-2.17943000	-2.23585800
H	-6.00811900	-2.33207500	-1.43535000
H	-5.06574900	-3.14264000	-2.70193000
H	-5.70205600	-1.48153100	-2.95856400
C	-4.07356100	1.15545500	2.20076800
O	-3.30559300	2.12215900	2.46508800
O	-4.04914500	0.48350400	1.11607300
C	-5.08405800	0.72099300	3.23896800
H	-4.60637100	-0.01719200	3.89192900
H	-5.94669100	0.25399200	2.76263100
H	-5.38749600	1.57370000	3.84773200
C	2.26051700	2.56358600	1.26283300
H	2.85110100	3.45616300	1.47140400
H	2.21840400	1.92856600	2.14756700
S	3.33465600	1.64032000	0.07888500
O	4.69927900	2.15745900	0.16083000
O	2.69949900	1.42840700	-1.21722100
O	3.28731700	0.17040000	0.92958600
C	4.00279000	-0.89733600	0.41435500
C	3.28305500	-2.00877900	-0.05802800

C	5.39427500	-0.89001500	0.43437500
C	4.00038900	-3.13966200	-0.50311700
C	6.08827200	-2.01645800	-0.02996000
H	5.90121200	-0.01039500	0.80493300
C	5.38172700	-3.14469600	-0.49064000
H	3.45314500	-4.00456600	-0.86176700
H	5.94480700	-4.00515900	-0.83341900
C	1.86333200	-1.98927100	-0.11239900
N	0.70917700	-2.00708700	-0.18830000
O	7.43371100	-2.11398400	-0.06424400
C	8.21576300	-1.00143700	0.36848900
H	9.25485400	-1.29823000	0.22625200
H	8.00362100	-0.10904400	-0.23098500
H	8.04139900	-0.78159300	1.42808900
Cl	-0.04509000	0.63841800	1.95593600
Cl	2.01982800	5.09297700	-0.45305700
Pd	-1.23881300	-2.07936500	-0.62474400
C	-1.22750200	-3.19740400	2.07557900
O	-0.47076000	-2.32159700	2.47908400
O	-1.69015500	-3.34059900	0.85277000
C	-1.76284000	-4.29312500	2.99570200
H	-2.85285400	-4.22217300	3.05950400
H	-1.52508700	-5.27971400	2.58793900
H	-1.32648500	-4.18336800	3.98925600

F-TS1^p

C	0.85928900	-3.06468000	-0.42048900
C	-0.49304000	-3.32801800	-0.25879600
C	-1.26115000	-2.70958500	0.75137300
C	-0.57312200	-1.85576600	1.63654500
C	0.77313300	-1.55013700	1.47091400
C	1.50297000	-2.13664000	0.41981900
H	1.40515000	-3.55720000	-1.21674300
H	2.70758600	-2.42459500	0.77039200
Cl	-1.24674200	-4.47803800	-1.35910800
C	-2.73495100	-2.94123900	0.85870700
H	-3.03181100	-3.93054500	0.50546700
H	-3.12080000	-2.77788500	1.86513000
S	-3.74065500	-1.82858000	-0.19863200
O	-5.14085600	-2.23310900	-0.08782100
O	-3.14033400	-1.58166900	-1.50331400

O	-3.50187100	-0.44205700	0.74576100
C	-4.10580700	0.74242300	0.36536700
C	-3.27721700	1.85495400	0.13201900
C	-5.49231900	0.84762800	0.29845300
C	-3.88097500	3.09856300	-0.16093200
C	-6.06925900	2.08599400	-0.01711700
H	-6.08816100	-0.03299300	0.49177100
C	-5.25433700	3.21422200	-0.23740500
H	-3.24860700	3.96259200	-0.33367400
H	-5.72838700	4.16140200	-0.46738100
C	-1.85903900	1.75836000	0.15278200
N	-0.70053600	1.77604700	0.12120100
O	-7.39712600	2.29442300	-0.11892800
C	-8.28569400	1.19296800	0.07156100
H	-9.28741800	1.59231500	-0.08615400
H	-8.08998300	0.39501000	-0.65320500
H	-8.20856600	0.79256700	1.08880900
Cl	-1.39947100	-1.15458700	3.02364800
Pd	2.81184900	-0.72308100	-0.60409000
Pd	1.24261600	2.02565900	-0.34974600
C	0.85780200	0.15316100	-2.68529200
O	1.48829100	-0.81654100	-2.16242900
O	0.76487900	1.33709200	-2.24055200
C	3.99176700	1.86105900	-1.52125500
O	3.98953500	0.60371100	-1.67749000
O	3.11604200	2.57018200	-0.93597600
C	1.97758700	2.30804300	2.41818900
O	2.08871300	1.08553300	2.48870200
O	1.59260800	2.99064600	1.36833700
C	4.53652000	-1.71044700	1.48707300
O	3.83126400	-2.75825800	1.47923800
O	4.30969700	-0.68293800	0.76396700
C	2.32192900	3.21313900	3.59561900
H	2.32331600	2.63059500	4.51807700
H	3.32137900	3.63279300	3.43926100
H	1.62024800	4.04690500	3.67053400
C	5.71372800	-1.61850700	2.43135600
H	6.05607700	-2.61610700	2.70737400
H	6.52040500	-1.04101200	1.97735200
H	5.38522900	-1.09366000	3.33456500
H	1.24979300	-0.83512400	2.13388300

C	5.19194100	2.60580000	-2.07055400
H	5.97540200	2.60492900	-1.30531900
H	5.57921300	2.09496200	-2.95354700
H	4.93064300	3.63903400	-2.30156500
C	0.10181400	-0.15500500	-3.96064900
H	-0.06709200	0.75761300	-4.53341700
H	0.64367600	-0.89169400	-4.55589000
H	-0.86899800	-0.58279400	-3.68640700

G-TS1^m

C	-0.11206200	-4.68313400	-0.37213400
C	1.03627500	-4.18100100	-0.98310600
C	1.15268000	-2.83765500	-1.39333900
C	0.05726200	-2.00014400	-1.11393200
C	-1.11097100	-2.44818800	-0.46223000
C	-1.17028800	-3.81906100	-0.12759800
H	-0.16096600	-5.72999300	-0.09614100
H	-2.19782100	-1.96987200	-1.00206000
H	-2.06966400	-4.20740300	0.34208200
Cl	2.36387600	-5.29382700	-1.25463200
C	2.36590100	-2.35058900	-2.12196600
H	2.84452400	-3.13869800	-2.70388900
H	2.15108700	-1.49446300	-2.76141800
S	3.73619600	-1.77831300	-1.02580400
O	5.01499900	-2.17682900	-1.61009600
O	3.46320600	-2.00699900	0.38866700
O	3.51569600	-0.12242000	-1.33855700
C	4.39716600	0.77572100	-0.76054800
C	3.88702300	1.68606600	0.18242300
C	5.72812000	0.82094500	-1.16371600
C	4.75103600	2.67048300	0.70928400
C	6.57523100	1.79334800	-0.61246900
H	6.07308900	0.09945100	-1.89044300
C	6.07492400	2.72405500	0.31962000
H	4.36386900	3.38197900	1.43045100
H	6.74970300	3.47198700	0.71980500
C	2.53862200	1.60498500	0.62208600
N	1.45385000	1.56345500	1.02309100
O	7.88086100	1.92019700	-0.92394900
C	8.46327000	0.99765700	-1.84491300
H	9.51434900	1.27677600	-1.91635800

H	8.38050700	-0.03242600	-1.48082100
H	7.99690400	1.07672200	-2.83362400
Cl	0.10267900	-0.32600700	-1.60439100
Pd	-1.90459900	-1.27358200	1.19216500
Pd	-0.27468800	1.41637800	2.02098200
C	0.50641900	-1.38297700	2.94251400
O	-0.31792500	-2.03491200	2.22774900
O	0.58926100	-0.12574400	3.08308000
C	1.53524700	-2.21082300	3.68355700
H	2.37855800	-2.38165900	3.00538900
H	1.89540400	-1.67249500	4.56110900
H	1.11674900	-3.17805600	3.96580500
C	-2.69452500	0.52784500	3.51539200
O	-2.77650600	-0.59969700	2.94676500
O	-1.88329400	1.46780900	3.25398800
C	-3.65423100	0.77639300	4.66185900
H	-3.26614800	0.27769300	5.55625300
H	-3.73918500	1.84449300	4.86287200
H	-4.63013300	0.34590100	4.43089600
C	-1.73676000	4.66685500	-0.35966600
H	-1.22239900	5.47382900	0.17484600
H	-2.76195300	4.64821800	0.02931600
N	-1.71188200	4.88194500	-1.78900800
C	-1.05762600	3.32765200	-0.04315500
O	-0.60843300	2.62015400	-0.94387200
O	-1.04550500	3.09230300	1.23757100
C	-2.16173000	6.03061900	-2.35983600
O	-2.64698000	6.94923900	-1.70611900
C	-2.02665600	6.10357700	-3.87599500
H	-1.58439500	5.20887700	-4.32332300
H	-3.01683800	6.26765000	-4.31015000
H	-1.41248000	6.97121000	-4.13301300
C	-5.17241900	-0.12345900	-1.40584200
H	-5.02296400	0.95842200	-1.33464700
H	-5.97862300	-0.39855400	-0.72230900
N	-5.56280800	-0.50193700	-2.73930200
C	-3.89476500	-0.80071100	-0.90194100
O	-3.25089200	-1.56305600	-1.67519300
O	-3.57139000	-0.52186100	0.29406400
C	-6.33700000	-1.62472500	-2.93825700
O	-6.87288200	-2.21842800	-2.01351700

C	-6.47934100	-2.06013700	-4.38651000
H	-7.47601200	-2.48012100	-4.52978100
H	-6.31991300	-1.24347900	-5.09633000
H	-5.74841200	-2.84890900	-4.59500900
H	-1.27908200	4.13765800	-2.32106100
H	-4.98181100	-0.18703500	-3.50255300

G-TS1^p

C	-1.19594500	-3.12344300	0.06469900
C	-0.00080200	-3.64907600	-0.40846900
C	0.79663800	-2.96911000	-1.35422700
C	0.29035100	-1.74962400	-1.84856000
C	-0.89913100	-1.20495400	-1.37713800
C	-1.65275600	-1.87488100	-0.39496400
H	-1.76369600	-3.67739100	0.80289600
H	-2.94615400	-1.80475200	-0.64409800
Cl	0.49663300	-5.22273900	0.19611400
C	2.11059100	-3.52455800	-1.80887600
H	2.12278100	-4.61635600	-1.80981100
H	2.41142200	-3.15516900	-2.78937900
S	3.52193700	-3.11433600	-0.71323400
O	4.71737300	-3.75677000	-1.25352600
O	3.18992500	-3.22553100	0.70071700
O	3.56462300	-1.47113300	-1.10404300
C	4.48884500	-0.66644600	-0.45529500
C	4.00155400	0.38335000	0.34103500
C	5.85264400	-0.85107100	-0.65686700
C	4.92646100	1.27596800	0.92763600
C	6.75630700	0.03030800	-0.04474800
H	6.17866600	-1.66995900	-1.28260300
C	6.28317100	1.10041100	0.74071400
H	4.55352900	2.09903700	1.52733100
H	7.00463900	1.77435100	1.18809000
C	2.61304700	0.56377700	0.58079600
N	1.50849100	0.78742700	0.84627800
O	8.09563000	-0.06115800	-0.16352300
C	8.65032500	-1.12915100	-0.93194600
H	9.73148700	-1.00995200	-0.86410500
H	8.36199300	-2.10391200	-0.52301600
H	8.34143800	-1.06458400	-1.98149900
Cl	1.13259500	-0.87862300	-3.12083300

Pd	-2.54600200	-0.55230800	1.06248100
Pd	-0.24267100	1.46007700	1.56255500
C	-0.58476800	-0.98367400	3.26869600
O	-1.46411000	-1.50523700	2.51100900
O	-0.05536700	0.16099300	3.15470000
C	-2.94357300	1.85916300	2.77297800
O	-3.36619800	0.69608100	2.49122900
O	-1.83377900	2.37524500	2.44012500
C	0.44609300	3.69590800	-0.06209100
O	1.42485900	3.87155700	0.66247700
O	-0.43841600	2.74155700	0.03431900
C	-4.43671600	-0.44588700	-1.07618600
O	-4.12841100	-1.65923300	-1.26902300
O	-3.83938200	0.32457300	-0.25844800
C	0.13542700	4.64529100	-1.22330000
H	0.03767500	4.08156500	-2.15676800
H	-0.84291900	5.10799900	-1.03843700
C	-5.55594900	0.18445400	-1.89185600
H	-6.27833400	0.65056600	-1.21595900
H	-5.10402600	0.99073400	-2.48555300
H	-1.23925200	-0.25661500	-1.77885400
N	1.18791300	5.62962900	-1.33546200
C	1.39752800	6.33505000	-2.48023400
O	0.66387600	6.24151800	-3.45991800
C	2.60385700	7.26491900	-2.46209400
H	2.26018000	8.29026600	-2.62512900
H	3.17572500	7.22661600	-1.53081200
H	3.26002400	7.00589700	-3.29763900
H	1.85398500	5.62880800	-0.57353000
C	-0.09691500	-1.84809900	4.41196100
H	-0.90638300	-2.47749800	4.78482500
H	0.70090800	-2.49925700	4.03867200
H	0.30890300	-1.22531000	5.20988900
C	-3.87837100	2.74188000	3.57260100
H	-4.53513100	2.13266600	4.19495300
H	-3.30977500	3.44796700	4.17903600
H	-4.49815800	3.30876300	2.86981300
N	-6.26934700	-0.76522400	-2.70987500
C	-7.62870100	-0.92738700	-2.57816900
C	-8.22187800	-2.08290600	-3.36636100
H	-7.51663900	-2.55039000	-4.05877800

H	-8.58228100	-2.83961700	-2.66290300
H	-9.08646800	-1.71751300	-3.92509800
O	-8.31409700	-0.18912400	-1.88387800
H	-5.72868100	-1.49261700	-3.15396500
H-TS1^m			
C	-1.03722100	3.76081000	2.49354500
C	-2.25479800	3.33436700	1.96433300
C	-2.37574700	2.81244500	0.65938500
C	-1.18813700	2.72333400	-0.09059000
C	0.06813600	3.14712100	0.39589300
C	0.09950800	3.67772000	1.70483900
H	-0.99970300	4.16438900	3.49851500
H	0.71528600	3.81221300	-0.45093300
H	1.04412900	4.03782700	2.10076100
Cl	-3.67712400	3.50991300	2.96853300
C	-3.72165100	2.47129500	0.09457800
H	-4.49176200	3.16485800	0.43662800
H	-3.72201000	2.43586800	-0.99440700
S	-4.40819400	0.84701600	0.61601200
O	-5.86675500	0.93785800	0.59411000
O	-3.70893200	0.27227400	1.75631700
O	-3.92287600	-0.00082000	-0.77293700
C	-4.16048400	-1.36694400	-0.79606700
C	-3.04879100	-2.22038900	-0.89180900
C	-5.45864900	-1.86708900	-0.79343000
C	-3.26427400	-3.61102400	-1.00330200
C	-5.65222800	-3.25363600	-0.88150700
H	-6.28323800	-1.17226700	-0.72009300
C	-4.54765000	-4.12098700	-0.99542000
H	-2.40840700	-4.27125800	-1.09059200
H	-4.73040500	-5.18647900	-1.07358700
C	-1.72862100	-1.69946000	-0.87981500
N	-0.63350400	-1.32661800	-0.87909100
O	-6.86361400	-3.84674000	-0.87697800
C	-8.02866600	-3.03477100	-0.73452000
H	-8.87073200	-3.72672600	-0.72501500
H	-8.00683800	-2.46991000	0.20409000
H	-8.13556800	-2.34211500	-1.57736200
Cl	-1.26148600	2.14133700	-1.74156300
Pd	1.89607800	1.97347800	0.03386100
Pd	1.32592600	-0.96057700	-0.95114600

C	1.55872000	-0.22162600	1.98027700
O	1.52037300	1.04124000	1.81619000
O	1.47573400	-1.12027700	1.09905700
C	1.72957500	-0.68741200	3.42955500
H	2.27667100	0.09429100	3.96537700
H	0.73687100	-0.78994300	3.88245900
C	4.09341700	-0.04987000	-0.42204700
O	3.77309100	1.06954000	0.06491500
O	3.36466400	-0.87974000	-1.03486800
C	5.56947500	-0.44504100	-0.24941800
H	6.14761700	-0.00404600	-1.06675800
H	5.92084100	-0.01556000	0.68913200
C	1.12342600	-2.03094700	-3.54756600
O	0.98144600	-3.11325500	-2.98602300
O	1.26513600	-0.86940600	-2.94583000
C	2.08695500	4.00552500	-2.04948300
O	1.20684000	4.66797200	-1.43850900
O	2.51873800	2.85965600	-1.68151300
C	1.15882700	-1.89529000	-5.06567900
H	0.40991700	-1.17132300	-5.39949600
H	2.13751000	-1.51982100	-5.37991400
H	0.97215900	-2.86611300	-5.52621800
C	2.67315800	4.55607100	-3.33156800
H	3.71745600	4.25698600	-3.43192700
H	2.11535400	4.13387800	-4.17408800
H	2.57443400	5.64170200	-3.35465700
N	5.77505400	-1.87863600	-0.23852500
C	5.29018400	-2.62250500	0.80268600
O	4.88483400	-2.09451100	1.83836900
C	5.28857300	-4.12374100	0.59838900
H	5.95425400	-4.44818800	-0.20555800
H	5.58151500	-4.61034000	1.53068500
H	4.26868100	-4.44116900	0.35618700
H	5.85780800	-2.33956700	-1.13330000
N	2.37839900	-1.96852800	3.53901100
C	1.68023500	-3.07473900	3.94154000
O	0.52600100	-3.02643200	4.35382800
C	2.45712300	-4.38033400	3.87125500
H	2.47621700	-4.83418600	4.86588100
H	1.92412600	-5.06840800	3.20870000
H	3.48066300	-4.25234100	3.51081100

H	3.27301300	-2.08887100	3.07201800
H-TS1^p			
C	0.15341400	-2.07798500	2.59202000
C	-1.22270100	-2.17292800	2.74481600
C	-2.06585300	-1.04378600	2.65833800
C	-1.43765100	0.20275100	2.46490200
C	-0.06368400	0.31633200	2.28379400
C	0.75073000	-0.83051500	2.32974000
H	0.75854400	-2.97412800	2.66108000
H	1.86262500	-0.60477400	2.94370100
Cl	-1.90490300	-3.75993700	3.07761400
C	-3.55309100	-1.16848700	2.76878400
H	-3.85738500	-1.99663200	3.41227700
H	-4.03134300	-0.24844700	3.10485600
S	-4.39774900	-1.56676400	1.19211500
O	-5.83234800	-1.65316300	1.45804500
O	-3.71904700	-2.60427800	0.42856600
O	-4.07197500	-0.08185200	0.44513700
C	-4.52365900	0.13094800	-0.84501900
C	-3.57369900	0.48452500	-1.82026500
C	-5.88147900	0.07571000	-1.14661100
C	-4.02505700	0.79866000	-3.12244900
C	-6.30441700	0.36733700	-2.45138700
H	-6.57628400	-0.19092000	-0.36299800
C	-5.36753900	0.73852100	-3.43629100
H	-3.29902500	1.08059600	-3.87719900
H	-5.72443400	0.97056300	-4.43302800
C	-2.17923500	0.51327200	-1.54693400
N	-1.02634700	0.55024000	-1.43462100
O	-7.59052400	0.33125000	-2.85186400
C	-8.59615700	-0.05735300	-1.91544900
H	-9.53500500	-0.04141000	-2.46867300
H	-8.41254000	-1.06711600	-1.53209100
H	-8.65349500	0.64871500	-1.07925500
Cl	-2.37798900	1.68864500	2.48050800
Pd	2.35894200	-0.81399400	0.87349300
Pd	0.96570300	0.39591100	-1.67164600
C	1.06254800	-2.57409000	-1.15778800
O	1.54005500	-2.47690700	0.01791400
O	0.73736900	-1.62470100	-1.93369600

C	3.82418900	-0.45217800	-1.72151400
O	3.86508800	-0.91299300	-0.54829200
O	2.90545900	0.22022000	-2.27424900
C	1.07089900	3.11282300	-0.68405400
O	0.75573200	2.72827900	0.44326700
O	1.20908300	2.38644600	-1.75344300
C	3.48701500	0.70849100	3.01853500
O	2.82344900	-0.05565800	3.77437200
O	3.40767500	0.69826800	1.74204700
C	1.35290500	4.59339000	-0.96001700
H	2.37859000	4.69774400	-1.33421000
H	0.69756800	4.94489800	-1.76541100
C	4.46098500	1.69130800	3.62745300
H	5.42187500	1.18474200	3.76793400
H	4.61184600	2.54166700	2.96181800
H	4.10139000	2.01832800	4.60399500
H	0.36461600	1.29017300	2.07642400
C	5.05203000	-0.71184000	-2.60995800
H	4.68875400	-0.84311300	-3.63029800
H	5.69072400	0.17594600	-2.58724700
C	0.90480100	-3.97364900	-1.70286700
H	0.10950300	-4.00720800	-2.44836600
H	1.85510600	-4.23345500	-2.18353800
H	0.71038300	-4.68015500	-0.89450800
N	1.15166800	5.35150700	0.25372000
C	1.31147700	6.70078600	0.30007400
C	1.05979200	7.34314900	1.65834300
H	0.27393300	8.09600200	1.55139300
H	0.76839600	6.63132500	2.43579900
H	1.96760100	7.86462300	1.97457100
O	1.63743600	7.36169800	-0.68170800
N	5.82446000	-1.86637500	-2.20786600
C	5.24093600	-3.10838800	-2.24932100
O	4.15265700	-3.29018300	-2.78514400
C	6.02764900	-4.22822600	-1.59363400
H	5.91799300	-5.13339900	-2.19361400
H	7.08952900	-3.99594500	-1.47500500
H	5.60003600	-4.42766000	-0.60516800
H	6.58078600	-1.72292900	-1.55511000
H	0.87899800	4.80351500	1.05929700

I-TS1^m

Pd	2.99761300	0.31453400	0.12852900
C	1.66405600	2.04534100	-0.26589700
C	0.75985700	3.79120200	1.19674400
H	0.89897000	4.54790500	1.95999700
C	-0.50927100	3.56632000	0.66826500
C	-0.75281500	2.60874600	-0.33676800
C	0.36103200	1.86491800	-0.77066300
O	2.53303100	0.58105200	2.08424600
C	1.78122200	-0.23585200	2.74479500
C	1.82548000	3.04082100	0.72064500
O	1.16157500	-1.21456500	2.28959700
H	2.56391600	2.03373600	-1.17591500
H	2.81770900	3.22203100	1.12102300
C	1.69362800	0.06313100	4.23386200
H	2.34094800	-0.64125100	4.76689200
H	0.66972700	-0.09675900	4.57816900
H	2.01949400	1.07890700	4.46084600
C	4.26503400	-2.35925300	0.39175100
O	4.36358600	-1.11502000	0.68076800
O	3.25165700	-2.95529300	-0.04500300
C	5.53821000	-3.16542800	0.59066700
H	6.22666800	-2.65565200	1.26544900
H	6.02586900	-3.28535400	-0.38265600
H	5.29208200	-4.15963600	0.96881200
C	3.77141700	1.02816300	-2.57176000
O	3.31281500	2.17852000	-2.31598400
O	3.69524000	0.03218500	-1.77906600
C	4.48573300	0.80038300	-3.88560100
H	4.44416300	-0.25269000	-4.16573700
H	5.53599600	1.08617400	-3.76317400
H	4.05017500	1.42873800	-4.66395100
Ag	1.19234700	-2.18088400	0.14695300
C	-2.11062500	2.47750800	-0.95611900
H	-2.60957300	3.44322300	-1.05012900
H	-2.08184200	1.98350700	-1.92652500
S	-3.33325300	1.50899200	0.02752300
O	-4.64788900	2.13115500	-0.12183600
O	-2.83509200	1.11972300	1.33900000
O	-3.30451900	0.12726000	-0.97150500
C	-4.10862900	-0.94054500	-0.60926500

C	-3.48157100	-2.17278800	-0.34914400
C	-5.49465700	-0.81435600	-0.57256900
C	-4.28560100	-3.29487000	-0.05600900
C	-6.27364300	-1.93660800	-0.25686700
H	-5.93319100	0.15049900	-0.78315300
C	-5.66103000	-3.18024700	-0.00652800
H	-3.80888400	-4.24929400	0.13898300
H	-6.29013200	-4.03202000	0.22491700
C	-2.06486200	-2.28037700	-0.37386000
N	-0.90874300	-2.39007200	-0.39248500
O	-7.62048900	-1.92165400	-0.18050400
C	-8.30906600	-0.68873300	-0.38867200
H	-9.36555100	-0.91287400	-0.24176900
H	-7.99070200	0.07100500	0.33372800
H	-8.15432500	-0.31415100	-1.40709800
Cl	0.13949100	0.69603600	-2.06601700
Cl	-1.82957800	4.54877500	1.27245800

I-TS1^p

Pd	3.16753300	0.24339000	0.29080300
C	0.96051700	1.56094900	-1.31788500
C	1.12540800	2.48275900	0.90765000
H	1.69469900	2.70918900	1.80095500
C	-0.21841700	2.83109200	0.84675700
C	-1.02408100	2.54106100	-0.27547700
C	-0.38122700	1.92117700	-1.36505400
O	2.48178600	0.20939700	2.19670300
C	1.69042100	-0.69201300	2.67915000
C	1.73362300	1.81656000	-0.16972500
O	1.13726900	-1.61103200	2.04934400
H	2.95976200	2.17564000	-0.50593700
C	1.41144600	-0.53395600	4.16607500
H	2.24235700	-0.04326700	4.67525400
H	1.21321300	-1.51177300	4.60816100
H	0.51497500	0.08350400	4.28932800
C	4.25492400	-2.48429600	0.19063400
O	4.42614800	-1.32634100	0.71139100
O	3.25518100	-2.87685300	-0.46069700
C	5.38450300	-3.47351000	0.42278400
H	5.58718400	-4.01727400	-0.50268800
H	5.06069500	-4.20314900	1.17227200

H	6.28588700	-2.97299800	0.77693400
C	4.43517100	1.61116500	-1.85280700
O	3.98703100	2.64149900	-1.26593900
O	4.11766900	0.41693100	-1.52864400
C	5.41705300	1.77860500	-2.98817700
H	6.42998200	1.75725900	-2.57187600
H	5.26681900	2.73909700	-3.48240000
H	5.32406200	0.95438800	-3.69678200
Ag	1.22497700	-2.01633200	-0.27007800
C	-2.47518000	2.90511200	-0.31227700
H	-2.68791600	3.81267600	0.25652300
H	-2.85979800	3.01326900	-1.32656300
S	-3.60311900	1.69115800	0.47242000
O	-4.94949600	2.26062500	0.45957600
O	-3.05498900	1.10161200	1.68517800
O	-3.50401000	0.52828400	-0.75795100
C	-4.18316800	-0.66582800	-0.58108400
C	-3.43762900	-1.85748600	-0.63235100
C	-5.56714300	-0.68490800	-0.43187500
C	-4.12343200	-3.08842100	-0.53770500
C	-6.22485900	-1.91784900	-0.31747400
H	-6.09894900	0.25560800	-0.40565000
C	-5.49452600	-3.12102000	-0.37897900
H	-3.55641400	-4.01184300	-0.58253400
H	-6.03072600	-4.05944500	-0.29751900
C	-2.02222000	-1.84097100	-0.76422700
N	-0.86594400	-1.88666100	-0.87166600
O	-7.55732900	-2.04936700	-0.15803900
C	-8.36034300	-0.87291800	-0.06063000
H	-9.38050000	-1.22462800	0.09248900
H	-8.05436400	-0.25232000	0.78886800
H	-8.31279600	-0.28228400	-0.98270200
Cl	-1.25255700	1.61442100	-2.86309100
Cl	-0.90610500	3.68302700	2.22354900
H	1.41104100	1.09166600	-2.18556800

J-TS1^m

Pd	2.52539700	-0.79625200	0.79907800
C	1.43728300	0.97258900	1.52581400
C	0.40489600	1.58685300	3.66379300
H	0.44396300	1.65411800	4.74481500

C	-0.72851100	2.02696700	2.98369900
C	-0.83443700	1.97848300	1.57949600
C	0.26837300	1.43854100	0.88993700
O	1.77923700	-1.74884300	2.42099200
C	0.90098500	-2.69471000	2.34127300
C	1.46794700	1.07521400	2.93318900
O	0.29451400	-3.06638400	1.32119800
H	2.52750500	1.41118300	0.92906100
H	2.35386600	0.73743800	3.46105300
C	0.64172700	-3.40680200	3.66004500
H	0.86044000	-2.76092600	4.51178300
H	1.29773200	-4.28226700	3.71508100
H	-0.39272400	-3.75258800	3.69513400
C	3.45849500	-3.18859800	-0.69657300
O	3.62716900	-2.47337200	0.35445500
O	2.47757100	-3.16023200	-1.47668200
C	4.60118500	-4.13970200	-1.01118700
H	4.21469500	-5.04290800	-1.48652600
H	5.16486400	-4.38722000	-0.11071700
H	5.27701400	-3.64487900	-1.71705500
C	3.83277000	1.31985400	-0.67292000
O	3.45461900	2.08532600	0.26843800
O	3.51669800	0.09890200	-0.77583100
C	4.75485500	1.87612900	-1.74383100
H	5.70938800	1.33745400	-1.65553200
H	4.35745100	1.63647800	-2.73430400
Ag	0.48951400	-2.37289400	-0.91131000
C	-2.02729600	2.55762200	0.88175800
H	-2.39301000	3.45649700	1.38049900
H	-1.83384500	2.77307500	-0.16821800
S	-3.52741400	1.48498700	0.87247100
O	-4.70870800	2.33383200	1.01754700
O	-3.37165400	0.27706000	1.67049900
O	-3.41297000	1.04295400	-0.76945600
C	-4.37888200	0.18410600	-1.26810900
C	-3.95306000	-1.05929100	-1.76937100
C	-5.71467300	0.57021800	-1.33357400
C	-4.90716800	-1.91733000	-2.35643000
C	-6.65031200	-0.30646200	-1.90153200
H	-5.99507500	1.53590600	-0.93797600
C	-6.23693000	-1.54967500	-2.41970200

H	-4.58469100	-2.87441300	-2.75161900
H	-6.98169600	-2.20124900	-2.86199800
C	-2.58800800	-1.44258000	-1.67655800
N	-1.47645100	-1.77182800	-1.61114600
O	-7.96818000	-0.03861300	-2.00529400
C	-8.46565100	1.19113800	-1.47805400
H	-9.54180600	1.17121300	-1.64955800
H	-8.26633500	1.27233200	-0.40374500
H	-8.02957600	2.05156800	-1.99846000
Cl	0.22326100	1.40449900	-0.86890800
Cl	-2.04425300	2.68932400	3.93344900
N	4.92005800	3.30696300	-1.62963200
C	5.07187600	4.09315900	-2.73899500
O	5.16792900	3.62469600	-3.86687900
C	5.12888500	5.58970200	-2.47415400
H	5.01383300	5.85688800	-1.42010900
H	6.08689200	5.97400600	-2.83497000
H	4.34273000	6.07824600	-3.05609700
H	4.72731100	3.71775900	-0.72786900

J-TS1^p

Pd	-2.79217700	0.74780700	0.67879700
C	-0.93595200	-1.52139400	-0.16700400
C	-0.93219800	-1.15483500	2.22201400
H	-1.40885700	-0.80239400	3.12853800
C	0.34480900	-1.69799000	2.28945100
C	1.03842600	-2.13983800	1.14303600
C	0.34237000	-2.06205100	-0.07976900
O	-1.94020300	1.58104800	2.31513500
C	-1.04260700	2.51191700	2.27387500
C	-1.58492000	-1.03014400	0.98319700
O	-0.47514900	2.95354400	1.25961000
H	-2.89225200	-1.35135500	0.90743000
C	-0.65427000	3.04959800	3.64288800
H	-1.49493100	3.00447000	4.33734500
H	-0.28979200	4.07341900	3.54634500
H	0.15738300	2.43281300	4.04401600
C	-3.58695200	3.23272100	-0.68712200
O	-3.83198100	2.49113000	0.32867100
O	-2.61803000	3.12957600	-1.47921200
C	-4.57622600	4.36273000	-0.91900100

H	-5.48931600	4.21791100	-0.34115700
H	-4.80486000	4.43306400	-1.98487700
H	-4.10652900	5.30483300	-0.61766900
C	-4.32417700	-1.29936900	-0.55050600
O	-3.98744600	-1.96490900	0.47521100
O	-3.89911600	-0.13518100	-0.82324100
C	-5.31956700	-1.90646100	-1.53961800
H	-5.08436900	-1.50413500	-2.52650700
H	-6.32345600	-1.56814300	-1.26528400
Ag	-0.68919600	2.17001700	-0.95924600
C	2.42589100	-2.69345600	1.23140300
H	2.60531000	-3.21458700	2.17419500
H	2.67190000	-3.35217900	0.39832500
S	3.76543900	-1.44188900	1.22893300
O	5.03315200	-2.14343700	1.42549500
O	3.44287500	-0.25605300	2.00941800
O	3.63045400	-1.03268400	-0.41134900
C	4.45434800	-0.03439300	-0.90289900
C	3.84588100	1.09302300	-1.48342600
C	5.83873600	-0.18128700	-0.88851500
C	4.66962700	2.08034000	-2.06721400
C	6.63822000	0.82225200	-1.45349100
H	6.26038800	-1.06812900	-0.43715700
C	6.04419200	1.95127200	-2.05099100
H	4.20776700	2.94936200	-2.52298200
H	6.68667400	2.70617500	-2.48934600
C	2.43361100	1.25731400	-1.47962100
N	1.28709300	1.44391500	-1.50447900
O	7.98624000	0.78619300	-1.48144400
C	8.65952000	-0.31470500	-0.87104200
H	9.72376000	-0.10985200	-0.98672700
H	8.41352400	-0.38987900	0.19398200
H	8.41336000	-1.25807200	-1.37186600
Cl	1.05966200	-2.69383300	-1.55599600
Cl	1.08975200	-1.84433800	3.87792100
H	-1.43930700	-1.51820300	-1.12789800
N	-5.29505900	-3.35165500	-1.56941500
C	-4.13319100	-3.97995700	-1.94707000
O	-3.18509000	-3.34856600	-2.39828200
C	-4.10836200	-5.48679800	-1.77002100
H	-5.10567600	-5.92687100	-1.68471100

H	-3.58566300	-5.93060400	-2.61918500
H	-3.54018500	-5.72827700	-0.86550100
H	-5.94272000	-3.85217800	-0.97922500

K-TS1^m

C	1.07204200	3.25891600	0.48400800
C	-0.21715300	3.31391500	-0.04950000
C	-0.69803900	2.35463600	-0.96193800
C	0.21288700	1.34685200	-1.34460800
C	1.47556900	1.15471100	-0.72753800
C	1.87073600	2.16677300	0.18482500
H	1.41026000	4.04402300	1.15065100
H	2.54701900	0.65000800	-1.41295000
H	2.85144400	2.08695900	0.64669600
Cl	-1.23100300	4.66183000	0.42497400
C	-2.09691700	2.40953200	-1.49159200
H	-2.47148100	3.43077100	-1.58789900
H	-2.21074700	1.89222700	-2.44334500
S	-3.38417600	1.66229200	-0.41008400
O	-4.68278800	2.01280400	-0.98568200
O	-3.12584200	1.85477400	1.00943900
O	-3.06502500	0.02746500	-0.77487500
C	-3.87099200	-0.94595800	-0.20348600
C	-3.24152700	-2.00935500	0.47668200
C	-5.25504500	-0.92137000	-0.36124300
C	-4.03861200	-3.05151700	0.99637200
C	-6.02813900	-1.95642500	0.18317100
H	-5.70121300	-0.09894700	-0.90084500
C	-5.41200800	-3.02688500	0.85940100
H	-3.55562000	-3.87430800	1.51218800
H	-6.03458400	-3.81834400	1.26021200
C	-1.82922200	-2.03789200	0.62866300
N	-0.67175700	-2.05260600	0.74510100
O	-7.37279500	-2.01613600	0.09532900
C	-8.06971600	-0.95792500	-0.56266900
H	-9.12742000	-1.20926700	-0.48491000
H	-7.88385100	0.00500800	-0.07418300
H	-7.78695000	-0.89317200	-1.61958500
Cl	-0.21049700	0.34496900	-2.73220500
C	2.52794600	-2.51456700	-1.31203700
O	3.36639500	-2.46543700	-0.38919000

O	1.40070100	-1.87729700	-1.34593000
O	3.53395900	0.43864800	-2.15662400
C	4.69833800	0.46085300	-1.61089600
O	4.93322700	0.47502000	-0.37671400
C	5.87434600	0.44599600	-2.57031300
H	5.59175700	0.83953000	-3.54776800
H	6.70560500	1.01464400	-2.14872100
H	6.20768000	-0.59045700	-2.69415300
Pd	0.96585300	-0.74398400	0.26204000
O	0.48162600	0.26830400	1.96899100
C	1.31273900	0.28231400	2.95176200
O	2.49241400	-0.14629200	2.93602100
Ag	3.67691900	-0.67816400	1.11724500
C	0.78432000	0.91877900	4.22263600
H	-0.29056500	0.75775000	4.31967400
H	1.31684000	0.52131600	5.08788700
H	0.96142100	1.99878400	4.17334800
C	2.80295700	-3.35200000	-2.54463800
H	1.87834700	-3.75930200	-2.95787000
H	3.25688300	-2.70272800	-3.30085500
H	3.50333100	-4.15265000	-2.30187300

K-TS1^p

C	-1.26248700	2.09030700	-0.06811500
C	-0.03413900	2.72339500	0.03669100
C	0.90852600	2.37192200	1.03232100
C	0.46289800	1.49384200	2.03416100
C	-0.77070400	0.85211200	1.94512600
C	-1.63760200	1.07769400	0.84750200
H	-1.91145300	2.34231900	-0.90104400
H	-3.02711200	0.88705800	1.12334600
Cl	0.37091300	3.95974300	-1.15111100
C	2.32915400	2.82938100	0.97952000
H	2.44396800	3.81991600	0.53371000
H	2.82340600	2.80359500	1.95001600
S	3.42080400	1.81316700	-0.10363000
O	4.79358900	2.25543800	0.14200700
O	2.91876700	1.69783500	-1.46509400
O	3.17962900	0.31522300	0.66577600
C	3.91591900	-0.78593700	0.25462900
C	3.22627800	-1.98933800	-0.00985100

C	5.30685300	-0.73314700	0.18241800
C	3.97711700	-3.13791700	-0.34683400
C	6.02589400	-1.88080700	-0.17817000
H	5.80216000	0.19965000	0.40749700
C	5.35324000	-3.08984800	-0.43668000
H	3.45039500	-4.06566300	-0.54240400
H	5.93395300	-3.96554000	-0.70235700
C	1.80874400	-2.08508400	0.04698300
N	0.65134200	-2.20722300	0.07383100
O	7.36944900	-1.92167200	-0.28928800
C	8.11815400	-0.72636200	-0.06754600
H	9.15927400	-0.99338200	-0.24849500
H	7.81588600	0.06621200	-0.76092200
H	8.00626200	-0.37301000	0.96387300
Cl	1.49201000	1.10441100	3.41123200
C	-3.15284400	-2.36882700	1.36796900
O	-3.72744500	-2.30154500	0.26615100
O	-1.98864000	-1.85297800	1.63347800
O	-4.11723900	0.93462700	1.62620700
C	-5.15812600	0.92005400	0.86262300
O	-5.16706300	0.66643300	-0.36298200
C	-6.46437400	1.23880100	1.56264100
H	-7.27501600	1.31672600	0.83803600
H	-6.69048100	0.44169700	2.27821800
H	-6.36782700	2.16805600	2.13019300
Pd	-1.12169700	-0.93355700	0.06587800
O	-0.18576300	-0.12638000	-1.55768000
C	-0.77830500	-0.05403300	-2.69723200
O	-1.98915300	-0.30141300	-2.92027100
Ag	-3.55513800	-0.51496400	-1.36761200
C	0.11383500	0.34673400	-3.85473500
H	1.00372000	0.86647500	-3.49790400
H	0.42338500	-0.56050700	-4.38518800
H	-0.44729100	0.96895900	-4.55473600
H	-1.04718600	0.13510400	2.71087200
C	-3.80851300	-3.06513100	2.54253700
H	-4.52753700	-3.80187800	2.18124900
H	-3.06352300	-3.53665000	3.18632800
H	-4.34356600	-2.31434100	3.13406800

L-TS1^m

C	0.09801000	-3.70369900	-0.29678800
C	1.30863900	-3.34668400	-0.89385100
C	1.49852900	-2.10449700	-1.52979100
C	0.37781900	-1.24744600	-1.57389900
C	-0.82397100	-1.49136100	-0.86028800
C	-0.91750800	-2.76317900	-0.23987700
H	-0.01221000	-4.68625000	0.14754400
H	-2.03716900	-1.04864800	-1.31440300
H	-1.83339900	-3.01398100	0.29001500
Cl	2.60226100	-4.52775600	-0.86398200
C	2.81998400	-1.72207400	-2.11922700
H	3.37252200	-2.57995500	-2.50805700
H	2.73656200	-0.96392300	-2.89692500
S	4.03850700	-1.02749100	-0.92850600
O	5.32056400	-0.93743400	-1.62735900
O	3.95483900	-1.63075800	0.39370500
O	3.38015300	0.54259300	-0.82053500
C	4.04157500	1.48354800	-0.04581300
C	3.29551800	2.18196200	0.92690600
C	5.38191500	1.78990400	-0.27050400
C	3.93082000	3.19981700	1.67003400
C	5.99759800	2.78946600	0.49579000
H	5.91761300	1.24416900	-1.03316400
C	5.26282000	3.49873000	1.46540400
H	3.35676000	3.74394700	2.41214800
H	5.76243900	4.27373900	2.03496600
C	1.92647600	1.87451900	1.14967800
N	0.80501300	1.61605200	1.32189700
O	7.29065000	3.14865600	0.36254900
C	8.10387000	2.46108700	-0.58877700
H	9.09809900	2.89792300	-0.49613600
H	8.15139100	1.38872000	-0.36953800
H	7.73330800	2.61054200	-1.60928500
Cl	0.45536200	0.14375000	-2.65219300
C	-3.16915600	3.02966400	-1.15160700
H	-3.34906600	2.57833300	-2.13056900
H	-2.45419200	3.84901200	-1.28702500
N	-4.43698200	3.50963400	-0.64845300
C	-2.54076800	1.97655100	-0.23380100
O	-3.11412200	1.61708100	0.80856300
O	-1.39962700	1.54007800	-0.65875300

C	-5.61974800	3.10702100	-1.21651500
O	-5.67592500	2.53028000	-2.29790400
C	-6.86679800	3.43826500	-0.41411600
H	-7.19855000	2.53645100	0.11161100
H	-6.70707400	4.23113700	0.32180100
H	-7.66018900	3.73367700	-1.10298600
H	-4.46024400	3.75096400	0.33260700
O	-3.09901000	-0.83511900	-1.94508100
C	-4.25087600	-1.02693800	-1.41453800
O	-4.47759400	-1.27669300	-0.19752500
C	-5.43173800	-0.90495300	-2.35262300
H	-6.30386800	-1.40741000	-1.93127600
H	-5.65828200	0.16049500	-2.47882600
H	-5.18395500	-1.31559000	-3.33360600
Pd	-0.59417300	0.15974300	0.57649200
O	0.21224600	-1.12802500	1.94356100
C	-0.50198300	-1.49677300	2.94677100
O	-1.74003200	-1.32440300	3.08382200
Ag	-3.16612100	-0.81566500	1.48374400
C	0.26498100	-2.17496400	4.06440900
H	-0.39066200	-2.85516900	4.61026500
H	1.13500300	-2.70345600	3.67141100
H	0.61973500	-1.40630900	4.75961200

L-TS1^P

C	0.63370100	-2.19521100	1.29253600
C	-0.63767200	-2.34025400	1.82460900
C	-1.36838400	-1.23845200	2.33113700
C	-0.66692200	-0.02853800	2.46210500
C	0.61353400	0.13106300	1.93548400
C	1.27024900	-0.93071800	1.26582000
H	1.11346400	-3.05873900	0.84210300
H	2.69424000	-0.88499700	1.29053600
Cl	-1.37468400	-3.93886900	1.80118100
C	-2.82987400	-1.32248700	2.62712000
H	-3.13897200	-2.30965600	2.97814200
H	-3.16862200	-0.56053600	3.32808200
S	-3.92352300	-1.09757600	1.15963300
O	-5.29277500	-0.99300100	1.66323900
O	-3.60808500	-2.01196500	0.07181600
O	-3.38531700	0.45170300	0.70570900

C	-4.02628200	1.11564200	-0.33005500
C	-3.23446200	1.67257200	-1.35841300
C	-5.40746100	1.30017100	-0.31772900
C	-3.87306800	2.42103300	-2.37298000
C	-6.01872200	2.02668300	-1.34914900
H	-5.97958200	0.87379600	0.49299000
C	-5.24183400	2.59401900	-2.37701000
H	-3.26658400	2.85666400	-3.15962700
H	-5.73836100	3.16029700	-3.15636000
C	-1.82394100	1.50555900	-1.40939000
N	-0.66842900	1.38807000	-1.49173800
O	-7.34648700	2.24368400	-1.43037600
C	-8.20210600	1.68142400	-0.43459500
H	-9.21478900	1.95907200	-0.72640500
H	-8.11379500	0.58984700	-0.40550000
H	-7.98186400	2.09394500	0.55652100
Cl	-1.41933300	1.37081500	3.22461200
C	3.26779800	1.59254900	-0.79719300
O	3.63676600	0.68756000	-1.56009700
O	2.12214500	1.64181400	-0.18391800
O	3.84222300	-0.79226600	1.64177000
C	4.75356000	-1.45806100	1.01815900
O	4.59613100	-2.10311700	-0.04529600
C	6.12821000	-1.41429800	1.65272100
H	6.76281600	-2.19620700	1.23469300
H	6.58144400	-0.43971500	1.44139400
H	6.05179700	-1.51470000	2.73753000
Pd	0.88788000	0.11041400	-0.65538600
O	-0.39771200	-1.35433700	-1.24181300
C	-0.02263500	-2.24992400	-2.08694600
O	1.15129500	-2.43795000	-2.49090400
Ag	2.97261100	-1.70130500	-1.48942500
C	-1.13757800	-3.11672300	-2.63378800
H	-2.02090100	-3.06291100	-1.99671600
H	-1.39693700	-2.75824900	-3.63589000
H	-0.78797000	-4.14691500	-2.72898400
H	1.09425500	1.10063600	2.00886900
C	4.20321600	2.76411100	-0.53501200
H	4.51579800	3.16349100	-1.50761200
H	5.11292100	2.37254500	-0.06449700
N	3.60518000	3.78955700	0.29361900

C	4.35536100	4.81247000	0.79325900
O	5.54711100	4.93495200	0.53137200
C	3.61702600	5.78981400	1.69641800
H	3.75186000	6.80094300	1.30356500
H	2.54723600	5.58262100	1.79019300
H	4.07246300	5.76340100	2.69051000
H	2.63964000	3.66113900	0.55677600

A-TS1^{m'}

C	-0.88699500	3.28310500	-1.42268000
C	0.25432100	3.38269000	-0.63013400
C	0.45906700	2.56971000	0.50644300
C	-0.59396600	1.70169800	0.85112500
C	-1.73183600	1.52053800	0.04437100
C	-1.84526700	2.32710000	-1.10477000
H	-1.00378100	3.93509600	-2.28056500
H	-3.02085800	1.21334400	0.50483000
H	-2.73465600	2.22196100	-1.71958700
Cl	1.43935600	4.59608900	-1.06979000
C	1.75270600	2.59329900	1.26144800
H	2.21496900	3.58248500	1.28527700
H	1.66294800	2.21062500	2.27758200
S	3.06951200	1.56853600	0.49405500
O	4.25879900	1.64597800	1.33892700
O	3.16520800	1.76734900	-0.94596300
O	2.32888600	0.06568700	0.75211200
C	2.83142700	-1.03657300	0.08011500
C	1.90983400	-1.84745000	-0.61066300
C	4.18012500	-1.37162800	0.14264900
C	2.37561500	-3.02202300	-1.23966400
C	4.62613600	-2.52816200	-0.51369300
H	4.85156600	-0.73492800	0.70214500
C	3.71450900	-3.35485900	-1.20042800
H	1.66679400	-3.65881800	-1.75722200
H	4.08809400	-4.24972500	-1.68438000
C	0.53671400	-1.49369500	-0.64295500
N	-0.58279700	-1.19633700	-0.65323500
O	5.91025700	-2.93722000	-0.52797600
C	6.89515900	-2.14822500	0.14009800
H	7.84359600	-2.65862700	-0.02645700
H	6.94422600	-1.13674700	-0.27818400

H	6.69507700	-2.09192200	1.21611300
Cl	-0.49624000	0.78884800	2.35111800
Pd	-2.39478500	-0.54663900	-0.12429800
C	-2.85119900	-3.36746500	0.27256300
O	-3.32417300	-2.32424900	-0.37807000
O	-1.85483800	-3.37136100	0.98594400
O	-4.98167100	1.52537400	-1.10189100
C	-5.06095700	0.72286700	-0.19633800
O	-4.04282900	0.49561400	0.68859100
C	-6.26647900	-0.13111800	0.10557800
H	-7.09303500	0.14668600	-0.54855900
H	-5.99299800	-1.17950800	-0.05303600
H	-6.55375900	-0.02266600	1.15493600
C	-3.69965000	-4.61538200	0.04755800
H	-3.23972300	-5.46697100	0.55018400
H	-4.70671600	-4.45577300	0.44507500
H	-3.79989700	-4.81920600	-1.02237800

A-TS1^{m''}

C	-1.00108000	2.93822500	-1.43884200
C	0.21596100	3.20901600	-0.82239100
C	0.60530400	2.55772100	0.36300300
C	-0.31481600	1.64481800	0.91870900
C	-1.48381100	1.26369700	0.24782200
C	-1.83461700	1.94765200	-0.92147800
H	-1.27736800	3.46804600	-2.34324900
H	-2.22206400	0.44640700	1.57464100
H	-2.75008500	1.67597300	-1.43978000
Cl	1.25973100	4.41492300	-1.55685600
C	1.97092000	2.74239800	0.94792200
H	2.39957200	3.72244100	0.72937500
H	2.01953600	2.55372500	2.01981600
S	3.21263800	1.59816400	0.21863200
O	4.49189200	1.80426200	0.89252200
O	3.13365200	1.54297300	-1.23426300
O	2.52720000	0.16162800	0.82479500
C	2.91632500	-1.05200700	0.29598300
C	1.89910300	-1.99446400	0.03571200
C	4.25517200	-1.36817600	0.08726500
C	2.26056700	-3.27327100	-0.44342200
C	4.58918900	-2.63549300	-0.41225700

H	5.01067000	-0.63133100	0.32319900
C	3.58378700	-3.58990200	-0.66997000
H	1.48116500	-4.00121400	-0.64030500
H	3.87556100	-4.56339900	-1.04619500
C	0.53598300	-1.66064700	0.24347700
N	-0.57616900	-1.38726900	0.41678100
O	5.84987900	-3.03540200	-0.66349200
C	6.92469700	-2.11761500	-0.45394400
H	7.82774500	-2.65056400	-0.75062300
H	6.80646500	-1.22179300	-1.07323000
H	7.00050600	-1.82978100	0.60062600
Cl	0.00386500	1.00208400	2.53233100
Pd	-2.45610200	-0.56966300	0.45570400
C	-3.29816000	-2.82171200	-0.60243100
O	-3.34461800	-2.51655400	0.64756200
O	-2.79204600	-2.03583900	-1.43607700
O	-4.58478800	0.70232600	-1.52370100
C	-5.00402900	0.54869300	-0.38601200
O	-4.30307000	0.14896700	0.66290300
C	-6.45640500	0.79822300	0.00031300
H	-6.96902300	1.29314000	-0.82524700
H	-6.94277100	-0.15862500	0.21339700
H	-6.51634000	1.40629200	0.90636700
C	-3.90279400	-4.14459200	-1.02364700
H	-4.99253800	-4.04131100	-1.05046500
H	-3.55151300	-4.42190000	-2.01817100
H	-3.66154900	-4.92472600	-0.29803600

A-TS1^{m''}

C	1.11615200	-2.20445800	-2.13737300
C	-0.05666700	-2.72463200	-1.59562700
C	-0.46200200	-2.45003400	-0.27057100
C	0.40374000	-1.64648700	0.49361100
C	1.58554400	-1.05688200	-0.01426300
C	1.90794000	-1.37577200	-1.35258300
H	1.39401100	-2.45178900	-3.15523700
H	2.58072200	-1.08084300	0.83147400
H	2.82829300	-0.98973900	-1.77938600
Cl	-1.00774000	-3.79230300	-2.60626800
C	-1.74646100	-2.99890500	0.27463500
H	-1.98841100	-3.98345400	-0.13113900

H	-1.76129800	-3.04358200	1.36333600
S	-3.23072200	-2.01713900	-0.16724400
O	-4.41029200	-2.70397400	0.35169700
O	-3.19386300	-1.52550600	-1.53788500
O	-2.90014600	-0.70262600	0.85468000
C	-3.54069900	0.49423400	0.59003100
C	-2.73318300	1.62388500	0.36366300
C	-4.92784900	0.58777900	0.60754900
C	-3.35472000	2.87407100	0.15738300
C	-5.52745600	1.83551400	0.38066400
H	-5.50755600	-0.30566600	0.79675500
C	-4.73142200	2.97854400	0.16214300
H	-2.73830100	3.74959600	-0.01412300
H	-5.22490700	3.92946100	-0.00186000
C	-1.32109500	1.48676900	0.34327900
N	-0.17061800	1.35820100	0.33327800
O	-6.85927200	2.03996200	0.36497000
C	-7.73195100	0.92623400	0.55779400
H	-8.74236900	1.32790000	0.48414800
H	-7.58203100	0.16600800	-0.21682500
H	-7.58903300	0.47693500	1.54712100
Cl	0.04451000	-1.39511600	2.19511600
Pd	1.80481300	1.15294900	0.22632200
C	1.74201600	3.84613300	-0.69730100
O	1.97940200	3.16902900	0.39966100
O	1.46563300	3.35613200	-1.79203400
O	5.39517000	-0.07358600	-1.06557000
C	4.54575200	0.87062600	-0.92373500
O	3.81773600	0.90482300	0.11584300
C	4.49405800	1.93397400	-1.98543200
H	3.46449100	2.23917700	-2.18862400
H	5.02324800	2.81431800	-1.60245200
H	4.99544400	1.59306900	-2.89155800
C	1.86458700	5.35184900	-0.48899800
H	2.89574500	5.60449400	-0.22323800
H	1.58388000	5.87437600	-1.40419100
H	1.22946500	5.67451300	0.34068300
C	4.58841600	-1.87658200	1.68861600
O	3.38031200	-1.49907200	1.80155000

O	5.35510300	-1.72756500	0.69172100
C	5.18647200	-2.57083500	2.89868000
H	5.72407500	-1.82517000	3.49498300
H	4.40728400	-3.01420800	3.51955900
H	5.90819400	-3.32519400	2.57926300
H	5.29318700	-0.84400500	-0.21699400

TS15'

C	0.47871300	0.44244900	-1.20202500
C	-0.76994900	0.00694500	-1.63146000
C	-1.16925800	-1.33644200	-1.50202200
C	-0.22888900	-2.22680300	-0.94041400
C	1.04388800	-1.83261500	-0.50922400
C	1.40009300	-0.45986600	-0.65107600
H	0.75083100	1.48453400	-1.32831200
H	2.64146000	-0.05783100	-1.27571400
Cl	-1.82772500	1.18972800	-2.37952600
C	-2.51725400	-1.80816200	-1.95801700
H	-2.96199200	-1.15723600	-2.71111800
H	-2.48900100	-2.83236800	-2.33338200
S	-3.78848400	-1.91511700	-0.63680200
O	-3.20817700	-2.27941700	0.65197700
O	-4.94505300	-2.63090200	-1.16325300
O	-4.14711800	-0.27138600	-0.59220100
C	-5.35479700	0.11103400	-0.02134300
C	-6.28339800	0.76298300	-0.84693400
C	-5.59088500	-0.09451400	1.33522600
C	-7.48114900	1.22273100	-0.26388400
C	-6.79766300	0.35461200	1.88749600
H	-4.83485500	-0.59545700	1.92450300
C	-7.73882400	1.01993900	1.08002400
H	-8.20608900	1.73474100	-0.88717400
H	-8.66026000	1.36497700	1.53521600
C	-6.01229600	0.95341400	-2.23651800
N	-5.79928500	1.11525400	-3.36919600
O	-7.14010800	0.20299900	3.18756900
C	-6.23915500	-0.47834300	4.05674500
H	-6.72602800	-0.49783700	5.03204200
H	-6.05715400	-1.50497500	3.71845700
H	-5.28369400	0.05334800	4.13811100
Cl	-0.67565900	-3.92349500	-0.77232400

Pd	2.86190500	0.05996000	0.72651500
C	2.30270800	3.11965800	0.45457900
O	2.63847100	2.14996400	1.18898300
O	2.38228200	3.15559300	-0.81330200
C	3.12641900	-1.95614100	0.87550700
C	4.43132400	-2.54971900	0.28052100
C	2.78733200	-3.77870900	-0.68841100
C	1.99174500	-2.77424500	0.20200100
C	3.99073000	-2.93098000	-1.14852800
H	4.74881300	-3.52973300	-1.66582300
H	3.72690500	-2.08180900	-1.77749200
C	4.62374500	-3.96302900	0.90812700
H	5.60831300	-4.35280300	0.62957000
H	4.57400500	-3.95899600	2.00035100
C	3.47302700	-4.79771200	0.25489300
H	3.87337500	-5.63938100	-0.31867000
H	2.78103600	-5.20717200	0.99678800
H	5.30375300	-1.89947900	0.38073300
H	2.18378600	-4.23383900	-1.47533200
H	1.42058000	-3.32074200	0.96081100
O	3.85067800	-0.71867400	2.69844300
C	3.09232000	-1.84977000	2.37128800
O	2.50231400	-2.49302300	3.20209300
C	3.80268700	-0.28623200	4.07822300
H	4.40422700	0.61997200	4.12209800
H	2.77150700	-0.08327500	4.37377900
H	4.22231700	-1.06555200	4.71656600
O	4.19732900	2.16600100	-2.07951400
C	4.19927600	0.99919800	-2.60989200
O	3.38358300	0.07053300	-2.35494300
C	5.30046900	0.73094800	-3.60214200
H	5.57096600	1.64589100	-4.13061300
H	6.18222300	0.38091300	-3.05318300
H	4.99826600	-0.05051500	-4.29973500
C	1.72537300	4.33488300	1.16588100
H	0.80338500	4.01757300	1.67334500
H	2.41140300	4.64494400	1.96145400
N	1.48738700	5.42686300	0.25045000
C	1.28410300	6.69776500	0.70086700
O	1.25106000	6.96923300	1.89657900
C	1.09359800	7.75358400	-0.37790500

H	1.18085300	7.36477900	-1.39615200
H	0.10627000	8.20757200	-0.25526500
H	1.83505900	8.54351100	-0.23100300
H	1.57348200	5.21293000	-0.73284900
H	3.34889100	2.46770900	-1.45910700

TS15''

C	-1.29513900	-1.47136400	0.22899200
C	-2.61417800	-1.81738700	0.49244100
C	-3.36946400	-1.14234600	1.47611500
C	-2.72201000	-0.10661900	2.18282100
C	-1.40612400	0.28786300	1.91419200
C	-0.66810200	-0.43134400	0.93978300
H	-0.73310200	-2.04692500	-0.49925300
H	0.54107100	-0.91170000	1.22329200
Cl	-3.29624900	-3.16500900	-0.39599700
C	-4.79005500	-1.52548800	1.76919700
H	-5.02073400	-2.54583400	1.46273900
H	-5.04232900	-1.39634100	2.82341100
S	-6.06225200	-0.50204600	0.93429500
O	-5.74665700	0.92062700	1.00675100
O	-7.37703600	-0.99275100	1.32983700
O	-5.72509900	-1.03239100	-0.62251400
C	-6.64601800	-0.73525000	-1.62245200
C	-7.26063400	-1.81336400	-2.27727100
C	-6.88411000	0.58593100	-1.99090800
C	-8.13872100	-1.52735900	-3.34194800
C	-7.77620900	0.84466100	-3.04007600
H	-6.37285800	1.37504500	-1.45689100
C	-8.39809200	-0.22117700	-3.71655500
H	-8.61656600	-2.34958000	-3.86326700
H	-9.07693800	0.00702900	-4.53044300
C	-6.99376700	-3.15884100	-1.87839500
N	-6.78012500	-4.25979100	-1.56749800
O	-8.09170600	2.08492800	-3.47778100
C	-7.51051400	3.20973000	-2.82182800
H	-7.91963600	4.08787600	-3.32187700
H	-7.77932500	3.23512500	-1.75956100
H	-6.41869600	3.21004900	-2.92126700
Cl	-3.58908800	0.71662900	3.47426200
Pd	0.87757200	0.71964600	0.10538700

C	3.58925000	1.95383400	-1.28981800
O	2.58273300	1.23438800	-1.03463600
O	4.72019000	1.48831900	-1.62235200
C	0.30107700	2.10381600	1.53458300
C	1.49842500	2.38733000	2.45840200
C	-0.00376200	1.40336700	3.84888000
C	-0.77791200	1.52120900	2.49539300
C	1.45647500	1.16451700	3.40171800
H	2.16595700	1.24879200	4.23202300
H	1.63088300	0.21887700	2.88690800
C	1.09295900	3.53346700	3.44212700
H	1.98697400	3.89496800	3.95963900
H	0.65492700	4.39093000	2.92610700
C	0.10251100	2.83348900	4.42794400
H	0.51085600	2.80483100	5.44309900
H	-0.86924500	3.33353300	4.47994900
H	2.43591700	2.57874700	1.93512500
H	-0.43644900	0.67241000	4.53595000
H	-1.57675300	2.26157600	2.60198900
O	0.75845000	4.06604100	0.28293200
C	-0.22215300	3.21252800	0.64932200
O	-1.38392800	3.34308000	0.31529900
C	0.37171000	5.16726700	-0.56903000
H	1.30097300	5.68412400	-0.80982800
H	-0.11888500	4.79057900	-1.46985900
H	-0.32108400	5.82418800	-0.03749400
O	2.87236400	-3.33250300	2.32047600
C	1.82636100	-2.62761100	2.26325900
O	1.61663300	-1.79003000	1.32284500
C	0.79855900	-2.79728400	3.36357000
H	0.70839400	-1.86632900	3.93182000
H	-0.18060500	-3.01048000	2.92498500
H	1.08718200	-3.60499200	4.03530300
C	3.42425800	3.46016600	-1.24414700
H	2.65822800	3.72640600	-1.98442000
H	3.00240100	3.74329200	-0.27608100
N	4.65981600	4.16270600	-1.50410200
C	4.68644100	5.52300400	-1.51570800
O	3.68238100	6.19662500	-1.28838700
C	6.03056800	6.16004800	-1.82486400
H	6.30461700	6.82151900	-0.99866800

H	6.83323500	5.43491200	-1.98342900
H	5.92897600	6.78138200	-2.71896000
H	5.46850600	3.60229500	-1.73236100
O	5.46026400	-2.54110200	-2.53515700
O	5.71388300	-3.84296300	-0.69645400
C	5.88137600	-3.56702000	-1.92120200
C	6.70417300	-4.55127300	-2.73485900
H	6.61295400	-5.55898400	-2.32754400
H	6.40110500	-4.52662000	-3.78254400
H	7.75678900	-4.25255900	-2.67870900
Ag	4.91003900	-0.62864400	-1.84880600
Ag	4.25232400	-3.28616900	0.70240900