

Insights of Disilylation and Distannation: Sequence Influence and Ligand/Steric Effect in Pd-Catalyzed Difunctionalization of Carbenes

Electronic Supplementary Information

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1. Complete reference for Gaussian 09

Gaussian 09, Revision D.01, M. J. Frisch, G. W. T., H. B. Schlegel, G. E., M. A. R. Scuseria, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, J. B. A. F. Izmaylov, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, R. F. K. Toyota, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O., H. N. Kitao, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, J. J. H. M. Bearpark, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B., V. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, A. J. A. O. Yazyev, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, V. G. Z. K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, and A. D. D. S. Dapprich, ©. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, **2013**.

2. Computational Methods.

All the DFT calculations were carried out with the GAUSSIAN 09 series of programs. Density functional theory B3LYP¹ with a standard 6-31G(d) basis set was used for geometry optimizations. Harmonic frequency calculations were performed for all stationary points to confirm them as a local minima or transition structures and to derive the thermochemical corrections for the enthalpies and free energies. M11-L² functional with basis set 6-311+G(d,p) was employed to calculate the solvation single point energies to give more accurate energy information. The solvent effects were considered by single point calculations on the gas-phase stationary points with a SMD continuum solvation model³. The energies given in this paper are M11-L calculated Gibbs free energies.

3. Details for Direct Silyl Group Migration Step in Oxidation Addition & Carbonation Pathway

Details for direct silyl group migration step in oxidation addition & carbonation pathway is shown in Figure S1. The process undergoes via a three-membered ring **43-ts**. The energy barrier for this transformation is 41.1 kcal/mol, and the relative free energy for 43-ts is 55.5 kcal/mol. These results shows this pathway is unfavorable.

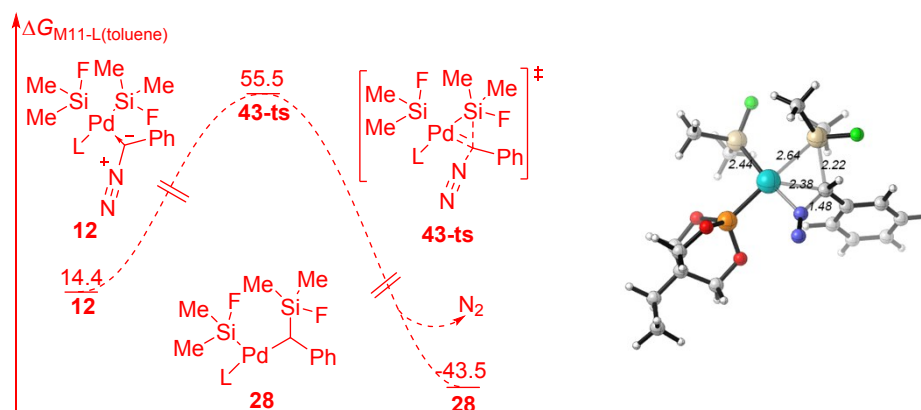


Fig S1. Free energy profiles for direct silyl group migration process of Pd-catalyzed disilylation of carbene. The energies are in kcal/mol and represent the relative free energies, which were calculated using the M11-L method in toluene solvent. The bond lengths are in angstroms.

3. Absolute calculation energies, enthalpies, and free energies.

Geometry	$E_{\text{(elec-B3LYP)}}^1$	$G_{\text{(corr-B3LYP)}}^2$	$H_{\text{(corr-B3LYP)}}^3$	$E_{\text{(solv,M11)}}^4$	IF ⁵
1	-1731.438337	0.295461	0.375499	-1731.651244	-
2	-938.493005	0.11626	0.17039	-938.505070	-
L	-802.3086098	0.139115	0.184948	-802.321792	-
3-ts	-2669.92776	0.433155	0.5467	-2670.158029	-56.2
4	-2669.950774	0.434308	0.547405	-2670.159995	-
5	-1867.61778	0.272641	0.360414	-1867.816567	-
6	-379.7929796	0.082719	0.123185	-379.813719	-
7	-1445.090475	0.214493	0.29798	-1445.309907	-
8-ts	-1445.065	0.211493	0.295844	-1445.27234	-450.6
9	-1335.562091	0.210401	0.284781	-1335.773738	-
10	-2137.907148	0.370372	0.473556	-2138.126722	-
11-ts	-1867.58898	0.273746	0.35919	-1867.808394	-45.4
12	-2247.424413	0.377419	0.485667	-2247.647453	-
13-ts	-2247.399937	0.376931	0.483571	-2247.620043	-465.7
14	-2111.2356	0.393314	0.499832	-2111.47161	-
15	-1308.90109	0.237697	0.312889	-1309.131409	-
16-ts	-1308.88147	0.233484	0.310823	-1309.101276	-498.3
17	-1199.38883	0.230112	0.30096	-1199.607447	-
18-ts	-2137.87636	0.369333	0.472371	-2138.112072	-67.2
19-ts	-2111.21073	0.393913	0.497583	-2111.44134	-519.1
20	-2001.72804	0.390039	0.488084	-2001.954857	-
21	-2199.390778	0.472365	0.58783	-2199.6983	-
L'	-1036.281701	0.228068	0.291254	-1036.341102	-
22-ts	-2579.151393	0.57567	0.71004	-2579.491293	-540.6
23	-2469.67204	0.571785	0.700448	-2470.006357	-
24	-1433.365021	0.318555	0.407165	-1433.630626	-
25	-1542.874285	0.326098	0.418951	-1543.152097	-
26-ts	-1542.855868	0.324085	0.417105	-1543.123635	-511.9
27-ts	-2137.90159	0.373785	0.472881	-2138.12844	-131.5
28	-2137.97354	0.375226	0.474738	-2138.210194	-

29-ts	-2137.95455	0.376229	0.473702	-2138.19999	-110.1
30	-1208.87214	0.21734	0.285197	-1208.91466	-
31	-929.08131	0.13725	0.188163	-929.2950536	-
32	-246.257941	0.169892	0.235707	-246.287176	-
33-ts	-1445.64898	0.421874	0.538794	-1445.905733	-24.1
34	-1445.67584	0.42663	0.539989	-1445.91923	-
35-ts	-1445.67586	0.428686	0.539144	-1445.92259	-20.4
36	-1445.70393	0.425353	0.539563	-1445.95052	-
37-ts	-1445.69657	0.428279	0.539147	-1445.94845	-76.7
38	-516.600934	0.267471	0.350379	-516.638171	-
39-ts	-1977.69922	0.486824	0.613136	-1977.94862	-25.2
40	-1977.71693	0.487314	0.61382	-1977.94361	-
41	-1555.18137	0.430102	0.551409	-1555.43041	-
42-ts	-1555.1599	0.429275	0.549348	-1555.39943	-499.9
43-ts	-2247.34951	0.379798	0.484068	-2247.58434	-248.7
N₂	-109.520718	-0.012849	0.008905	-109.514488	-

¹The electronic energy calculated by B3LYP in gas phase. ²The thermal correction to Gibbs free energy calculated by B3LYP in gas phase. ³The thermal correction to enthalpy calculated by B3LYP in gas phase. ⁴The electronic energy calculated by M11-L in toluene solvent. ⁵The B3LYP calculated imaginary frequencies for the transition states.

4. B3LYP geometries for all the optimized compounds and transition states.

1				C	7.27878000	-1.22416500	0.25888600
				H	6.90282200	0.87129000	0.60362600
P	2.26616400	0.12370100	-0.03405400	H	6.88186700	0.41773700	-1.09053000
O	3.05568200	1.52063200	-0.42633000	H	8.36318600	-1.09032400	0.18381200
O	3.04273200	-0.26242700	1.37121500	H	7.06007800	-1.55023300	1.28138900
O	3.00171900	-0.92698700	-1.07429800	H	7.00307200	-2.03942000	-0.41872700
C	4.47288800	-0.44788200	1.28435000	P	-2.26616000	0.12395300	0.03426300
H	4.92066200	0.10452700	2.11921000	O	-3.05581800	1.52111100	0.42533700
H	4.68411100	-1.51491400	1.41943300	O	-3.04233300	-0.26333600	-1.37087400
C	4.43845500	-0.81991700	-1.18568700	O	-3.00170100	-0.92601700	1.07520200
H	4.83312700	-1.83976500	-1.13732500	C	-4.47270900	-0.44743100	-1.28471300
H	4.67965900	-0.39901300	-2.17066400	H	-4.91973200	0.10592400	-2.11935800
C	4.49044000	1.49765800	-0.27408700	H	-4.68477300	-1.51418300	-1.42062500
H	4.91722200	1.93595300	-1.18395900	C	-4.43864600	-0.82028200	1.18525800
H	4.75872600	2.13502500	0.57856000	H	-4.83246500	-1.84040900	1.13580200
C	5.02202800	0.06295800	-0.06352400	H	-4.68104500	-0.40029000	2.17032400
C	6.56461700	0.08958500	-0.09098800	C	-4.49070600	1.49763100	0.27436400

H	-4.91694700	1.93516400	1.18486900	C	6.63114500	-3.12290200	0.92051000
H	-4.75990200	2.13548800	-0.57762400	H	6.86805100	-1.31074600	-0.23474800
C	-5.02202400	0.06291400	0.06325300	H	6.31743500	-2.68933500	-1.16876500
C	-6.56463500	0.08945000	0.09043900	H	7.67857700	-3.40919100	0.77821800
C	-7.27877900	-1.22447000	-0.25883600	H	6.55141700	-2.65763100	1.90890300
H	-6.90274800	0.87079000	-0.60462700	H	6.03997200	-4.04484800	0.93590200
H	-6.88206100	0.41809900	1.08976000	P	-2.12125900	-0.69903800	0.05484200
H	-8.36319600	-1.09044300	-0.18423800	O	-3.04854700	-0.31543800	1.37494200
H	-7.05976400	-1.55125300	-1.28104300	O	-3.17180100	-0.28620200	-1.15635200
H	-7.00342200	-2.03930400	0.41942000	O	-2.30491000	-2.34017700	0.04941700
Pd	0.00002100	0.15271000	0.00011000	C	-4.54645100	-0.70069200	-0.99079600
2				H	-5.15573500	0.19151100	-0.79587400
Si	0.28937500	1.14266600	-0.03696600	H	-4.86155600	-1.13494500	-1.94498000
Si	-0.28937500	-1.14266600	-0.03696600	C	-3.65705400	-2.84039600	-0.05871300
C	0.28937500	-2.00569000	1.53743900	H	-3.77026600	-3.29429300	-1.04982600
H	0.04661900	-3.07484400	1.50191600	H	-3.77109900	-3.62434000	0.69950200
H	1.37240800	-1.91597200	1.67909300	C	-4.32054900	-0.99130300	1.47497600
H	-0.20117900	-1.58259200	2.42319700	H	-4.26852300	-1.70649800	2.30608000
C	2.13509400	1.42144500	-0.28532700	H	-5.07102600	-0.22995800	1.71762000
H	2.49319500	0.94987400	-1.20686000	C	-4.68845100	-1.71533900	0.16180100
H	2.36064100	2.49340000	-0.34223500	C	-6.12804300	-2.25929300	0.27616300
H	2.71028900	1.00255900	0.55009300	C	-6.61579100	-3.15294600	-0.87356400
C	-2.13509400	-1.42144500	-0.28532700	H	-6.80799300	-1.40252300	0.38078200
H	-2.49319500	-0.94987400	-1.20686000	H	-6.20482300	-2.82095400	1.21765200
H	-2.36064100	-2.49340000	-0.34223500	H	-7.65533100	-3.45000100	-0.69914400
H	-2.71028900	-1.00255900	0.55009300	H	-6.58072600	-2.64033600	-1.84091600
C	-0.28937500	2.00569000	1.53743900	H	-6.02421000	-4.07071700	-0.95940700
H	-0.04661900	3.07484400	1.50191600	Pd	0.01495400	0.08975600	-0.04205900
H	-1.37240800	1.91597200	1.67909300	Si	0.17823600	2.90384200	-1.15944100
H	0.20117900	1.58259200	2.42319700	Si	-0.28133700	2.86224600	1.19982800
F	-0.49233100	1.85426600	-1.28892700	F	-0.65322500	4.31155100	-1.39964800
F	0.49233100	-1.85426600	-1.28892700	F	0.59825300	4.22667200	1.50715500
3-ts				C	-2.09425500	3.30175900	1.47609000
P	2.16230400	-0.65927300	-0.10584200	H	-2.72546400	2.40771900	1.41241300
O	3.15378100	-0.19373500	-1.35097800	H	-2.23101800	3.74380900	2.47112900
O	3.14313800	-0.30953100	1.18093600	H	-2.43450800	4.02600300	0.72882700
O	2.36299900	-2.29654200	-0.18590700	C	-0.50248900	1.80028500	-2.53217300
C	4.52941900	-0.70238700	1.06467600	H	-0.33248600	2.32927000	-3.48116800
H	5.13724400	0.20491200	0.95291100	H	-0.00741400	0.82472600	-2.59875300
H	4.79897700	-1.18763900	2.00807900	H	-1.57790600	1.62984800	-2.42656400
C	3.71259300	-2.79129200	-0.03433500	C	0.30969400	1.68834800	2.55548100
H	3.77825500	-3.30039400	0.93404100	H	1.37044300	1.43809300	2.46361800
H	3.87532600	-3.53024000	-0.82808900	H	0.16840500	2.21845200	3.50897400
C	4.43692900	-0.85163900	-1.42171800	H	-0.26429000	0.75692900	2.60294200
H	4.43694500	-1.51758900	-2.29429700	C	1.99736800	3.29448400	-1.45876100
H	5.19020700	-0.07088500	-1.57921300	H	2.60131200	2.37989600	-1.45990800
C	4.74265400	-1.64811300	-0.13478100	H	2.12363200	3.78861200	-2.43050400
C	6.19109800	-2.17576800	-0.20534400	H	2.37860200	3.96611700	-0.68224900

4				C	-2.64207700	3.62963900	0.08674100
P	1.81403500	-0.46450900	-0.11055700	H	-3.36908100	2.83687000	-0.12424800
O	3.31667500	0.03855300	-0.58154100	H	-3.13570400	4.40092500	0.69218000
O	2.14933000	-0.99542300	1.41353400	H	-2.32871000	4.08058100	-0.85931100
O	1.73095200	-1.90415400	-0.91856200	C	1.67455900	2.26057600	-2.69991300
C	3.35259800	-1.78268800	1.56867200	H	2.09260100	3.08177300	-3.29784700
H	4.09455700	-1.17783100	2.10529800	H	2.43511800	1.47880300	-2.60675600
H	3.08484200	-2.64111500	2.19234600	H	0.81987900	1.84836500	-3.24842100
C	2.75537900	-2.87557300	-0.59952000	C	-1.67487700	2.26036300	2.69941000
H	2.28334800	-3.68636500	-0.03336800	H	-0.82119300	1.84569700	3.24763800
H	3.12298000	-3.27888300	-1.55032100	H	-2.09133300	3.08176000	3.29817900
C	4.35566200	-0.96532300	-0.55998200	H	-2.43708900	1.48027000	2.60520800
H	4.62016100	-1.21093200	-1.59637500	C	2.64417500	3.62701800	-0.08639200
H	5.22745900	-0.51182700	-0.07489700	H	3.37039500	2.83335500	0.12378500
C	3.90571000	-2.23108200	0.20051400	H	3.13850000	4.39839400	-0.69112300
C	5.11327300	-3.18056900	0.34968300	H	2.33134000	4.07734000	0.86013600
C	4.82301100	-4.57138600	0.93215500	5			
H	5.86588000	-2.67821700	0.97274100	P	1.33428500	0.27275500	0.18047800
H	5.57435600	-3.30102400	-0.64057700	O	2.07738500	0.19947900	1.64627300
H	5.75474900	-5.14021900	1.01885500	O	2.01447300	-1.02106500	-0.57599900
H	4.37903900	-4.51873700	1.93225500	O	2.16268700	1.51044000	-0.51995600
H	4.14582300	-5.15066200	0.29506000	C	3.45380300	-1.14885700	-0.45296500
P	-1.81425800	-0.46405100	0.11030900	H	3.66463200	-2.03388600	0.15978000
O	-3.31732900	0.04061500	0.57848000	H	3.83934800	-1.32067900	-1.46225300
O	-2.14783900	-0.99702700	-1.41341500	C	3.59959600	1.34434900	-0.61743300
O	-1.73322800	-1.90248100	0.92070700	H	3.84949000	1.25164200	-1.67957900
C	-3.35158600	-1.78344000	-1.56899300	H	4.05711400	2.26071800	-0.22732600
H	-4.09248400	-1.17861300	-2.10714400	C	3.52420700	0.23721000	1.61997600
H	-3.08389400	-2.64280700	-2.19138200	H	3.84701200	1.18080400	2.07644900
C	-2.75768800	-2.87378500	0.60148100	H	3.87879700	-0.59224100	2.24191600
H	-2.28526600	-3.68558400	0.03710200	C	4.07484500	0.11278300	0.18193900
H	-3.12682600	-3.27565500	1.55230300	C	5.61500400	0.02541700	0.24603300
C	-4.35686300	-0.96278000	0.55729300	C	6.35999500	0.02395700	-1.09664200
H	-4.62247700	-1.20670200	1.59379700	H	5.88034100	-0.88172800	0.80601300
H	-5.22784800	-0.50941100	0.07062700	H	5.97617200	0.86870000	0.85078200
C	-3.90664100	-2.22978400	-0.20095400	H	7.43720500	-0.06523000	-0.92189300
C	-5.11455800	-3.17877100	-0.35031400	H	6.06378600	-0.81465400	-1.73596200
C	-4.82432200	-4.57059200	-0.93038000	H	6.19752800	0.94917400	-1.65983200
H	-5.86606700	-2.67690000	-0.97508600	Pd	-1.04917700	0.43239700	0.09495800
H	-5.57700800	-3.29751600	0.63951600	Si	-3.31552900	1.06315100	-0.09330400
H	-5.75625100	-5.13906300	-1.01741600	Si	-1.96430300	-1.69820000	-0.05913700
H	-4.37907300	-4.51964100	-1.93000100	F	-4.18359100	0.39872400	-1.32409500
H	-4.14823900	-5.14929600	-0.29159900	F	-3.45191700	-1.96377800	0.59207600
Pd	0.00020800	1.07611500	-0.00005200	C	-2.07639000	-2.25526600	-1.85651300
Si	1.14925200	2.92391100	-0.99805700	H	-1.10970700	-2.14831600	-2.36195300
Si	-1.14804200	2.92432900	0.99820100	H	-2.38332400	-3.30799800	-1.91295300
F	0.21697300	4.22332100	-1.41014800	H	-2.81495200	-1.64854900	-2.38903300
F	-0.21460300	4.22257000	1.41151400	C	-3.08313500	2.88425700	-0.60100200

H	-4.06777200	3.35548900	-0.72808200	F	-1.94216800	2.50029500	-0.56274100
H	-2.53710400	3.45492500	0.16068400	N	1.04026100	3.71359500	1.01312000
H	-2.54195500	2.97617000	-1.54917800	N	1.21161700	2.89558600	0.24186700
C	-0.83056600	-2.83234400	0.94875000	C	1.39509200	1.92352000	-0.63342800
H	-0.79839700	-2.52524500	1.99965000	H	1.07198700	2.17247200	-1.63829500
H	-1.20952400	-3.86241800	0.90624700	C	2.35334100	0.83738900	-0.36128400
H	0.19180700	-2.82329100	0.55607500	C	2.66137200	-0.06238200	-1.40630500
C	-4.41389900	0.98879900	1.43788300	C	2.94657100	0.63478700	0.90363500
H	-3.92508500	1.48030300	2.28843800	C	3.54684300	-1.11848800	-1.18978900
H	-5.36896600	1.49741700	1.25280300	H	2.21795700	0.08463100	-2.38728900
H	-4.61849600	-0.04918100	1.71359900	C	3.82954500	-0.42315400	1.10418800
6				H	2.72206000	1.31093500	1.72409000
N	3.42215400	0.63372500	0.00030400	C	4.13671200	-1.30325300	0.06187200
N	2.52736300	-0.08435900	0.00001400	H	3.77750000	-1.79460100	-2.00823100
C	1.49507300	-0.87629900	-0.00015400	H	4.28114800	-0.55901700	2.08282600
H	1.72276800	-1.93518900	-0.00047000	H	4.82823400	-2.12429400	0.22547500
C	0.12639700	-0.37388500	-0.00028200	8-ts			
C	-0.93287500	-1.30139300	-0.00003600	Pd	-0.31914600	0.04390500	-0.28162400
C	-0.18378600	0.99962300	-0.00010800	Si	-2.00809700	1.69577200	-0.12876500
C	-2.25639900	-0.86832800	0.00024100	Si	-1.88333800	-1.41633100	0.55740600
H	-0.71033200	-2.36575300	0.00011500	C	-1.63886800	2.92345800	1.26897400
C	-1.51002800	1.42399100	-0.00011800	H	-0.63170400	3.34640400	1.16396100
H	0.61556700	1.73624900	-0.00013000	H	-2.35776200	3.75342600	1.26134100
C	-2.55516300	0.49625200	0.00008000	H	-1.69181900	2.43547900	2.24860300
H	-3.05829100	-1.60205200	0.00044200	C	-2.05003500	2.64748200	-1.77537000
H	-1.72768400	2.48888400	-0.00010000	H	-2.35901700	1.99653300	-2.60092800
H	-3.58795400	0.83253900	0.00018900	H	-2.75691700	3.48618900	-1.71989800
7				H	-1.06248000	3.05685800	-2.02447400
Pd	-0.10798300	0.10610800	-0.12884500	C	-3.20869800	-1.93223300	-0.68056900
Si	-1.01017300	-1.98467200	0.26582900	H	-3.77754200	-2.78712600	-0.29205600
Si	-2.26082500	0.92675900	-0.13133500	H	-3.90004200	-1.10269100	-0.85613000
C	-0.81934900	-3.11242300	-1.24456800	H	-2.76499600	-2.22451600	-1.63827200
H	0.22869500	-3.16786500	-1.56371900	C	-2.60966100	-1.04043100	2.25655700
H	-1.15877700	-4.13018400	-1.00952800	H	-3.31983000	-0.21078600	2.19064800
H	-1.40859300	-2.74301000	-2.09107000	H	-3.13847400	-1.92227900	2.64101200
C	-0.11528400	-2.75952700	1.74707900	H	-1.82636100	-0.77294800	2.97378000
H	-0.33499200	-2.21103400	2.66962900	F	-3.58341300	1.24922400	0.12306700
H	-0.43344800	-3.80183100	1.88450600	F	-0.96120300	-2.77055100	0.79104900
H	0.97203200	-2.75054800	1.60225800	N	1.55796600	-2.35456200	-2.53546400
C	-3.10664800	1.04993200	1.55081700	N	1.75084400	-2.03263000	-1.48603800
H	-4.03211800	1.63483600	1.46821600	C	1.50582000	-1.01794900	-0.03025000
H	-3.35736300	0.05223500	1.92427400	H	1.41749000	-1.87287300	0.64374500
H	-2.45743500	1.54161500	2.28362800	C	2.77191800	-0.27661700	0.15560800
C	-3.45754400	0.31244600	-1.45613300	C	3.63796700	-0.58890600	1.22053500
H	-3.77774000	-0.71241300	-1.24346600	C	3.08632400	0.82285700	-0.66850300
H	-4.34801200	0.95419800	-1.48200400	C	4.76861800	0.18737900	1.46973100
H	-2.99570500	0.33301500	-2.44947500	H	3.41068500	-1.43936800	1.85842300
F	-2.61575500	-2.08881600	0.65281900	C	4.23164500	1.57914600	-0.43939200

H	2.42136200	1.07299500	-1.49248500	C	-4.05425900	-0.87672600	0.17748000
C	5.07065800	1.26678500	0.63594600	H	-4.58979500	-1.25254900	-0.69964100
H	5.42014600	-0.05562200	2.30437500	H	-4.43566500	-1.39071000	1.06859300
H	4.46615000	2.41920300	-1.08700000	C	-3.48406800	1.07025900	1.62118900
H	5.95765900	1.86580600	0.82294700	H	-4.00242400	0.66405600	2.49717800
9				H	-3.45383100	2.16365200	1.70879600
Pd	-0.41670100	-0.52433200	-0.60280300	C	-4.20578700	0.65020500	0.32237100
Si	-2.67860600	-0.82099300	0.16735000	C	-5.68572100	1.07920300	0.41556000
Si	-0.68489800	1.60998000	0.25829300	C	-6.54610200	0.86133900	-0.83760200
C	-4.04293000	-0.57257900	-1.12709700	H	-5.71286300	2.14482600	0.68246500
H	-3.83104900	-1.16324000	-2.02767600	H	-6.14032000	0.54552800	1.26142400
H	-5.01715100	-0.89330100	-0.73465800	H	-7.57427300	1.18296800	-0.64143500
H	-4.12768500	0.47590100	-1.43197500	H	-6.18194800	1.43949800	-1.69369100
C	-2.73096400	-2.64896800	0.71089200	H	-6.58594500	-0.19155400	-1.13634000
H	-2.06122700	-2.83374700	1.55831100	Pd	0.73854500	-0.44534400	0.27227400
H	-3.75012700	-2.92305900	1.01667400	Si	0.45032900	-2.70068400	-0.61912600
H	-2.43569000	-3.32265200	-0.10397600	Si	3.09233400	-1.03197600	0.37926100
C	-0.46294900	1.67324700	2.13005400	C	-0.43313300	-3.89969800	0.56053200
H	-0.42104100	2.71643900	2.46980600	H	-1.43433200	-3.52836100	0.80693000
H	-1.30244700	1.17593200	2.62437900	H	-0.53542600	-4.89313300	0.10386500
H	0.46619900	1.17942000	2.43470000	H	0.12469600	-4.01459200	1.49723800
C	-2.15310300	2.65041900	-0.31028800	C	-0.46536800	-2.71628900	-2.28748700
H	-3.08040900	2.31695900	0.16566600	H	0.05266100	-2.09755300	-3.03010100
H	-1.98405300	3.70060200	-0.03892700	H	-0.52106000	-3.73901500	-2.68362300
H	-2.28013500	2.59682200	-1.39684900	H	-1.48692900	-2.33398300	-2.18132500
F	-3.20590500	0.02028300	1.49349300	C	3.94304200	-1.15906200	-1.30225800
F	0.61799600	2.42145500	-0.35781600	H	5.02386500	-1.29605600	-1.16533400
C	1.49447700	-0.15767000	-1.21288900	H	3.55023300	-2.00797100	-1.86782500
H	1.63673400	0.38677600	-2.15753300	H	3.79335900	-0.24511800	-1.88901400
C	2.74143900	-0.27259200	-0.51557400	C	3.48659600	-2.49827000	1.50522500
C	3.95432900	0.21113500	-1.07563700	H	3.13471800	-3.43693300	1.07036400
C	2.79741700	-0.91675200	0.74971400	H	4.57272100	-2.56394800	1.65368600
C	5.16276100	0.04666700	-0.41203400	H	3.02020800	-2.37095100	2.48894200
H	3.92098800	0.71417800	-2.03854100	F	1.85343400	-3.51433800	-0.99370700
C	4.00399200	-1.07064000	1.41751100	F	3.92560000	0.19871100	1.12789000
H	1.86639100	-1.27808300	1.17725500	C	1.48235300	1.29358300	0.93975200
C	5.18505800	-0.59116700	0.83499200	H	1.69341300	1.38136300	2.01309600
H	6.08529500	0.41618700	-0.85007700	C	1.90166800	2.47830000	0.23654000
H	4.03684600	-1.56050100	2.38618500	C	2.45778000	3.58163700	0.93068000
H	6.12991900	-0.71343900	1.35819500	C	1.73977300	2.58260000	-1.16827700
10				C	2.82322300	4.74060100	0.25568700
P	-1.54651600	-0.05997100	0.26183100	H	2.59899500	3.50666900	2.00566800
O	-2.12489500	0.57979100	1.66646500	C	2.11280000	3.73705700	-1.84298900
O	-2.05657100	1.07109600	-0.82249900	H	1.31778700	1.73467000	-1.69994000
O	-2.66531000	-1.24494900	0.00336100	C	2.65295400	4.81644600	-1.13111000
C	-3.48263400	1.32122400	-0.86389200	H	3.24799600	5.58001000	0.79877000
H	-3.61708000	2.40878000	-0.83465700	H	1.98751200	3.80537600	-2.91979300
H	-3.85992900	0.94707000	-1.82170400	H	2.94522700	5.71927000	-1.66124500

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P	-1.34185000	-0.44171100	-0.02344700
O	-1.80984800	0.37596300	-1.38255600
O	-2.45491100	-1.66127900	-0.02292400
O	-1.98927600	0.54365900	1.13702500
C	-3.82325700	-1.28725600	-0.30681800
H	-4.08720300	-1.67099600	-1.30072800
H	-4.44612700	-1.79205500	0.43820600
C	-3.41998900	0.74955200	1.08304000
H	-3.86796300	0.22928900	1.93716700
H	-3.59471600	1.82579900	1.19870200
C	-3.17242000	0.85602100	-1.39600900
H	-3.15321300	1.95049600	-1.31545100
H	-3.59789800	0.58583700	-2.36925000
C	-4.00645800	0.24294500	-0.25069000
C	-5.48248400	0.65641800	-0.43016400
C	-6.44543400	0.27001500	0.70178200
H	-5.84419800	0.22590200	-1.37409800
H	-5.51502300	1.74663400	-0.56481300
H	-7.46085000	0.59649700	0.45370400
H	-6.48191300	-0.81249200	0.86456400
H	-6.17381900	0.74286900	1.65170100
Pd	0.79209300	-0.96191200	0.19197900
Si	2.36078100	1.58425800	0.10223900
Si	3.42163600	-0.54772700	-0.18389600
F	3.74998400	2.47847800	0.13070900
F	3.59674700	-0.77401900	-1.79924900
C	5.15642600	-0.32403000	0.52469800
H	5.11895100	-0.17465700	1.61101900
H	5.77288300	-1.20888800	0.32417400
H	5.64219500	0.55344200	0.08849700
C	1.53920000	1.98165300	1.75197700
H	1.48569300	3.07237200	1.86928000
H	0.52459100	1.57675500	1.82036200
H	2.12109900	1.58892400	2.59402900
C	2.89238300	-2.25155000	0.54223500
H	1.85770400	-2.66802700	0.51506300
H	3.47750200	-2.96792700	-0.04852900
H	3.22476500	-2.30482900	1.58408900
C	1.41898900	2.23027000	-1.39265900
H	0.41870100	1.79457000	-1.47536200
H	1.32352400	3.32173000	-1.32248000
H	1.96289800	1.99981900	-2.31583700

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P	1.11651200	-0.67587900	0.01608700
O	1.89846500	-0.11378100	-1.31547300
O	2.06237200	-0.05653600	1.21916100
O	1.63511800	-2.24205400	0.02180100

C	3.46034600	-0.43514600	1.19614300
H	4.04342600	0.48278100	1.33372100
H	3.64074500	-1.09752200	2.04953400
C	3.04788500	-2.44717200	-0.22773900
H	3.39336000	-3.16705500	0.51999400
H	3.15862000	-2.89403700	-1.22362000
C	3.34117900	-0.20740000	-1.28547500
H	3.65408300	-0.60905800	-2.25565300
H	3.74405900	0.80674100	-1.17653200
C	3.82802500	-1.11876000	-0.13668300
C	5.35006300	-1.33243400	-0.27767300
C	6.04524500	-2.09024200	0.86276200
H	5.82098100	-0.34552000	-0.38635400
H	5.53249300	-1.85843100	-1.22469100
H	7.11056700	-2.20466800	0.63702400
H	5.97002000	-1.55783500	1.81700500
H	5.63307100	-3.09486700	1.00602100
Pd	-1.21473200	-0.16895200	0.15591500
Si	-1.96741200	-2.24954300	-0.59540300
Si	-3.55699400	0.34096300	0.21519700
C	-1.18929500	-2.68836100	-2.26571600
H	-0.09696600	-2.72813900	-2.19616500
H	-1.54895000	-3.67043500	-2.60021600
H	-1.45507100	-1.95011900	-3.03021600
C	-1.58924600	-3.58634700	0.68972500
H	-2.11824000	-3.38524100	1.62780700
H	-1.91354600	-4.56807900	0.31943400
H	-0.51655500	-3.63410900	0.90440400
C	-4.64548500	-0.56547600	1.47007700
H	-5.61576100	-0.06194000	1.56960300
H	-4.82332600	-1.59853300	1.15678100
H	-4.17074000	-0.58311400	2.45803300
C	-4.46053500	0.54536200	-1.43545800
H	-4.60578700	-0.42456800	-1.91931300
H	-5.44400700	1.00663100	-1.27717700
H	-3.89273600	1.18832500	-2.11832900
F	-3.58884100	-2.42928300	-0.87944600
F	-3.55034600	1.91077900	0.81297100
N	0.20664200	1.65657300	3.32713900
N	-0.17209600	1.91353100	2.28691700
C	-0.59390600	2.16719400	1.05657200
H	-1.66984800	2.32606900	1.01475100
C	0.29891800	2.88127600	0.12116700
C	-0.24244800	3.30882200	-1.10440900
C	1.64825800	3.15931900	0.39748900
C	0.54729900	3.98961500	-2.02775700
H	-1.28583200	3.10194100	-1.32627100
C	2.43176400	3.84385600	-0.53132500

H	2.08481600	2.84681200	1.34183600	N	-0.98653000	2.63030200	-2.07487000
C	1.88924000	4.26059300	-1.74900500	N	0.05429200	2.32512500	-1.82197000
H	0.10972400	4.31215700	-2.96870400	C	1.37106200	1.40276700	-1.03525500
H	3.47026200	4.06280400	-0.29467500	H	1.95729700	1.33341300	-1.94947100
H	2.50218400	4.79569700	-2.46877000	C	1.95820500	2.37119400	-0.07635100
13-ts				C	3.27738400	2.82339800	-0.26781100
P	-1.59066700	-0.09378200	0.02091100	C	1.25761200	2.78132100	1.07464500
O	-2.00443400	1.37783100	0.66034200	C	3.88606900	3.64883400	0.67695300
O	-2.38956900	-0.01390800	-1.41991300	H	3.82837000	2.48952100	-1.14180500
O	-2.60788500	-1.06827100	0.87706200	C	1.85754200	3.63395200	1.99737900
C	-3.76017200	0.45449500	-1.37722500	H	0.24145300	2.43034100	1.23105000
H	-3.79983400	1.43006100	-1.87704600	C	3.17483900	4.06407500	1.80493500
H	-4.35355700	-0.26055500	-1.95481900	H	4.91140500	3.97586900	0.52737800
C	-4.02429500	-0.78292600	0.77801000	H	1.30452800	3.95330500	2.87669100
H	-4.49182200	-1.60941200	0.23223100	H	3.64528800	4.71767900	2.53472800
H	-4.42063700	-0.76752800	1.79966900	14			
C	-3.42136900	1.63696400	0.79386500	P	2.28473900	-0.52641100	0.07404900
H	-3.66398500	1.66596200	1.86337600	O	3.32723800	0.58688600	0.75821500
H	-3.60878100	2.62817700	0.36507600	O	2.84546400	-1.89734700	0.81190400
C	-4.26998000	0.56600300	0.07431200	O	2.99907900	-0.68049200	-1.41064400
C	-5.75436000	0.98653100	0.13176300	C	4.23013000	-2.23563200	0.58256000
C	-6.77484900	-0.02030200	-0.41886000	H	4.65605700	-2.52091400	1.55215000
H	-5.85883300	1.93709100	-0.40891900	H	4.26238500	-3.10715200	-0.08171000
H	-6.00330500	1.20665800	1.17915900	C	4.43981700	-0.77497500	-1.43141200
H	-7.78374600	0.39952600	-0.34923700	H	4.69006600	-1.58516100	-2.12398100
H	-6.59434200	-0.26093000	-1.47201500	H	4.84525700	0.16328300	-1.83337500
H	-6.77380100	-0.95929100	0.14491000	C	4.71113200	0.19514200	0.84539800
Pd	0.70863500	-0.49466100	-0.26423400	H	5.31329500	1.04802700	0.50883200
Si	0.62195200	-2.59373000	0.88845600	H	4.95430500	-0.00689000	1.89731900
Si	2.95378400	-1.22466700	-0.77978700	C	5.00434500	-1.04707000	-0.02239400
C	0.13431000	-2.32451600	2.70416000	C	6.52698600	-1.29565000	-0.04573900
H	-0.86750400	-1.88942600	2.78797600	C	7.00103000	-2.58958200	-0.72346200
H	0.13932200	-3.28185400	3.24229300	H	6.88774300	-1.28878300	0.99246900
H	0.84134600	-1.65338300	3.20532600	H	7.00496900	-0.43618800	-0.53606000
C	-0.55899800	-3.85472500	0.10089700	H	8.09486900	-2.64179000	-0.70337800
H	-0.26547400	-4.08043100	-0.93054000	H	6.62248500	-3.48247600	-0.21431700
H	-0.54644500	-4.79371700	0.67002100	H	6.69102100	-2.64611800	-1.77241000
H	-1.58673400	-3.47558400	0.08679700	Pd	0.08485200	-0.04837600	0.21396700
C	3.09542800	-2.77933600	-1.85316900	C	0.10196600	2.23252400	1.57375400
H	4.12499500	-2.88560900	-2.21951000	H	1.10120800	1.97003000	1.90285700
H	2.83452400	-3.67806300	-1.28787900	C	-0.11972200	3.07552700	0.39224500
H	2.43368100	-2.71239800	-2.72472300	C	0.99614500	3.46337800	-0.37406300
C	4.21031100	-1.24528100	0.63498700	C	-1.39787700	3.51192000	-0.00275000
H	3.97504500	-2.03391000	1.35435400	C	0.83430100	4.27090700	-1.49725800
H	5.21950500	-1.42221400	0.24036200	H	1.98518800	3.11754500	-0.08533100
H	4.21793800	-0.28369300	1.16129400	C	-1.54750800	4.32344600	-1.12484900
F	2.03315800	-3.45634900	1.02499500	H	-2.27409800	3.19905900	0.55808200
F	3.60405800	-0.06907400	-1.80149200	C	-0.43597000	4.71015900	-1.87824700

H	1.70737900	4.55927500	-2.07711600	Pd	0.77061400	-0.53631700	-0.30596400
H	-2.54239200	4.65146100	-1.41516600	C	2.87675700	-1.10596600	-0.61204100
H	-0.55897800	5.34153000	-2.75373100	H	2.75643200	-1.28802400	-1.68302600
N	-0.83120900	2.08232600	2.48261100	C	3.73714800	0.02935700	-0.17677000
N	-1.66308200	1.93821000	3.25508300	C	3.99748600	1.05779800	-1.09816800
P	-2.05167300	-0.73181400	-0.12894000	C	4.29199600	0.11440600	1.11017200
O	-2.52632400	-1.09515300	-1.67146200	C	4.79410800	2.14246800	-0.73826000
O	-2.53820600	-2.10462800	0.65459200	H	3.56564700	1.00696800	-2.09418000
O	-3.29126700	0.29006700	0.30377800	C	5.09151000	1.20077900	1.46130200
C	-3.94081200	-2.43645600	0.57023100	H	4.09585400	-0.66440600	1.84263100
H	-4.00510900	-3.50467000	0.32939600	C	5.34717800	2.22041600	0.54196500
H	-4.38723800	-2.27515300	1.55848700	H	4.98332300	2.92914800	-1.46367100
C	-4.62690200	-0.11917200	-0.05618000	H	5.51303500	1.25001100	2.46170900
H	-5.25587800	0.03814100	0.82651300	H	5.96811600	3.06688600	0.82070900
H	-4.98852700	0.53426400	-0.86185300	N	3.00530100	-2.26648700	0.05421400
C	-3.82855100	-1.69783100	-1.80897000	N	3.14051300	-3.23189200	0.63648500
H	-4.33976900	-1.17785000	-2.62807600	16-ts			
H	-3.69589500	-2.74978000	-2.09476600	P	1.45488700	0.27798200	-0.03247400
C	-4.65323500	-1.59336500	-0.50726700	O	2.42316900	1.45201200	0.62195800
C	-6.08747900	-2.09098000	-0.78169500	O	1.95388600	-1.02422100	0.86143200
C	-7.01839500	-2.20607300	0.43391200	O	2.27671700	-0.01432600	-1.43924200
H	-6.01854200	-3.07440000	-1.26767300	C	3.35368400	-1.36533100	0.77855000
H	-6.54458700	-1.42083300	-1.52303500	H	3.70185600	-1.55196600	1.80194500
H	-8.01061500	-2.54157800	0.11352400	H	3.44543700	-2.29553100	0.20534400
H	-6.64956800	-2.93182300	1.16674900	C	3.71376100	-0.09722600	-1.34101500
H	-7.14848500	-1.24811300	0.94868200	H	4.02018900	-0.96674800	-1.93174500
15				H	4.14785400	0.80291000	-1.79671300
P	-1.36203800	-0.04402500	-0.10399600	C	3.79826300	1.08526000	0.84850000
O	-1.80865400	1.55086500	-0.16294900	H	4.41739100	1.91186800	0.47945500
O	-2.40287900	-0.66335600	-1.23537100	H	3.96087600	0.98668500	1.93028300
O	-2.14758200	-0.50222500	1.28098300	C	4.16742100	-0.22901900	0.12699900
C	-3.81223600	-0.48598100	-0.98071200	C	5.68815800	-0.45830700	0.24480200
H	-4.27185500	-0.16039500	-1.92196500	C	6.22027700	-1.80442800	-0.26845700
H	-4.23486900	-1.46002600	-0.70672200	H	5.96764900	-0.34750900	1.30202500
C	-3.49571600	-0.01500200	1.44966600	H	6.19769500	0.35674200	-0.28776100
H	-4.09437700	-0.86214600	1.80020200	H	7.31030900	-1.83811400	-0.16670500
H	-3.49426600	0.75662600	2.23128800	H	5.81381000	-2.64979100	0.29730000
C	-3.22454900	1.81171700	-0.21937000	H	5.98576400	-1.96650600	-1.32621000
H	-3.43255300	2.61854600	0.49370100	Pd	-0.73501300	0.66242600	-0.20732800
H	-3.47573400	2.16731700	-1.22772700	C	-2.74998600	0.77811900	-0.63095000
C	-4.05212000	0.55644600	0.12993800	H	-2.97794200	1.23244700	-1.60117600
C	-5.53873600	0.95097800	0.24930800	C	-3.74648100	-0.26322500	-0.26593600
C	-6.54016000	-0.19846100	0.43370000	C	-4.82253400	-0.56220000	-1.12157000
H	-5.81286000	1.51764100	-0.65179600	C	-3.59098900	-1.01722700	0.91251500
H	-5.63868100	1.65387300	1.08812100	C	-5.70769700	-1.59598900	-0.81933400
H	-7.55425800	0.20248100	0.53592400	H	-4.95570200	0.01680000	-2.03261500
H	-6.54376900	-0.88100100	-0.42300700	C	-4.49168000	-2.03055900	1.22899300
H	-6.33065800	-0.78987700	1.33152600	H	-2.74187700	-0.80427400	1.55624600

C	-5.54827100	-2.32576600	0.36115400	C	3.49823800	1.58590500	-1.30472900
H	-6.52557300	-1.82557400	-1.49692500	H	4.09645700	1.22714800	-2.15058100
H	-4.36150200	-2.60423500	2.14248200	H	3.43635000	2.67901500	-1.35914700
H	-6.24177500	-3.12708800	0.60211800	C	3.29754500	1.75096700	1.18097600
N	-3.25485800	2.18333600	0.29466300	H	3.43670800	2.83568400	1.22546100
N	-3.33241000	2.96469900	1.08650300	H	3.60015800	1.32138600	2.14517800
17				C	3.95107000	-0.40576800	0.12032700
P	1.22247500	-0.40692100	-0.11619000	H	4.45777500	-0.79666900	1.01062700
O	1.81338400	-0.64444100	1.40618100	H	4.37863600	-0.89211700	-0.76598600
O	2.44078500	-1.08746300	-1.00779600	C	4.11593100	1.12648800	0.03192300
O	1.57691500	1.19365400	-0.32187800	C	5.61483700	1.47711500	0.13232000
C	3.75852900	-0.51966700	-0.83637100	C	5.99114100	2.95056300	-0.07981400
H	4.45718400	-1.35583300	-0.71188700	H	6.15611900	0.86401100	-0.60167100
H	4.01858000	0.01795700	-1.75559000	H	5.97443400	1.15268500	1.11873100
C	2.88641300	1.62177700	0.11201500	H	7.07153500	3.08024300	0.04407900
H	3.28943800	2.25541600	-0.68461900	H	5.73413500	3.30082300	-1.08534200
H	2.77052300	2.23230500	1.01724000	H	5.49864000	3.61215200	0.64099400
C	3.21479700	-0.35453500	1.59082800	Pd	-0.77353300	0.05210300	-0.32889100
H	3.30166900	0.24026900	2.50772500	Si	-0.79816400	-2.45358400	1.38621400
H	3.74788700	-1.30268400	1.73964900	Si	-0.91184300	-2.82097900	-1.00128800
C	3.80607900	0.41506400	0.38964700	C	0.79102400	-3.26546000	2.00268700
C	5.24481800	0.85307200	0.73362500	H	1.66144800	-2.68161400	1.68285200
C	6.05938300	1.48569100	-0.40414700	H	0.79104200	-3.31920100	3.09852500
H	5.78690500	-0.02582100	1.10956100	H	0.90324900	-4.28324200	1.61475400
H	5.19351800	1.55760600	1.57525800	C	-1.20683800	-1.01667200	2.54533800
H	7.04463900	1.78786700	-0.03343800	H	-2.17536900	-0.56244900	2.32023900
H	6.22307700	0.78585000	-1.23075800	H	-1.26312200	-1.45022000	3.55495400
H	5.57657600	2.37982400	-0.81330800	H	-0.44607700	-0.23030200	2.55618000
Pd	-0.93952500	-1.02095600	-	C	-2.58111200	-2.56644900	-1.84029200
0.41406900				H	-2.64609400	-3.20121300	-2.73330800
C	-2.78396300	-1.07359600	0.26641800	H	-3.39068200	-2.85455500	-1.15842200
H	-3.05157000	-1.87705200	0.97071300	H	-2.74077200	-1.52601700	-2.13233600
C	-3.85495400	-0.10566400	0.21138900	C	-0.56683600	-4.68765700	-1.00439400
C	-5.04789800	-0.27692700	0.95917900	H	-1.26432500	-5.23122600	-0.35798500
C	-3.74954000	1.04194200	-0.61497700	H	-0.68169900	-5.06772500	-2.02786600
C	-6.08499700	0.64558100	0.88046400	H	0.45280900	-4.91827700	-0.67753600
H	-5.14283200	-1.15051900	1.59967700	F	-2.03973600	-3.50685100	1.67895200
C	-4.78239900	1.96788900	-0.68854000	F	0.28168500	-2.22487600	-1.96137400
H	-2.83230700	1.17185600	-1.18234300	C	-2.28834400	1.11699600	-1.01666400
C	-5.95129600	1.76948000	0.05714700	H	-2.48294600	1.07702800	-2.10069700
H	-6.99415800	0.49880200	1.45713000	C	-3.11828000	2.14420100	-0.42499900
H	-4.68665300	2.84375700	-1.32421500	C	-4.07536500	2.85385700	-1.19383600
H	-6.75996200	2.49351700	-0.00290800	C	-3.01892400	2.45483200	0.95463900
18-ts				C	-4.90067800	3.81110500	-0.61358700
P	1.45423900	0.40332300	-0.13916000	H	-4.16083100	2.63288300	-2.25520200
O	2.56177700	-0.78135000	0.22382500	C	-3.83424700	3.41943100	1.53282100
O	2.16535400	1.05492000	-1.47573600	H	-2.27931300	1.91969600	1.54268600
O	1.88128700	1.52458200	1.00194900	C	-4.77898000	4.09611500	0.75069100

H	-5.63303900	4.34041700	-1.21711200	C	4.52415200	0.08888100	1.16991800
H	-3.74287000	3.64814400	2.59110300	H	5.30244000	0.82201000	0.93275100
H	-5.41929300	4.84772300	1.20531700	H	4.53691600	-0.09195100	2.25349500
19-ts				C	3.67993200	-2.23370600	0.89280700
P	-1.63479700	-0.86405900	-0.12098200	H	3.87731300	-2.52421200	1.93211000
O	-2.11501400	-1.17681800	1.43473900	H	3.69355800	-3.13984500	0.27175400
O	-3.11497100	-0.50535200	-0.79521400	C	4.74505000	-1.23030000	0.40319500
O	-1.46283900	-2.41750000	-0.68163300	C	6.14803600	-1.82006900	0.65543200
C	-4.12748300	-1.52891700	-0.72765400	C	7.33655400	-1.03065500	0.08731200
H	-5.05908800	-1.04512600	-0.40772000	H	6.16824000	-2.83720200	0.23935500
H	-4.27580500	-1.93330000	-1.73646800	H	6.27905600	-1.93644000	1.74034900
C	-2.48715100	-3.35998700	-0.30423400	H	8.27608300	-1.52779500	0.35185500
H	-2.73609800	-3.93311800	-1.20380600	H	7.29972900	-0.96270200	-1.00534200
H	-2.06991900	-4.04995800	0.44191300	H	7.38400300	-0.01075700	0.48413400
C	-3.31218000	-1.96369700	1.58592600	20			
H	-3.10512400	-2.71950200	2.35340300	P	-1.84553500	-0.27827800	-0.29445900
H	-4.11718600	-1.31116600	1.95029300	O	-3.19897600	0.25605600	-1.08554000
C	-3.72814500	-2.64140200	0.26214300	O	-1.90468300	-1.88255800	-0.71205400
C	-4.88820200	-3.61903000	0.54166900	O	-2.42891300	-0.36535600	1.25100800
C	-5.55535300	-4.25759200	-0.68518400	C	-3.08495900	-2.60965300	-0.31027300
H	-5.65311800	-3.08198100	1.12021400	H	-3.40293100	-3.21218000	-1.17016600
H	-4.51340400	-4.41280300	1.20277300	H	-2.80640600	-3.28733500	0.50572100
H	-6.33971100	-4.95217300	-0.36556300	C	-3.75265900	-0.92019700	1.40487400
H	-6.02533500	-3.50863900	-1.33169400	H	-3.70630200	-1.60721100	2.25605200
H	-4.84410900	-4.82573900	-1.29457000	H	-4.44689800	-0.10592700	1.65227700
Pd	0.09245700	0.58516300	-0.43103700	C	-4.36502200	-0.58589700	-0.98654600
C	-0.65178600	2.42126400	-1.12657500	H	-5.21714500	0.07048400	-0.77349900
H	-1.14274100	2.33722100	-2.10187600	H	-4.53308900	-1.06898200	-1.95836100
C	-1.45933200	3.26173600	-0.19344000	C	-4.20923000	-1.64717000	0.12305500
C	-2.78136600	3.61503200	-0.51391000	C	-5.55736600	-2.37104900	0.31853700
C	-0.94637100	3.64765300	1.05875600	C	-5.55622500	-3.57973200	1.26586900
C	-3.57566800	4.31158200	0.39690500	H	-5.91369800	-2.69665200	-0.66886400
H	-3.18996300	3.32635500	-1.47936800	H	-6.29065000	-1.63422400	0.67470700
C	-1.72915900	4.37029200	1.95553200	H	-6.56864100	-3.98915100	1.34986400
H	0.06991700	3.36496400	1.32085400	H	-4.90758800	-4.38447200	0.90318300
C	-3.04915600	4.69922900	1.63066400	H	-5.22663900	-3.31435800	2.27625100
H	-4.60052200	4.56426800	0.13726000	Pd	0.06862700	0.95108900	-0.59579600
H	-1.31547300	4.66568400	2.91616500	C	0.27068400	2.85737600	-1.02816300
H	-3.66270500	5.25311600	2.33634000	H	0.31559100	3.12950400	-2.09492300
N	0.58562200	3.48612600	-1.67492900	C	0.38842800	4.06062100	-0.22192600
N	1.62662700	3.87994900	-1.80063600	C	0.52832000	5.33878400	-0.81430400
P	2.18100100	-0.26041100	-0.01262900	C	0.36583700	3.99258400	1.19252700
O	2.35723600	-1.66808800	0.85180400	C	0.63939200	6.48894200	-0.03779300
O	3.10282000	-0.64012000	-1.33981100	H	0.54788600	5.41234900	-1.89932200
O	3.26314600	0.69351600	0.81555900	C	0.47738400	5.13877800	1.96979000
C	4.48576600	-0.96786100	-1.09456800	H	0.25834700	3.01368200	1.65163600
H	4.71628700	-1.86249600	-1.68647000	C	0.61423300	6.39070700	1.35651400
H	5.10307100	-0.13953000	-1.46302600	H	0.74590800	7.46055800	-0.51336500

H	0.45853000	5.06536300	3.05404700	H	4.61426900	-4.62137500	-2.53837600
H	0.70125300	7.28704100	1.96555000	C	3.09286300	-0.01038100	1.67406000
P	1.70149800	-0.63198300	-0.29497700	C	2.42877200	0.68388400	2.69900400
O	2.12316700	-1.53595700	-1.61444600	C	4.29377700	-0.67140000	1.97378500
O	3.19367600	-0.07146200	0.15618100	C	2.96332700	0.73384100	3.98644500
O	1.51308700	-1.83611700	0.82991900	H	1.48230700	1.17262200	2.47995500
C	4.18527500	-1.06774200	0.48437000	C	4.82372100	-0.62761100	3.26572300
H	5.11877600	-0.76544200	-0.00575600	H	4.81520900	-1.22832000	1.20097300
H	4.34099300	-1.05226600	1.56968400	C	4.16270200	0.07714200	4.27313400
C	2.50809500	-2.88138500	0.82442700	H	2.43720900	1.27593900	4.76791500
H	2.76940200	-3.07348200	1.87035500	H	5.75282100	-1.14822300	3.48361700
H	2.05724300	-3.79109700	0.40544800	H	4.57526900	0.10768800	5.27822200
C	3.31098200	-2.34036300	-1.47148900	C	-3.09350200	-0.49121400	1.60352900
H	3.08009500	-3.32802600	-1.88800900	C	-2.43338500	-1.46183900	2.37525600
H	4.11355500	-1.88950100	-2.07027600	C	-4.29307700	0.05441200	2.08517200
C	3.74652000	-2.46594300	0.00513500	C	-2.97056000	-1.89168500	3.58869500
C	4.88402700	-3.50301800	0.10508600	H	-1.48783400	-1.86606400	2.02152900
C	5.56595800	-3.64099000	1.47393500	C	-4.82534800	-0.37046800	3.30503200
H	5.64544800	-3.24555000	-0.64461700	H	-4.81068700	0.81746400	1.51176600
H	4.48181300	-4.47982800	-0.19768700	C	-4.16840100	-1.34611500	4.05683300
H	6.33177800	-4.42297100	1.43283800	H	-2.44788400	-2.64411300	4.17351000
H	6.06193000	-2.71363900	1.78015000	H	-5.75324600	0.06451900	3.66769400
H	4.85826900	-3.91764800	2.26295700	H	-4.58298500	-1.67373100	5.00664500
21				C	-3.10498200	-1.14460200	-1.22614000
P	2.31500800	-0.00119700	-0.00613100	C	-4.30377600	-1.83366900	-0.98652100
P	-2.31363000	-0.00134200	-0.00276200	C	-2.45554100	-1.32543500	-2.45880600
Pd	0.00046600	-0.00436200	-0.00963100	C	-4.84581300	-2.67338800	-1.96285900
C	3.10164100	1.45849800	-0.82995200	H	-4.81346400	-1.72138900	-0.03438800
C	2.44143700	2.01012600	-1.94039300	C	-3.00250800	-2.15707300	-3.43590300
C	4.30605100	2.03798700	-0.40286300	H	-1.51100100	-0.81763300	-2.63907200
C	2.98346400	3.10089800	-2.62029800	C	-4.19975400	-2.83368600	-3.18973900
H	1.49217000	1.58443800	-2.25678500	H	-5.77294300	-3.20402200	-1.76141000
C	4.84267100	3.13675700	-1.07846000	H	-2.48825300	-2.28528700	-4.38482200
H	4.82298300	1.63674200	0.46362300	H	-4.62192700	-3.48931700	-3.94690900
C	4.18557600	3.66778100	-2.18972500	C	-3.09908900	1.63365100	-0.37648200
H	2.46082400	3.51549400	-3.47836900	C	-4.29685300	1.77845800	-1.09279400
H	5.77376100	3.57879100	-0.73285700	C	-2.44404300	2.78760800	0.08554900
H	4.60333400	4.52433900	-2.71240200	C	-4.83139300	3.04711300	-1.33155100
C	3.10573700	-1.44777100	-0.84907500	H	-4.81171400	0.90125500	-1.47255500
C	4.30852700	-1.37012200	-1.56761300	C	-2.98396300	4.05293100	-0.14490500
C	2.45009300	-2.68700200	-0.75937600	H	-1.50063900	2.68451500	0.61640300
C	4.84715500	-2.50831900	-2.17296600	C	-4.17920200	4.18580200	-0.85581200
H	4.82369100	-0.41895900	-1.66275900	H	-5.75751000	3.14344700	-1.89257500
C	2.99440600	-3.82465300	-1.35527500	H	-2.46551400	4.93539500	0.22095500
H	1.50226200	-2.74723500	-0.22980700	H	-4.59570400	5.17193400	-1.04409900
C	4.19448600	-3.73754800	-2.06511300	22-ts			
H	5.77713600	-2.43166600	-2.73067400	P	1.84388300	0.91016000	-0.13918100
H	2.47469200	-4.77595400	-1.27610600	Pd	0.04618900	-0.54999000	-0.52690700

C	0.68083300	-2.36736500	-1.37323700	H	-5.80419700	-1.83784100	-4.08732200
H	1.12989100	-2.22962000	-2.36339800	C	1.53636200	2.63146500	-0.76473800
C	1.51139100	-3.30721300	-0.55343300	C	0.84947500	2.76073300	-1.98418300
C	2.73383200	-3.80609000	-1.03618600	C	1.92991500	3.79751500	-0.09093100
C	1.11284500	-3.66469800	0.74825300	C	0.58133100	4.01802800	-2.52526800
C	3.54317900	-4.61694500	-0.23891600	H	0.51385200	1.86448600	-2.50032300
H	3.05439500	-3.54486400	-2.04166100	C	1.64551400	5.05766300	-0.62432000
C	1.90941000	-4.49126400	1.53735500	H	2.45497000	3.72637200	0.85616200
H	0.17727800	-3.27150800	1.13727100	C	0.97586500	5.17192400	-1.84351000
C	3.13091200	-4.96644100	1.04860400	H	0.05150300	4.09700400	-3.47102600
H	4.48893800	-4.98583100	-0.62797900	H	1.95290600	5.95059800	-0.08551000
H	1.58458200	-4.75642100	2.54012900	H	0.75676500	6.15281900	-2.25719000
H	3.75581000	-5.60432000	1.66816300	C	2.26999700	1.15901100	1.64964200
N	-0.59940000	-3.34896500	-1.91148300	C	3.52227700	1.62471800	2.08513700
N	-1.66987100	-3.69090900	-1.96000000	C	1.29193900	0.86196900	2.61176800
P	-2.20997100	0.04510900	-0.00458700	C	3.78032700	1.80466800	3.44518600
C	-2.75400900	-0.80082500	1.55282100	H	4.30213200	1.83888900	1.36020600
C	-2.68574600	-2.20571300	1.60900900	C	1.54966100	1.04401100	3.97207500
C	-3.13532300	-0.10425000	2.70871900	H	0.33023500	0.47436700	2.28564200
C	-3.00170800	-2.89048100	2.78141400	C	2.79386500	1.51737900	4.39169900
H	-2.39729700	-2.76542600	0.72292800	H	4.75454800	2.16564600	3.76527100
C	-3.43882800	-0.79173500	3.88781900	H	0.78004100	0.80599100	4.70168600
H	-3.19913800	0.97899900	2.69119800	H	2.99816800	1.65397500	5.45054300
C	-3.37514600	-2.18421900	3.92897600	C	3.51853100	0.54268000	-0.85867600
H	-2.95403400	-3.97638200	2.80010300	C	4.17086700	-0.63250400	-0.44360300
H	-3.73198900	-0.23287200	4.77310500	C	4.13472700	1.33894700	-1.83569500
H	-3.61547200	-2.71717200	4.84512600	C	5.40741300	-0.99001300	-0.97821000
C	-2.81446400	1.78512000	0.25356100	H	3.70887600	-1.27248900	0.30263400
C	-1.89193700	2.74423900	0.69654800	C	5.36904200	0.97186900	-2.38039300
C	-4.14371700	2.18176500	0.03289000	H	3.65644800	2.25242100	-2.17363100
C	-2.28670200	4.06362100	0.92810500	C	6.01134600	-0.18960300	-1.95243000
H	-0.85632700	2.45732900	0.84870300	H	5.89506400	-1.89983400	-0.63767400
C	-4.53716500	3.50177300	0.25681400	H	5.82930200	1.60292300	-3.13674700
H	-4.87360600	1.46066100	-0.32166100	H	6.97280200	-0.47122800	-2.37399800
C	-3.61055000	4.44557900	0.70702100	23			
H	-1.55375700	4.79186700	1.26451400	P	2.01139200	-0.26871300	0.06512900
H	-5.56901600	3.79354100	0.07740200	Pd	-0.06261800	0.80364700	0.51424200
H	-3.91875900	5.47406500	0.87708700	C	-0.31788500	2.62448600	1.21141100
C	-3.41430900	-0.59162300	-1.26467800	H	-0.39533600	2.73445800	2.30654500
C	-4.65169900	-1.17556300	-0.95023300	C	-0.48316700	3.93691700	0.59971800
C	-3.05190800	-0.47588200	-2.61719300	C	-0.73935000	5.09244500	1.37844000
C	-5.50550800	-1.62219100	-1.96170400	C	-0.40015200	4.10642300	-0.80464300
H	-4.94945600	-1.28849700	0.08783400	C	-0.90711400	6.34374800	0.79130700
C	-3.90931900	-0.91200500	-3.62765000	H	-0.80669100	4.98826500	2.45924500
H	-2.08453100	-0.04954300	-2.87278700	C	-0.56537700	5.35487600	-1.39324100
C	-5.13928800	-1.48825900	-3.30188500	H	-0.19777700	3.22767100	-1.41047800
H	-6.45820600	-2.07562300	-1.69975900	C	-0.82062700	6.47872300	-0.59755200
H	-3.61235000	-0.81164300	-4.66851700	H	-1.10405700	7.21470200	1.41149400

H	-0.49505100	5.46016600	-2.47297100	C	4.11729700	0.59390200	-1.68802500
H	-0.94960700	7.45461400	-1.05884600	C	1.86450000	0.73270700	-2.54771900
P	-1.87435500	-0.67222400	0.07427800	C	4.60561800	1.09903100	-2.89522000
C	-3.16935200	0.09714800	-1.01079800	H	4.81098300	0.35711400	-0.88694200
C	-3.35624100	1.48736800	-0.93215900	C	2.35334800	1.23005100	-3.75643900
C	-3.96871700	-0.64208600	-1.89791500	H	0.79331300	0.61968000	-2.40070300
C	-4.32693700	2.11916700	-1.71007300	C	3.72643800	1.41457700	-3.93285600
H	-2.72711500	2.06872600	-0.26472000	H	5.67481500	1.24838700	-3.02228300
C	-4.93417200	-0.00552800	-2.68163800	H	1.66097000	1.48323800	-4.55518200
H	-3.83840600	-1.71627900	-1.98154500	H	4.10838300	1.80990500	-4.87047500
C	-5.11724500	1.37516000	-2.58904500	C	3.31313600	0.12625700	1.33173600
H	-4.45618300	3.19577300	-1.63551500	C	3.26224900	1.37403000	1.97413800
H	-5.54284400	-0.59227700	-3.36515600	C	4.35031900	-0.76057600	1.66407300
H	-5.86751700	1.86857400	-3.20162200	C	4.23139900	1.73108800	2.91206400
C	-1.72955500	-2.36978200	-0.66188500	H	2.44808200	2.05458600	1.73916500
C	-0.95616000	-2.51074200	-1.82639700	C	5.31396300	-0.40469500	2.61092700
C	-2.33354200	-3.51240800	-0.11648000	H	4.40835800	-1.73390600	1.18732800
C	-0.80783500	-3.75261900	-2.44112300	C	5.25888900	0.84206600	3.23562100
H	-0.45948900	-1.64155100	-2.24992400	H	4.17698900	2.70215500	3.39758300
C	-2.17492200	-4.76006500	-0.72616200	H	6.10714000	-1.10555300	2.85901300
H	-2.93304600	-3.43229300	0.78463500	H	6.00804100	1.11689400	3.97371700
C	-1.41664000	-4.88343300	-1.89046300	24			
H	-0.20601000	-3.84004000	-3.34164600	P	-1.05904700	-0.02891500	0.03550600
H	-2.64953100	-5.63505000	-0.28888600	Pd	1.14556700	-0.63129900	0.65412900
H	-1.29505600	-5.85420600	-2.36384900	C	2.97998500	-1.27067400	0.48240700
C	-2.78024600	-0.98267600	1.65864700	H	3.13451500	-2.35838000	0.39237000
C	-4.17119200	-1.15738900	1.72601100	C	4.23907500	-0.59308500	0.25578100
C	-2.03389700	-1.03892400	2.84660400	C	5.42717700	-1.31429200	-0.02394300
C	-4.79775700	-1.39226500	2.95190300	C	4.32515100	0.81976800	0.32669000
H	-4.76831100	-1.10415300	0.82051500	C	6.63843800	-0.66013100	-0.22096400
C	-2.65954000	-1.28117400	4.07017000	H	5.37872300	-2.39920900	-0.08121900
H	-0.96091500	-0.86715400	2.80757600	C	5.53396800	1.47509400	0.12763300
C	-4.04389900	-1.45801100	4.12536500	H	3.41278400	1.36840800	0.54155800
H	-5.87660800	-1.52024300	2.98893100	C	6.69176700	0.73611400	-0.14599500
H	-2.06715400	-1.32029700	4.98063900	H	7.54001000	-1.22843300	-0.43314600
H	-4.53366400	-1.63791500	5.07884800	H	5.58394700	2.55904300	0.18492800
C	2.22215100	-2.10232400	-0.12016100	H	7.63726100	1.24979800	-0.30081100
C	1.60779200	-2.92601500	0.83792400	C	-1.87627400	-1.20889500	-1.12857600
C	2.94608700	-2.70671600	-1.15864100	C	-1.07390500	-1.83882800	-2.09385900
C	1.73037000	-4.31283800	0.77303200	C	-3.24897300	-1.49819800	-1.09275100
H	1.02230100	-2.47604400	1.63596500	C	-1.63619000	-2.72249600	-3.01535500
C	3.05944500	-4.09787100	-1.23019500	H	-0.00507700	-1.64127300	-2.10698000
H	3.42668700	-2.09382400	-1.91455500	C	-3.80817300	-2.38969500	-2.01123700
C	2.45681200	-4.90379000	-0.26414600	H	-3.88228600	-1.03381100	-0.34264900
H	1.24830600	-4.93263800	1.52427200	C	-3.00456900	-3.00029400	-2.97575400
H	3.62365100	-4.54924900	-2.04263700	H	-1.00319600	-3.20221100	-3.75724000
H	2.54642200	-5.98546000	-0.32079400	H	-4.87213500	-2.60836800	-1.96962100
C	2.74017500	0.39834100	-1.50161200	H	-3.44107100	-3.69566700	-3.68796200

C	-1.25108000	1.60897800	-0.79901700	H	-2.72890900	-1.13361700	-4.56593900
C	-2.23384500	1.87501000	-1.76470300	H	-5.70513600	-1.50280600	-1.48046300
C	-0.36120500	2.63289600	-0.43692100	H	-5.05810000	-1.67484100	-3.87540800
C	-2.32989500	3.14113200	-2.34630500	C	-1.34554200	1.84663200	0.00686500
H	-2.92102200	1.09142500	-2.06934500	C	-0.27134600	2.61881000	0.47932600
C	-0.46372800	3.89965500	-1.01240400	C	-2.51218700	2.50112200	-0.41699400
H	0.41982500	2.42302200	0.28962700	C	-0.36816400	4.00886600	0.54414900
C	-1.44824900	4.15601400	-1.96948700	H	0.64547600	2.12022400	0.78489600
H	-3.09276500	3.33231600	-3.09663100	C	-2.60456400	3.89409400	-0.36048800
H	0.23179200	4.68256300	-0.72163600	H	-3.34944800	1.92483000	-0.79890600
H	-1.52290300	5.13983700	-2.42535100	C	-1.53544600	4.65036500	0.12261500
C	-2.23515300	0.05938300	1.46156700	H	0.47202000	4.59110600	0.91356200
C	-2.09491400	-0.90828700	2.47159900	H	-3.51313000	4.38692300	-0.69722000
C	-3.23074700	1.03858300	1.59555500	H	-1.60822500	5.73409300	0.16340800
C	-2.94369300	-0.90815800	3.57814900	C	-1.81114900	-0.52493400	1.61724500
H	-1.31149800	-1.65812300	2.38878500	C	-1.45107300	-1.79779700	2.08935900
C	-4.07484900	1.04125200	2.70885000	C	-2.65319600	0.27388300	2.40574800
H	-3.34665500	1.80289700	0.83327600	C	-1.93528100	-2.26795700	3.30998200
C	-3.93585700	0.06787800	3.69956600	H	-0.77784100	-2.41129500	1.49542500
H	-2.82331700	-1.66375500	4.34992400	C	-3.12957900	-0.19389900	3.63317500
H	-4.84057100	1.80729300	2.80068900	H	-2.93377400	1.26650700	2.06671900
H	-4.59228500	0.07376200	4.56573100	C	-2.77488500	-1.46539200	4.08647100
25				H	-1.64793600	-3.25608000	3.65995200
P	-1.13164100	0.00585700	-0.02333000	H	-3.77649400	0.43904200	4.23537800
Pd	0.98185900	-0.69185800	-0.47187100	H	-3.14421900	-1.82648800	5.04281000
C	3.02413400	-1.31439800	-0.96345900	26-ts			
H	2.85136200	-1.34770200	-2.04211400	P	-1.19697500	0.00233800	-0.03482200
C	3.97736400	-0.30473000	-0.42752900	Pd	0.96453400	-0.76690000	-0.30294100
C	4.26791400	0.82177300	-1.21639900	C	2.92103500	-1.11835800	-0.77586500
C	4.59553700	-0.42943400	0.82738500	H	3.06954500	-1.48650600	-1.79742200
C	5.15195000	1.79626700	-0.75885900	C	4.04299000	-0.23123100	-0.35476000
H	3.78928000	0.93365000	-2.18570300	C	5.07627300	0.09030800	-1.25254800
C	5.48122400	0.54841600	1.27727500	C	4.05619700	0.35569000	0.92429200
H	4.38212300	-1.28826200	1.45847500	C	6.08192200	0.98748800	-0.89312700
C	5.76469700	1.66643400	0.48989900	H	5.08254300	-0.36206900	-2.24168600
H	5.36278000	2.66039900	-1.38334500	C	5.07692000	1.22702800	1.29468600
H	5.94973100	0.43449000	2.25125700	H	3.24316000	0.12864900	1.60839900
H	6.45391600	2.42719800	0.84500600	C	6.08900300	1.55084300	0.38463400
N	3.09199800	-2.55675100	-0.45402300	H	6.86491200	1.23691500	-1.60426600
N	3.18743700	-3.59910700	-0.01045100	H	5.07593700	1.66970100	2.28713300
C	-2.44007000	-0.54577900	-1.21461700	H	6.87663600	2.24313100	0.67005400
C	-2.08338900	-0.65847300	-2.56839200	N	3.28440800	-2.63567400	-0.01773800
C	-3.75512000	-0.85580800	-0.83587700	N	3.25649700	-3.49511400	0.69545000
C	-3.02144700	-1.05290900	-3.52218100	C	-2.30810200	-1.06958700	0.98911700
H	-1.05906100	-0.44516000	-2.86450600	C	-1.73103500	-1.75559600	2.07069800
C	-4.69176200	-1.26052900	-1.79049500	C	-3.67893300	-1.23435400	0.73903600
H	-4.04970700	-0.78896000	0.20703800	C	-2.50889000	-2.56935800	2.89420200
C	-4.32889700	-1.35706600	-3.13470700	H	-0.66398400	-1.65417800	2.25381800

C	-4.45529500	-2.05680800	1.55927200	H	6.34302000	1.06485600	1.67153600
H	-4.14244300	-0.72567200	-0.10079200	H	6.70651400	-0.01350000	0.31561500
C	-3.87395000	-2.72264400	2.63955500	Pd	-0.54687000	-0.45971400	-0.30751700
H	-2.04696900	-3.09236200	3.72756800	Si	0.23441800	-2.59527300	0.60080500
H	-5.51519500	-2.17803600	1.35038200	Si	-3.08992500	-1.16865300	-0.37984100
H	-4.47920700	-3.36396200	3.27495400	C	0.90188600	-3.81902200	-0.69043800
C	-1.33303300	1.65806900	0.78377100	H	1.82348700	-3.42878900	-1.13758400
C	-2.37562500	2.01302500	1.65304200	H	1.12532300	-4.79016200	-0.22888900
C	-0.32787600	2.60113200	0.51189700	H	0.18376300	-3.98773800	-1.50082900
C	-2.41648000	3.28536800	2.22904800	C	1.46789800	-2.56711700	2.04729600
H	-3.15480800	1.29423200	1.88807600	H	1.15744700	-1.87125100	2.83468800
C	-0.37511400	3.87411200	1.08022500	H	1.55765600	-3.56748900	2.49045500
H	0.49763300	2.32301800	-0.13897400	H	2.46148600	-2.25750000	1.70249500
C	-1.41957500	4.21901100	1.94177800	C	-3.63809000	-1.36751100	1.40319500
H	-3.22797900	3.54424600	2.90448500	H	-4.64353000	-1.80707500	1.43392100
H	0.40939700	4.59294300	0.85825700	H	-2.94735800	-2.03167500	1.92995200
H	-1.45190100	5.20769200	2.39223700	H	-3.67686000	-0.40336200	1.92058800
C	-2.15083100	0.23037200	-1.60556400	C	-2.99022700	-2.77663700	-1.35728500
C	-1.89099200	-0.66080100	-2.65959500	H	-2.38430600	-3.51845300	-0.83214100
C	-3.10894400	1.23822600	-1.79385300	H	-4.00513300	-3.17628100	-1.48640600
C	-2.58597400	-0.55933500	-3.86491000	H	-2.56353800	-2.61149600	-2.35259100
H	-1.12930300	-1.42573800	-2.52951100	F	-1.07910600	-3.37889100	1.25814100
C	-3.79786900	1.34440500	-3.00451000	F	-4.31409200	-0.37043300	-1.13753200
H	-3.31446400	1.94753600	-0.99776300	C	-1.92990900	0.83184900	-0.91845200
C	-3.54089600	0.44492700	-4.04066800	H	-2.21366900	0.84269500	-1.97769300
H	-2.37357400	-1.25759600	-4.67037200	C	-2.58451200	1.92000000	-0.20244800
H	-4.53375700	2.13344800	-3.13724300	C	-3.40957800	2.84048800	-0.88970200
H	-4.07601100	0.53085800	-4.98283500	C	-2.37360600	2.13230800	1.18165100
27-ts				C	-3.97104000	3.93384100	-0.23617200
P	1.55454100	0.25112100	-0.30146900	H	-3.60125100	2.68296600	-1.94777200
O	1.88783000	1.58052800	-1.21541100	C	-2.94429300	3.21677500	1.83664200
O	2.15668300	0.72552200	1.15141100	H	-1.74072200	1.43433900	1.72374700
O	2.74741300	-0.75863700	-0.82208100	C	-3.74348500	4.12408100	1.12956800
C	3.57258300	1.03483200	1.17403100	H	-4.59582400	4.63222400	-0.78661600
H	3.68272400	1.96422400	1.74353700	H	-2.76713900	3.36247000	2.89896900
H	4.08223700	0.22891100	1.71345300	H	-4.18847100	4.97211400	1.64335400
C	4.06336200	-0.16971400	-0.96201100	28			
H	4.76790300	-0.88468500	-0.52704700	P	1.64308000	0.14164900	0.06808400
H	4.28371500	-0.06536000	-2.03159800	O	2.14375300	1.39616800	1.01361900
C	3.19815600	2.16109700	-1.01840400	O	2.40585800	-1.10490200	0.81929800
H	3.59980700	2.38333700	-2.01324200	O	2.58856700	0.36232900	-1.25244300
H	3.07858000	3.10388400	-0.46995600	C	3.85122900	-1.03487400	0.84951200
C	4.13274800	1.19913900	-0.25472200	H	4.16106700	-1.30324200	1.86577600
C	5.56411500	1.77597900	-0.25461600	H	4.23745700	-1.78553200	0.15178800
C	6.59846800	1.03684900	0.60679900	C	3.98591900	0.64361000	-0.99482700
H	5.50852500	2.82194300	0.07722900	H	4.55948500	-0.00191800	-1.66611100
H	5.91686600	1.80840100	-1.29461500	H	4.17929300	1.69024800	-1.26129700
H	7.58028900	1.50863000	0.49533500	C	3.55277300	1.39310300	1.34417300

H	3.92119400	2.41142800	1.17701800	O	-2.67261900	-1.19681500	0.49678700
H	3.65532000	1.15384200	2.41013200	O	-2.84913200	1.32856800	0.47393900
C	4.34182200	0.38130200	0.48266300	C	-4.11920700	-1.19493700	0.49398100
C	5.85046000	0.56127400	0.75420400	H	-4.44170600	-2.17992400	0.13634100
C	6.79040100	-0.45832800	0.09457200	H	-4.45756800	-1.07077700	1.52877900
H	6.00389000	0.53335200	1.84199700	C	-4.26802300	1.28025600	0.19726200
H	6.13574500	1.57341400	0.43595000	H	-4.77835600	1.45922400	1.14869800
H	7.83011500	-0.21803000	0.34019500	H	-4.51330500	2.10041600	-0.48976000
H	6.60045000	-1.47890800	0.44367100	C	-3.97923500	-0.19886700	-1.78779000
H	6.70451000	-0.45646000	-0.99732000	H	-4.39404800	0.53046700	-2.49296100
Pd	-0.61135900	-0.03256000	-	H	-4.12147500	-1.20491600	-2.20279200
0.21579400				C	-4.67205100	-0.07721600	-0.41301600
Si	-0.52640500	-2.26774300	-0.90102800	C	-6.19864100	-0.19043800	-0.61008800
Si	-3.71672000	-0.51420300	1.04203800	C	-7.05307900	-0.23186600	0.66541700
C	-0.53302200	-3.49272700	0.54050500	H	-6.39835400	-1.09574400	-1.20004900
H	-1.44752200	-3.42136300	1.13929100	H	-6.52396700	0.65325500	-1.23416100
H	-0.44419800	-4.52289100	0.17079600	H	-8.11436500	-0.28259200	0.40039100
H	0.31830200	-3.29117300	1.19985400	H	-6.82903300	-1.10862500	1.28250500
C	-1.77060600	-2.77299300	-2.23175500	H	-6.91412300	0.65960800	1.28626300
H	-1.70733300	-2.10120000	-3.09502400	Pd	0.26131000	0.30871400	0.03679300
H	-1.55877500	-3.79211900	-2.58087600	Si	1.20231700	-1.83485000	0.73397300
H	-2.79903800	-2.74609300	-1.85682600	Si	3.95694800	-0.71151100	-0.65706500
C	-2.86118100	-0.57784200	2.71974800	C	0.49821200	-1.96636700	2.48340000
H	-3.53117000	-1.03303500	3.45996300	H	-0.57537500	-1.75244200	2.48904100
H	-1.94334400	-1.17523000	2.67948900	H	0.65616700	-2.97991100	2.87458600
H	-2.59745900	0.41847400	3.09192800	H	0.98766000	-1.26317800	3.16703900
C	-4.43205300	-2.20320900	0.61288200	C	0.31655500	-2.95547900	-0.51109000
H	-3.66365100	-2.97570200	0.50079300	H	0.61072700	-2.73867700	-1.54275900
H	-5.11746100	-2.52926000	1.40452500	H	0.56283800	-4.00480200	-0.30092600
H	-5.00410100	-2.16057100	-0.32169100	H	-0.76671400	-2.82297500	-0.43270500
F	0.93303000	-2.50129600	-1.63239400	C	3.49842900	-1.88535700	-2.05232300
F	-5.01651300	0.46429200	1.26050700	H	4.35832600	-2.00120100	-2.72322600
C	-2.72252600	0.15289400	-0.39468200	H	3.21873000	-2.87567000	-1.68235900
H	-3.12759200	-0.23631600	-1.33362800	H	2.66567400	-1.49241000	-2.64770400
C	-2.38625100	1.58906700	-0.50466900	C	5.39269200	-1.32631300	0.38660600
C	-2.50610400	2.29483300	-1.73219500	H	5.11877600	-2.22947600	0.93891800
C	-1.79980900	2.28877000	0.58449500	H	6.25933600	-1.55295800	-0.24588400
C	-2.09581800	3.61309200	-1.84990000	H	5.70085200	-0.56070200	1.10885300
H	-2.94257900	1.78227700	-2.58580200	F	2.64262500	-2.67028200	0.88332600
C	-1.37478900	3.61926900	0.45136900	F	4.52081400	0.61905400	-1.43073800
H	-1.73769500	1.81001100	1.55755400	C	2.52442300	-0.09917400	0.46155200
C	-1.52327400	4.28683700	-0.75753300	H	2.85803100	-0.29042000	1.48960800
H	-2.21815100	4.12985600	-2.79863100	C	2.25372900	1.39368400	0.38390500
H	-0.94070400	4.12626400	1.30899600	C	2.19221500	2.16884500	1.56996400
H	-1.20308700	5.31993000	-0.85956700	C	2.07123700	2.08306200	-0.84464500
29-ts				C	1.99156100	3.54520600	1.53076400
P	-1.93065900	0.12145300	-0.17667100	H	2.32693300	1.67210600	2.52800900
O	-2.56019100	0.05868300	-1.70039600	C	1.86350000	3.46658300	-0.87264800

H	2.15521000	1.54348200	-1.78208700	H	2.19496400	-1.28036700	-1.57461200
C	1.83015200	4.20531800	0.30787500	H	1.86998000	0.37003800	-2.15540000
H	1.96516200	4.10749400	2.46073000	C	1.54371200	1.62566400	0.19091000
H	1.74406900	3.96291100	-1.83210800	H	1.93259300	2.34440500	-0.53996400
H	1.67958100	5.28078300	0.27990400	H	1.74466700	2.01160600	1.19903700
30				C	2.20770000	0.24569800	-0.00082600
C	-3.11127500	0.28350100	1.19719900	C	3.74068400	0.41913200	0.00446200
C	-1.73603600	0.26966300	0.95986200	C	4.57497900	-0.87015300	-0.00238300
C	-1.22260100	0.03048500	-0.32778200	H	4.01230300	1.01120000	0.88975300
C	-2.14083100	-0.19866400	-1.36505300	H	4.01709300	1.03273100	-0.86420700
C	-3.51622300	-0.18635200	-1.12977900	H	5.64188100	-0.62431900	-0.02887800
C	-4.00969700	0.05590400	0.15320700	H	4.40124100	-1.47515800	0.89399100
H	-3.47940300	0.47364500	2.20222100	H	4.36213300	-1.49635200	-0.87549900
H	-1.05154300	0.44885400	1.78559900	Pd	-2.70451400	-0.11943900	0.00022300
H	-1.77031800	-0.39400300	-2.36874200	32			
H	-4.20260500	-0.36800700	-1.95292500	Sn	-1.42750200	-0.00004200	-0.00019500
H	-5.08038800	0.06614800	0.33769900	Sn	1.42750500	0.00006500	0.00025800
C	0.27328600	0.00792900	-0.59564600	C	2.21148300	1.86440700	0.76520600
H	0.42849200	-0.02625900	-1.68650100	H	1.87997400	2.03727000	1.79458400
Si	1.04520700	-1.62694500	0.00329500	H	3.30739300	1.84539700	0.75764600
Si	1.17954800	1.57620200	-0.03203300	H	1.88032100	2.71008600	0.15314800
C	2.88632000	-1.71986900	-0.36747200	C	2.21072600	-1.59524300	1.23195000
H	3.46389500	-1.04349900	0.27327900	H	1.88093300	-2.57287900	0.86451800
H	3.24912600	-2.73833000	-0.18352300	H	3.30658500	-1.57814900	1.22146300
H	3.10846500	-1.47496500	-1.41237600	H	1.87752100	-1.49029300	2.26992800
F	1.64646900	1.33275800	1.52205800	C	2.21232400	-0.26972300	-1.99666300
F	0.34045000	-2.79185100	-0.90076300	H	1.88003100	0.53438600	-2.66180800
C	0.70219200	-2.01451600	1.80366600	H	3.30816700	-0.26516500	-1.97577000
H	-0.37161000	-2.08321600	2.00431900	H	1.88277600	-1.22330200	-2.42274000
H	1.15969100	-2.97222500	2.07890300	C	-2.21068500	1.59739500	-1.22917500
H	1.12239000	-1.23740800	2.45249800	H	-1.87737100	1.49425900	-2.26729700
C	0.08430200	3.09939700	-0.06240200	H	-3.30654200	1.58021100	-1.21882700
H	-0.79197200	2.98712800	0.58280600	H	-1.88098200	2.57441900	-0.86002700
H	0.64451800	3.98196200	0.26843800	C	-2.21132400	-1.86304100	-0.76871500
H	-0.27742800	3.29431800	-1.07960400	H	-1.88031200	-2.70987300	-0.15817000
C	2.73233500	1.88108700	-1.04856700	H	-3.30723400	-1.84404000	-0.76136800
H	3.43950600	1.04709300	-1.00619900	H	-1.87957800	-2.03400100	-1.79833700
H	2.47904600	2.05268500	-2.10242700	C	-2.21253600	0.26609200	1.99708600
H	3.25066400	2.77692300	-0.68617600	H	-1.88309700	1.21892200	2.42492800
31				H	-3.30838000	0.26151500	1.97605900
P	-0.54795200	0.04514700	-0.00014900	H	-1.88028300	-0.53923400	2.66078300
O	0.11493200	1.56188700	-0.00081600	33-ts			
O	0.28090000	-0.62296100	1.26734400	P	1.95761200	0.93148500	-0.34602000
O	0.28058900	-0.62521000	-1.26696100	O	2.77402200	1.92978800	-1.37451700
C	1.71947200	-0.67091600	1.13916200	O	2.70621600	1.30450200	1.08114600
H	2.13737800	-0.34991400	2.10086800	O	2.71107300	-0.50701200	-0.69153100
H	2.01172900	-1.71263200	0.96242900	C	4.13584000	1.09284300	1.13255600
C	1.69504800	-0.33675200	-1.33334100	H	4.57602400	1.98675400	1.59020200

H	4.32710000	0.23500400	1.78733800	H	1.48373600	-3.05959200	2.70264600
C	4.15114800	-0.46679500	-0.81973300	H	1.16090800	-3.98907900	1.22349600
H	4.53878300	-1.32526500	-0.26248100	H	1.92980500	-2.39173700	1.11216100
H	4.40944900	-0.59194400	-1.87922400	C	-0.72947000	-0.27310100	2.74036400
C	4.20421600	1.99520500	-1.18963500	H	0.04075800	0.43323500	2.41728300
H	4.65847400	1.92409200	-2.18459200	H	-1.69815200	0.23543500	2.71994000
H	4.45356200	2.97500800	-0.76202300	H	-0.51747800	-0.57607700	3.77371200
C	4.71755400	0.86062400	-0.27721800	34			
C	6.26055600	0.87556800	-0.27855900	P	1.90443600	0.64933200	-0.30273700
C	6.95704100	-0.08424200	0.69711700	O	2.27418600	2.10745400	-0.98620000
H	6.58957800	1.90134600	-0.06104800	O	2.65309000	0.81817000	1.15098400
H	6.60217500	0.66073900	-1.30053300	O	2.96752200	-0.31444100	-1.10952200
H	8.04364000	-0.00031700	0.58921400	C	4.08837900	1.01065300	1.09977500
H	6.71491100	0.14243500	1.74103500	H	4.32552900	1.80262500	1.81882100
H	6.69114300	-1.13037800	0.51122700	H	4.56196400	0.07973400	1.42902700
Pd	-0.29388000	1.14662900	-0.42687000	C	4.31201900	0.20469100	-1.25785800
C	-1.73603300	2.39661100	-0.92697700	H	4.98748200	-0.62440200	-1.02802700
H	-2.04751200	2.43121300	-1.98302200	H	4.45632700	0.49645400	-2.30561900
C	-2.36975000	3.47661800	-0.20534100	C	3.63650800	2.55454700	-0.80330500
C	-3.26864400	4.36732900	-0.84607100	H	3.97846900	2.93865300	-1.77101000
C	-2.12687400	3.66323700	1.17947900	H	3.63649200	3.37994600	-0.07983700
C	-3.89811500	5.38649600	-0.14024700	C	4.54747900	1.40643400	-0.31990700
H	-3.46370200	4.23902900	-1.90815400	C	6.01608100	1.87939000	-0.34326700
C	-2.75155500	4.68449600	1.88404500	C	7.05219300	0.92011700	0.26032300
H	-1.43451000	2.98394200	1.66837500	H	6.07047600	2.84015300	0.18735600
C	-3.63837300	5.54594600	1.22555900	H	6.28742400	2.09518000	-1.38585900
H	-4.58647900	6.05846000	-0.64542200	H	8.05624200	1.34532500	0.15915000
H	-2.55448900	4.81601500	2.94437200	H	6.87828300	0.74501400	1.32747900
H	-4.12733300	6.34394200	1.77853000	H	7.05820900	-0.05333100	-0.24169200
Sn	-1.64500400	-2.03703900	-1.23331000	Pd	-0.27265800	0.11873700	-0.31028500
Sn	-0.76258000	-2.04461500	1.50348200	C	-1.46585200	1.61834000	-0.83151800
C	-3.55028200	-1.06626400	-1.54406200	H	-1.72188400	1.74056400	-1.89164900
H	-3.89154700	-1.23032800	-2.57318100	C	-2.03676900	2.69193400	-0.03766000
H	-4.30631300	-1.47328400	-0.86365000	C	-2.70770200	3.77339300	-0.65909400
H	-3.46477300	0.00905500	-1.36646000	C	-1.88662300	2.73046400	1.37131800
C	-2.02469800	-4.15647100	-1.54294200	C	-3.18763900	4.84731000	0.08566100
H	-2.76817300	-4.53649800	-0.83402700	H	-2.83685800	3.76034200	-1.73848700
H	-2.40564700	-4.31771800	-2.55888100	C	-2.37913800	3.79486100	2.11521200
H	-1.10749900	-4.74451200	-1.42637800	H	-1.36943400	1.90750000	1.85724500
C	-0.26500200	-1.50699400	-2.80875200	C	-3.02939600	4.85808900	1.47445900
H	-0.32290100	-0.43840900	-3.03381100	H	-3.69145200	5.67167200	-0.41164700
H	0.76392300	-1.73781100	-2.51794800	H	-2.25534500	3.80583700	3.19462700
H	-0.51602800	-2.07833800	-3.71093100	H	-3.41143500	5.69125800	2.05830900
C	-2.16910300	-3.37364100	2.48673800	Sn	-2.90981200	-0.67312700	-
H	-3.18123800	-2.95446400	2.47389600	0.40565800			
H	-2.19738300	-4.35241600	1.99639100	Sn	0.48320200	-2.37704800	0.47878000
H	-1.87373200	-3.52033000	3.53266400	C	-3.70759700	-0.72165600	1.60040800
C	1.18220500	-2.98078100	1.65137700	H	-4.76109200	-1.02429000	1.57148500

H	-3.15588200	-1.42567600	2.22844900	C	-2.78919200	3.65559200	-0.63073500
H	-3.64911100	0.27295800	2.05454500	C	-2.04580600	2.58782500	1.41194500
C	-3.03016600	-2.61853800	-1.35285500	C	-3.26583900	4.73660000	0.10689200
H	-2.46739400	-3.38162100	-0.81116000	H	-2.88954600	3.65268100	-1.71340800
H	-4.08532800	-2.91559800	-1.39381500	C	-2.53523900	3.65964200	2.14831400
H	-2.64621900	-2.56248200	-2.37642900	H	-1.55857700	1.75429200	1.91123300
C	-4.37450200	0.43085200	-1.56880400	C	-3.14561100	4.74074900	1.49909000
H	-4.56136800	1.42803000	-1.16004900	H	-3.73846100	5.57275100	-0.40172600
H	-4.06085100	0.53425800	-2.61359400	H	-2.43872300	3.66098600	3.23078300
H	-5.31595000	-0.13190700	-1.55376800	H	-3.52545900	5.57903800	2.07686400
C	-0.87295800	-3.39308100	1.85195400	Sn	-2.97301900	-0.65073200	-0.42697500
H	-0.99506800	-2.81022100	2.77207700	Sn	0.62994800	-2.38273600	0.48241100
H	-1.86581000	-3.57253900	1.42755900	C	-3.67269100	-0.92569300	1.59293000
H	-0.43743900	-4.36367900	2.12187400	H	-4.63040300	-1.45916300	1.57848300
C	0.76935700	-3.73411400	-1.19603800	H	-2.95752500	-1.50329900	2.18309900
H	1.01030400	-4.74018000	-0.83046500	H	-3.82800800	0.04426900	2.07567400
H	-0.12406300	-3.79998900	-1.82500100	C	-2.87868300	-2.51381400	-1.52406000
H	1.60056400	-3.38499900	-1.81866600	H	-2.27665600	-3.26165500	-1.00380600
C	2.35559000	-2.52766600	1.58164400	H	-3.89725700	-2.89981100	-1.65151500
H	3.20566300	-2.30722400	0.92713400	H	-2.44414700	-2.34623000	-2.51455900
H	2.37855600	-1.82907500	2.42468900	C	-4.55668100	0.40255500	-1.46241100
H	2.47224400	-3.54701500	1.97025900	H	-4.76243900	1.37311700	-1.00265800
35-ts				H	-4.30381500	0.55948600	-2.51655500
P	1.87593700	0.68449100	-0.29614200	H	-5.46638700	-0.20826900	-1.41745300
O	2.19222500	2.14506300	-0.99820800	C	-0.73674200	-3.48051900	1.78203100
O	2.62661700	0.89102200	1.15088700	H	-0.88412800	-2.95105100	2.73020200
O	2.96543000	-0.25328500	-1.09916700	H	-1.71855100	-3.65023100	1.32833900
C	4.05457300	1.13152600	1.08723500	H	-0.29238700	-4.45864800	2.00716300
H	4.26909000	1.93789300	1.79721500	C	0.98619400	-3.68917600	-1.21883900
H	4.56138100	0.22029300	1.42203600	H	1.23396000	-4.70040500	-0.87248400
C	4.28931300	0.31167500	-1.26487400	H	0.11089700	-3.75354900	-1.87322400
H	4.99536700	-0.49122200	-1.03426800	H	1.82709900	-3.30996300	-1.80977900
H	4.41383300	0.59915800	-2.31631800	C	2.48113700	-2.48920800	1.62229700
C	3.53908600	2.64141400	-0.82674600	H	3.33633900	-2.23742700	0.98576200
H	3.86171600	3.02853300	-1.79981100	H	2.46611200	-1.79526300	2.46940700
H	3.51388600	3.47258200	-0.11046700	H	2.62402800	-3.50628800	2.00787200
C	4.49099300	1.52919100	-0.33924600	36			
C	5.94307400	2.04981900	-0.37758900	P	-1.54010600	-0.52679400	0.38292900
C	7.01380800	1.13271200	0.23106500	O	-1.61447800	-2.03368400	1.05839700
H	5.96902700	3.01847100	0.14065600	O	-2.72549300	0.22305800	1.24076900
H	6.20079500	2.26126100	-1.42449400	O	-2.30555100	-0.81384500	-1.04443400
H	8.00296900	1.58814200	0.11579600	C	-4.05522300	-0.33583400	1.10301400
H	6.85370400	0.96769000	1.30195800	H	-4.49005800	-0.36640800	2.10822600
H	7.04713000	0.15272500	-0.25703700	H	-4.64299900	0.35023300	0.48370300
Pd	-0.25541500	0.07635100	-0.27837200	C	-3.50629200	-1.62151400	-0.96982000
C	-1.57763200	1.47950900	-0.79355300	H	-4.24724500	-1.12768400	-1.60486000
H	-1.81382700	1.61228500	-1.85691200	H	-3.28449800	-2.61010600	-1.39097800
C	-2.15599300	2.55765100	-0.00020000	C	-2.94633200	-2.55971300	1.26684800

H	-2.93181200	-3.60246500	0.93089500	H	0.98174100	-1.25253500	-2.55959000
H	-3.16143000	-2.54101900	2.34263800	H	2.70259400	-0.87421800	-2.76839900
C	-4.00151100	-1.74855700	0.48566900	37-ts			
C	-5.36176600	-2.47208700	0.57093400	P	-2.45929700	0.27641800	-0.18488900
C	-6.57023000	-1.72625600	-0.01325800	O	-2.79947800	-0.88367700	-1.32020700
H	-5.56051100	-2.69645300	1.62810600	O	-3.45057400	-0.23444700	1.03872900
H	-5.26171300	-3.44520900	0.07059500	O	-3.36426000	1.52384600	-0.78625700
H	-7.46808800	-2.34685200	0.07506100	C	-4.86217800	-0.31048400	0.73822400
H	-6.76987800	-0.78767500	0.51492600	H	-5.22188800	-1.27013100	1.12829400
H	-6.43940600	-1.49126400	-1.07495400	H	-5.36761600	0.49776300	1.27904400
Pd	0.43117500	0.45717300	0.29827300	C	-4.69570800	1.19817400	-1.24482400
C	1.92802400	-1.04194000	1.04158300	H	-5.36207800	1.96769700	-0.84228200
H	1.66235200	-1.55120700	1.97125800	H	-4.71182100	1.26212100	-2.34086900
C	2.50405300	0.25435800	1.24025000	C	-4.19190500	-1.22747200	-1.48096500
C	2.70988400	0.82636100	2.54724800	H	-4.39505700	-1.25250400	-2.55802100
C	2.67604400	1.14895900	0.11957800	H	-4.35017900	-2.23477100	-1.07372500
C	3.15929400	2.11452900	2.70419600	C	-5.11658500	-0.20986800	-0.77968100
H	2.53650400	0.19398100	3.41429600	C	-6.58154000	-0.52811100	-1.14577200
C	3.15527500	2.47462200	0.31686600	C	-7.66196100	0.28891200	-0.42249900
H	2.71164200	0.73907100	-0.88822300	H	-6.75524000	-1.59569600	-0.95130000
C	3.40036900	2.95345400	1.58271900	H	-6.69695200	-0.39743200	-2.23062300
H	3.33861600	2.50008800	3.70497100	H	-8.65389900	-0.00446300	-0.78219800
H	3.33904300	3.09769100	-0.55436300	H	-7.64590500	0.12432700	0.66025400
H	3.77072700	3.96347100	1.73109600	H	-7.55584100	1.36469100	-0.59927400
Sn	2.38741600	-2.43329400	-0.52314900	Pd	-0.35822800	0.67838100	0.31636000
Sn	-0.59041200	2.72671500	-0.66648800	C	2.12393200	0.21393800	0.61663300
C	0.42699400	3.36031800	-2.48232100	H	2.77935500	-0.08350400	1.44449700
H	-0.00253600	4.30369000	-2.84226400	C	1.66204800	1.62156900	0.90627300
H	1.49708000	3.51634300	-2.30650600	C	1.59895900	2.09654300	2.24700200
H	0.31822000	2.61145200	-3.27476800	C	1.30434400	2.55319100	-0.11022200
C	-2.69529200	2.76452200	-1.20802800	C	1.25202200	3.40808900	2.54406000
H	-3.32073400	2.62507200	-0.31963900	H	1.85682100	1.41308700	3.05310300
H	-2.94950600	3.73007100	-1.66263900	C	0.94733600	3.87529400	0.20358800
H	-2.93070500	1.97082100	-1.92513000	H	1.38711200	2.27397400	-1.15696200
C	-0.36075400	4.34977400	0.75734700	C	0.92883000	4.31303100	1.52237000
H	-0.56557600	5.31377800	0.27512800	H	1.23678400	3.73316200	3.58144500
H	-1.06030300	4.22590400	1.59159600	H	0.69926800	4.55790400	-0.60509600
H	0.65514500	4.37331500	1.16449000	H	0.66300300	5.33897500	1.75992100
C	4.47417900	-2.98170500	-0.42292100	Sn	0.84189700	-1.75316000	1.02903900
H	4.72278100	-3.70918900	-1.20430800	Sn	3.29666500	0.01396300	-1.21180100
H	5.11409200	-2.10281300	-0.55805300	C	2.54739600	-2.80147000	1.86614300
H	4.71064000	-3.42745400	0.54946700	H	2.24913700	-3.82610600	2.12049900
C	1.17636700	-4.17338700	-0.16264100	H	3.39446600	-2.85687600	1.17672700
H	0.14820300	-3.87117200	0.05890300	H	2.88531100	-2.31402200	2.78888900
H	1.17046000	-4.83503300	-1.03589800	C	0.24692500	-2.90156300	-0.69940600
H	1.55876700	-4.74108900	0.69296400	H	0.96298700	-2.77759900	-1.51908900
C	1.99399100	-1.66462000	-2.49713200	H	0.21069400	-3.96630100	-0.43839700
H	2.08750200	-2.46619400	-3.23906300	H	-0.73749400	-2.58274600	-1.05158900

C	-0.56663300	-1.90766400	2.66781000	C	2.02499400	-1.05018800	2.01251000
H	-0.28070900	-1.23032500	3.47955600	H	1.40422400	-1.93959700	2.16674400
H	-1.58261800	-1.65745000	2.35494400	H	3.05283400	-1.30489900	2.29484600
H	-0.54301000	-2.93490000	3.05356700	H	1.67436600	-0.26625100	2.69238300
C	4.31020000	-1.88444300	-1.30675100	C	3.31985700	1.25927100	-0.28920100
H	3.61053900	-2.72582200	-1.32394300	H	4.32768100	0.98360900	0.04052500
H	4.90551800	-1.92077200	-2.22683600	H	3.37335800	1.56154000	-1.34059100
H	4.99050000	-2.01929900	-0.45953300	H	2.98720600	2.12220200	0.29607000
C	2.06058900	0.19536000	-2.96794900	39-ts			
H	1.04850900	-0.17204700	-2.76913500	P	-2.18916100	-1.48536600	-0.13486100
H	1.98704200	1.23699200	-3.29892000	O	-2.51801400	-2.83082400	-1.03374700
H	2.48588300	-0.39078600	-3.79046900	O	-2.95251000	-1.87960600	1.27576300
C	4.80098200	1.55812600	-1.20979400	O	-3.30345700	-0.43769600	-0.77722600
H	5.49047800	1.42153500	-0.36948200	C	-3.86994300	-3.33013700	-0.95521600
H	5.38277500	1.52714600	-2.13810900	H	-4.19623600	-3.53576900	-1.98141700
H	4.34612900	2.54953800	-1.11959200	H	-3.85719700	-4.27567300	-0.39763500
38				C	-4.81827100	-2.31658700	-0.27897100
C	-0.56997700	3.51852900	1.27790600	C	-6.26684100	-2.83699800	-0.39021700
C	-0.30834500	2.17672400	0.99859700	C	-7.34365000	-2.03421500	0.35411100
C	-0.31793800	1.68297100	-0.32199900	H	-6.28337700	-3.87378800	-0.02620600
C	-0.60599600	2.60413300	-1.34768800	H	-6.52830300	-2.88839200	-1.45623300
C	-0.86842800	3.94635600	-1.07108600	H	-8.32780400	-2.48290100	0.18221100
C	-0.85251400	4.41431200	0.24445400	H	-7.17426400	-2.02407000	1.43622000
H	-0.55148100	3.86395600	2.30877600	H	-7.39541000	-0.99441400	0.01371100
H	-0.09222200	1.49681200	1.82015300	Pd	0.00004100	-0.89743900	-0.00016400
H	-0.62194900	2.25796100	-2.37913800	Sn	0.37827800	2.41875400	-1.38331700
H	-1.08535400	4.62877000	-1.88934000	Sn	-0.37840600	2.41855400	1.38339900
H	-1.05568300	5.45937300	0.46087600	C	2.52779600	2.38138600	-1.63068400
C	-0.03655900	0.23585100	-0.63478300	H	2.77963400	2.35070800	-2.69739300
H	-0.02834000	0.11041900	-1.72758400	H	2.97582900	3.28267900	-1.19728900
Sn	1.96354000	-0.39173700	-0.03970900	H	2.96634500	1.50797100	-1.14032300
Sn	-1.68430100	-1.04906300	-0.00741000	C	-0.25589400	4.38783700	-2.05012500
C	-2.06583500	-0.89402400	2.10437300	H	0.18060700	5.17672100	-1.42796400
H	-2.88999500	-1.55988900	2.38423200	H	0.06230200	4.55182700	-3.08695000
H	-1.18512800	-1.17805300	2.68971300	H	-1.34667000	4.48381300	-2.00973100
H	-2.34624700	0.12829900	2.37654900	C	-0.50330400	1.05404200	-2.80623000
C	-1.22886600	-3.10164300	-0.48985600	H	-0.08080400	0.04898100	-2.70812700
H	-2.09886500	-3.73767300	-0.29091200	H	-1.58564800	0.98574500	-2.66380200
H	-0.96641500	-3.20934500	-1.54789200	H	-0.30118200	1.42545600	-3.81887600
H	-0.39302000	-3.47880500	0.10939000	C	0.25570000	4.38756300	2.05049400
C	-3.43610900	-0.43619400	-1.09868400	H	1.34650200	4.48343100	2.01052800
H	-3.33672800	-0.68076000	-2.16197400	H	-0.18048200	5.17651200	1.42819100
H	-4.33143200	-0.93777300	-0.71505300	H	-0.06288100	4.55155500	3.08720100
H	-3.58224200	0.64522100	-1.00901700	C	-2.52793100	2.38119000	1.63071100
C	2.56865500	-2.02037100	-1.31517800	H	-2.77976800	2.34979900	2.69740000
H	3.57932600	-2.35532100	-1.05603400	H	-2.97584800	3.28285200	1.19796100
H	1.89174600	-2.87546000	-1.21743300	H	-2.96660900	1.50818500	1.13973900
H	2.57480300	-1.70868900	-2.36556500	C	0.50316200	1.05371800	2.80619400

H	0.08064600	0.04867200	2.70803800	H	2.45398300	6.40501400	-0.26456900
H	1.58550200	0.98542400	2.66374100	H	4.27452600	6.89804000	1.35613200
H	0.30106600	1.42507800	3.81886500	H	4.04317300	5.34432000	2.16000900
P	2.18924700	-1.48531600	0.13467000	H	4.63323800	5.40234200	0.49222100
O	2.95279600	-1.87935400	-1.27590300	P	1.48268300	-1.53595900	-0.03981800
O	3.30344900	-0.43769500	0.77729600	O	1.34060500	-3.15556100	0.27158800
C	4.36896900	-2.15687300	-1.18806800	O	2.10377700	-1.59839900	-1.56747700
H	4.55095300	-3.08003600	-1.75109000	O	2.84974300	-1.19956400	0.82734700
H	4.90394500	-1.33659000	-1.68008800	C	3.35954200	-2.29752500	-1.72309000
C	4.63490000	-0.96031500	0.98915700	H	3.25661600	-2.95108300	-2.59715600
H	5.33132100	-0.20947000	0.60301500	H	4.13575800	-1.55275600	-1.93201900
H	4.79840700	-1.06602800	2.06951400	C	3.93948400	-2.14304300	0.70375800
C	3.86997100	-3.33014000	0.95501600	H	4.84763400	-1.55172900	0.55000400
H	4.19613300	-3.53588500	1.98123600	H	4.03335600	-2.68882500	1.65139900
H	3.85731600	-4.27561100	0.39732600	C	2.46461100	-3.97705300	-0.11241300
C	4.81836300	-2.31649200	0.27901600	H	2.68226600	-4.63957300	0.73323900
C	6.26692600	-2.83689600	0.39037800	H	2.16409000	-4.59204200	-0.97016000
C	7.34383600	-2.03395600	-0.35363600	C	3.70023900	-3.12159100	-0.46409400
H	6.28353600	-3.87361700	0.02617300	C	4.90597600	-4.05758900	-0.69011900
H	6.52823500	-2.88848800	1.45642100	C	6.19928600	-3.40355900	-1.19807800
H	8.32796300	-2.48269300	-0.18171500	H	4.60061100	-4.83692300	-1.40211400
H	7.17458600	-2.02356100	-1.43576300	H	5.11325100	-4.57878800	0.25474300
H	7.39556900	-0.99423300	-0.01299300	H	6.98524200	-4.16009900	-1.29424000
O	2.51802100	-2.83086800	1.03343200	H	6.06833000	-2.94270500	-2.18309700
C	-4.36868900	-2.15714400	1.18807700	H	6.57092500	-2.63285000	-0.51410300
H	-4.55058100	-3.08038700	1.75100100	Pd	-0.36807800	-0.09079200	-0.00034000
H	-4.90362300	-1.33693900	1.68027000	Sn	-2.67777700	0.72883400	-1.04530800
C	-4.63491700	-0.96031600	-0.98897400	Sn	-2.04908500	-1.87286200	1.04491300
H	-5.33131900	-0.20954000	-0.60266000	C	-1.93081500	1.69817500	-2.84357100
H	-4.79857100	-1.06591700	-2.06932000	H	-2.77950000	1.98251900	-3.47863800
40				H	-1.36114400	2.59644300	-2.58981700
P	0.62107800	2.03887800	0.03869500	H	-1.28484100	1.02336700	-3.41515800
O	-0.24859700	3.40991900	-0.28392100	C	-4.14198300	-0.64470800	-1.88045800
O	1.13364600	2.38351400	1.56913800	H	-4.71607300	-1.18548400	-1.12255500
O	1.99686700	2.36952100	-0.81756900	H	-4.84607700	-0.07021100	-2.49609900
C	1.61388700	3.72797500	1.79815500	H	-3.64936700	-1.37928400	-2.52734700
H	0.87451800	4.26070300	2.40988400	C	-3.78927400	2.21206200	0.07005400
H	2.53969300	3.63310900	2.37401800	H	-4.58946100	2.63032000	-0.55290800
C	2.71126500	3.57083200	-0.44355100	H	-4.24180700	1.77820400	0.96750300
H	3.63807800	3.26824800	0.05704400	H	-3.12114200	3.02439800	0.37280600
H	2.96895300	4.09331300	-1.37233000	C	-2.39458800	-3.68840800	-0.07951000
C	0.47943600	4.65525500	-0.21545300	H	-2.89903000	-4.43105800	0.55079800
H	0.60396000	5.04115500	-1.23534400	H	-3.01940000	-3.50024100	-0.95809200
H	-0.14238700	5.35822100	0.35049400	H	-1.43893900	-4.10495600	-0.41326800
C	1.85146700	4.47129700	0.46717800	C	-0.92176900	-2.42622200	2.82090900
C	2.49412500	5.85704300	0.68720300	H	-1.54721300	-3.06092800	3.46154400
C	3.94066700	5.86643700	1.20262800	H	-0.01907100	-2.97885500	2.54644700
H	1.85871500	6.41966300	1.38493700	H	-0.62999400	-1.54028600	3.39496600

C	-3.95926200	-1.29956900	1.91035800	H	5.26660400	-0.67603800	-1.80204700
H	-3.83485700	-0.42365200	2.55694200	H	4.38627200	-1.94436700	-0.92745200
H	-4.72492300	-1.06901000	1.16402600	H	3.80779400	-1.39674900	-2.51135800
H	-4.32553200	-2.12827200	2.52979800	C	3.19705600	2.06284200	-2.19454100
41				H	3.04224800	3.06768600	-1.78212600
P	-1.78475900	-0.39820400	-0.15055700	H	4.20314500	2.04037600	-2.63143500
O	-2.67016500	-0.29516100	1.23477600	H	2.47733800	1.90497900	-3.00562300
O	-2.76363400	0.44750300	-1.18621800	Sn	1.31800600	-2.06365000	0.83256200
O	-2.14755900	-1.93931700	-0.62115000	C	-0.16787400	-2.60856500	2.32037800
C	-4.10559900	-0.06616200	-1.36304500	H	-0.33449500	-1.79428200	3.03272900
H	-4.78743000	0.79018100	-1.30062400	H	-1.12340900	-2.85276300	1.84775000
H	-4.17285000	-0.49526800	-2.36879300	H	0.18785400	-3.48752400	2.87263800
C	-3.53376300	-2.33808200	-0.49856500	C	3.15329300	-2.21094800	1.98263600
H	-3.78590400	-2.86871800	-1.42140100	H	4.05662600	-2.02778700	1.39421700
H	-3.61886500	-3.03761800	0.34278900	H	3.13678300	-1.50469900	2.81994300
C	-4.09288400	-0.50337200	1.09258600	H	3.21548900	-3.22551000	2.39672400
H	-4.39907300	-1.17506900	1.90234300	C	1.34691100	-3.64775900	-0.63891500
H	-4.59571600	0.46237500	1.22905100	H	2.13072200	-3.48025900	-1.38391600
C	-4.44561200	-1.11286600	-0.28221200	H	1.53087400	-4.61252000	-0.15035100
C	-5.94049200	-1.49551200	-0.29330200	H	0.38148100	-3.69324900	-1.15255700
C	-6.51369800	-1.98146000	-1.63265400	42-ts			
H	-6.51642400	-0.62211400	0.04307400	P	-2.03091800	0.03790800	-0.04744100
H	-6.09778200	-2.27119500	0.46867300	O	-2.76600700	1.29257800	0.75123900
H	-7.56781900	-2.25128400	-1.50959100	O	-2.70049400	0.22577000	-1.54578900
H	-6.46373900	-1.20858300	-2.40729100	O	-2.92739100	-1.22697500	0.51793200
H	-5.99231900	-2.86789100	-2.00936200	C	-4.14580000	0.20296800	-1.62215500
Pd	0.47788200	0.20267300	-0.20171500	H	-4.45183900	1.08247900	-2.20062600
N	-1.03042200	2.51915800	-2.97118900	H	-4.43380300	-0.69780300	-2.17458000
N	-0.54215900	2.59129900	-1.94763400	C	-4.36652100	-1.06272900	0.52061400
C	0.00767500	2.61948300	-0.73872100	H	-4.78469200	-1.95212900	0.03964000
H	1.07071100	2.82572400	-0.79282800	H	-4.70342000	-1.03721400	1.56443000
C	-0.77196700	3.15672000	0.39815400	C	-4.19295900	1.42521400	0.55531500
C	-0.09057500	3.41003700	1.60174000	H	-4.65135300	1.50460000	1.54789900
C	-2.14880500	3.42556900	0.32918400	H	-4.37430600	2.35941600	0.00929700
C	-0.77087100	3.91995900	2.70523300	C	-4.78190900	0.22507500	-0.21773500
H	0.97332500	3.19829300	1.66936900	C	-6.31652700	0.38371500	-0.28136400
C	-2.82159200	3.93769300	1.43771000	C	-7.08226700	-0.65757700	-1.11059800
H	-2.69458900	3.23117800	-0.58926000	H	-6.53646900	1.38427400	-0.67892700
C	-2.13996400	4.18746600	2.63055000	H	-6.70128200	0.37769800	0.74765900
H	-0.22663300	4.10995400	3.62633500	H	-8.15643000	-0.44962000	-1.06550600
H	-3.88562200	4.14803200	1.36471300	H	-6.79127700	-0.63930600	-2.16632400
H	-2.66829800	4.58764500	3.49111100	H	-6.93221300	-1.67678900	-0.73881300
Sn	3.07915500	0.50161100	-0.66123500	Pd	0.28524800	0.12350600	-0.23588400
C	4.27018900	1.31487800	0.96295500	C	0.72685800	2.14345700	-0.77467300
H	4.35388300	0.60509600	1.79164000	H	1.34994100	2.30431200	-1.65523900
H	5.28007600	1.55245600	0.60662800	C	1.13406200	3.02822000	0.35047100
H	3.82111500	2.23710400	1.35026500	C	2.34843000	3.73590100	0.28694800
C	4.26829300	-1.06873800	-1.57259700	C	0.36262800	3.11040700	1.52594300

C	2.79852200	4.47612500	1.37973800	H	-4.70814100	-1.29108900	1.17323200
H	2.94627000	3.69057600	-0.62005600	H	-4.12589800	0.02870400	2.21864600
C	0.79886200	3.87661200	2.60369800	C	-4.45435400	0.61961400	0.13854000
H	-0.58001600	2.57295300	1.57922700	C	-5.95110900	0.95914000	0.30593600
C	2.02165900	4.55268900	2.53781400	C	-6.50485300	2.07524900	-0.59157700
H	3.74706600	5.00299900	1.32239800	H	-6.12041300	1.23228000	1.35668000
H	0.19140900	3.93798200	3.50254900	H	-6.52882400	0.04010000	0.13712100
H	2.36585400	5.13847700	3.38585900	H	-7.57442200	2.20880800	-0.39902900
Sn	2.72311200	-0.46576800	-1.12344900	H	-6.01702400	3.03717400	-0.40114500
C	4.42047500	-0.05322900	0.16049500	H	-6.39167900	1.84666400	-1.65667100
H	4.40995200	-0.68838700	1.05083700	Pd	0.44270100	-0.50605400	-0.35802600
H	5.35531000	-0.23345500	-0.38445000	Si	0.35939200	-2.66898700	0.77632200
H	4.40870100	0.99275800	0.48699600	Si	3.03158300	-0.92773800	-0.66743000
C	3.01962000	-2.43728100	-1.98826600	C	0.02574200	-2.52326500	2.64303500
H	3.99916100	-2.47188900	-2.48148300	H	-0.91169300	-1.98475800	2.82494100
H	2.98123000	-3.23947100	-1.24577300	H	-0.05573800	-3.51807800	3.10112900
H	2.25037500	-2.63454300	-2.74347200	H	0.83025200	-1.98152900	3.15404600
C	3.09582100	0.79064100	-2.87527500	C	-0.98292400	-3.80762700	0.04824200
H	3.37494700	1.81636000	-2.60586500	H	-0.81346900	-3.99790400	-1.01813000
H	3.93143200	0.35866300	-3.43986200	H	-0.98171200	-4.77529800	0.56758300
H	2.22621200	0.83183100	-3.54118700	H	-1.97916800	-3.36388800	0.15730900
Sn	0.60267400	-2.17691700	1.07982700	C	2.88811700	-2.34778000	-1.90355100
C	-0.49370400	-1.89434700	2.93704800	H	3.89306100	-2.63226900	-2.24014800
H	-0.10152500	-1.03792600	3.49702400	H	2.40018900	-3.21220000	-1.45207500
H	-1.55613800	-1.72727700	2.73880000	H	2.31514000	-2.03821900	-2.78576300
H	-0.38752800	-2.78920200	3.56350800	C	3.63936600	-1.18165000	1.09473400
C	2.51559000	-2.88202200	1.83507900	H	3.23162700	-2.09971700	1.52063300
H	3.23376100	-3.13065200	1.04888400	H	4.73434900	-1.24191400	1.09052600
H	2.97174100	-2.13690500	2.49609100	H	3.35014300	-0.33398800	1.72472400
H	2.32948400	-3.78829600	2.42591700	F	1.70522300	-3.64896500	0.71089400
C	-0.28615600	-3.87602900	0.06822300	F	4.34099400	-0.14132100	-1.33415800
H	0.26216000	-4.11808000	-0.84811300	N	0.08032700	2.04648800	-2.15970900
H	-0.27384300	-4.75660300	0.72239600	N	0.70475600	1.33192700	-1.48631900
H	-1.32434100	-3.65169400	-0.19712800	C	2.09835900	1.04070100	-1.09613700
N	-0.66578800	2.95403600	-1.47218700	H	2.65034100	1.04903000	-2.03261200
N	-1.74141000	3.12145200	-1.71832900	C	2.57843300	2.01419000	-0.06733800
43-ts				C	3.79843200	2.67952300	-0.26967800
P	-1.80762500	-0.06327000	-0.07354100	C	1.83221800	2.29510000	1.08850700
O	-2.69912600	-0.88814600	1.03323700	C	4.25210300	3.61381900	0.66033700
O	-2.15452700	1.48472000	0.36214000	H	4.39515600	2.44949100	-1.14602600
O	-2.73617100	-0.23746200	-1.41418900	C	2.28806400	3.23753200	2.01004600
C	-3.55492000	1.86063700	0.31654100	H	0.89341300	1.77460100	1.26197800
H	-3.77863000	2.37259000	1.25936300	C	3.49950700	3.89993300	1.80145500
H	-3.67980500	2.56927100	-0.50881600	H	5.19916300	4.11880900	0.49018200
C	-4.15656400	-0.00027500	-1.24235500	H	1.69655300	3.44685200	2.89728300
H	-4.46004400	0.66558000	-2.05521200	H	3.85686400	4.62771900	2.52463400
H	-4.67621600	-0.95920300	-1.35794400	L			
C	-4.05559300	-0.41237000	1.21716900	P	-1.98445000	-0.27994800	0.00024700

O	-1.51761100	1.31361100	0.02123700	C	1.46543500	2.36341900	-1.03255300
O	-1.06544900	-0.85399500	1.25832700	C	0.26396600	3.35024600	1.27917200
O	-1.07378500	-0.81798100	-1.27961100	H	-0.91976500	1.55422200	1.25459000
C	0.35964300	-0.64192700	1.18261800	C	1.87255600	3.58928900	-0.50574900
H	0.67736200	-0.19151600	2.13173300	H	1.92569400	1.99144700	-1.94517700
H	0.84063100	-1.62247200	1.08699300	C	1.27019600	4.08720700	0.65199600
C	0.31487600	-0.42764100	-1.30847400	H	-0.21249500	3.73409700	2.17782900
H	0.90092100	-1.33877900	-1.47117700	H	2.65155500	4.16011200	-1.00456700
H	0.46786400	0.24015600	-2.16689400	H	1.57869100	5.04671700	1.05874200
C	-0.10419800	1.56991200	0.12465000	C	-1.62140000	-0.40061500	-0.40320300
H	0.16275800	2.27321300	-0.67419500	C	-2.77983700	0.08512100	-1.03380000
H	0.08820100	2.05577100	1.09060400	C	-1.76570400	-1.17389400	0.75928300
C	0.72984600	0.27599800	-0.00034000	C	-4.04497600	-0.17535900	-0.50691000
C	2.22669300	0.65084800	0.00332300	H	-2.68799400	0.66795900	-1.94755000
C	3.23052500	-0.51137900	-0.00290400	C	-3.03307500	-1.44445700	1.28089200
H	2.41685000	1.27712400	0.88617400	H	-0.88570100	-1.56984700	1.25716000
H	2.41770100	1.29355100	-0.86732700	C	-4.17467400	-0.94375900	0.65233700
H	4.25298400	-0.11926700	-0.02404100	H	-4.92900700	0.21205800	-1.00680100
H	3.14077300	-1.13860000	0.89053400	H	-3.12699600	-2.04732600	2.18070400
H	3.11115600	-1.15790700	-0.87896600	H	-5.15982600	-1.15635300	1.05921300

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P	-0.00001100	-0.00016200	-1.20708900
C	1.15743000	-1.20387500	-0.40297100
C	1.31616300	-2.45003000	-1.03349900
C	1.89920900	-0.94204500	0.75946500
C	2.17437100	-3.41529100	-0.50648300
H	0.76553300	-2.66202500	-1.94724800
C	2.76737000	-1.90414100	1.28114700
H	1.80175400	0.01804100	1.25722400
C	2.90468200	-3.14317700	0.65271000
H	2.28098300	-4.37464100	-1.00626300
H	3.33642700	-1.68390300	2.18092700
H	3.58152400	-3.88990500	1.05958800
C	0.46376000	1.60431100	-0.40323300
C	-0.13550600	2.11734500	0.75772500

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