

Supporting Information

Mechanistic Insights into the Stereocontrolling Non-Covalent π Interactions in Pd-Catalyzed Redox-Relay Heck Arylation Reaction

Xiaoxiao Hu^{a,b}, Boming Shen^b, Jin Zhang^b and Peiyuan Yu^{*b}

^a*School of Chemistry and Chemical Engineering, Harbin Institute of Technology, Harbin 150001, China;*

^b*Department of Chemistry and Shenzhen Grubbs Institute, Southern University of Science and Technology, Shenzhen, Guangdong 518055, China;*

Contents

I. Computational details.....	2
II. Free energy profiles for the disfavored γ -insertion pathway and two possible alkene β -insertion pathways	3
III. DFT-optimized structure of transition state TS1	4
IV. Free energy profiles of alternative β -hydride elimination and reinsertion pathways with the ligand L2 ...	4
V. DFT-optimized geometries of selected transition states	5
VI. Free energy profiles for all the possible pathways leading to the product with the ligand L2	5
VII. Free energy profiles of alternative β -hydride elimination and reinsertion pathways with the ligand L1 .	7
VIII. The configurations with the alkyl chain in the <i>cis</i> position to the oxazoline group on the ligand L1	8
IX. DFT-optimized structures of selected transition states with the ligand L1	8
X. Energies and Cartesian coordinates of all the structures.....	9

I. Computational details

Density functional theory (DFT) computations were performed using the Gaussian 16 program.¹ Geometry optimizations were conducted using the B3LYP functional² with Grimme's dispersion corrections (with Beck-Johnson damping)³ and def2-SVP basis sets.⁴ Frequency computations were performed at the same level of theory as geometry optimization to confirm whether optimized stationary points were either local minimum (zero imaginary frequencies) or transition structures (a single imaginary frequency). The transition-state structures were further confirmed by intrinsic reaction coordinate (IRC) calculations, thereby enabling the identification of the forward and reverse species. To obtain electronic energies of higher accuracy, single-point energy calculations were executed on the optimized structures using the M06 functional⁵ and def2-TZVP basis sets.⁴ A mixed solvent with methanol and methyl tert-butyl ether in a ratio of 3:1, was described by the SMD implicit solvation model for all calculations.⁶ Several conformations for the intermediates and transition state structures have been conducted but only the optimal energy conformers are shown in this work. Independent gradient model based on Hirshfeld partition (IGMH) analysis was performed using Multiwfn program⁷ and the results were presented by VMD program.⁸ Molecular structures were visualized using CYLview software.⁹

1. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, D. J. Fox, *Gaussian 16, Revision C.01*, Gaussian, Inc., Wallingford, CT, 2019.
2. (a) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785; (b) A. D. Becke, *J. Chem. Phys.*, 1992, **96**, 2155; (c) P. J. Stephens, F. J. Devlin, C. F. Chabalowski and M. J. Frisch, *J. Phys. Chem.*, 1994, **98**, 11623.
3. (a) S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104; (b) S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.*, 2011, **32**, 1456–1465.
4. (a) F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297; (b) F. Weigend, *Phys. Chem. Chem. Phys.*, 2006, **8**, 1057.
5. (a) Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215; (b) Y. Zhao and D. G. Truhlar, *Acc. Chem. Res.*, 2008, **41**, 157.
6. A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378.
7. T. Lu and F. Chen, *J. Comput. Chem.*, 2012, **33**, 580.
8. W. Humphrey, A. Dalke and K. Schulten, *J. Mol. Graphics*, 1996, **14**, 33.
9. C. Y. Legault, *CYLview*, version 1.0b; Université de Sherbrooke, 2009 (<http://www.cylview.org>).

II. Free energy profiles for the disfavored γ -insertion pathway and two possible alkene β -insertion pathways

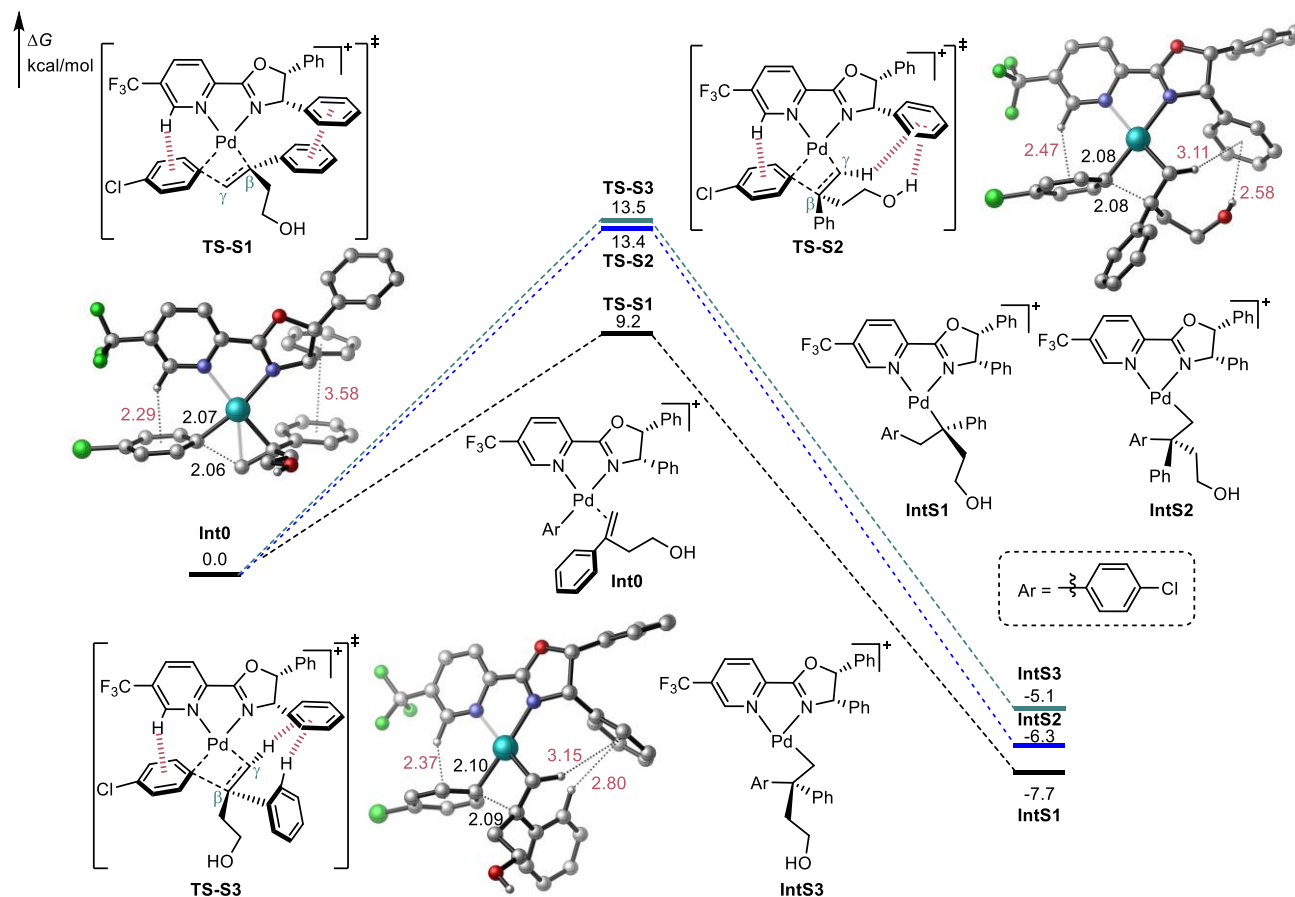


Fig. S1. Free energy profiles for the disfavored γ -insertion pathway and two possible alkene β -insertion pathways.

Complex **Int0** undergoes γ -insertion via **TS-S1** to give complex **IntS1**. **TS-S1** is higher than **TS1** by 2.1 kcal/mol, and the *R/S* configurations of the carbons coordinated to palladium center are different. We calculated the enantiomeric transition states (**TS-S2** and **TS-S3**) with the stereogenic centers being established on the β -carbon atoms. The free energy of activation of **Int0** to **IntS2** via **TS-S2** is 13.4 kcal/mol and the activation barrier to **IntS3** via **TS-S3** is 13.5 kcal/mol.

III. DFT-optimized structure of transition state TS1

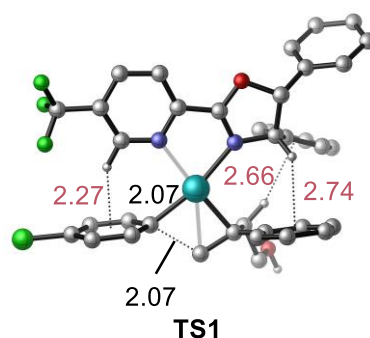


Fig. S2. Optimized geometry of transition state **TS1**, with selected bond lengths in Å. Irrelevant hydrogen atoms are omitted for clarity.

IV. Free energy profiles of alternative β -hydride elimination and reinsertion pathways with the ligand **L2**

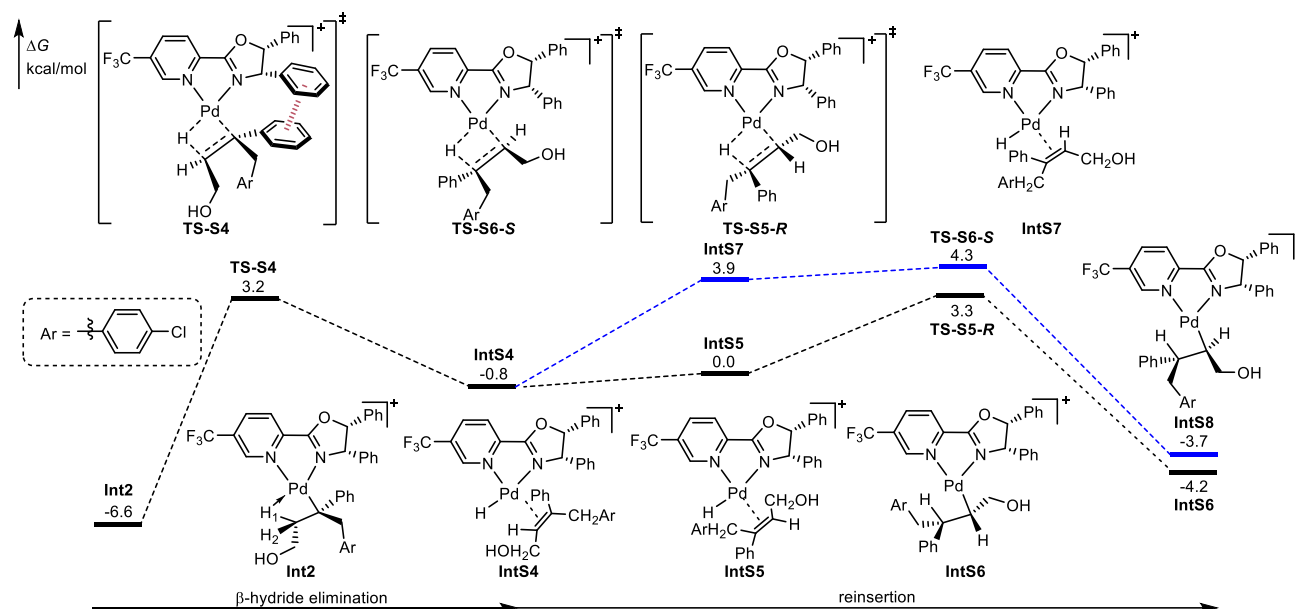


Fig. S3. Free energy profiles of alternative β -hydride elimination and reinsertion pathways with the ligand **L2**.

V. DFT-optimized geometries of selected transition states

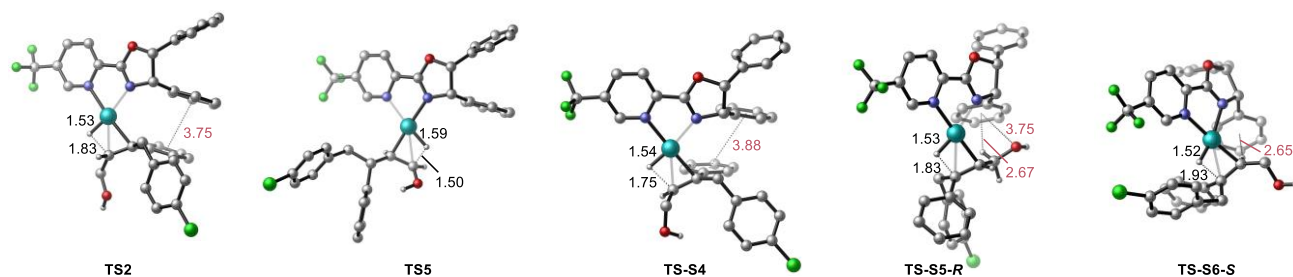


Fig. S4. DFT-optimized structures of selected transition states, with selected bond lengths given in Å. Irrelevant hydrogen atoms are omitted for clarity.

VI. Free energy profiles for all the possible pathways leading to the product with the ligand L2

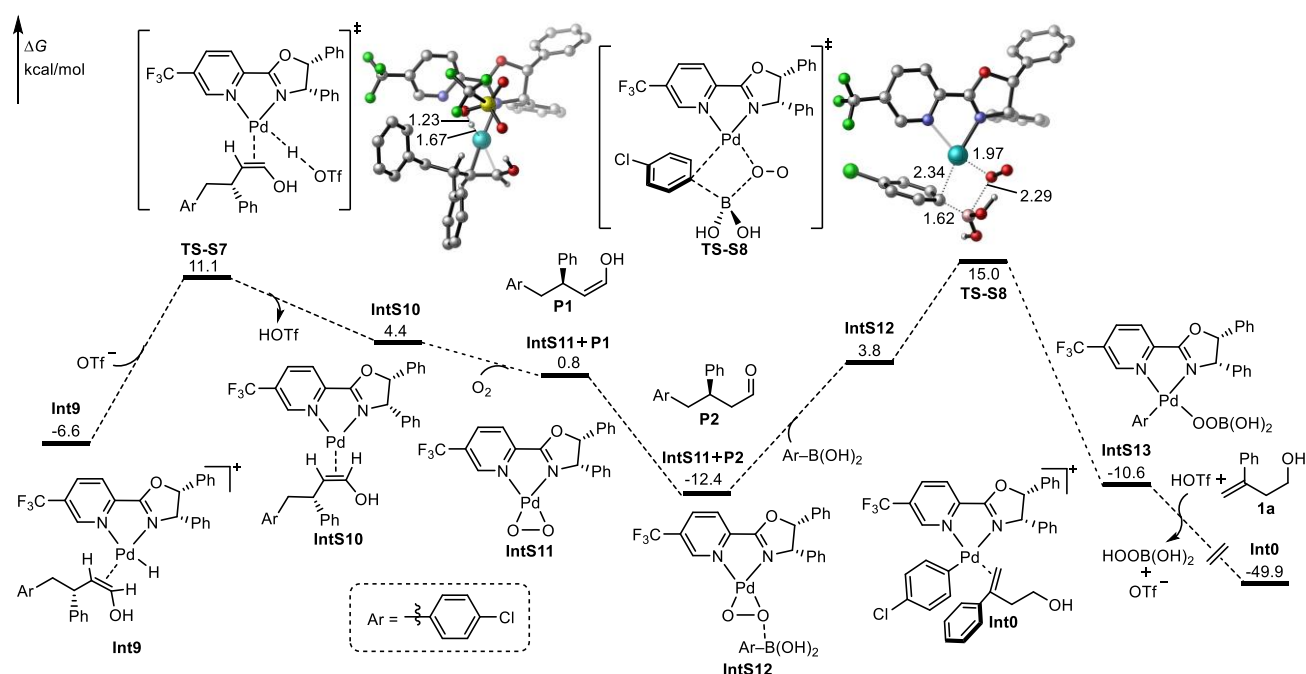


Fig. S5. Free energy profiles for deprotonation, oxidation (O_2 , triplet) and transmetalation with the ligand PhPyrOx **L2**, leading to the formation of the final product, and selected bond lengths are given in Å.

Int9 undergoes the OTf-aided deprotonation via **TS-S7** with a 17.7 kcal/mol energy barrier to give the Pd(0) species **IntS10**, and subsequent oxidation generates a palladium peroxo complex **IntS11**. The enol **P1** tautomerizes to the ketone product **P2** by a large thermodynamic driving force of 13.2 kcal/mol. The ensuing transmetalation of **IntS11** via **TS-S8** requires an activation free energy of 27.4 kcal/mol to afford the intermediate **IntS13**. The intermediate **IntS13** undergoes ligand exchange to generate a more stable complex **Int0**.

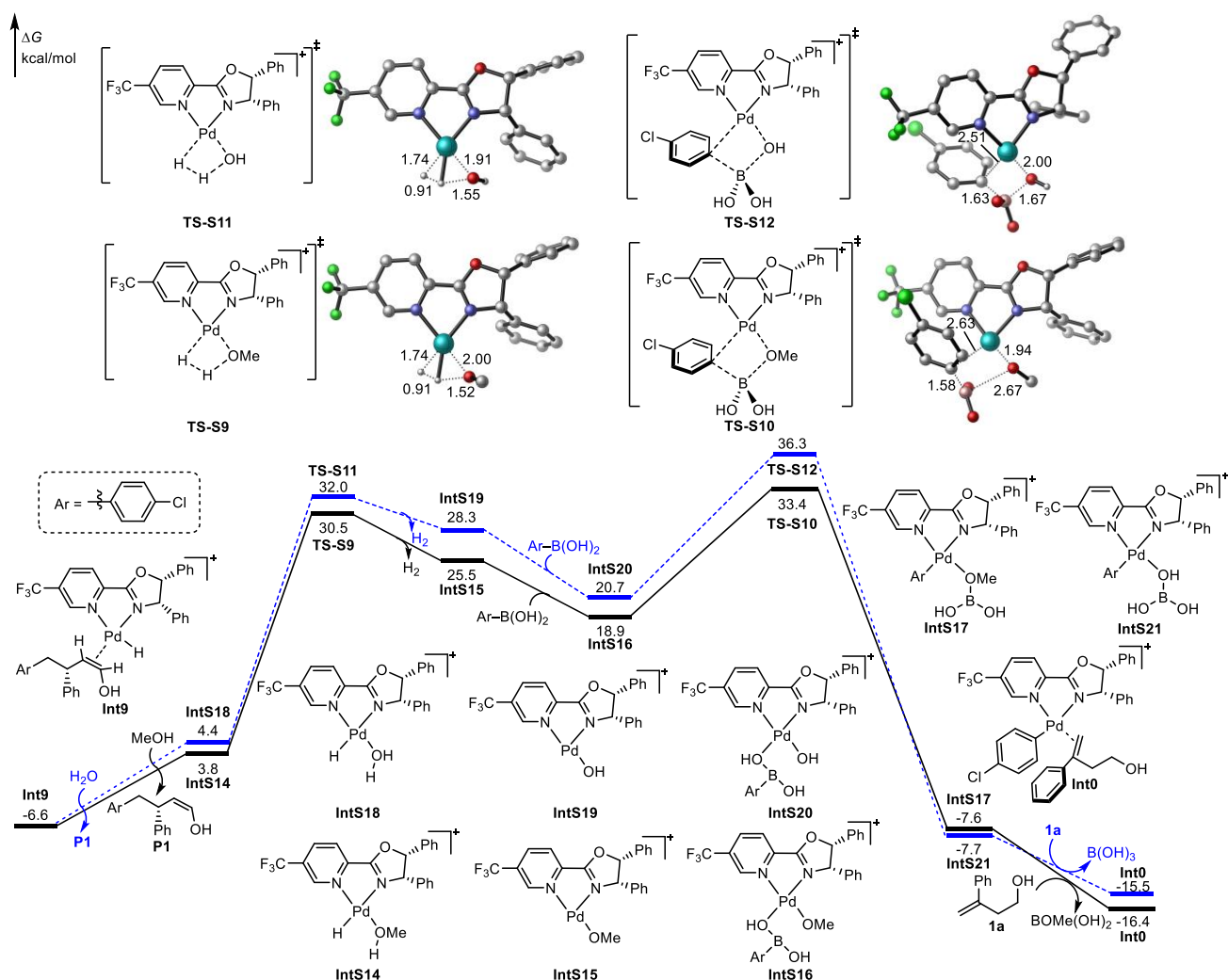


Fig. S6. Free energy profiles for the generation of the final product, and selected bond lengths are given in Å.

The intermediate **Int9** releases the enol **P1**, then the metal center coordinates with the solvent MeOH to form the intermediate **IntS14**. The enol **P1** rapidly tautomerizes to the final product ketone **P2**. Following this, the intermediate **IntS14** underwent deprotonation through the transition state **TS-S9**, resulting in the release of hydrogen and the formation of the intermediate **IntS15**. The intermediate **IntS15** undergoes transmetalation to generate the intermediate **Int17**, which further undergoes ligand exchange to produce the species **Int0**, thus completing the catalytic cycle. Notably, if water is used instead of MeOH, the process remains similar, however, the transition state **TS-S11** for deprotonation is 1.5 kcal/mol higher in energy than **TS-S9** (32.0 vs 30.5 kcal/mol), while the transmetalation transition state **TS-S12** requires an energy barrier of 42.9 kcal/mol compared to **Int9**, which is less favorable than the transition state **TS-S10**.

VII. Free energy profiles of alternative β -hydride elimination and reinsertion pathways with the ligand L1

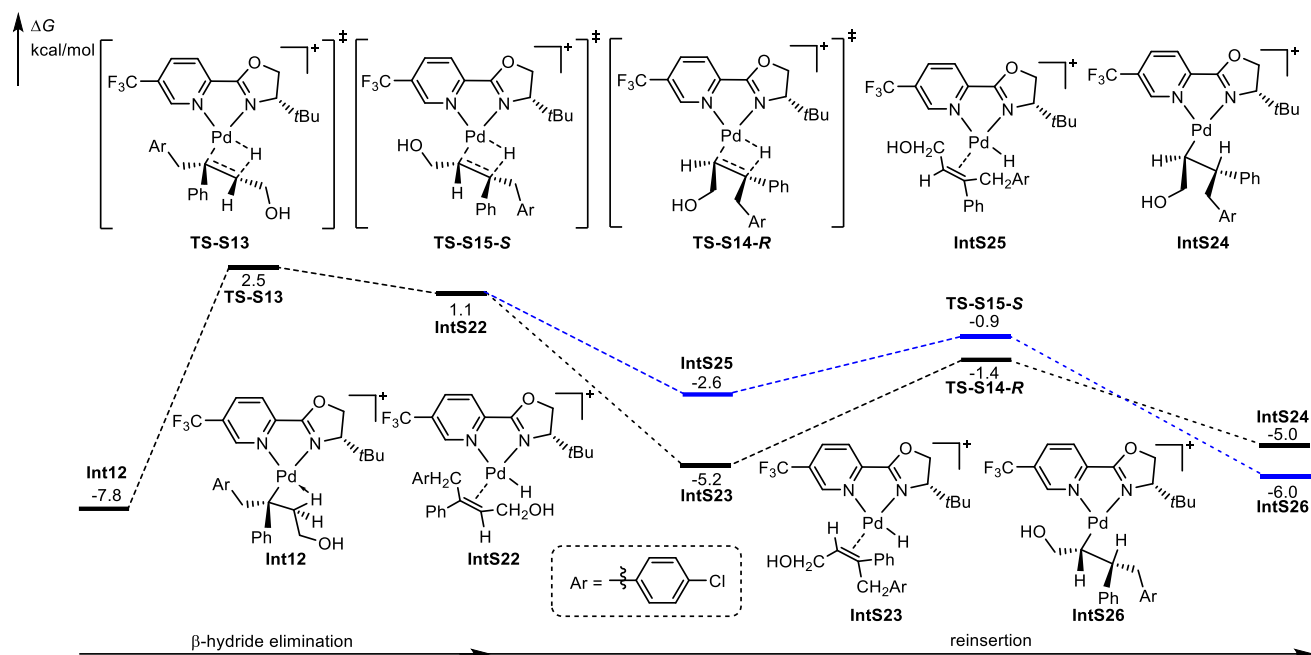


Fig. S7. Free energy profiles of alternative β -hydride elimination and reinsertion pathways with the ligand L1.

VIII. The configurations with the alkyl chain in the *cis* position to the oxazoline group on the ligand L1

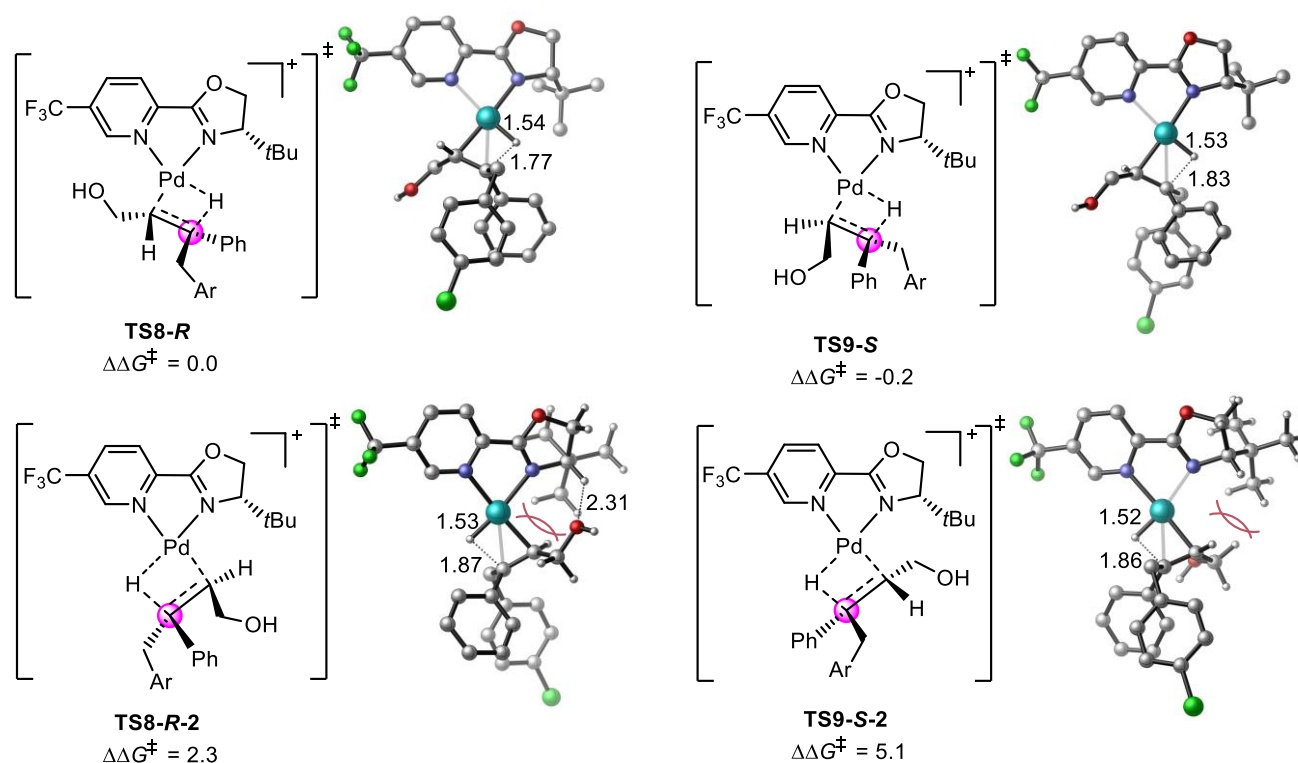


Fig. S8. The alternative configurations with the alkyl chain in the *cis* position to the oxazoline group on the ligand **L1**. Relative energies are given in kcal/mol.

IX. DFT-optimized structures of selected transition states with the ligand L1

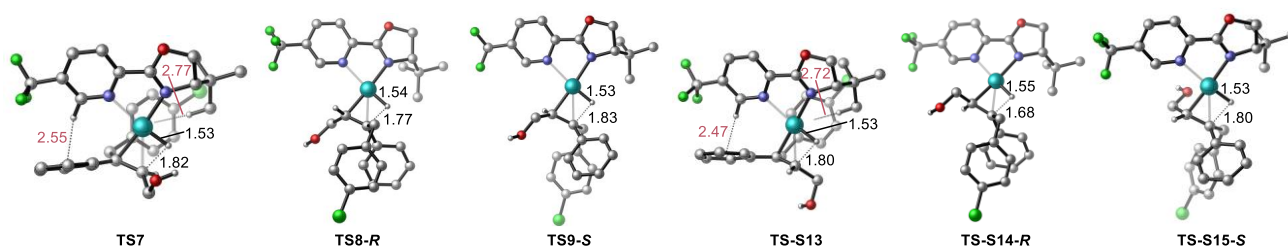


Fig. S9. DFT-optimized structures of selected transition states, with selected bond lengths given in Å. Irrelevant hydrogen atoms are omitted for clarity.

X. Energies and Cartesian coordinates of all the structures

Tables S1. Energies and Cartesian coordinates of all the structures reported in the text of this manuscript.

1a

H = -463.121476

G = -463.169659

Esol = -463.328010

Cartesian coordinates

C	-2.288264	-0.617690	0.686338
H	-2.433174	0.052779	1.558077
H	-1.421936	-1.267536	0.918837
C	-1.977339	0.231120	-0.542761
H	-1.867921	-0.452662	-1.401821
H	-2.851466	0.863180	-0.759500
C	-0.745561	1.091131	-0.377058
C	-0.834502	2.432201	-0.388466
H	-1.799355	2.931476	-0.509546
O	-3.447745	-1.375159	0.405861
H	-3.648000	-1.922229	1.174817
C	0.561703	0.403839	-0.185973
C	0.848739	-0.810482	-0.836889
C	1.551191	0.950101	0.652900
C	2.084081	-1.440081	-0.675345
H	0.102954	-1.262973	-1.492835
C	2.785452	0.321064	0.817136
H	1.336563	1.870433	1.199629
C	3.059752	-0.877025	0.151208
H	2.285364	-2.377154	-1.200346
H	3.534414	0.763861	1.478470
H	4.024563	-1.372680	0.282179

H	0.048439	3.069712	-0.301383
---	----------	----------	-----------

Ar-BOH2

H = -867.649531

G = -867.69577

Esol = -867.775254

Cartesian coordinates

O	-3.260914	1.216395	-0.075091
B	-2.636305	0.008087	-0.001904
O	-3.414887	-1.114551	0.072656
H	-2.918777	-1.936508	0.153643
C	-1.065625	-0.015650	-0.003559
C	-0.343408	1.192029	0.033808
C	-0.326186	-1.210842	-0.042417
C	1.050803	1.212663	0.037529
H	-0.893263	2.135319	0.060652
C	1.068822	-1.217635	-0.041588
H	-0.838414	-2.178357	-0.081352
C	1.749122	0.002164	-0.000024
H	1.601987	2.153724	0.068351
H	1.630949	-2.151924	-0.073930
H	-4.222867	1.127217	-0.057471
Cl	3.495714	0.012881	0.003330

BOH3

H = -252.444401

G = -252.476129

Esol = -252.498786

Cartesian coordinates

O	1.364017	0.093587	-0.000009
B	-0.000033	0.000112	-0.000039
O	-0.763161	1.134464	-0.000125
H	-1.706758	0.932966	0.001008
O	-0.600935	-1.228009	-0.000080
H	0.044866	-1.944846	0.000503
H	1.662687	1.010992	0.000388

BOMeOH2

H = -291.691311

G = -291.728382

Esol = -291.775252

Cartesian coordinates

O	-0.505191	1.361573	-0.000002
B	-0.519576	-0.004243	-0.000005
O	-1.710832	-0.678094	0.000010
H	-1.575648	-1.633806	-0.000062
O	0.649285	-0.706894	0.000002
H	-1.398009	1.726871	-0.000005
C	1.896669	-0.044363	0.000002
H	2.017638	0.593624	-0.892033
H	2.017368	0.594173	0.891677
H	2.690415	-0.806150	0.000351

H2

H = -1.157753

G = -1.172591

Esol = -1.170996

Cartesian coordinates

H	0.000000	0.000000	0.380436
H	0.000000	0.000000	-0.380436

H₂O

H = -76.445214

G = -76.466657

Esol = -76.470226

Cartesian coordinates

O	-0.000000	0.000000	0.120211
H	-0.000000	0.757010	-0.480842
H	-0.000000	-0.757010	-0.480842

HOBOH₂

H = -327.552143

G = -327.588717

Esol = -327.610916

Cartesian coordinates

O	-0.646957	-0.767818	-0.062191
B	0.488871	0.023046	-0.004446
O	0.423574	1.376137	-0.011218
H	1.303202	1.771232	0.031523
O	1.684008	-0.636088	0.012812
H	1.578519	-1.595057	0.056247
O	-1.860485	-0.028965	0.148243
H	-2.127206	0.162469	-0.766712

HOTf

H = -962.065503

G = -962.107347

Esol = -962.113086

Cartesian coordinates

S	-0.860388	-0.144737	0.082101
C	1.005788	0.001679	-0.002939
F	1.356518	1.239271	0.338944
F	1.538209	-0.862048	0.847509
F	1.427307	-0.256066	-1.229484
O	-1.249208	0.216822	1.434328
O	-1.230347	-1.375467	-0.576118
O	-1.246385	1.074911	-0.922589
H	-1.359306	1.885180	-0.393671

Int0

H = -2574.91054

G = -2575.033123

Esol = -2575.552349

Cartesian coordinates

Pd	0.338346	-0.170293	-0.010356
C	-0.650854	2.486028	-0.932714
C	-0.741984	3.836068	-1.259237
C	0.392792	4.636902	-1.106378
C	1.565088	4.051920	-0.632417
C	1.579318	2.684573	-0.331047
N	0.495461	1.921360	-0.480927
H	0.367095	5.698734	-1.356494
H	-1.686648	4.238527	-1.625657
H	2.484120	2.190432	0.025607
C	2.817101	4.873033	-0.395878
F	2.820102	5.972083	-1.156735
F	2.891004	5.254040	0.885442
F	3.913362	4.158024	-0.676036

C	-1.789382	1.561804	-1.046336
O	-2.961867	2.018317	-1.463736
N	-1.691741	0.319186	-0.737344
C	-3.930909	0.931263	-1.300343
H	-4.421875	0.801433	-2.273111
C	-3.000187	-0.313239	-0.992812
H	-2.903900	-0.909742	-1.913339
C	4.889715	-0.431359	1.396315
C	4.576442	-0.399301	0.034091
C	3.239504	-0.310255	-0.359642
C	2.218560	-0.255665	0.597071
C	2.546488	-0.252100	1.956929
C	3.883933	-0.342883	2.361293
H	5.373429	-0.463698	-0.707727
H	3.005434	-0.318041	-1.426720
H	1.768531	-0.190944	2.722179
H	4.146198	-0.353974	3.420449
C	-0.999595	-4.290284	-1.599875
H	-1.343681	-4.624788	-0.601304
H	-0.171944	-4.955445	-1.908987
C	-0.509565	-2.844011	-1.499729
H	-0.087417	-2.548389	-2.470185
H	-1.395760	-2.229082	-1.334491
C	0.463344	-2.629659	-0.366489
C	-0.031357	-2.153777	0.846920
H	-1.111270	-2.105788	0.998969
O	-2.053387	-4.281746	-2.540413
H	-2.331300	-5.190631	-2.711991
C	-4.943627	1.282035	-0.244048
C	-6.123322	0.528652	-0.177817

C	-4.711015	2.282620	0.705723
C	-7.048943	0.758737	0.839328
H	-6.313374	-0.253344	-0.917326
C	-5.642570	2.516984	1.720862
H	-3.805237	2.888363	0.650737
C	-6.808734	1.752247	1.793819
H	-7.963145	0.163317	0.885765
H	-5.456630	3.303215	2.455853
H	-7.535229	1.935237	2.588377
C	-3.429211	-1.232326	0.123159
C	-3.861501	-2.531155	-0.171248
C	-3.384189	-0.807873	1.459106
C	-4.255975	-3.392107	0.857829
H	-3.852902	-2.890663	-1.203312
C	-3.776926	-1.666900	2.484682
H	-3.040707	0.199108	1.699658
C	-4.217312	-2.961321	2.185618
H	-4.588924	-4.404571	0.619020
H	-3.742567	-1.325876	3.521573
H	-4.526067	-3.633392	2.989291
Cl	6.552083	-0.600411	1.892269
C	1.850803	-3.111555	-0.526014
C	2.430561	-3.228139	-1.805078
C	2.644028	-3.434259	0.594467
C	3.760014	-3.619858	-1.956288
H	1.850001	-2.982472	-2.694454
C	3.972096	-3.818403	0.444268
H	2.219852	-3.382473	1.596351
C	4.537959	-3.907033	-0.832167
H	4.192418	-3.694087	-2.956266

H	4.573075	-4.047216	1.326359
H	5.582315	-4.204603	-0.948335
H	0.579036	-2.198784	1.748818

Int10

H = -2270.238174

G = -2270.350578

Esol = -2270.82576

Cartesian coordinates

Pd	-0.475573	-0.239585	0.424642
C	-1.460108	2.304191	-0.738832
C	-1.526002	3.573063	-1.307975
C	-0.377475	4.368513	-1.298480
C	0.783393	3.859573	-0.720163
C	0.775799	2.565369	-0.186222
N	-0.321324	1.806474	-0.200522
H	-0.384500	5.368178	-1.735898
H	-2.463828	3.920663	-1.741406
H	1.675425	2.124753	0.244439
C	2.048962	4.688734	-0.626491
F	2.068396	5.640402	-1.564854
F	2.132550	5.281918	0.570339
F	3.132557	3.917524	-0.779928
C	-2.631604	1.420915	-0.636103
O	-3.784166	1.818616	-1.159399
N	-2.601700	0.293271	-0.016327
C	-4.703296	0.700505	-0.981357
H	-4.805549	0.200396	-1.955674
C	-4.003403	-0.180055	0.079999
H	-4.054210	-1.241122	-0.202969

C	4.227018	-0.578248	1.156672
C	3.732399	-0.433845	-0.143213
C	2.355114	-0.324592	-0.344068
C	1.473123	-0.360004	0.742449
C	1.980739	-0.470523	2.041086
C	3.360632	-0.582316	2.252094
H	4.421699	-0.425819	-0.988402
H	1.979685	-0.242597	-1.366385
H	1.314133	-0.482010	2.907132
H	3.762880	-0.680440	3.261656
C	-1.894840	-4.231250	-1.480707
H	-2.024603	-4.790610	-0.531963
H	-1.063187	-4.710502	-2.030500
C	-1.541983	-2.775572	-1.160348
H	-1.321765	-2.258105	-2.105948
H	-2.444104	-2.310751	-0.747618
C	-0.406545	-2.648482	-0.174833
C	-0.701457	-2.295687	1.142239
H	-1.743127	-2.298171	1.462303
O	-3.081350	-4.185648	-2.236994
H	-3.321751	-5.082557	-2.502069
C	-4.576861	-0.034153	1.523373
Cl	5.940429	-0.770437	1.407674
C	0.938108	-3.084208	-0.599535
C	1.310565	-3.043168	-1.958275
C	1.892766	-3.523907	0.340119
C	2.597292	-3.399267	-2.358244
H	0.599139	-2.701380	-2.710729
C	3.178408	-3.874348	-0.058508
H	1.628665	-3.593217	1.394708

C	3.537654	-3.808108	-1.408899
H	2.869442	-3.351735	-3.414681
H	3.907408	-4.198416	0.686534
H	4.548573	-4.080213	-1.719901
H	0.041620	-2.419121	1.930037
H	-5.671228	1.109197	-0.674282
C	-6.018357	-0.571762	1.514428
H	-6.052831	-1.619799	1.175976
H	-6.440327	-0.534595	2.529801
H	-6.685069	0.017161	0.866072
C	-3.742181	-0.874597	2.499753
H	-4.172802	-0.816894	3.510423
H	-3.734614	-1.936802	2.206897
H	-2.704103	-0.516791	2.556671
C	-4.560189	1.432947	1.981143
H	-3.533813	1.828925	2.027621
H	-5.153861	2.087006	1.324653
H	-4.986579	1.514864	2.991947

Int11

H = -2270.257889

G = -2270.368699

Esol = -2270.846534

Cartesian coordinates

Pd	-0.303805	-0.608348	-0.110578
C	0.567881	2.243119	-0.665328
C	1.282694	3.377403	-1.050969
C	2.675690	3.303746	-1.098833
C	3.291632	2.103157	-0.745633
C	2.496498	1.010217	-0.387655

N	1.168675	1.070844	-0.360697
H	3.272354	4.166520	-1.400706
H	0.746406	4.293979	-1.297162
H	2.952837	0.063960	-0.105798
C	4.799284	1.978032	-0.701473
F	5.276822	2.439950	0.461962
F	5.177405	0.695898	-0.817842
F	5.367923	2.678392	-1.687039
C	-0.891632	2.251811	-0.490495
O	-1.571504	3.372694	-0.713683
N	-1.538178	1.230389	-0.056936
C	-2.973451	3.026819	-0.504772
H	-3.443098	2.929277	-1.494837
C	-2.909327	1.680835	0.253984
H	-3.633585	0.972167	-0.162024
C	-3.813471	-1.135681	-1.599168
C	-3.871606	-1.788659	-0.355047
C	-2.745898	-2.434433	0.130420
C	-1.538629	-2.467436	-0.613017
C	-1.525700	-1.837197	-1.889713
C	-2.659479	-1.164848	-2.373707
H	-4.799042	-1.772854	0.218434
H	-2.791559	-2.941197	1.096931
H	-0.665243	-1.957515	-2.549735
H	-2.642756	-0.682369	-3.351409
C	-0.334749	-3.294952	-0.161652
H	-0.109392	-4.062212	-0.917104
C	0.850095	-2.333855	0.010873
C	1.891938	-2.460736	-1.083723
H	2.604857	-1.625912	-1.077778

H	1.404419	-2.430925	-2.069994
C	2.710972	-3.754790	-1.031723
H	3.222099	-3.838441	-0.052962
H	2.034929	-4.629223	-1.113558
O	3.620496	-3.689562	-2.102288
H	4.152464	-4.495161	-2.119378
C	-3.145941	1.774505	1.792225
Cl	-5.204023	-0.246124	-2.153677
H	-0.576369	-3.824525	0.767580
C	1.311576	-2.044396	1.391978
C	0.385563	-2.010148	2.465892
C	2.650028	-1.685558	1.678200
C	0.769731	-1.597800	3.741095
H	-0.649747	-2.310810	2.304082
C	3.033016	-1.286964	2.957316
H	3.411721	-1.748110	0.901231
C	2.093821	-1.228330	3.992578
H	0.031040	-1.573991	4.545025
H	4.076322	-1.027872	3.150691
H	2.397356	-0.913540	4.993076
H	-3.442559	3.848443	0.046574
C	-2.930250	0.393350	2.429570
H	-3.109396	0.447870	3.514080
H	-3.622533	-0.350805	2.011294
H	-1.903700	0.031469	2.273053
C	-4.604631	2.206290	2.017078
H	-5.306067	1.507145	1.533896
H	-4.834239	2.223239	3.093069
H	-4.808913	3.215121	1.626351
C	-2.184983	2.782431	2.441897

H	-1.135885	2.467978	2.327844
H	-2.289400	3.795186	2.023822
H	-2.388705	2.853813	3.520792

Int12

H = -2270.256264

G = -2270.362943

Esol = -2270.843898

Cartesian coordinates

Pd	0.244185	-0.352145	0.705417
C	-0.774186	2.372152	0.069447
C	-1.587784	3.436680	-0.311034
C	-2.820588	3.154707	-0.906408
C	-3.183453	1.822112	-1.095284
C	-2.300985	0.810068	-0.702365
N	-1.127624	1.081221	-0.135521
H	-3.490383	3.959208	-1.214515
H	-1.258112	4.459628	-0.128007
H	-2.560750	-0.241273	-0.836731
C	-4.534333	1.434231	-1.658622
F	-4.433798	0.342390	-2.430199
F	-5.391739	1.151553	-0.666722
F	-5.057793	2.422834	-2.388736
C	0.516920	2.545923	0.754604
O	0.986280	3.764428	0.989455
N	1.209729	1.542074	1.154650
C	2.206362	3.585152	1.770829
H	2.010721	3.974811	2.779313
C	2.460959	2.050971	1.743133
H	2.546480	1.651507	2.765395

C	3.693256	-1.365819	-2.258858
C	2.577110	-0.580361	-2.556852
C	1.311689	-1.023523	-2.175614
C	1.134621	-2.250992	-1.514354
C	2.266534	-3.045892	-1.284863
C	3.544243	-2.609085	-1.641531
H	2.705282	0.368841	-3.077203
H	0.440475	-0.406819	-2.409413
H	2.156378	-4.032085	-0.826415
H	4.421535	-3.226612	-1.445144
C	0.398913	-2.556750	1.412797
H	1.172780	-1.669521	1.535310
C	-0.614329	-2.192452	0.363345
C	-0.247377	-2.662276	-1.056008
H	-0.354844	-3.760369	-1.107352
C	-2.076456	-2.140690	0.662411
C	-2.568818	-1.462530	1.801346
C	-3.023319	-2.656216	-0.248039
C	-3.936456	-1.271606	1.988661
C	-4.393834	-2.468506	-0.053396
H	-2.700094	-3.214010	-1.125922
C	-4.857517	-1.760530	1.056363
H	-4.287094	-0.726649	2.868102
H	-5.100239	-2.872455	-0.781506
H	-0.977472	-2.246142	-1.762362
C	3.719669	1.597422	0.948689
Cl	5.288280	-0.776427	-2.643697
H	-5.927409	-1.594828	1.197032
H	2.992688	4.182765	1.296270
C	4.961205	2.159499	1.659954

H	5.873381	1.839513	1.134445
H	4.969480	3.260602	1.683049
H	5.027066	1.795897	2.698048
C	3.794850	0.062179	0.953938
H	3.774796	-0.336774	1.981111
H	2.964640	-0.385399	0.390646
H	4.727587	-0.271008	0.476392
C	3.659013	2.105340	-0.499263
H	3.701019	3.203901	-0.559454
H	4.508463	1.711160	-1.075763
H	2.740310	1.765130	-0.998868
C	0.006280	-2.889529	2.850815
H	-0.961327	-3.423616	2.855864
H	1.102268	-3.302156	1.017364
H	-1.867197	-1.058602	2.530884
O	-0.053778	-1.685514	3.593204
H	0.771973	-3.567154	3.268442
H	-0.333599	-1.883017	4.497372

Int13

H = -2270.241813

G = -2270.351084

Esol = -2270.827432

Cartesian coordinates

Pd	1.226956	1.046923	-0.096627
C	0.175902	-1.537724	-1.310439
C	-0.582727	-2.623072	-1.735675
C	-1.975006	-2.544474	-1.622821
C	-2.533184	-1.378796	-1.110194
C	-1.691195	-0.345226	-0.676458

N	-0.369623	-0.426174	-0.763914
H	-2.610844	-3.372844	-1.937384
H	-0.089614	-3.501403	-2.151913
H	-2.108772	0.559949	-0.242067
C	-4.029475	-1.166724	-1.049356
F	-4.693204	-2.321756	-1.135007
F	-4.387522	-0.560272	0.096731
F	-4.430786	-0.376386	-2.055879
C	1.637737	-1.487351	-1.436917
O	2.287851	-2.476712	-2.029501
N	2.333817	-0.491942	-1.005344
C	3.673060	-2.036598	-2.150669
H	3.844152	-1.783580	-3.206847
C	3.765100	-0.808001	-1.207837
H	4.240286	0.043388	-1.716156
C	-1.316672	-2.358777	2.065170
C	-2.317599	-1.404908	2.256660
C	-1.961738	-0.066955	2.444767
C	-0.620102	0.332631	2.448664
C	0.366678	-0.662905	2.348901
C	0.031636	-2.000921	2.150444
H	-3.365750	-1.701136	2.224481
H	-2.755465	0.672286	2.557854
H	1.421068	-0.385255	2.415310
H	0.803089	-2.765287	2.049145
C	1.217279	3.078535	0.870459
H	2.453458	1.932526	0.089297
C	-0.019046	2.440339	1.093756
C	-0.204922	1.788591	2.477879
H	0.746890	1.874423	3.019918

C	-1.244933	2.750887	0.288536
C	-1.213396	2.806509	-1.121709
C	-2.487501	2.944129	0.917866
C	-2.371939	3.020507	-1.864527
C	-3.651788	3.157077	0.173783
H	-2.559629	2.937915	2.004435
C	-3.602509	3.186948	-1.220024
H	-2.317063	3.040008	-2.955027
H	-4.602613	3.295707	0.692433
H	-0.932780	2.381974	3.051321
C	4.539604	-1.072149	0.119728
Cl	-1.751633	-4.003202	1.681113
H	-4.514056	3.337243	-1.801669
H	4.313358	-2.878479	-1.869035
C	5.998141	-1.396995	-0.250058
H	6.089554	-2.307956	-0.861127
H	6.463560	-0.566138	-0.804006
H	6.589071	-1.560963	0.663244
C	4.534269	0.184410	1.004339
H	4.883565	1.071885	0.453387
H	3.531469	0.403798	1.395402
H	5.204452	0.036933	1.864548
C	3.912370	-2.241448	0.894171
H	4.459448	-2.409715	1.833699
H	2.864922	-2.028135	1.154596
H	3.939182	-3.186087	0.329621
C	1.501408	4.248222	-0.035079
H	0.820338	4.280345	-0.897917
H	1.925462	3.042893	1.704297
H	-0.275109	2.620597	-1.648099

O	2.856245	4.175467	-0.418082
H	1.301633	5.154806	0.573911
H	3.099292	4.984213	-0.887003

Int14

H = -2270.241139

G = -2270.354817

Esol = -2270.826583

Cartesian coordinates

Pd	-0.823345	-0.547354	-0.245238
C	-3.588468	0.581030	-0.538319
C	-4.715071	1.394209	-0.633689
C	-4.590775	2.742078	-0.287681
C	-3.347808	3.214562	0.130424
C	-2.266761	2.326445	0.200481
N	-2.385909	1.040329	-0.121887
H	-5.448507	3.414869	-0.339172
H	-5.661770	0.971839	-0.971467
H	-1.288017	2.673550	0.536305
C	-3.134863	4.676309	0.470030
F	-4.269169	5.240332	0.892561
F	-2.209137	4.808459	1.430028
F	-2.709326	5.349225	-0.605612
C	-3.603856	-0.850093	-0.876757
O	-4.722475	-1.426514	-1.279715
N	-2.548872	-1.584771	-0.787750
C	-4.368155	-2.797444	-1.638331
H	-4.415193	-2.870090	-2.733928
C	-2.933583	-2.983871	-1.073307
H	-2.258232	-3.379559	-1.845828

H	0.077497	-1.742368	-0.494365
C	-2.838481	-3.913095	0.174914
C	0.579247	0.960853	1.957166
C	0.761497	0.709931	0.479303
H	0.644938	1.605212	-0.144275
C	1.556165	-0.308418	-0.060941
C	2.103385	-0.155368	-1.475011
C	2.284282	-1.309929	0.778933
C	2.287839	-2.678085	0.466006
C	3.126011	-0.844720	1.803559
C	3.091833	-3.568987	1.175235
H	1.647334	-3.052049	-0.336719
C	3.938246	-1.737947	2.506347
H	3.157945	0.221810	2.030066
C	3.921649	-3.099561	2.198869
H	3.073511	-4.632568	0.927753
H	4.594196	-1.362165	3.294580
H	2.072985	-1.121201	-1.997231
H	4.556479	-3.795409	2.751610
H	-5.121194	-3.457117	-1.195369
C	-3.308466	-5.315413	-0.251804
H	-2.699128	-5.706089	-1.082597
H	-3.209886	-6.015429	0.591027
H	-4.363834	-5.334602	-0.564160
C	-1.380833	-4.012339	0.650948
H	-1.299936	-4.761866	1.452408
H	-0.711572	-4.324921	-0.166448
H	-1.008793	-3.058129	1.048669
C	-3.714495	-3.380351	1.318916
H	-3.374378	-2.388359	1.654941

H	-4.776542	-3.304800	1.037525
H	-3.656927	-4.057166	2.184245
C	3.537286	0.328560	-1.379231
C	4.605433	-0.563674	-1.536861
C	3.816109	1.660975	-1.045459
C	5.924476	-0.141003	-1.375035
H	4.406442	-1.609702	-1.781067
C	5.129028	2.100317	-0.879699
H	2.999082	2.372618	-0.902825
C	6.180136	1.192769	-1.043891
H	6.754898	-0.836769	-1.500764
H	5.344713	3.138328	-0.623804
H	1.482355	0.554564	-2.041478
Cl	7.822678	1.729633	-0.832022
H	0.694287	0.017828	2.519189
O	1.545067	1.929576	2.320508
H	1.465897	2.118596	3.265509
H	-0.444942	1.333697	2.150591

Int15

H = -2270.248399

G = -2270.359896

Esol = -2270.835054

Cartesian coordinates

Pd	-0.847990	-0.411316	-0.238103
C	-3.618757	0.590115	-0.479035
C	-4.739370	1.415145	-0.519568
C	-4.593905	2.755920	-0.156074
C	-3.333175	3.214060	0.223857
C	-2.256622	2.320282	0.242317

N	-2.399171	1.037768	-0.095105
H	-5.448453	3.434695	-0.165906
H	-5.699761	1.003659	-0.830926
H	-1.263009	2.653122	0.544491
C	-3.098471	4.669963	0.575911
F	-4.205470	5.224544	1.075868
F	-2.116638	4.785605	1.480416
F	-2.739214	5.361840	-0.511466
C	-3.655522	-0.833772	-0.845224
O	-4.799132	-1.387519	-1.219154
N	-2.604281	-1.571871	-0.807904
C	-4.473725	-2.755039	-1.612454
H	-4.569641	-2.813284	-2.705745
C	-3.017023	-2.956784	-1.113364
H	-2.378073	-3.343122	-1.921608
H	0.552015	-1.381973	-0.481642
C	-2.864463	-3.904394	0.112807
C	0.841562	1.082408	1.718900
C	0.811082	0.631363	0.276859
H	0.895359	1.487023	-0.407046
C	1.475477	-0.604826	-0.196959
C	2.178456	-0.478039	-1.581493
C	2.259890	-1.456623	0.780589
C	2.086930	-2.846180	0.815420
C	3.269320	-0.874434	1.563574
C	2.892168	-3.645465	1.629547
H	1.318767	-3.312812	0.195229
C	4.073113	-1.674562	2.377458
H	3.424793	0.203863	1.529205
C	3.887849	-3.059246	2.414953

H	2.742716	-4.727207	1.647673
H	4.857467	-1.210947	2.979799
H	2.241864	-1.478382	-2.033085
H	4.520854	-3.680946	3.051779
H	-5.210697	-3.417377	-1.145740
C	-3.317484	-5.310654	-0.314609
H	-2.728227	-5.678838	-1.169782
H	-3.179734	-6.019373	0.515551
H	-4.381788	-5.344092	-0.594524
C	-1.386395	-3.960446	0.523480
H	-1.239830	-4.697494	1.327090
H	-0.749373	-4.259245	-0.324574
H	-1.031268	-2.989397	0.898426
C	-3.705671	-3.408603	1.298673
H	-3.378488	-2.412132	1.634214
H	-4.779627	-3.357856	1.061151
H	-3.595647	-4.094451	2.151797
C	3.560522	0.110823	-1.449155
C	4.679868	-0.727275	-1.349423
C	3.751080	1.495965	-1.348470
C	5.957062	-0.205562	-1.149440
H	4.551324	-1.810206	-1.415090
C	5.020807	2.035468	-1.145145
H	2.898812	2.174443	-1.428176
C	6.120585	1.178383	-1.041881
H	6.824604	-0.861922	-1.072291
H	5.165463	3.113730	-1.068916
H	1.546562	0.141520	-2.236459
Cl	7.709145	1.842526	-0.781035
H	0.946832	0.214715	2.392835

O	1.916438	1.994186	1.840106
H	2.024522	2.237895	2.769430
H	-0.119755	1.573514	1.970945

Int16

H = -2270.242779

G = -2270.356345

Esol = -2270.828873

Cartesian coordinates

Pd	1.074281	-0.601137	0.772753
C	3.134839	1.426068	-0.146229
C	3.879385	2.559350	-0.467238
C	3.234492	3.798521	-0.468768
C	1.881323	3.847717	-0.139371
C	1.213127	2.657956	0.177918
N	1.819966	1.473792	0.163867
H	3.778932	4.713292	-0.709445
H	4.939579	2.463181	-0.702261
H	0.159341	2.680554	0.460185
C	1.113685	5.154592	-0.160475
F	1.918266	6.186479	0.106128
F	0.564684	5.353627	-1.364648
F	0.125751	5.138132	0.744538
C	3.733676	0.082215	-0.090762
O	5.020265	-0.066444	-0.347025
N	3.057148	-0.972260	0.215162
C	5.336438	-1.467432	-0.086469
H	5.966416	-1.497547	0.813206
C	3.952711	-2.147069	0.106161
H	3.917381	-2.695427	1.058840

H	0.848056	-2.011489	1.261566
C	3.548002	-3.131766	-1.030915
C	-0.915500	-0.770851	3.112860
C	-0.775864	-0.098859	1.770368
H	-0.741161	0.994601	1.847079
C	-1.203538	-0.613871	0.540280
C	-1.528857	0.344146	-0.593003
H	-1.117539	-0.025532	-1.542975
C	-1.730538	-1.993673	0.335388
C	-2.657635	-2.552477	1.230919
C	-1.387889	-2.709294	-0.825057
C	-3.201136	-3.814721	0.980386
H	-2.977407	-1.980255	2.102397
C	-1.921245	-3.973885	-1.064539
C	-2.829837	-4.531965	-0.158824
H	-3.929656	-4.234549	1.677416
H	-1.634426	-4.523890	-1.963467
H	-3.257062	-5.518812	-0.349548
H	-0.685745	-2.277082	-1.540960
H	5.907525	-1.837797	-0.944028
C	3.467306	-2.399533	-2.378751
H	3.214555	-3.109593	-3.180112
H	2.686170	-1.623382	-2.366165
H	4.420696	-1.923487	-2.658034
C	4.608712	-4.246029	-1.088291
H	4.703305	-4.758878	-0.117667
H	4.317086	-4.999807	-1.834529
H	5.603775	-3.875377	-1.378236
C	2.189792	-3.771076	-0.709012
H	1.942854	-4.530670	-1.465956

H	2.200841	-4.269582	0.273194
H	1.378114	-3.033690	-0.701122
C	-3.036578	0.480330	-0.720763
C	-3.680276	0.182694	-1.927274
C	-3.812185	0.874674	0.379703
C	-5.066111	0.292215	-2.049325
H	-3.093793	-0.142889	-2.790015
C	-5.197726	0.986182	0.273964
H	-3.342220	1.075552	1.345452
C	-5.820158	0.695426	-0.944381
H	-5.564860	0.063344	-2.991893
H	-5.800420	1.291385	1.130224
H	-1.076196	1.326266	-0.400158
Cl	-7.550295	0.829260	-1.081911
H	-0.800001	-1.864350	3.019057
O	-2.198073	-0.409981	3.598091
H	-2.275651	-0.676368	4.524279
H	-0.116543	-0.403814	3.782623

Int17

H = -2270.248924

G = -2270.360832

Esol = -2270.835734

Cartesian coordinates

Pd	0.821427	-0.385757	0.080622
C	3.728045	0.131587	0.168572
C	4.972065	0.754386	0.205021
C	5.022525	2.148884	0.134720
C	3.827471	2.857894	0.025665
C	2.615423	2.158058	0.006069

N	2.567600	0.827789	0.081945
H	5.977017	2.677006	0.167104
H	5.875233	0.149006	0.286009
H	1.665490	2.688813	-0.063618
C	3.815413	4.368034	-0.108392
F	4.892682	4.907539	0.466972
F	3.808058	4.723293	-1.398218
F	2.720280	4.883946	0.466595
C	3.556809	-1.329150	0.202881
O	4.611483	-2.122431	0.308479
N	2.395218	-1.869948	0.117011
C	4.089796	-3.484701	0.382930
H	4.302965	-3.862593	1.392014
C	2.568890	-3.333055	0.090566
H	1.972963	-3.766281	0.908869
H	-0.613753	-1.287619	0.017807
C	2.078496	-3.972876	-1.240588
C	-0.859429	1.837588	1.250381
C	-0.771230	0.879732	0.087297
H	-0.782447	1.413155	-0.873631
C	-1.488849	-0.416615	0.077977
C	-2.238000	-0.758002	-1.244677
H	-2.329711	-1.850702	-1.321857
C	-2.216862	-0.861130	1.331252
C	-3.299867	-0.112367	1.819220
C	-1.872644	-2.058308	1.972969
C	-4.017246	-0.561643	2.929264
H	-3.567398	0.825904	1.335167
C	-2.592473	-2.507145	3.082679
C	-3.669656	-1.758401	3.562253

H	-4.858312	0.028711	3.299535
H	-2.310959	-3.441852	3.572428
H	-4.235978	-2.105745	4.429070
H	-1.029430	-2.648838	1.602121
H	4.634634	-4.085842	-0.353516
C	2.842284	-3.393334	-2.440534
H	2.480437	-3.848411	-3.374535
H	2.691894	-2.305521	-2.523330
H	3.924451	-3.588962	-2.385125
C	2.302499	-5.491312	-1.142608
H	1.752515	-5.922911	-0.290931
H	1.944087	-5.986432	-2.057326
H	3.366106	-5.752642	-1.028770
C	0.575256	-3.701160	-1.415928
H	0.186498	-4.268048	-2.274948
H	0.000683	-4.006704	-0.526485
H	0.377854	-2.636535	-1.607484
C	-3.608392	-0.131168	-1.298547
C	-4.743331	-0.888407	-0.977815
C	-3.773399	1.227947	-1.600249
C	-6.012806	-0.312055	-0.951449
H	-4.634202	-1.947083	-0.730708
C	-5.034471	1.821702	-1.575358
H	-2.908124	1.845141	-1.849565
C	-6.151245	1.047031	-1.245792
H	-6.892862	-0.905588	-0.701181
H	-5.159451	2.879447	-1.809757
H	-1.615185	-0.418204	-2.086925
Cl	-7.728842	1.783208	-1.205605
H	-0.936975	1.282037	2.201246

O	-1.986741	2.660146	1.017494
H	-2.136797	3.220834	1.790503
H	0.066167	2.445031	1.299178

Int1

H = -2574.925218

G = -2575.044029

Esol = -2575.568725

Cartesian coordinates

Pd	0.666505	0.951397	0.047948
C	1.062875	-2.121353	0.496405
C	1.509841	-3.429767	0.675646
C	2.871126	-3.695068	0.503701
C	3.715829	-2.642890	0.161069
C	3.176850	-1.357302	0.001628
N	1.883802	-1.101163	0.167742
H	3.268044	-4.702883	0.632984
H	0.800822	-4.213359	0.943343
H	3.817634	-0.520594	-0.270077
C	5.204909	-2.837302	-0.035048
F	5.893805	-2.127433	0.868946
F	5.550429	-4.122141	0.089762
F	5.577849	-2.416953	-1.251424
C	-0.353061	-1.755050	0.646045
O	-1.233062	-2.696309	0.956963
N	-0.789938	-0.555991	0.470055
C	-2.508269	-2.014858	1.208718
H	-2.590514	-1.928944	2.302526
C	-2.255097	-0.585718	0.597926
H	-2.571520	0.174603	1.321130

C	4.515481	1.748571	-0.488332
C	4.119321	2.128032	0.803546
C	2.858928	2.681035	0.994872
C	1.966352	2.879422	-0.090204
C	2.390253	2.462015	-1.377861
C	3.656400	1.901370	-1.577701
H	4.806141	1.995617	1.640307
H	2.565115	3.010152	1.993919
H	1.755385	2.650021	-2.245267
H	3.982050	1.602584	-2.574638
C	-2.023180	3.915227	-1.747116
H	-1.703389	4.264093	-2.746263
H	-1.837268	4.743722	-1.046141
C	-1.189480	2.659615	-1.359545
H	-1.848345	1.789151	-1.452169
H	-0.405823	2.520588	-2.118700
C	-0.518990	2.663276	0.010715
C	0.658979	3.650040	0.103160
H	0.573239	4.433089	-0.666005
O	-3.415677	3.687974	-1.723921
H	-3.628962	2.974741	-2.342991
C	-1.388737	2.599615	1.225954
C	-0.805486	2.418240	2.500299
C	-2.790867	2.687910	1.151941
C	-1.588541	2.294741	3.644969
H	0.279962	2.345406	2.594362
C	-3.574539	2.586403	2.305996
H	-3.280152	2.861827	0.194606
C	-2.983573	2.376780	3.553145
H	-1.110604	2.141167	4.615043

H	-4.660280	2.677702	2.223274
H	0.678789	4.155084	1.075910
C	-3.668274	-2.784107	0.658721
C	-4.899343	-2.714280	1.321937
C	-3.570212	-3.492022	-0.545749
C	-6.027261	-3.334328	0.779756
H	-4.977861	-2.172266	2.268465
C	-4.694749	-4.120581	-1.080755
H	-2.610940	-3.555907	-1.061279
C	-5.926115	-4.037527	-0.423130
H	-6.984142	-3.276237	1.302808
H	-4.611345	-4.676842	-2.016900
H	-6.805706	-4.528231	-0.845376
C	-2.938843	-0.312018	-0.723382
C	-4.211291	0.270508	-0.722201
C	-2.337215	-0.635999	-1.946259
C	-4.865594	0.547220	-1.923930
H	-4.688765	0.521486	0.226464
C	-2.987429	-0.358856	-3.150473
H	-1.342197	-1.084195	-1.962819
C	-4.251194	0.240225	-3.142826
H	-5.856353	1.006507	-1.908864
H	-2.506274	-0.609609	-4.098340
H	-4.761499	0.456137	-4.084232
Cl	6.084164	1.039260	-0.724455
H	-3.599993	2.291873	4.450757

Int2

H = -2574.921235

G = -2575.043742

Esol = -2575.562526

Cartesian coordinates

Pd	0.784647	-1.298667	-0.225071
C	3.376480	0.167989	-0.750338
C	4.709337	0.547222	-0.891240
C	5.696907	-0.422084	-0.700522
C	5.307564	-1.723000	-0.384271
C	3.943215	-2.017155	-0.260256
N	3.000880	-1.092818	-0.439677
H	6.754601	-0.169547	-0.792495
H	4.955872	1.579069	-1.143092
H	3.611821	-3.025437	-0.004656
C	6.330171	-2.828819	-0.217486
F	7.503722	-2.338800	0.191898
F	5.910451	-3.732465	0.678610
F	6.527054	-3.464407	-1.378975
C	2.255689	1.103169	-0.936256
O	2.488385	2.351453	-1.301855
N	1.033768	0.737268	-0.761819
C	1.180463	2.961364	-1.590571
H	1.095757	2.969169	-2.686895
C	0.165240	1.897511	-0.996775
H	-0.565077	1.644476	-1.778072
C	-6.266936	-1.645569	-1.495708
C	-5.490497	-2.645035	-0.904990
C	-4.115712	-2.455905	-0.747906
C	-3.503875	-1.270703	-1.173890
C	-4.303472	-0.277270	-1.759431
C	-5.676515	-0.454253	-1.926609

H	-5.964756	-3.567016	-0.565726
H	-3.536138	-3.238621	-0.259433
H	-3.846710	0.660060	-2.089904
H	-6.291433	0.322759	-2.382623
C	-0.973341	-4.047756	1.088116
H	-0.342164	-4.926946	0.850717
C	-0.746563	-2.995856	-0.001458
H	0.458517	-3.007941	-0.071180
H	-1.019867	-3.418449	-0.978281
C	-1.243652	-1.589370	0.124901
C	-2.006173	-1.020147	-1.066088
H	-1.859365	0.068338	-1.062336
C	-1.546621	-1.033842	1.475892
C	-0.673407	-1.250969	2.565741
C	-2.693380	-0.250474	1.705445
C	-0.954593	-0.745125	3.833068
H	0.255296	-1.807097	2.421068
C	-2.980376	0.244433	2.976846
H	-3.385968	-0.043422	0.893200
C	-2.121875	-0.007812	4.048344
H	-0.260267	-0.929606	4.655791
H	-3.884438	0.837356	3.127120
H	-1.523365	-1.394429	-1.985885
C	1.091776	4.356086	-1.057089
C	0.377463	5.314292	-1.786273
C	1.632457	4.696978	0.189400
C	0.189970	6.597794	-1.268599
H	-0.035784	5.057208	-2.765498
C	1.453485	5.981694	0.701257
H	2.197348	3.957314	0.758227

C	0.726472	6.931985	-0.023047
H	-0.368258	7.339860	-1.843205
H	1.880602	6.243357	1.671678
H	0.585110	7.936527	0.381521
C	-0.575374	2.338272	0.243201
C	-1.773485	3.047353	0.095862
C	-0.043757	2.147500	1.523340
C	-2.416807	3.587089	1.210616
H	-2.196759	3.197379	-0.900873
C	-0.687046	2.684880	2.638129
H	0.876446	1.575804	1.653850
C	-1.868484	3.413758	2.483560
H	-3.345920	4.146843	1.084118
H	-2.368965	3.836689	3.357225
Cl	-7.982669	-1.878946	-1.689162
H	-2.352783	0.379502	5.043042
O	-2.339279	-4.372751	1.071972
H	-2.543974	-4.954603	1.815306
H	-0.655389	-3.664596	2.069528
H	-0.267276	2.527689	3.633074

Int3

H = -2574.907708

G = -2575.029555

Esol = -2575.547602

Cartesian coordinates

Pd	0.944687	-1.388353	-0.253439
C	3.324880	0.318413	-0.784326
C	4.632561	0.771471	-0.936191
C	5.677465	-0.132341	-0.734083

C	5.367817	-1.448635	-0.394086
C	4.027078	-1.824960	-0.255904
N	3.028360	-0.958203	-0.446694
H	6.717632	0.182075	-0.835257
H	4.813042	1.812237	-1.206223
H	3.757686	-2.843959	0.020641
C	6.457804	-2.487256	-0.213789
F	7.588410	-1.920994	0.217161
F	6.083725	-3.420143	0.671266
F	6.715355	-3.100465	-1.374756
C	2.152714	1.183373	-0.978403
O	2.330837	2.454211	-1.295481
N	0.951449	0.741814	-0.840868
C	0.999017	3.003832	-1.589526
H	0.923800	3.023745	-2.686719
C	0.038754	1.882257	-1.022109
H	-0.698125	1.636492	-1.798177
C	-6.211740	-1.688049	-1.495477
C	-5.355133	-2.708029	-1.074692
C	-3.997876	-2.441079	-0.882987
C	-3.484444	-1.156757	-1.106571
C	-4.363872	-0.144260	-1.519363
C	-5.720004	-0.398817	-1.719839
H	-5.753186	-3.707391	-0.893841
H	-3.356570	-3.249587	-0.529785
H	-3.984180	0.868007	-1.683526
H	-6.398104	0.392370	-2.042312
C	-0.716930	-4.041098	0.730739
H	0.090888	-4.724638	0.408498
C	-0.744462	-2.825857	-0.176297

H	1.239845	-2.837567	0.100145
H	-0.823089	-3.103906	-1.233922
C	-1.289214	-1.572753	0.155329
C	-2.009909	-0.812307	-0.945618
H	-1.940489	0.261114	-0.744037
C	-1.529561	-1.147225	1.564680
C	-0.585225	-1.380912	2.585656
C	-2.722905	-0.486843	1.911016
C	-0.838324	-1.004345	3.903220
H	0.374996	-1.838921	2.341958
C	-2.979053	-0.119934	3.231845
H	-3.473183	-0.277020	1.151809
C	-2.044808	-0.382050	4.235248
H	-0.087680	-1.195179	4.673364
H	-3.918832	0.380026	3.474273
H	-1.493393	-1.002562	-1.901193
C	0.834144	4.383453	-1.035155
C	0.083907	5.317740	-1.759118
C	1.337432	4.727780	0.226101
C	-0.176742	6.580332	-1.221569
H	-0.300231	5.058461	-2.749578
C	1.085548	5.991998	0.757661
H	1.928682	4.006414	0.791567
C	0.322456	6.917761	0.038468
H	-0.762797	7.303919	-1.792034
H	1.483489	6.256711	1.739585
H	0.123802	7.906090	0.458591
C	-0.687584	2.246292	0.252728
C	-1.903891	2.935055	0.163332
C	-0.138209	1.988287	1.513438

C	-2.551864	3.378653	1.316666
H	-2.339391	3.142394	-0.817734
C	-0.785639	2.430601	2.667562
H	0.798007	1.434998	1.600631
C	-1.989446	3.131431	2.571699
H	-3.496403	3.920579	1.235010
H	-2.495573	3.476309	3.475774
Cl	-7.905096	-2.019482	-1.732738
H	-2.248653	-0.091986	5.268271
O	-1.987438	-4.637565	0.573379
H	-2.054734	-5.409000	1.151257
H	-0.525398	-3.757346	1.776761
H	-0.352527	2.217146	3.645974

Int4

H = -2574.910628

G = -2575.034359

Esol = -2575.550727

Cartesian coordinates

Pd	-0.875324	-0.998182	0.708654
C	-3.509090	0.275693	0.235047
C	-4.848742	0.490092	-0.075236
C	-5.620958	-0.600452	-0.482941
C	-5.021470	-1.856484	-0.558640
C	-3.667764	-1.992026	-0.228067
N	-2.931438	-0.948434	0.161481
H	-6.673270	-0.474960	-0.743364
H	-5.265906	1.494369	0.003652
H	-3.168420	-2.959635	-0.282019
C	-5.820268	-3.085378	-0.947739

F	-6.853985	-2.755063	-1.726964
F	-5.051589	-3.961149	-1.606949
F	-6.298495	-3.695972	0.142599
C	-2.607670	1.353697	0.674400
O	-3.099170	2.561996	0.900591
N	-1.353376	1.154155	0.869757
C	-1.968725	3.433686	1.234496
H	-2.207522	3.895787	2.200834
C	-0.775351	2.399544	1.404349
H	-0.599417	2.236617	2.479833
H	-0.821795	-2.514640	0.697488
C	-1.785851	4.489116	0.178586
C	-1.009232	5.613293	0.489024
C	-2.300794	4.343104	-1.114108
C	-0.730850	6.567868	-0.488574
H	-0.606107	5.736630	1.497336
C	-2.028451	5.304521	-2.090858
H	-2.922369	3.480988	-1.361126
C	-1.237614	6.413585	-1.782766
H	-0.119823	7.437760	-0.238990
H	-2.438087	5.186739	-3.096450
H	-1.023122	7.163012	-2.547557
C	0.532055	2.796396	0.768669
C	1.592313	3.223904	1.576456
C	0.686904	2.804161	-0.624735
C	2.788336	3.665066	1.001988
H	1.482511	3.217740	2.664405
C	1.880917	3.239027	-1.198968
H	-0.133315	2.475472	-1.264441
C	2.933152	3.674131	-0.386652

H	3.608591	3.996991	1.641941
H	1.992924	3.238752	-2.285024
H	3.868485	4.011199	-0.837849
C	1.127092	-1.615753	2.925529
C	1.087669	-0.887862	1.605867
H	1.230301	0.194749	1.691355
C	1.383062	-1.453617	0.361049
C	1.744635	-0.550702	-0.806254
C	1.748513	-2.886317	0.160239
C	1.228317	-3.618806	-0.919994
C	2.737104	-3.469880	0.968674
C	1.662922	-4.918782	-1.170136
H	0.465101	-3.169749	-1.560091
C	3.180183	-4.769363	0.706574
H	3.170524	-2.893976	1.787515
C	2.643844	-5.497673	-0.356369
H	1.239836	-5.483144	-2.004075
H	3.956088	-5.210440	1.336153
H	2.991569	-6.513382	-0.557011
H	1.350675	0.458052	-0.640608
C	3.255146	-0.499679	-0.932062
C	4.001098	0.301642	-0.057205
C	3.933137	-1.286648	-1.871122
C	5.393274	0.331261	-0.122889
H	3.490860	0.918074	0.684992
C	5.325932	-1.268370	-1.950141
H	3.368005	-1.930250	-2.549101
C	6.050676	-0.456968	-1.072609
H	5.973193	0.958946	0.554895
H	5.853191	-1.878797	-2.684261

Cl	7.790234	-0.427205	-1.161386
H	1.306801	-0.945128	-1.734164
H	0.874075	-2.681280	2.784725
O	2.432825	-1.437725	3.445894
H	2.480399	-1.846237	4.320849
H	0.367335	-1.176143	3.599620

Int5

H = -2574.91915

G = -2575.04122

Esol = -2575.560174

Cartesian coordinates

Pd	-0.546842	-0.688404	0.394476
C	-3.562881	-0.645951	0.358934
C	-4.918014	-0.930422	0.215269
C	-5.281087	-2.183270	-0.286382
C	-4.275953	-3.089131	-0.621051
C	-2.934939	-2.715577	-0.455964
N	-2.587340	-1.522844	0.023175
H	-6.330805	-2.449733	-0.420543
H	-5.662808	-0.183607	0.492273
H	-2.127994	-3.398521	-0.728393
C	-4.608425	-4.480432	-1.122216
F	-5.797421	-4.499346	-1.730838
F	-3.679528	-4.907303	-1.987822
F	-4.648444	-5.347098	-0.102816
C	-3.057647	0.635278	0.876142
O	-3.874967	1.643067	1.123763
N	-1.799466	0.821915	1.067927
C	-3.042317	2.818234	1.420929

H	-3.373321	3.190063	2.398975
C	-1.587181	2.200242	1.540508
H	-1.307745	2.149295	2.604096
H	0.610351	-1.780422	-0.267765
C	-3.228020	3.873557	0.365121
C	-2.771857	5.170449	0.636625
C	-3.775003	3.583021	-0.889278
C	-2.843314	6.160215	-0.342968
H	-2.346308	5.406414	1.615393
C	-3.852160	4.577817	-1.867847
H	-4.151418	2.581548	-1.102872
C	-3.381348	5.864771	-1.599577
H	-2.481802	7.167109	-0.124209
H	-4.285530	4.345661	-2.843112
H	-3.440929	6.640792	-2.365579
C	-0.467559	2.875222	0.786931
C	0.575299	3.486541	1.489473
C	-0.419307	2.835391	-0.614656
C	1.661434	4.042192	0.807754
H	0.554171	3.509273	2.582071
C	0.658814	3.396112	-1.297726
H	-1.223673	2.358263	-1.175997
C	1.704425	3.997677	-0.586751
H	2.478629	4.499061	1.368779
H	0.687458	3.362180	-2.388913
H	2.552220	4.429775	-1.122771
C	1.671617	0.254687	2.162946
C	1.316796	0.024737	0.714419
H	1.413886	0.946761	0.132628
C	1.676533	-1.214493	-0.015990

C	2.202295	-0.975173	-1.462387
C	2.402583	-2.316007	0.727836
C	1.881789	-3.615041	0.784177
C	3.656929	-2.057920	1.304312
C	2.594258	-4.644666	1.403171
H	0.904794	-3.827474	0.339031
C	4.368121	-3.087710	1.922728
H	4.063821	-1.047617	1.276920
C	3.842484	-4.381976	1.972641
H	2.173549	-5.651815	1.440475
H	5.343438	-2.876036	2.366689
H	4.403504	-5.184195	2.456858
H	1.554102	-0.223012	-1.937800
C	3.639989	-0.519778	-1.476078
C	3.975713	0.817259	-1.217709
C	4.675346	-1.440911	-1.686323
C	5.307391	1.225198	-1.158290
H	3.191965	1.558805	-1.054083
C	6.012932	-1.049084	-1.634326
H	4.434938	-2.488283	-1.883240
C	6.322949	0.286179	-1.362871
H	5.565326	2.265290	-0.955260
H	6.814743	-1.769882	-1.798664
Cl	7.989451	0.788265	-1.283920
H	2.100464	-1.910420	-2.031323
H	1.710327	-0.702214	2.710979
O	2.918850	0.927507	2.175644
H	3.263603	0.932998	3.078385
H	0.886133	0.878226	2.628847

Int6

H = -2574.912037

G = -2575.034623

Esol = -2575.551985

Cartesian coordinates

Pd	-0.694443	0.903348	0.267456
C	-3.294712	-0.031381	-0.860282
C	-4.637346	-0.107483	-1.219865
C	-5.471754	0.969273	-0.909272
C	-4.929382	2.071687	-0.251181
C	-3.570955	2.067475	0.088167
N	-2.774489	1.039208	-0.214402
H	-6.531411	0.949051	-1.169374
H	-5.009037	-0.996093	-1.730553
H	-3.119707	2.904712	0.621532
C	-5.773542	3.290397	0.067414
F	-7.063278	2.961132	0.182517
F	-5.374010	3.859125	1.210687
F	-5.661686	4.201499	-0.907191
C	-2.333781	-1.111597	-1.140071
O	-2.765895	-2.224464	-1.718249
N	-1.090752	-1.024805	-0.829299
C	-1.660904	-3.184934	-1.669212
H	-1.539366	-3.581126	-2.684897
C	-0.432945	-2.262312	-1.282346
H	0.129517	-2.019209	-2.198527
H	-0.698924	2.207798	1.030221
C	-1.968289	-4.291809	-0.697807
C	-1.250977	-5.490750	-0.802793
C	-2.879440	-4.124366	0.351274

C	-1.425989	-6.501090	0.142596
H	-0.541065	-5.631604	-1.621699
C	-3.060148	-5.140135	1.293395
H	-3.460925	-3.204405	0.431241
C	-2.329333	-6.326326	1.195465
H	-0.859554	-7.430510	0.054577
H	-3.777794	-5.004887	2.105542
H	-2.470241	-7.119067	1.933213
C	0.526259	-2.838531	-0.272093
C	1.728469	-3.410448	-0.703753
C	0.215106	-2.845552	1.094586
C	2.611002	-3.983967	0.215546
H	1.984562	-3.399769	-1.766547
C	1.097387	-3.412646	2.014632
H	-0.723183	-2.408160	1.439316
C	2.297536	-3.984246	1.576717
H	3.548360	-4.422465	-0.132808
H	0.845352	-3.416634	3.077353
H	2.985780	-4.431209	2.297347
C	1.080238	1.256449	2.788499
H	2.082215	1.121860	3.250178
C	1.149491	0.616075	1.416185
H	1.229810	-0.476124	1.458171
C	1.519051	1.221921	0.214204
C	2.047041	0.367374	-0.935464
H	1.726704	0.799676	-1.894878
C	1.913638	2.664169	0.117321
C	3.013016	3.117669	0.865494
C	1.298389	3.540387	-0.787267
C	3.463332	4.434620	0.735460

H	3.538062	2.426462	1.528739
C	1.746725	4.856197	-0.914568
C	2.827448	5.307903	-0.150323
H	4.320287	4.773740	1.321314
H	1.250239	5.533491	-1.612868
H	3.177411	6.337372	-0.250886
H	0.452972	3.190041	-1.384312
O	0.652780	2.587762	2.852143
H	0.383513	0.667838	3.404918
H	1.299039	3.152733	2.403114
C	3.558942	0.310157	-0.865976
C	4.355161	1.192920	-1.606210
C	4.183425	-0.590097	0.009451
C	5.745072	1.179588	-1.485473
H	3.884306	1.910318	-2.282409
C	5.571607	-0.615632	0.142265
H	3.579905	-1.290572	0.591425
C	6.347899	0.274489	-0.607149
H	6.363988	1.866247	-2.064303
H	6.057869	-1.320524	0.817976
Cl	8.081514	0.252211	-0.445026
H	1.641899	-0.646261	-0.854417

Int7

H = -2574.918966

G = -2575.040831

Esol = -2575.559972

Cartesian coordinates

Pd	-0.125596	0.544217	-0.385072
C	-2.878871	1.654659	-0.862098

C	-4.007620	2.461194	-0.985888
C	-3.883100	3.821302	-0.692555
C	-2.640448	4.310520	-0.291145
C	-1.558137	3.426842	-0.189585
N	-1.676112	2.130388	-0.471321
H	-4.741420	4.491047	-0.768297
H	-4.955193	2.024145	-1.302111
H	-0.577579	3.781113	0.133750
C	-2.433980	5.784678	-0.007322
F	-3.562684	6.351374	0.427900
F	-1.483414	5.961426	0.920631
F	-2.047695	6.425973	-1.117033
C	-2.889620	0.209348	-1.131857
O	-3.996403	-0.374566	-1.553342
N	-1.841466	-0.520096	-0.964439
C	-3.738436	-1.817686	-1.605771
H	-3.972843	-2.138236	-2.628824
C	-2.173007	-1.903257	-1.351071
H	-1.664390	-2.108073	-2.306080
H	1.308791	1.420911	-0.072337
C	-4.606149	-2.541858	-0.614228
C	-4.807830	-3.917655	-0.784487
C	-5.143996	-1.899871	0.506631
C	-5.520531	-4.647151	0.166769
H	-4.394186	-4.425900	-1.659190
C	-5.865936	-2.629555	1.454021
H	-5.006812	-0.825727	0.640930
C	-6.049313	-4.004364	1.290193
H	-5.668142	-5.720246	0.028694
H	-6.287189	-2.120923	2.323877

H	-6.610986	-4.574494	2.033188
C	-1.739896	-2.934048	-0.343496
C	-1.194539	-4.145007	-0.786465
C	-1.913886	-2.716274	1.028531
C	-0.828484	-5.131333	0.132899
H	-1.052148	-4.318188	-1.856810
C	-1.544067	-3.697219	1.947007
H	-2.317624	-1.768246	1.384472
C	-1.003812	-4.907330	1.501311
H	-0.402168	-6.073097	-0.219304
H	-1.664935	-3.510187	3.015320
H	-0.713255	-5.674828	2.221974
C	1.313575	-1.764742	0.865834
H	2.303682	-2.224450	1.055613
C	1.448390	-0.749589	-0.249209
H	1.609337	-1.220431	-1.228013
C	2.158630	0.541595	-0.054866
C	3.034785	1.007215	-1.256956
H	3.175092	2.095269	-1.181523
C	2.781242	0.810206	1.303992
C	3.829954	-0.001780	1.768270
C	2.358723	1.885634	2.097433
C	4.431864	0.259096	3.001390
H	4.186224	-0.834556	1.162336
C	2.961382	2.148076	3.329593
C	4.000780	1.332946	3.785180
H	5.246054	-0.380853	3.347968
H	2.615657	2.988161	3.935572
H	4.472873	1.533240	4.749221
H	1.536589	2.519893	1.753454

O	0.744161	-1.248489	2.047351
H	0.661317	-2.574619	0.518734
H	1.419125	-0.740056	2.518071
C	4.379700	0.327625	-1.304139
C	5.511012	0.954388	-0.763371
C	4.521264	-0.965253	-1.829554
C	6.748173	0.311405	-0.730271
H	5.423449	1.960916	-0.347762
C	5.749337	-1.626117	-1.800450
H	3.662807	-1.469313	-2.280145
C	6.859930	-0.984164	-1.242569
H	7.624498	0.804770	-0.308172
H	5.856414	-2.629749	-2.213955
Cl	8.395225	-1.802676	-1.197189
H	2.468186	0.812833	-2.180555

Int8

H = -2574.917419

G = -2575.042066

Esol = -2575.557578

Cartesian coordinates

Pd	0.484225	-0.618746	-0.303999
C	1.582609	2.083487	0.269030
C	1.792600	3.458511	0.322641
C	0.860534	4.300842	-0.288702
C	-0.229867	3.728023	-0.940864
C	-0.372247	2.335883	-0.944070
N	0.502392	1.531801	-0.338422
H	0.981682	5.385116	-0.260642
H	2.674768	3.847510	0.832037

H	-1.221419	1.867444	-1.437958
C	-1.245784	4.577083	-1.678525
F	-0.892774	4.721049	-2.961785
F	-2.455179	3.999803	-1.648274
F	-1.339952	5.792210	-1.133736
C	2.531296	1.105900	0.824487
O	3.661875	1.506888	1.377565
N	2.308836	-0.156042	0.730137
C	4.337861	0.295901	1.881629
H	4.172986	0.298123	2.968581
C	3.489525	-0.871842	1.225837
H	3.184371	-1.573395	2.015318
H	-2.260070	-1.398767	0.712566
C	5.803020	0.321913	1.579159
C	6.697547	-0.208285	2.516398
C	6.284768	0.783284	0.347078
C	8.060086	-0.292296	2.220447
H	6.328659	-0.559133	3.484123
C	7.646463	0.708870	0.056443
H	5.594062	1.204450	-0.384795
C	8.535465	0.164916	0.989361
H	8.751705	-0.707637	2.956384
H	8.017100	1.073754	-0.903820
H	9.601076	0.104331	0.757958
C	4.180654	-1.647960	0.126372
C	4.986530	-2.740516	0.470765
C	4.089595	-1.261854	-1.217113
C	5.702132	-3.428341	-0.509758
H	5.064236	-3.049643	1.516200
C	4.798214	-1.955895	-2.200961

H	3.465369	-0.412501	-1.501732
C	5.609383	-3.037157	-1.848787
H	6.331973	-4.274935	-0.228502
H	4.720060	-1.647444	-3.245880
H	6.167142	-3.577168	-2.616872
C	-6.717534	0.340516	2.055914
C	-6.801952	0.254256	0.663573
C	-5.631442	0.269056	-0.094886
C	-4.374258	0.372276	0.514873
C	-4.315475	0.462865	1.912487
C	-5.475158	0.448275	2.687885
H	-7.778362	0.173327	0.184352
H	-5.700366	0.186049	-1.181937
H	-3.344691	0.545890	2.410351
H	-5.425780	0.522312	3.775030
C	-0.522457	-2.541131	-1.079643
H	0.591842	-2.300448	-0.574946
H	-0.145282	-2.917904	-2.047329
C	-1.259107	-1.263513	-1.168441
C	-2.520541	-1.136179	-0.325050
C	-3.104767	0.295271	-0.295240
H	-2.353276	0.965865	0.146927
O	-0.986106	-3.534155	-0.242028
H	-1.951903	-3.605985	-0.348651
C	-3.567532	-2.148169	-0.783106
C	-3.934034	-2.252756	-2.134481
C	-4.225821	-2.953621	0.159119
C	-4.935837	-3.139640	-2.532735
H	-3.444324	-1.628315	-2.885667
C	-5.228143	-3.842856	-0.238600

H	-3.965377	-2.865064	1.216833
C	-5.585414	-3.937368	-1.585317
H	-5.212985	-3.207710	-3.587093
H	-5.734979	-4.457265	0.508547
H	-3.293000	0.636476	-1.326850
Cl	-8.172814	0.316493	3.013545
H	-6.369414	-4.630422	-1.897679
H	-1.321384	-0.831214	-2.176616

Int9

H = -2574.917915

G = -2575.043644

Esol = -2575.557541

Cartesian coordinates

Pd	0.449537	-0.547257	-0.578423
C	1.600911	2.118973	0.264660
C	1.877892	3.461864	0.511555
C	1.016119	4.424712	-0.019550
C	-0.078706	4.001398	-0.772086
C	-0.282515	2.629679	-0.967786
N	0.536039	1.710428	-0.463271
H	1.188297	5.488052	0.156172
H	2.747457	3.734456	1.110408
H	-1.143729	2.277314	-1.537369
C	-1.025213	4.996890	-1.411324
F	-0.600636	5.327372	-2.637175
F	-2.254145	4.473689	-1.530411
F	-1.107826	6.114332	-0.685101
C	2.436986	1.022970	0.777977
O	3.546017	1.277291	1.445450

N	2.126369	-0.211813	0.572237
C	4.056293	-0.020941	1.929257
H	3.747998	-0.080423	2.983361
C	3.214849	-1.057502	1.082314
H	2.798371	-1.816260	1.758724
H	-2.205402	-1.478930	0.224336
C	5.545800	-0.100826	1.818905
C	6.261421	-0.780194	2.811997
C	6.223350	0.410886	0.704451
C	7.640545	-0.962504	2.685901
H	5.739253	-1.171060	3.689657
C	7.601672	0.237805	0.584763
H	5.672142	0.946967	-0.069130
C	8.311516	-0.454926	1.571098
H	8.192106	-1.494261	3.464006
H	8.125606	0.641958	-0.283987
H	9.390489	-0.592518	1.472901
C	3.969095	-1.750287	-0.030202
C	4.671668	-2.925757	0.262737
C	4.048741	-1.208414	-1.319022
C	5.455179	-3.542894	-0.712832
H	4.616082	-3.355814	1.265956
C	4.825733	-1.830355	-2.299065
H	3.502254	-0.296088	-1.565508
C	5.534320	-2.995596	-1.996747
H	6.003503	-4.455855	-0.471267
H	4.880004	-1.401323	-3.302067
H	6.144909	-3.479891	-2.761794
C	-6.178315	-0.300337	2.868131
C	-6.554679	-0.075644	1.541069

C	-5.571678	0.181554	0.585406
C	-4.214820	0.221841	0.933984
C	-3.862606	-0.003358	2.272237
C	-4.831612	-0.263134	3.241758
H	-7.609437	-0.105288	1.265026
H	-5.868119	0.343993	-0.453381
H	-2.809372	0.025526	2.567318
H	-4.554375	-0.433242	4.282925
C	-0.895483	-1.765794	-2.348518
H	0.604127	-2.057197	-0.479980
H	-0.185793	-1.579967	-3.161225
C	-1.459332	-0.712097	-1.630693
C	-2.606026	-0.937295	-0.648024
C	-3.147998	0.411266	-0.112542
H	-2.302182	0.973982	0.314748
O	-1.209758	-3.038344	-2.235082
H	-2.012072	-3.152984	-1.686498
C	-3.716387	-1.801581	-1.228666
C	-4.267958	-1.521929	-2.489312
C	-4.238799	-2.869413	-0.484144
C	-5.318782	-2.290091	-2.990974
H	-3.874685	-0.693392	-3.084374
C	-5.290520	-3.642662	-0.986846
H	-3.834429	-3.081125	0.509257
C	-5.832657	-3.353528	-2.240092
H	-5.739911	-2.060642	-3.972336
H	-5.689767	-4.467304	-0.392558
H	-3.541562	0.999684	-0.957740
Cl	-7.397439	-0.626885	4.069315
H	-6.654618	-3.954858	-2.634235

H	-1.420876	0.250267	-2.152364
---	-----------	----------	-----------

IntS10

H = -2574.488239

G = -2574.613795

Esol = -2575.117015

Cartesian coordinates

Pd	0.535981	-0.903449	-0.419346
C	1.328627	2.064219	0.283610
C	1.266394	3.400553	0.693381
C	0.156833	4.155762	0.320951
C	-0.834042	3.549307	-0.458552
C	-0.668179	2.215780	-0.851025
N	0.380294	1.483455	-0.480443
H	0.058091	5.198312	0.627405
H	2.069527	3.818505	1.300789
C	-2.090785	4.297216	-0.823638
F	-2.640417	3.829140	-1.951899
F	-3.016880	4.181476	0.150982
F	-1.854838	5.608303	-0.987134
C	2.416756	1.164772	0.679469
O	3.526232	1.667326	1.247912
N	2.348439	-0.103168	0.502631
C	4.326686	0.524022	1.663859
H	4.173543	0.411527	2.748577
C	3.625092	-0.684987	0.915135
H	3.437676	-1.495578	1.633594
H	-2.238107	-1.121263	0.574269
C	5.780728	0.742438	1.372547
C	6.742707	0.250998	2.262058

C	6.194745	1.348165	0.178997
C	8.103014	0.345653	1.957546
H	6.425142	-0.215273	3.198955
C	7.552249	1.448940	-0.122718
H	5.447595	1.734475	-0.515273
C	8.509882	0.942756	0.762467
H	8.845684	-0.043815	2.657702
H	7.865932	1.919454	-1.057360
H	9.572810	1.018395	0.521649
C	4.400331	-1.247936	-0.258326
C	5.452172	-2.140797	-0.014905
C	4.134697	-0.849438	-1.573314
C	6.243411	-2.608632	-1.063823
H	5.662494	-2.462587	1.008105
C	4.921334	-1.324492	-2.626342
H	3.298803	-0.178012	-1.774859
C	5.981220	-2.198226	-2.374664
H	7.065460	-3.298292	-0.858534
H	4.700564	-1.011029	-3.649470
H	6.597670	-2.566263	-3.198242
C	-6.613872	1.057412	0.515431
C	-6.781501	-0.161481	-0.145572
C	-5.679845	-0.767729	-0.751610
C	-4.408628	-0.177623	-0.708433
C	-4.270977	1.041981	-0.029638
C	-5.359656	1.668940	0.576504
H	-7.767238	-0.627366	-0.181753
H	-5.809306	-1.724986	-1.261580
H	-3.291221	1.518235	0.031883
H	-5.239330	2.626408	1.084455

C	-0.106132	-2.893408	-0.242229
H	0.589233	-3.527138	-0.803364
C	-1.081455	-2.130440	-0.937819
C	-2.420081	-1.743099	-0.317824
C	-3.207478	-0.852689	-1.313773
H	-2.505751	-0.097962	-1.700591
O	-0.276583	-3.398213	1.032663
H	-1.082714	-3.025993	1.414888
C	-3.270532	-2.921567	0.135688
C	-3.347329	-4.099282	-0.622573
C	-4.039941	-2.829569	1.304751
C	-4.175814	-5.150884	-0.227863
H	-2.739602	-4.192943	-1.525377
C	-4.867832	-3.881671	1.706665
H	-3.997643	-1.913525	1.900146
C	-4.940521	-5.045993	0.939001
H	-4.220688	-6.062033	-0.829976
H	-5.459413	-3.788734	2.620872
H	-3.509614	-1.474371	-2.171676
Cl	-7.990767	1.829188	1.272449
H	-5.585381	-5.871465	1.250130
H	-1.090648	-2.248783	-2.029117
H	-1.408432	1.725558	-1.485947

IntS11

H = -1571.19679

G = -1571.284322

Esol = -1571.548611

Cartesian coordinates

O	1.167504	-3.591777	0.742461
---	----------	-----------	----------

O	-0.156303	-3.638467	0.377645
Pd	0.609389	-1.875299	-0.089813
C	1.502246	0.906877	-0.749626
C	2.258807	2.071005	-0.887941
C	3.598993	2.037032	-0.508400
C	4.123902	0.842237	-0.004011
C	3.298562	-0.280878	0.102485
N	2.012946	-0.249607	-0.262200
H	4.232106	2.920280	-0.606133
H	1.793621	2.972666	-1.287203
H	3.673986	-1.231261	0.486071
C	5.558869	0.782065	0.462454
F	6.016394	-0.474998	0.500224
F	6.358596	1.492755	-0.349595
F	5.684489	1.299399	1.695792
C	0.086925	0.803941	-1.102715
O	-0.597378	1.862579	-1.551037
N	-0.541115	-0.307569	-0.967547
C	-2.003348	1.467379	-1.542113
H	-2.431969	1.772553	-2.504876
C	-1.915121	-0.110447	-1.440124
H	-1.974643	-0.537675	-2.455476
C	-2.729954	2.130280	-0.401188
C	-4.124023	2.251405	-0.467040
C	-2.061617	2.539264	0.758498
C	-4.842212	2.753914	0.617758
H	-4.654162	1.930771	-1.366938
C	-2.780041	3.048558	1.842758
H	-0.975035	2.464035	0.818268
C	-4.171354	3.151305	1.777994

H	-5.929829	2.834415	0.557761
H	-2.248707	3.363443	2.743800
H	-4.732687	3.543899	2.628859
C	-2.969532	-0.760394	-0.583774
C	-4.173831	-1.165764	-1.170975
C	-2.795826	-0.903549	0.797430
C	-5.202828	-1.690201	-0.386367
H	-4.307527	-1.072570	-2.252696
C	-3.820427	-1.434785	1.581116
H	-1.851374	-0.611567	1.258124
C	-5.027805	-1.822428	0.993509
H	-6.138035	-2.005984	-0.854550
H	-3.670927	-1.553095	2.656428
H	-5.827723	-2.239901	1.609459

IntS12

H = -2438.845362

G = -2438.954338

Esol = -2439.324509

Cartesian coordinates

C	0.871288	1.398245	0.500783
C	1.491173	2.596812	0.164723
C	2.840003	2.756961	0.481535
C	3.503119	1.717547	1.133006
C	2.798245	0.557624	1.473174
N	1.511046	0.401940	1.166891
H	3.376188	3.664815	0.205932
H	0.933528	3.357929	-0.380457
H	3.284058	-0.274798	1.985735
C	-0.484798	1.031016	0.085371

N	-0.925843	-0.149196	0.331039
C	-2.368732	1.022484	-1.125859
C	-2.249078	-0.304567	-0.267251
Pd	0.514486	-1.469360	1.012627
O	0.318976	-3.408594	0.567024
B	0.303016	-3.429091	-1.315717
O	-1.076195	-3.219545	-1.504106
H	-1.539378	-4.063058	-1.427258
O	0.757715	-4.717434	-1.597737
H	1.712279	-4.803042	-1.506337
C	1.188514	-2.138014	-1.711572
C	2.549039	-1.983447	-1.375528
C	0.585385	-1.074845	-2.409702
C	3.254807	-0.809169	-1.651490
H	3.059928	-2.780230	-0.831554
C	1.264583	0.110421	-2.699780
H	-0.458431	-1.181936	-2.713263
C	2.596640	0.239006	-2.297856
H	4.297843	-0.691600	-1.353282
H	0.776676	0.930983	-3.229508
O	-1.257014	1.846603	-0.627557
H	-2.122870	0.794368	-2.172926
H	-2.215959	-1.183583	-0.929625
C	-3.668243	1.761413	-1.046445
C	-3.994296	2.536373	0.074230
C	-4.610690	1.599013	-2.067945
C	-5.250662	3.132745	0.172699
H	-3.262303	2.666378	0.872357
C	-5.872706	2.189662	-1.966046
H	-4.357818	1.000376	-2.947348

C	-6.195109	2.955898	-0.843958
H	-5.498027	3.733561	1.050772
H	-6.602744	2.054409	-2.767272
H	-7.180888	3.419535	-0.762046
C	-3.332056	-0.506087	0.769097
C	-4.573038	-1.012636	0.361484
C	-3.147633	-0.148301	2.108865
C	-5.621749	-1.134707	1.272515
H	-4.720868	-1.303759	-0.681267
C	-4.194464	-0.279852	3.025372
H	-2.176653	0.224452	2.439144
C	-5.435521	-0.765430	2.608475
H	-6.586850	-1.524462	0.940730
H	-4.036974	-0.003487	4.070580
H	-6.254854	-0.865135	3.324205
C	4.987484	1.778571	1.396738
F	5.295286	1.233662	2.583335
F	5.438284	3.040814	1.388994
F	5.667302	1.099273	0.457019
Cl	3.458463	1.735994	-2.622869
O	1.544707	-3.181149	1.170098

IntS13

H = -2438.864034

G = -2438.97728

Esol = -2439.343417

Cartesian coordinates

C	0.147491	-2.214580	-0.370079
C	0.135651	-3.604628	-0.449338
C	-1.065699	-4.278190	-0.229758

C	-2.209599	-3.530559	0.052999
C	-2.126621	-2.135456	0.102184
N	-0.974739	-1.489508	-0.096622
H	-1.117348	-5.366454	-0.288091
H	1.060148	-4.132149	-0.685611
H	-3.005267	-1.517408	0.293825
C	1.348456	-1.398940	-0.592341
N	1.283389	-0.133027	-0.429867
C	3.358208	-0.758856	-1.343393
C	2.581751	0.464463	-0.706893
Pd	-0.690517	0.578872	-0.188058
O	-0.063242	2.475632	-0.523880
B	-0.633882	3.753995	-0.282376
O	-0.393876	4.674358	-1.225344
H	0.108775	4.122080	-1.890131
O	-1.347450	3.958739	0.852933
H	-1.562191	3.133152	1.305701
C	-2.589569	1.136101	-0.027436
C	-3.396306	0.817998	1.076888
C	-3.150412	1.890859	-1.071797
C	-4.737426	1.219635	1.133241
H	-2.985771	0.257094	1.922327
C	-4.488055	2.290872	-1.031616
H	-2.532057	2.182935	-1.925433
C	-5.275223	1.948134	0.071519
H	-5.360922	0.975673	1.995187
H	-4.920755	2.875542	-1.845081
O	2.509428	-1.917838	-0.989322
H	3.311810	-0.684972	-2.439976
H	2.397056	1.274457	-1.433722

C	4.770801	-0.967391	-0.893957
C	5.061273	-1.553134	0.345001
C	5.816777	-0.478115	-1.684724
C	6.380743	-1.641470	0.787198
H	4.249289	-1.935322	0.964656
C	7.138022	-0.558475	-1.238172
H	5.595544	-0.024033	-2.654460
C	7.421871	-1.139219	-0.000202
H	6.598294	-2.097921	1.755487
H	7.946857	-0.170094	-1.861199
H	8.454329	-1.203907	0.350882
C	3.210342	1.054721	0.535845
C	4.219233	2.015008	0.389487
C	2.853950	0.632074	1.821409
C	4.878246	2.526437	1.507231
H	4.490264	2.361591	-0.610417
C	3.506000	1.150358	2.943273
H	2.054384	-0.100127	1.948997
C	4.524477	2.093319	2.788798
H	5.665521	3.272803	1.378815
H	3.214463	0.817418	3.942281
H	5.035659	2.498157	3.665318
C	-3.526349	-4.211991	0.347270
F	-3.632894	-4.497434	1.655099
F	-3.632390	-5.367047	-0.326167
F	-4.564454	-3.435921	0.015318
Cl	-6.951820	2.447249	0.128335
O	0.544507	2.422569	-1.864034

H = -1536.946511

G = -1537.036441

Esol = -1537.358058

Cartesian coordinates

Pd	-0.642879	1.757078	-0.089159
C	-1.618341	-0.910974	-0.717661
C	-2.441309	-2.024944	-0.840014
C	-3.784045	-1.910175	-0.472156
C	-4.243530	-0.684999	0.007113
C	-3.357914	0.394026	0.107235
N	-2.072130	0.284784	-0.246051
H	-4.464338	-2.758605	-0.563136
H	-2.025826	-2.957867	-1.222500
H	-3.690547	1.364375	0.473463
C	-5.679247	-0.515183	0.467793
F	-6.091382	0.744362	0.286775
F	-6.493008	-1.332551	-0.205890
F	-5.785524	-0.802479	1.770534
C	-0.195760	-0.916539	-1.090309
O	0.414685	-2.030920	-1.464599
N	0.497695	0.162852	-1.040518
C	1.853252	-1.722596	-1.507905
H	2.229036	-2.110114	-2.462417
C	1.854598	-0.139836	-1.506794
H	1.935578	0.218265	-2.546273
C	2.564235	-2.361133	-0.346428
C	3.955890	-2.509894	-0.419830
C	1.893836	-2.722518	0.828023
C	4.670726	-2.994633	0.675256
H	4.486486	-2.235584	-1.335176

C	2.610449	-3.214443	1.922200
H	0.807799	-2.636598	0.889655
C	3.999177	-3.344877	1.850740
H	5.755025	-3.105699	0.609291
H	2.079816	-3.501877	2.832492
H	4.557934	-3.729575	2.706493
C	2.913308	0.549604	-0.682338
C	4.035385	1.106406	-1.307548
C	2.790045	0.642611	0.714423
C	5.025239	1.742698	-0.552858
H	4.135175	1.047992	-2.394513
C	3.774742	1.287721	1.467701
H	1.930628	0.194038	1.215563
C	4.895594	1.837194	0.835001
H	5.895966	2.172460	-1.052408
H	3.672833	1.349172	2.553406
H	5.667240	2.336515	1.424716
O	0.949207	3.128688	0.064656
H	-1.591230	2.730779	0.617178
H	1.769020	2.609462	0.165886
C	0.973981	4.264798	0.945898
H	0.929231	3.950310	1.999679
H	1.890649	4.843528	0.760406
H	0.099195	4.879948	0.707040

IntS15

H = -1535.740185

G = -1535.829328

Esol = -1536.129789

Cartesian coordinates

Pd	-0.974701	1.872695	-0.362390
C	-1.549367	-0.999504	-0.404228
C	-2.176316	-2.237648	-0.322474
C	-3.535158	-2.269993	0.002010
C	-4.203755	-1.065622	0.224802
C	-3.500585	0.140882	0.127407
N	-2.201952	0.171040	-0.180144
H	-4.067377	-3.219216	0.085671
H	-1.604920	-3.148133	-0.507559
H	-3.997582	1.096487	0.308096
C	-5.691188	-1.046445	0.529632
F	-6.043956	-2.131904	1.222194
F	-6.015216	0.040101	1.239276
F	-6.395382	-1.027487	-0.606472
C	-0.134761	-0.800937	-0.727127
O	0.698355	-1.794171	-0.919718
N	0.337657	0.401938	-0.808334
C	1.985351	-1.192401	-1.351509
H	2.001008	-1.308843	-2.444358
C	1.792199	0.340332	-0.995205
H	2.073626	0.941399	-1.870963
C	3.150292	-1.890031	-0.731360
C	4.304856	-2.087431	-1.499018
C	3.139750	-2.269135	0.618149
C	5.446510	-2.645695	-0.919660
H	4.313837	-1.804113	-2.555053
C	4.276197	-2.836861	1.191620
H	2.242053	-2.122593	1.220169
C	5.433059	-3.019353	0.426110
H	6.343842	-2.797141	-1.523029

H	4.262467	-3.135732	2.241764
H	6.323408	-3.460397	0.879349
C	2.553971	0.835398	0.212426
C	3.875690	1.266557	0.036909
C	2.003624	0.815391	1.499132
C	4.640655	1.660615	1.134480
H	4.313806	1.283982	-0.964259
C	2.765806	1.220973	2.597456
H	0.974917	0.485469	1.655833
C	4.085873	1.639704	2.417971
H	5.671488	1.989531	0.987885
H	2.325945	1.208749	3.596854
H	4.682060	1.954411	3.276992
O	-0.038523	3.500016	-0.441210
C	1.101116	3.839824	-1.160167
H	2.013736	3.386070	-0.729576
H	1.023416	3.592881	-2.237026
H	1.220005	4.937485	-1.083192

IntS16

H = -2403.427382

G = -2403.535558

Esol = -2403.945524

Cartesian coordinates

C	-1.621663	-2.206120	0.011538
C	-2.264152	-3.180335	0.764561
C	-3.572695	-2.929551	1.190618
C	-4.176589	-1.718466	0.851684
C	-3.464090	-0.779293	0.096336
N	-2.221013	-1.031399	-0.315829

H	-4.114219	-3.663910	1.789438
H	-1.743167	-4.106077	1.012152
H	-3.884760	0.193078	-0.168165
C	-0.244461	-2.276265	-0.484132
N	0.215320	-1.295279	-1.193326
C	1.834878	-2.993576	-0.924684
C	1.659353	-1.490201	-1.387527
Pd	-1.058520	0.263993	-1.385363
O	-0.140891	1.723612	-2.412954
B	-0.996859	2.874230	-1.753393
O	-2.221847	1.939551	-1.451771
H	-2.780178	1.984697	-2.246709
O	-1.311868	3.799166	-2.746680
H	-1.334828	4.708429	-2.428370
C	-0.326589	3.341745	-0.379713
C	0.800612	4.183269	-0.392469
C	-0.751158	2.860635	0.871778
C	1.505629	4.495633	0.771648
H	1.155916	4.601434	-1.338740
C	-0.068580	3.162250	2.051121
H	-1.645867	2.236002	0.932243
C	1.074199	3.962888	1.987437
H	2.390730	5.132644	0.741639
H	-0.406920	2.778721	3.015178
O	0.570559	-3.258920	-0.191196
H	1.796097	-3.650259	-1.805227
H	1.897596	-1.424946	-2.458204
C	3.029338	-3.309345	-0.085395
C	3.083895	-2.953850	1.269285
C	4.145469	-3.896056	-0.694362

C	4.246480	-3.181747	2.003853
H	2.216325	-2.501420	1.751257
C	5.313733	-4.112481	0.039996
H	4.103610	-4.186123	-1.747781
C	5.365047	-3.754503	1.389059
H	4.283081	-2.907987	3.060290
H	6.180994	-4.569878	-0.440501
H	6.276016	-3.927811	1.965921
C	2.472804	-0.461600	-0.633903
C	3.761565	-0.159042	-1.091541
C	1.989208	0.168023	0.519999
C	4.557194	0.758046	-0.404077
H	4.147310	-0.645194	-1.991291
C	2.783433	1.088756	1.206942
H	0.983796	-0.040750	0.889294
C	4.067252	1.385957	0.745550
H	5.560626	0.986761	-0.769222
H	2.399585	1.581500	2.099945
H	4.681958	2.111813	1.281928
C	-5.608541	-1.414482	1.255726
F	-5.935040	-2.069794	2.371670
F	-6.450854	-1.788401	0.287116
F	-5.769835	-0.103218	1.463742
Cl	2.001736	4.256199	3.438440
C	1.239240	1.896083	-2.693628
H	1.829920	2.017132	-1.774476
H	1.599951	1.024665	-3.257073
H	1.342039	2.791207	-3.325427

H = -2403.465162

G = -2403.577704

Esol = -2403.983414

Cartesian coordinates

C	0.071013	2.364880	-0.490002
C	0.232727	3.731051	-0.288849
C	1.515831	4.223942	-0.036768
C	2.580512	3.326266	-0.001080
C	2.342948	1.962800	-0.208771
N	1.113678	1.491283	-0.436445
H	1.686332	5.290550	0.118285
H	-0.637827	4.385924	-0.337285
H	3.155383	1.236862	-0.188180
C	-1.226732	1.744232	-0.794604
N	-1.298720	0.505088	-1.130228
C	-3.446211	1.536240	-1.081493
C	-2.714407	0.136197	-1.242034
Pd	0.588161	-0.484628	-0.743376
O	-0.068774	-2.463503	-1.124012
B	-0.378792	-3.315130	-0.039037
O	0.299808	-3.206375	1.120143
O	-1.361643	-4.214085	-0.253639
H	-1.540902	-4.772612	0.513077
C	2.347038	-1.218104	-0.200379
C	2.845454	-0.996056	1.094211
C	3.086238	-2.012065	-1.089063
C	4.065321	-1.555103	1.495776
H	2.290365	-0.384444	1.811436
C	4.310437	-2.562298	-0.700668
H	2.715577	-2.211914	-2.097223

C	4.794474	-2.332439	0.592344
H	4.450376	-1.388663	2.503020
H	4.891207	-3.173262	-1.393552
O	-2.346433	2.436596	-0.691473
H	-3.782097	1.886222	-2.067469
H	-2.908219	-0.243218	-2.255581
C	-4.572558	1.598564	-0.096498
C	-4.336820	1.753079	1.275376
C	-5.882508	1.418331	-0.556954
C	-5.401687	1.723889	2.176040
H	-3.319957	1.907713	1.639472
C	-6.946710	1.377989	0.346309
H	-6.074492	1.310412	-1.628022
C	-6.707135	1.529946	1.714212
H	-5.212867	1.852329	3.243975
H	-7.965706	1.237788	-0.020301
H	-7.539140	1.505399	2.421182
C	-3.089246	-0.939175	-0.246094
C	-4.089967	-1.861357	-0.574295
C	-2.481026	-1.011410	1.014170
C	-4.482699	-2.836772	0.343579
H	-4.570710	-1.814763	-1.555058
C	-2.865579	-1.991800	1.930264
H	-1.697784	-0.301790	1.287254
C	-3.869959	-2.904363	1.597510
H	-5.266120	-3.548979	0.076380
H	-2.375789	-2.044218	2.904493
H	-4.176498	-3.667620	2.316403
C	3.992068	3.787394	0.308398
F	4.887330	3.059024	-0.367975

F	4.249206	3.647163	1.614978
F	4.156025	5.073262	-0.012762
Cl	6.313983	-3.023273	1.079302
H	1.091334	-2.645746	1.078694
C	-0.689838	-2.704671	-2.400566
H	-1.757029	-2.449392	-2.353695
H	-0.175989	-2.082934	-3.143557
H	-0.585882	-3.765303	-2.661459

IntS18

H = -1497.699082

G = -1497.78462

Esol = -1498.080527

Cartesian coordinates

Pd	-0.646203	1.872356	0.070337
C	-1.568660	-0.770615	-0.703252
C	-2.367243	-1.895455	-0.875593
C	-3.709598	-1.829367	-0.494299
C	-4.194035	-0.639021	0.044514
C	-3.329138	0.449592	0.204437
N	-2.043995	0.386832	-0.162244
H	-4.367744	-2.692209	-0.609548
H	-1.932719	-2.799938	-1.302693
H	-3.674884	1.384547	0.643238
C	-5.655136	-0.492902	0.427841
F	-6.165241	-1.669002	0.803884
F	-5.797736	0.376599	1.434595
F	-6.365723	-0.043465	-0.612134
C	-0.148912	-0.723608	-1.083135
O	0.484442	-1.799694	-1.523385

N	0.519404	0.367389	-0.974661
C	1.915766	-1.455260	-1.555698
H	2.294367	-1.778666	-2.532659
C	1.880276	0.124589	-1.463522
H	1.946971	0.543851	-2.480913
C	2.648094	-2.142211	-0.436035
C	4.041605	-2.260133	-0.527421
C	1.994357	-2.579034	0.722123
C	4.774414	-2.789494	0.534694
H	4.559388	-1.927009	-1.430484
C	2.728976	-3.115540	1.782809
H	0.907437	-2.517522	0.796371
C	4.119289	-3.215394	1.694302
H	5.859997	-2.876180	0.454883
H	2.211411	-3.461881	2.680019
H	4.692158	-3.635056	2.523885
C	2.927898	0.788661	-0.605242
C	4.041918	1.390268	-1.200891
C	2.803572	0.809879	0.794365
C	5.023429	2.001877	-0.415088
H	4.142634	1.387494	-2.289353
C	3.778867	1.431600	1.579476
H	1.953676	0.319201	1.272192
C	4.892364	2.027350	0.975199
H	5.888287	2.467232	-0.892431
H	3.678034	1.435459	2.667169
H	5.657014	2.507548	1.589359
O	0.898472	3.294245	0.306050
H	-1.607687	2.787247	0.837795
H	0.755902	3.975297	0.979996

H	1.739602	2.844360	0.520086
---	----------	----------	----------

IntS19

H = -1496.489491

G = -1496.573935

Esol = -1496.849652

Cartesian coordinates

Pd	0.605024	-1.885016	-0.021697
C	1.600720	0.791525	-0.659216
C	2.392051	1.924250	-0.806002
C	3.732419	1.848390	-0.415348
C	4.217225	0.647175	0.101675
C	3.352286	-0.447286	0.229214
N	2.073878	-0.375141	-0.144623
H	4.390676	2.714251	-0.506546
H	1.961645	2.838417	-1.217083
H	3.701827	-1.393172	0.648894
C	5.677531	0.499659	0.492641
F	6.167250	1.661586	0.930600
F	5.817914	-0.416976	1.456403
F	6.400180	0.110374	-0.561939
C	0.184866	0.705678	-1.025082
O	-0.501446	1.709597	-1.513715
N	-0.442543	-0.412071	-0.855216
C	-1.920004	1.282448	-1.559846
H	-2.269906	1.499146	-2.576059
C	-1.826059	-0.287664	-1.338991
H	-1.878104	-0.794470	-2.315134
C	-2.720647	2.036978	-0.538545
C	-4.111010	2.098214	-0.702979

C	-2.134176	2.596791	0.602721
C	-4.907804	2.694146	0.274083
H	-4.575904	1.666706	-1.592917
C	-2.933025	3.201843	1.575718
H	-1.050868	2.576081	0.733559
C	-4.320169	3.244975	1.417048
H	-5.990695	2.734222	0.140436
H	-2.469183	3.643967	2.459989
H	-4.943675	3.716315	2.179592
C	-2.846310	-0.900431	-0.418354
C	-3.927558	-1.602728	-0.962693
C	-2.746396	-0.756126	0.973537
C	-4.905852	-2.148767	-0.127922
H	-4.003464	-1.731503	-2.045512
C	-3.718460	-1.309782	1.807404
H	-1.913336	-0.201906	1.409111
C	-4.801980	-2.003700	1.257562
H	-5.744868	-2.697029	-0.561024
H	-3.634126	-1.194649	2.889976
H	-5.563089	-2.434753	1.911288
O	-0.655615	-3.281523	0.073346
H	-1.504865	-3.033396	0.475989

IntS1

H = -2574.926179

G = -2575.045477

Esol = -2575.568575

Cartesian coordinates

Pd	-0.668705	-0.984555	0.262715
C	-0.872667	2.068469	0.568366

C	-1.268442	3.387016	0.783660
C	-2.593400	3.735753	0.506255
C	-3.451628	2.752811	0.021494
C	-2.964042	1.451276	-0.170044
N	-1.707773	1.113271	0.100551
H	-2.951156	4.754425	0.662112
H	-0.548572	4.114726	1.159046
H	-3.615403	0.670970	-0.558744
C	-4.904152	3.037007	-0.299826
F	-5.707313	2.290812	0.472207
F	-5.206883	4.322693	-0.099627
F	-5.172261	2.733768	-1.576501
C	0.506234	1.615708	0.797969
O	1.449047	2.498413	1.081965
N	0.860475	0.381520	0.670867
C	2.664346	1.717030	1.370152
H	2.675300	1.576690	2.462402
C	2.331618	0.343400	0.681851
H	2.690228	-0.482034	1.309440
C	-4.401659	-1.544297	-0.883047
C	-4.266521	-1.860277	0.477351
C	-3.103390	-2.477268	0.921930
C	-2.049402	-2.803961	0.029508
C	-2.216261	-2.456220	-1.335002
C	-3.380360	-1.829104	-1.790786
H	-5.076993	-1.627765	1.169072
H	-3.019643	-2.756700	1.972627
H	-1.460524	-2.752276	-2.063821
H	-3.503959	-1.583345	-2.845993
C	-0.544930	-2.183853	3.251000

H	-1.295820	-2.997015	3.296307
H	-1.064409	-1.282357	2.863081
C	0.602217	-2.567462	2.323504
H	1.391223	-1.819066	2.486054
H	1.013734	-3.523093	2.696195
C	0.322176	-2.702750	0.830077
C	-0.846038	-3.642716	0.475501
H	-1.127157	-4.263522	1.338345
O	0.033912	-1.948163	4.512449
H	-0.664248	-1.817905	5.166049
C	3.896650	2.434269	0.921119
C	5.068551	2.302983	1.675834
C	3.923269	3.154572	-0.280556
C	6.262908	2.870738	1.225667
H	5.049663	1.752446	2.620538
C	5.113273	3.730550	-0.722915
H	3.012612	3.258815	-0.871348
C	6.286386	3.583872	0.024823
H	7.173529	2.763756	1.818867
H	5.127960	4.292897	-1.658928
H	7.218157	4.032781	-0.326126
C	2.899106	0.197740	-0.715286
C	4.241840	-0.172823	-0.854072
C	2.159484	0.520685	-1.859150
C	4.842780	-0.200463	-2.111492
H	4.827200	-0.427533	0.031297
C	2.756933	0.481247	-3.121359
H	1.108250	0.799206	-1.773000
C	4.101719	0.127152	-3.250073
H	5.893699	-0.482582	-2.203330

H	2.169353	0.732867	-4.007164
H	4.571439	0.104590	-4.235830
Cl	-5.845503	-0.750783	-1.434126
H	-0.563751	-4.325664	-0.335577
C	1.558533	-2.910893	0.001013
C	1.501278	-2.871622	-1.406553
C	2.805189	-3.199457	0.589146
C	2.625191	-3.114937	-2.190429
H	0.563661	-2.619234	-1.901491
C	3.931204	-3.458586	-0.195381
H	2.904930	-3.256657	1.672137
C	3.848573	-3.417383	-1.587012
H	2.549096	-3.056902	-3.277770
H	4.880077	-3.697266	0.290391
H	4.731605	-3.610659	-2.198980

IntS20

H = -2364.176671

G = -2364.281888

Esol = -2364.664873

Cartesian coordinates

C	1.744993	2.097451	-0.011897
C	2.419991	3.036096	0.757083
C	3.692456	2.706377	1.236348
C	4.228906	1.455104	0.933501
C	3.485709	0.555005	0.159595
N	2.279266	0.881103	-0.303554
H	4.256867	3.411443	1.849190
H	1.950550	3.995744	0.977347
H	3.853640	-0.445369	-0.077320

C	0.388047	2.244034	-0.548520
N	-0.090749	1.295962	-1.289623
C	-1.667663	3.011450	-0.998501
C	-1.542201	1.496484	-1.424666
Pd	1.078214	-0.328079	-1.440129
O	-0.043728	-1.645233	-2.486642
B	0.743992	-2.883981	-1.906490
O	2.052220	-2.113841	-1.468800
H	2.693316	-2.237195	-2.188582
O	1.067810	-3.724996	-2.975595
H	0.852902	-4.651589	-2.821481
C	-0.054561	-3.374069	-0.622870
C	-1.401526	-3.756138	-0.759552
C	0.489280	-3.360358	0.671785
C	-2.185427	-4.090010	0.343062
H	-1.863758	-3.765949	-1.750511
C	-0.278920	-3.683778	1.793636
H	1.536321	-3.079897	0.811062
C	-1.619466	-4.030574	1.618499
H	-3.234241	-4.365372	0.227035
H	0.147160	-3.657175	2.797873
H	0.107457	-1.611777	-3.446657
O	-0.406801	3.237577	-0.238890
H	-1.576525	3.645033	-1.892803
H	-1.841769	1.395589	-2.476087
C	-2.867603	3.397123	-0.197997
C	-2.958899	3.110575	1.170846
C	-3.955587	3.981079	-0.859140
C	-4.130447	3.403202	1.867555
H	-2.113348	2.661514	1.692498

C	-5.132702	4.261885	-0.162032
H	-3.884800	4.218068	-1.924252
C	-5.221034	3.972100	1.201530
H	-4.195634	3.182685	2.935009
H	-5.977870	4.716101	-0.683203
H	-6.139062	4.195798	1.749128
C	-2.311449	0.504270	-0.579748
C	-3.600917	0.133270	-0.977840
C	-1.794895	-0.000379	0.622283
C	-4.368783	-0.716887	-0.179515
H	-4.012898	0.518711	-1.913889
C	-2.559138	-0.854515	1.416550
H	-0.786889	0.260078	0.950428
C	-3.848814	-1.212640	1.018641
H	-5.374629	-0.997513	-0.499008
H	-2.145481	-1.257865	2.341419
H	-4.434430	-1.894681	1.638254
C	5.621174	1.063637	1.396719
F	5.946552	1.709645	2.518040
F	6.522754	1.370018	0.458111
F	5.687966	-0.252901	1.623044
Cl	-2.626406	-4.325411	3.017041

IntS21

H = -2364.216062

G = -2364.326924

Esol = -2364.704626

Cartesian coordinates

C	0.064595	2.343900	-0.697925
C	0.310524	3.711928	-0.664000

C	1.608501	4.153079	-0.392492
C	2.601608	3.203343	-0.163633
C	2.278508	1.841927	-0.200200
N	1.039389	1.420496	-0.466627
H	1.841775	5.218337	-0.352526
H	-0.508624	4.407882	-0.848136
H	3.029251	1.076002	-0.004859
C	-1.259027	1.770030	-0.977594
N	-1.419914	0.497324	-1.027973
C	-3.487676	1.639689	-1.175124
C	-2.815822	0.224416	-1.391408
Pd	0.373896	-0.544259	-0.458956
O	-0.508618	-2.451795	-0.319089
B	-0.131332	-3.755292	-0.703877
O	-1.145417	-4.648785	-0.747211
H	-0.859790	-5.541159	-0.982879
O	1.144467	-4.050534	-1.001905
H	1.783818	-3.339433	-0.839847
C	2.125686	-1.303232	0.069333
C	2.320213	-1.801967	1.365547
C	3.181164	-1.365919	-0.855297
C	3.554106	-2.341251	1.741209
H	1.510074	-1.777491	2.098518
C	4.417522	-1.913017	-0.488728
H	3.053723	-0.992451	-1.875350
C	4.598464	-2.394205	0.811380
H	3.709970	-2.725883	2.750345
H	5.237192	-1.968657	-1.206771
H	-1.456203	-2.377169	-0.099013
O	-2.320529	2.538025	-1.169902

H	-4.092786	1.917748	-2.046300
H	-2.832599	-0.014965	-2.467470
C	-4.273392	1.789256	0.098669
C	-3.703920	2.305773	1.268376
C	-5.590270	1.310464	0.125773
C	-4.440002	2.329567	2.456007
H	-2.688622	2.705244	1.255286
C	-6.321608	1.328955	1.313111
H	-6.043660	0.908865	-0.784004
C	-5.746183	1.835747	2.482476
H	-3.991829	2.740705	3.363165
H	-7.346144	0.951422	1.325075
H	-6.320165	1.854767	3.411289
C	-3.391087	-0.947512	-0.637236
C	-4.164385	-1.900568	-1.310490
C	-3.147760	-1.108423	0.737300
C	-4.690122	-2.999376	-0.625018
H	-4.348383	-1.790688	-2.382376
C	-3.667383	-2.210725	1.420096
H	-2.558043	-0.364984	1.276274
C	-4.440075	-3.158037	0.739582
H	-5.285874	-3.739625	-1.162740
H	-3.471498	-2.327918	2.487976
H	-4.842350	-4.021227	1.273552
C	4.040431	3.613097	0.087424
F	4.101264	4.835763	0.622138
F	4.727187	3.625228	-1.061195
F	4.640400	2.752499	0.917893
Cl	6.132196	-3.068825	1.275108

IntS22

H = -2270.243268

G = -2270.348846

Esol = -2270.829337

Cartesian coordinates

Pd	1.259078	1.041871	-0.354928
C	0.059218	-1.595535	-1.310893
C	-0.741861	-2.701127	-1.584650
C	-2.119046	-2.583395	-1.385994
C	-2.627039	-1.358123	-0.960012
C	-1.748794	-0.295735	-0.716683
N	-0.434144	-0.418477	-0.866466
H	-2.782285	-3.432152	-1.561259
H	-0.288271	-3.628710	-1.933638
H	-2.124444	0.666175	-0.376979
C	-4.112850	-1.184809	-0.738027
F	-4.575485	-2.117743	0.107878
F	-4.395306	0.018973	-0.216656
F	-4.786932	-1.308332	-1.886713
C	1.518408	-1.614135	-1.469063
O	2.121998	-2.670642	-1.989513
N	2.262647	-0.623686	-1.111091
C	3.523333	-2.295344	-2.151809
H	3.685755	-2.098953	-3.221494
C	3.677214	-1.029287	-1.271453
H	4.210968	-0.234608	-1.811664
C	-1.445219	-2.018401	2.195189
C	-2.400452	-1.009122	2.335606
C	-1.985129	0.323559	2.387425
C	-0.630186	0.666933	2.298425

C	0.312003	-0.373976	2.246768
C	-0.082645	-1.709604	2.188703
H	-3.458986	-1.265416	2.377108
H	-2.745257	1.100216	2.472546
H	1.378229	-0.137365	2.242914
H	0.653988	-2.511564	2.128868
C	1.276652	3.162133	0.366752
H	2.575329	1.791467	-0.275030
C	0.051574	2.602278	0.757651
C	-0.154427	2.103215	2.194883
H	0.787938	2.195308	2.746508
C	-1.164782	2.862722	-0.079915
C	-1.090110	2.906910	-1.488198
C	-2.420464	3.081945	0.512615
C	-2.224089	3.128375	-2.265211
H	-0.135497	2.726245	-1.987279
C	-3.559609	3.306032	-0.266073
H	-2.522628	3.100789	1.595793
C	-3.470359	3.319328	-1.657526
H	-2.137024	3.142967	-3.353746
H	-4.521515	3.468769	0.224203
H	-0.861969	2.777362	2.699607
C	4.411424	-1.274392	0.083368
Cl	-1.956306	-3.672086	1.992857
H	-4.361893	3.482087	-2.266384
C	2.440690	3.524830	1.268012
H	1.258346	3.756606	-0.553971
H	2.260255	4.549669	1.648119
O	3.686971	3.433793	0.616116
H	2.501293	2.863019	2.140667

H	4.133319	-3.148616	-1.839455
C	3.727963	-2.395865	0.881330
H	3.739650	-3.361928	0.354204
H	4.245130	-2.543899	1.840946
H	2.681475	-2.141794	1.107607
C	5.864406	-1.662516	-0.244347
H	6.426907	-1.830383	0.686001
H	5.934478	-2.588310	-0.835967
H	6.374109	-0.861067	-0.802423
C	4.430291	0.007160	0.930426
H	4.815615	0.873874	0.373389
H	3.426477	0.269051	1.292194
H	5.074043	-0.140438	1.810605
H	3.767614	4.150513	-0.028157

IntS23

H = -2270.248932

G = -2270.358905

Esol = -2270.835073

Cartesian coordinates

Pd	0.915816	0.998223	-0.883550
C	3.226561	-0.823939	-0.127114
C	4.085128	-1.879233	0.172971
C	3.558760	-3.173584	0.196301
C	2.205651	-3.349730	-0.086995
C	1.419465	-2.233006	-0.398788
N	1.917668	-0.999856	-0.414159
H	4.192417	-4.031086	0.429353
H	5.135488	-1.681709	0.388162
H	0.360292	-2.346363	-0.629558

C	1.559087	-4.717382	-0.012441
F	0.538759	-4.814010	-0.875891
F	2.440912	-5.682105	-0.288418
F	1.074590	-4.941094	1.218325
C	3.663530	0.580653	-0.125554
O	4.926514	0.881885	0.113682
N	2.844888	1.558564	-0.323089
C	5.042013	2.328845	-0.056221
H	5.579913	2.502964	-0.998788
C	3.572730	2.824748	-0.089303
H	3.403094	3.491803	-0.946502
H	0.509059	2.416239	-1.227093
C	3.103443	3.561093	1.202166
C	-0.888851	0.454802	-1.967792
C	-1.290114	0.584052	-0.632174
C	-2.006071	1.804146	-0.076648
C	-1.246805	1.400395	-3.096103
H	-0.655622	-0.563609	-2.305751
H	5.635454	2.711492	0.780281
C	3.944956	4.842140	1.340591
H	3.830516	5.492739	0.458893
H	3.616263	5.413715	2.221142
H	5.017595	4.633340	1.473886
C	1.624492	3.958159	1.075185
H	1.439224	4.542222	0.159920
H	0.965368	3.078962	1.054783
H	1.329886	4.579001	1.934546
C	3.284763	2.666470	2.438289
H	4.333349	2.370183	2.596293
H	2.961562	3.203753	3.342221

H	2.675438	1.751796	2.364771
H	-1.537249	2.099746	0.873258
H	-1.372338	2.427018	-2.729180
O	-2.478966	1.024518	-3.679800
H	-2.350198	0.251032	-4.244777
H	-0.432412	1.421463	-3.841347
C	-3.465120	1.469377	0.169991
C	-3.964208	1.372336	1.474682
C	-4.323766	1.199573	-0.906318
C	-5.294529	1.025364	1.712281
H	-3.306124	1.570489	2.324518
C	-5.655779	0.850799	-0.683096
H	-3.949917	1.248960	-1.931980
C	-6.135844	0.763901	0.627527
H	-5.682945	0.955608	2.729081
H	-6.326314	0.646097	-1.518803
Cl	-7.796752	0.323348	0.911054
H	-1.904644	2.656720	-0.760809
C	-1.363951	-0.632312	0.228141
C	-1.966012	-1.803380	-0.261735
C	-0.851334	-0.626556	1.536154
C	-2.020887	-2.955791	0.526251
H	-2.414891	-1.800228	-1.256848
C	-0.885906	-1.783926	2.313535
H	-0.394260	0.282100	1.934365
C	-1.464539	-2.953714	1.808103
H	-2.494905	-3.858445	0.135858
H	-0.463497	-1.775083	3.320637
H	-1.490155	-3.859220	2.417080

IntS24

H = -2270.246303

G = -2270.358506

Esol = -2270.833109

Cartesian coordinates

Pd	0.824678	0.321615	-0.293372
C	3.761583	-0.007870	-0.454865
C	5.049233	-0.536908	-0.431248
C	5.216909	-1.866880	-0.039112
C	4.090164	-2.607413	0.315769
C	2.829763	-2.002543	0.262219
N	2.668405	-0.736333	-0.123982
H	6.209934	-2.317974	0.000894
H	5.894877	0.092624	-0.709163
H	1.935558	-2.556859	0.546338
C	4.199876	-4.066880	0.710863
F	4.075446	-4.852077	-0.365854
F	5.380481	-4.321517	1.278535
F	3.229275	-4.397767	1.574169
C	3.474840	1.392403	-0.799832
O	4.457383	2.190822	-1.188271
N	2.289443	1.880862	-0.713393
C	3.827879	3.459486	-1.542869
H	3.877645	3.554981	-2.636566
C	2.377427	3.326383	-1.004257
H	1.646320	3.570790	-1.789549
H	-0.716296	1.039135	-0.389900
C	2.052976	4.201411	0.241267
C	-0.615454	-1.101647	-0.076041
C	-1.493969	0.084092	-0.212640

C	-2.373797	0.269467	-1.494178
C	-0.544677	-2.218105	-1.098711
H	-0.547845	-1.477672	0.955935
H	4.413668	4.260689	-1.079633
C	2.143384	5.677460	-0.180318
H	1.443063	5.903601	-1.000376
H	1.885994	6.328780	0.668186
H	3.155499	5.959995	-0.509402
C	0.622155	3.897671	0.706780
H	-0.101075	4.026246	-0.115144
H	0.532911	2.871863	1.091374
H	0.330744	4.581433	1.518113
C	3.032425	3.911156	1.388706
H	4.076470	4.132558	1.118205
H	2.786184	4.535101	2.260707
H	2.973375	2.859789	1.710838
H	-2.341388	1.333793	-1.768041
H	-0.605014	-1.829076	-2.123979
O	-1.610222	-3.135411	-0.957550
H	-1.525888	-3.605381	-0.116811
H	0.431505	-2.731367	-1.017802
C	-3.816864	-0.126521	-1.284240
C	-4.753476	0.844722	-0.900781
C	-4.242756	-1.455550	-1.410548
C	-6.078983	0.506648	-0.635567
H	-4.442330	1.886584	-0.795191
C	-5.567834	-1.809493	-1.152186
H	-3.528110	-2.232202	-1.683889
C	-6.480028	-0.826771	-0.758786
H	-6.802190	1.265681	-0.335164

H	-5.898157	-2.844237	-1.253054
Cl	-8.131812	-1.265341	-0.421290
H	-1.923575	-0.283581	-2.329324
C	-2.219082	0.500324	1.050379
C	-2.922201	-0.469299	1.778492
C	-2.318786	1.843525	1.429694
C	-3.702964	-0.100016	2.874439
H	-2.890966	-1.512322	1.457872
C	-3.093722	2.213896	2.530735
H	-1.795473	2.610732	0.856183
C	-3.787965	1.241869	3.255612
H	-4.256405	-0.862836	3.426099
H	-3.159191	3.265014	2.820065
H	-4.399611	1.530204	4.113069

IntS25

H = -2270.244834

G = -2270.354778

Esol = -2270.83096

Cartesian coordinates

Pd	0.813530	-1.024616	-0.081356
C	3.032278	1.027309	0.370848
C	3.821167	2.162933	0.548829
C	3.306375	3.394636	0.139258
C	2.031795	3.433086	-0.425348
C	1.309918	2.241590	-0.566668
N	1.798526	1.067357	-0.175616
H	3.889885	4.309951	0.254427
H	4.811081	2.073398	0.996581
H	0.308064	2.247576	-0.995780

C	1.409801	4.750661	-0.837114
F	0.860851	5.363909	0.222862
F	2.330072	5.572854	-1.350985
F	0.446409	4.569369	-1.749964
C	3.485652	-0.317807	0.760016
O	4.679761	-0.478683	1.302866
N	2.763728	-1.372369	0.586349
C	4.773780	-1.886710	1.679107
H	4.705967	-1.935742	2.775086
C	3.570968	-2.553384	0.960569
H	2.987407	-3.168002	1.661019
H	0.400862	-2.465279	0.076588
C	3.952795	-3.442085	-0.261845
C	-0.987724	-0.920104	-1.303167
C	-1.393025	-0.591727	-0.004387
C	-2.135617	-1.541914	0.929480
H	-1.872526	-1.301844	1.969534
C	-1.493882	0.852466	0.368720
C	-2.083850	1.774590	-0.511676
C	-1.032462	1.308195	1.615668
C	-2.180485	3.125684	-0.167881
H	-2.493632	1.426900	-1.461907
C	-1.111557	2.659527	1.951050
C	-1.681755	3.573738	1.057743
H	-2.645645	3.829801	-0.860587
H	-0.730083	3.003597	2.914872
H	-1.742646	4.631343	1.320280
H	-0.583320	0.600690	2.316355
C	-1.283761	-2.160719	-2.106787
H	-0.761418	-0.072947	-1.962099

H	5.755736	-2.248102	1.357185
C	4.801631	-4.614031	0.262367
H	5.060550	-5.289752	-0.566218
H	5.748577	-4.283391	0.716224
H	4.250323	-5.202614	1.013076
C	2.685050	-4.011268	-0.917549
H	2.050853	-4.536136	-0.185862
H	2.076891	-3.225651	-1.387111
H	2.964100	-4.733255	-1.699891
C	4.743699	-2.631793	-1.300363
H	4.144634	-1.798293	-1.699366
H	5.679695	-2.219874	-0.892031
H	5.017840	-3.274512	-2.150109
C	-3.626759	-1.360155	0.714446
C	-4.343772	-0.358343	1.383905
C	-4.305481	-2.166894	-0.211426
C	-5.702656	-0.160731	1.139309
H	-3.836035	0.280185	2.110173
C	-5.664675	-1.981904	-0.466753
H	-3.759298	-2.960487	-0.724880
C	-6.357520	-0.973066	0.208639
H	-6.259269	0.615475	1.666006
H	-6.193347	-2.616611	-1.179237
H	-1.849252	-2.576846	0.728901
Cl	-8.053290	-0.730631	-0.106437
H	-2.254502	-1.973717	-2.613514
O	-1.337263	-3.329886	-1.324308
H	-1.520703	-4.084302	-1.899219
H	-0.518549	-2.240731	-2.901419

IntS26

H = -2270.248835

G = -2270.360199

Esol = -2270.835883

Cartesian coordinates

Pd	0.780434	-0.401812	0.199443
C	3.685563	0.137837	0.165343
C	4.925581	0.770129	0.179836
C	4.962455	2.166325	0.202717
C	3.757909	2.867829	0.213336
C	2.552161	2.157302	0.205676
N	2.517532	0.825483	0.177651
H	5.913424	2.701379	0.220046
H	5.835894	0.170150	0.175187
H	1.596023	2.680723	0.230563
C	3.727224	4.382696	0.187538
F	4.833390	4.895280	0.730992
F	3.637094	4.826520	-1.072929
F	2.665324	4.846774	0.860828
C	3.527714	-1.324252	0.138817
O	4.594678	-2.108979	0.105989
N	2.367848	-1.874777	0.137355
C	4.091811	-3.478313	0.167141
H	4.389800	-3.894468	1.139236
C	2.551258	-3.331119	0.008048
H	2.027012	-3.822390	0.842180
H	-0.658295	-1.311867	0.275812
C	1.962200	-3.893201	-1.318973
C	-0.823257	0.856447	0.211843
C	-1.527673	-0.443454	0.338265

C	-2.415500	-0.968945	-0.832514
H	-2.578936	-2.042109	-0.653162
C	-2.120556	-0.719785	1.706047
C	-2.890273	0.258480	2.349587
C	-1.989947	-1.982082	2.300861
C	-3.513778	-0.020549	3.567996
H	-3.027907	1.236485	1.884648
C	-2.612260	-2.263111	3.518183
C	-3.377007	-1.280703	4.154967
H	-4.115324	0.749272	4.056074
H	-2.498311	-3.249533	3.972902
H	-3.864875	-1.498182	5.107451
H	-1.392298	-2.754691	1.807702
C	-0.921889	1.763988	-0.986840
H	-0.806017	1.435736	1.144128
H	4.578440	-4.043544	-0.635419
C	2.215330	-5.410094	-1.340942
H	1.786553	-5.851586	-2.252861
H	3.288106	-5.658068	-1.335264
H	1.746310	-5.906764	-0.476325
C	0.445813	-3.641365	-1.355205
H	-0.048022	-4.010148	-0.441392
H	0.216530	-2.572050	-1.467773
H	-0.003813	-4.165277	-2.211852
C	2.616291	-3.220280	-2.535024
H	2.433616	-2.134336	-2.536356
H	3.703763	-3.388924	-2.574805
H	2.192554	-3.627058	-3.465310
C	-3.747822	-0.267133	-0.942874
C	-4.807846	-0.584593	-0.078646

C	-3.962164	0.713626	-1.923236
C	-6.033526	0.073907	-0.167682
H	-4.679346	-1.363323	0.675203
C	-5.183167	1.381488	-2.027484
H	-3.162291	0.943114	-2.629709
C	-6.213771	1.063636	-1.138972
H	-6.853324	-0.178448	0.506044
H	-5.345395	2.138236	-2.796157
H	-1.853642	-0.862378	-1.766895
Cl	-7.739620	1.894296	-1.253306
H	-1.950803	2.173837	-1.031115
O	-0.588334	1.075059	-2.175782
H	-0.702838	1.668876	-2.929648
H	-0.248945	2.628665	-0.824879

IntS2

H = -2574.924383

G = -2575.043136

Esol = -2575.566755

Cartesian coordinates

Pd	0.540248	-0.260440	-0.594563
C	0.201709	2.789551	-0.621084
C	0.330886	4.175615	-0.576838
C	1.590606	4.715099	-0.299038
C	2.655089	3.844054	-0.085419
C	2.434276	2.460094	-0.156181
N	1.237010	1.943477	-0.411987
H	1.742032	5.794458	-0.253616
H	-0.538547	4.808484	-0.757000
H	3.255733	1.761870	-0.001958

C	4.048648	4.341165	0.241219
F	4.947053	3.803645	-0.593407
F	4.126090	5.671598	0.145805
F	4.389070	3.988963	1.488376
C	-1.079426	2.124227	-0.897335
O	-2.187501	2.832311	-1.030585
N	-1.174573	0.841048	-0.988797
C	-3.245627	1.892132	-1.434397
H	-3.340063	2.002769	-2.524792
C	-2.595041	0.490263	-1.111143
H	-2.737256	-0.179679	-1.970151
C	4.127544	-0.418948	0.580979
C	3.722623	-0.867040	-0.669312
C	2.530386	-1.608721	-0.780709
C	1.746633	-1.924896	0.363562
C	2.184396	-1.419028	1.617668
C	3.356703	-0.687651	1.728468
H	4.331191	-0.663691	-1.551145
H	2.300338	-2.081214	-1.737262
H	1.609165	-1.629629	2.517758
H	3.694164	-0.320169	2.698534
C	-1.373064	-4.100768	1.470136
H	-1.796955	-4.177948	2.488526
H	-0.987446	-5.097548	1.210804
C	-0.214387	-3.101125	1.512876
H	-0.587364	-2.126637	1.871189
C	0.542600	-2.887561	0.179054
C	-0.304427	-2.072657	-0.808071
H	-1.364847	-2.019299	-0.556684
O	-2.379051	-3.800289	0.522108

H	-2.978360	-3.138608	0.893279
C	-4.546264	2.203404	-0.763732
C	-5.738084	1.983066	-1.464534
C	-4.595427	2.619886	0.573056
C	-6.970188	2.160705	-0.830753
H	-5.705304	1.670987	-2.512060
C	-5.826102	2.807525	1.201496
H	-3.669505	2.801990	1.120315
C	-7.015091	2.571520	0.503503
H	-7.895861	1.987409	-1.383511
H	-5.859201	3.138201	2.241785
H	-7.977605	2.716554	0.998747
C	-3.123120	-0.191413	0.133996
C	-4.255699	-1.008513	0.028892
C	-2.542776	0.011517	1.391872
C	-4.805887	-1.607816	1.164266
H	-4.715837	-1.176891	-0.947422
C	-3.082610	-0.597124	2.527653
H	-1.654919	0.638097	1.490206
C	-4.215972	-1.407647	2.417841
H	-5.691663	-2.239147	1.069246
H	-2.617650	-0.436253	3.502665
H	-4.641520	-1.880805	3.305264
Cl	5.583926	0.520774	0.737703
H	-0.155190	-2.346756	-1.861874
C	1.015272	-4.232596	-0.374933
C	2.254297	-4.768806	0.003526
C	0.182425	-4.985806	-1.215187
C	2.659804	-6.023509	-0.457111
H	2.917274	-4.203078	0.662908

C	0.587965	-6.240068	-1.678372
H	-0.804319	-4.603409	-1.482604
C	1.828905	-6.761632	-1.304279
H	3.629890	-6.424535	-0.154714
H	-0.073360	-6.814522	-2.331008
H	0.494166	-3.477718	2.268790
H	2.146652	-7.740915	-1.668744

IntS3

H = -2574.920355

G = -2575.041199

Esol = -2575.56271

Cartesian coordinates

Pd	-0.520603	0.326435	-0.741392
C	-0.458377	-2.711409	-0.388200
C	-0.719077	-4.064829	-0.189033
C	-2.012353	-4.442526	0.184824
C	-2.976692	-3.450776	0.340573
C	-2.624947	-2.110795	0.118372
N	-1.397426	-1.747755	-0.237844
H	-2.264765	-5.490213	0.354213
H	0.077296	-4.797108	-0.325142
H	-3.362767	-1.319086	0.237964
C	-4.406258	-3.772316	0.726321
F	-4.543315	-5.059782	1.056459
F	-4.789148	-3.024832	1.770201
F	-5.236704	-3.508445	-0.290333
C	0.868429	-2.206919	-0.766285
O	1.901439	-3.026071	-0.866373
N	1.079749	-0.952198	-0.977243

C	3.020417	-2.228168	-1.394514
H	3.042255	-2.429949	-2.476195
C	2.523874	-0.750107	-1.159059
H	2.705081	-0.159085	-2.066640
C	-4.256539	0.880479	-0.064011
C	-3.747921	1.050622	-1.349198
C	-2.514296	1.696853	-1.518523
C	-1.780070	2.195143	-0.407074
C	-2.316615	1.960629	0.888203
C	-3.538182	1.323049	1.059520
H	-4.311241	0.696619	-2.213169
H	-2.170563	1.896929	-2.533958
H	-1.771219	2.317252	1.761187
H	-3.947387	1.165086	2.058210
C	0.397736	5.081406	-1.955305
H	1.289105	4.456876	-2.175598
H	0.645446	5.683904	-1.062102
C	-0.793609	4.179708	-1.662963
H	-1.644267	4.793677	-1.329915
H	-1.098897	3.734709	-2.621764
C	-0.493166	3.054528	-0.647039
C	0.446237	2.010582	-1.257268
H	0.447631	2.026041	-2.357504
O	0.039244	5.887284	-3.054256
H	0.723711	6.553122	-3.193994
Cl	-5.772772	0.060471	0.162806
C	4.322931	-2.613511	-0.766511
C	5.497375	-2.470117	-1.515984
C	4.399623	-3.032990	0.567323
C	6.739741	-2.727669	-0.932981

H	5.442538	-2.157261	-2.562417
C	5.640898	-3.301253	1.145043
H	3.486652	-3.158749	1.150260
C	6.812727	-3.142644	0.399143
H	7.651276	-2.614119	-1.523467
H	5.694542	-3.635097	2.183471
H	7.783250	-3.351138	0.854465
C	3.134853	-0.039252	0.028150
C	4.205366	0.839900	-0.173140
C	2.686816	-0.282725	1.333309
C	4.826928	1.459472	0.913008
H	4.560306	1.038326	-1.187654
C	3.310294	0.331501	2.420730
H	1.841587	-0.950538	1.509684
C	4.382847	1.202951	2.212833
H	5.660575	2.144050	0.743656
H	2.953205	0.133063	3.433475
H	4.870127	1.685611	3.062680
C	0.000259	3.620847	0.690033
C	-0.616557	4.762619	1.230927
C	1.008069	3.002297	1.442403
C	-0.231786	5.274678	2.470543
H	-1.417818	5.261642	0.684057
C	1.396143	3.512496	2.685506
H	1.503376	2.103968	1.079795
C	0.781167	4.651458	3.205171
H	-0.725915	6.166178	2.863232
H	2.188280	3.009368	3.243188
H	1.470326	1.987928	-0.873309
H	1.086221	5.052233	4.174232

IntS4

H = -2574.911783

G = -2575.034456

Esol = -2575.552339

Cartesian coordinates

Pd	0.791401	-1.272180	-0.516569
C	3.330766	0.276046	-0.642270
C	4.679969	0.617398	-0.672737
C	5.625861	-0.389346	-0.466269
C	5.181462	-1.691183	-0.240261
C	3.806775	-1.954002	-0.221820
N	2.903801	-0.989171	-0.418898
H	6.693746	-0.164575	-0.475106
H	4.969407	1.653052	-0.852300
H	3.428715	-2.959428	-0.036978
C	6.161933	-2.833655	-0.056684
F	7.317031	-2.393038	0.449965
F	5.660443	-3.761411	0.767530
F	6.418918	-3.420636	-1.231261
C	2.255671	1.262895	-0.825088
O	2.572155	2.542887	-0.943372
N	1.010740	0.932544	-0.828408
C	1.320488	3.253622	-1.239021
H	1.305167	3.388972	-2.331147
C	0.235196	2.185421	-0.834016
H	-0.532352	2.146484	-1.619270
C	-6.401817	-0.837065	-0.696534
C	-5.638128	-0.143005	-1.638526
C	-4.275895	0.056653	-1.400135

C	-3.660641	-0.428534	-0.235908
C	-4.451510	-1.110700	0.701479
C	-5.812354	-1.316622	0.478140
H	-6.109684	0.239650	-2.544571
H	-3.689211	0.615474	-2.134406
H	-4.002620	-1.486463	1.622277
H	-6.422879	-1.846964	1.210133
C	-1.067281	-2.078476	-1.365989
H	0.942365	-2.762358	-0.284183
C	-1.434139	-1.551845	-0.123361
C	-2.171805	-0.225733	-0.018138
H	-1.993616	0.227713	0.963100
C	-1.489965	-2.416825	1.090094
C	-1.876892	-3.764256	1.000557
C	-1.186360	-1.880725	2.355424
C	-1.946841	-4.558751	2.145492
H	-2.157115	-4.185794	0.033539
C	-1.245239	-2.679478	3.496963
H	-0.888369	-0.834177	2.444313
C	-1.626383	-4.021414	3.395661
H	-2.264629	-5.600296	2.062380
H	-0.997247	-2.252923	4.471344
H	-1.803910	0.478547	-0.767336
C	1.256726	4.579512	-0.548813
C	0.602278	5.641096	-1.185250
C	1.756478	4.751848	0.748557
C	0.433147	6.860604	-0.525442
H	0.222743	5.516409	-2.203242
C	1.597098	5.973516	1.401987
H	2.274138	3.930251	1.245182

C	0.929404	7.027328	0.769571
H	-0.078030	7.684391	-1.027968
H	1.993592	6.104606	2.411066
H	0.803331	7.982077	1.284630
C	-0.434645	2.425482	0.502237
C	-1.604111	3.193443	0.549910
C	0.097285	1.916099	1.692729
C	-2.237336	3.444452	1.767457
H	-2.027295	3.595796	-0.373848
C	-0.537069	2.163271	2.913064
H	1.003613	1.308580	1.674420
C	-1.707069	2.925838	2.952954
H	-3.150983	4.041964	1.791193
H	-0.115310	1.758548	3.835828
H	-2.205161	3.117256	3.905703
Cl	-8.097390	-1.097517	-0.981492
H	-1.682618	-4.644597	4.290737
C	-1.403669	-1.462818	-2.707500
H	-0.889081	-3.155370	-1.424132
H	-1.418426	-0.358792	-2.648997
O	-2.613494	-1.994791	-3.191148
H	-0.627705	-1.733260	-3.438464
H	-3.336323	-1.699876	-2.616237

IntS5

H = -2574.910353

G = -2575.033054

Esol = -2575.550644

Cartesian coordinates

Pd	0.907704	1.081626	0.787517
----	----------	----------	----------

C	3.284539	-0.567526	0.107562
C	4.567362	-0.966718	-0.257349
C	5.510294	0.018069	-0.559635
C	5.132290	1.357610	-0.477571
C	3.823988	1.678883	-0.098745
N	2.923233	0.734787	0.187543
H	6.524508	-0.251439	-0.859188
H	4.808246	-2.029115	-0.300819
H	3.495771	2.716069	-0.029645
C	6.126168	2.470412	-0.746411
F	6.723839	2.849226	0.389254
F	7.072670	2.068258	-1.599842
F	5.511586	3.540920	-1.265520
C	2.217391	-1.523565	0.445482
O	2.509964	-2.813075	0.521039
N	1.011831	-1.148205	0.687267
C	1.328709	-3.478929	1.086929
H	1.569004	-3.657330	2.145201
C	0.221691	-2.353110	0.988349
H	-0.235414	-2.211927	1.976010
H	1.159456	2.565927	0.941410
C	1.042689	-4.776112	0.396627
C	0.508068	-5.834481	1.141029
C	1.219255	-4.923395	-0.984990
C	0.137631	-7.023899	0.509607
H	0.380985	-5.730168	2.222124
C	0.858923	-6.115240	-1.613653
H	1.645832	-4.106187	-1.568347
C	0.311347	-7.164869	-0.869247
H	-0.278047	-7.845087	1.097326

H	1.004175	-6.226229	-2.690365
H	0.027727	-8.096289	-1.363978
C	-0.860687	-2.611935	-0.034006
C	-2.007417	-3.316579	0.355373
C	-0.719775	-2.227827	-1.372924
C	-2.994746	-3.636633	-0.578180
H	-2.123187	-3.626909	1.397007
C	-1.712797	-2.534567	-2.306140
H	0.167713	-1.675882	-1.688875
C	-2.851031	-3.242043	-1.911632
H	-3.881473	-4.191016	-0.263501
H	-1.596741	-2.221779	-3.346027
H	-3.626628	-3.483488	-2.641246
C	-1.029259	1.431475	1.726374
C	-1.211947	1.894648	0.418456
C	-1.839267	1.027493	-0.661619
C	-1.162058	3.357065	0.122892
C	-0.663484	3.833971	-1.102688
C	-1.681861	4.279889	1.044399
C	-0.660721	5.197855	-1.386649
H	-0.252136	3.132371	-1.831515
C	-1.688438	5.646437	0.755587
H	-2.114935	3.925480	1.981260
C	-1.174756	6.109923	-0.457202
H	-0.258199	5.553842	-2.337456
H	-2.107765	6.349732	1.478208
H	-1.181078	7.178236	-0.683641
C	-1.630833	0.169691	2.277932
H	-0.787455	2.174820	2.493424
H	-1.529165	-0.015331	-0.550107

H	-2.616979	0.438963	2.702259
C	-3.356791	1.096448	-0.608829
C	-4.093351	-0.035239	-0.232463
C	-4.051768	2.274011	-0.925601
C	-5.486780	0.000395	-0.162668
H	-3.576526	-0.970828	-0.011973
C	-5.443844	2.325306	-0.857109
H	-3.505068	3.165548	-1.236849
C	-6.157563	1.186591	-0.470159
H	-6.055252	-0.885980	0.122040
H	-5.981076	3.241175	-1.106767
Cl	-7.895769	1.244685	-0.380543
H	-1.482115	1.364094	-1.645263
O	-0.780034	-0.382513	3.270680
H	-1.320271	-0.742207	3.984988
H	-1.825006	-0.561545	1.478564

IntS6

H = -2574.917961

G = -2575.039873

Esol = -2575.558932

Cartesian coordinates

Pd	0.099649	0.803427	0.470532
C	2.936310	1.763191	0.154697
C	4.095622	2.505873	-0.054465
C	3.966258	3.813756	-0.527916
C	2.688243	4.317725	-0.767161
C	1.575525	3.497961	-0.537252
N	1.698378	2.249607	-0.088980
H	4.846531	4.431851	-0.712534

H	5.069621	2.060891	0.151208
H	0.564841	3.861988	-0.730732
C	2.484434	5.745698	-1.231716
F	2.332706	6.562607	-0.182209
F	3.532480	6.172764	-1.941785
F	1.385696	5.846155	-1.992176
C	2.946316	0.375512	0.641903
O	4.085664	-0.277595	0.777952
N	1.852190	-0.255104	0.902491
C	3.748593	-1.578803	1.387009
H	3.949653	-1.460857	2.462242
C	2.192587	-1.662623	1.158996
H	1.689799	-1.997260	2.073712
H	-1.373318	1.543683	-0.001486
C	4.582848	-2.682037	0.817474
C	5.003661	-3.717989	1.659807
C	4.871678	-2.742857	-0.552442
C	5.692873	-4.814903	1.136634
H	4.791953	-3.668983	2.731502
C	5.569644	-3.832357	-1.071760
H	4.550132	-1.935964	-1.212297
C	5.975222	-4.873510	-0.229948
H	6.017993	-5.619389	1.799670
H	5.796436	-3.872440	-2.139279
H	6.518857	-5.727507	-0.639781
C	1.756920	-2.560226	0.018407
C	1.626912	-3.935892	0.258503
C	1.518920	-2.071672	-1.270296
C	1.264296	-4.805434	-0.769307
H	1.827836	-4.330372	1.257902

C	1.148919	-2.941412	-2.302440
H	1.615183	-1.004997	-1.479049
C	1.019561	-4.308704	-2.055197
H	1.175115	-5.875588	-0.569841
H	0.965239	-2.545964	-3.303994
H	0.734305	-4.988722	-2.860665
C	-1.476763	-0.330814	1.074839
C	-2.210488	0.693739	0.297685
C	-2.741462	0.312716	-1.115149
C	-3.168849	1.559428	1.092820
C	-3.314639	2.922199	0.799914
C	-3.995424	0.978535	2.063330
C	-4.268617	3.694080	1.464191
H	-2.676155	3.387454	0.042329
C	-4.951699	1.749195	2.728825
H	-3.910962	-0.086945	2.284725
C	-5.091431	3.106599	2.430782
H	-4.369415	4.756035	1.230105
H	-5.593797	1.283820	3.479643
H	-5.839146	3.708355	2.951693
C	-1.492490	-1.800369	0.757458
H	-1.523041	-0.182343	2.162878
H	-1.949148	-0.226222	-1.654499
H	-2.545056	-2.147953	0.786112
C	-4.011933	-0.506362	-1.112412
C	-3.987371	-1.869655	-1.440468
C	-5.250310	0.079266	-0.802657
C	-5.151226	-2.639863	-1.435212
H	-3.043570	-2.342629	-1.722347
C	-6.421842	-0.676086	-0.789064

H	-5.307284	1.144405	-0.573380
C	-6.366450	-2.038752	-1.098029
H	-5.124118	-3.698549	-1.696175
H	-7.379980	-0.214603	-0.547040
Cl	-7.824460	-2.989552	-1.078197
H	-2.914472	1.252834	-1.661389
O	-0.719525	-2.447390	1.745904
H	-0.648397	-3.381593	1.512441
H	-1.110788	-2.003965	-0.258984

IntS7

H = -2574.90448

G = -2575.026875

Esol = -2575.5443

Cartesian coordinates

Pd	0.294023	-0.547689	-1.284743
C	0.472507	2.394312	-0.905765
C	0.955643	3.670088	-0.628909
C	2.326050	3.827422	-0.401075
C	3.151671	2.704690	-0.453459
C	2.593786	1.458459	-0.759254
N	1.286646	1.315421	-0.987297
H	2.745926	4.811027	-0.182971
H	0.264216	4.512242	-0.587633
H	3.210480	0.559946	-0.813181
C	4.631809	2.800366	-0.138049
F	5.320932	1.857727	-0.794079
F	5.116317	3.997503	-0.482150
F	4.838854	2.629218	1.172200
C	-0.955245	2.091354	-1.108082

O	-1.836663	3.077576	-1.168068
N	-1.380769	0.884023	-1.226814
C	-3.166926	2.455501	-1.197916
H	-3.707151	2.910772	-2.036931
C	-2.821962	0.942137	-1.517527
H	-2.935833	0.777519	-2.601714
H	1.612501	-1.226930	-1.539581
C	-3.890686	2.701214	0.097330
C	-5.282311	2.540968	0.122850
C	-3.209821	2.995163	1.284147
C	-5.981708	2.650038	1.324276
H	-5.821461	2.311438	-0.799536
C	-3.912141	3.112203	2.486185
H	-2.128461	3.141083	1.274474
C	-5.297044	2.932769	2.510191
H	-7.065521	2.517477	1.334861
H	-3.374724	3.347475	3.407505
H	-5.844958	3.022549	3.450600
C	-3.643845	-0.090282	-0.793769
C	-4.658794	-0.765079	-1.483471
C	-3.461389	-0.334203	0.574055
C	-5.495214	-1.661861	-0.813549
H	-4.800819	-0.585340	-2.552705
C	-4.304934	-1.217973	1.245171
H	-2.666869	0.173551	1.120999
C	-5.323868	-1.881896	0.554939
H	-6.282569	-2.184340	-1.360899
H	-4.164634	-1.387078	2.312806
H	-5.983449	-2.573191	1.084208
C	-0.773782	-2.412323	-1.536376

C	0.051510	-2.603018	-0.416980
C	1.312429	-3.477772	-0.440588
C	-0.529300	-2.388190	0.951224
C	-1.486245	-3.310202	1.401795
C	-0.113105	-1.362716	1.812930
C	-2.004214	-3.218863	2.694642
H	-1.825560	-4.104779	0.732843
C	-0.650612	-1.257079	3.097612
C	-1.590112	-2.190313	3.545104
H	-2.743606	-3.947643	3.033428
H	-0.323310	-0.450050	3.756872
H	1.053472	-4.378483	0.141648
H	-1.999277	-2.115194	4.554972
H	0.639214	-0.647599	1.477052
C	-0.582141	-3.049122	-2.896622
H	-1.810881	-2.127744	-1.325032
C	2.556270	-2.840196	0.138046
C	2.739618	-2.693764	1.519308
C	3.529836	-2.305558	-0.721699
C	3.822530	-1.974742	2.030114
H	2.021878	-3.133633	2.213269
C	4.622090	-1.588581	-0.228837
H	3.442854	-2.458078	-1.800866
C	4.748544	-1.404133	1.151898
H	3.952364	-1.852782	3.106282
H	5.376164	-1.178442	-0.901990
H	1.520468	-3.801920	-1.468583
Cl	6.074623	-0.465733	1.776928
H	0.488253	-3.154465	-3.148951
O	-1.277130	-4.275763	-2.964145

H	-0.805200	-4.930795	-2.432730
H	-1.026218	-2.398999	-3.664736

IntS8

H = -2574.918234

G = -2575.038996

Esol = -2575.559215

Cartesian coordinates

Pd	-0.132773	-0.341827	-0.491741
C	-0.123728	2.651343	-0.382495
C	0.230009	3.991838	-0.262500
C	1.548971	4.297086	0.092191
C	2.444599	3.253563	0.317766
C	1.997300	1.929870	0.204615
N	0.745559	1.642547	-0.142470
H	1.875599	5.333572	0.190591
H	-0.508891	4.770661	-0.454027
H	2.671503	1.090754	0.384406
C	3.905105	3.506651	0.634033
F	4.345969	2.645301	1.557248
F	4.649979	3.344841	-0.469745
F	4.095490	4.749775	1.084112
C	-1.456861	2.185316	-0.796210
O	-2.453936	3.033595	-0.973662
N	-1.693165	0.933173	-0.991522
C	-3.672095	2.226832	-1.147224
H	-4.187814	2.623172	-2.030128
C	-3.085611	0.787798	-1.444361
H	-3.059426	0.632333	-2.535420
H	1.111756	-1.376087	-0.000154

C	-4.543342	2.326404	0.074608
C	-5.896587	1.982766	-0.043479
C	-4.024847	2.662058	1.330591
C	-6.716440	1.954161	1.084271
H	-6.309869	1.722012	-1.020981
C	-4.848889	2.640333	2.458615
H	-2.978587	2.954452	1.433596
C	-6.192939	2.279958	2.339199
H	-7.768848	1.681142	0.983071
H	-4.438888	2.909571	3.434428
H	-6.835602	2.261780	3.221922
C	-3.805240	-0.373761	-0.812249
C	-4.690722	-1.138344	-1.580513
C	-3.623349	-0.686698	0.541454
C	-5.388878	-2.203684	-1.005301
H	-4.835212	-0.901982	-2.638540
C	-4.314652	-1.753390	1.115375
H	-2.938810	-0.094265	1.150290
C	-5.199680	-2.513636	0.343461
H	-6.077505	-2.794610	-1.612934
H	-4.165197	-1.991294	2.170663
H	-5.741122	-3.348039	0.794337
C	-0.707332	-2.266320	-0.803446
C	0.694903	-2.473347	-0.364167
C	1.778227	-2.827492	-1.422382
C	0.843548	-3.235726	0.937836
C	0.369460	-4.555777	0.980628
C	1.467068	-2.689095	2.064256
C	0.527486	-5.317062	2.139554
H	-0.124216	-4.973879	0.099462

C	1.620875	-3.451784	3.225512
C	1.153963	-4.767631	3.263438
H	0.155839	-6.343805	2.167522
H	2.107607	-3.016551	4.101035
H	1.930697	-3.914704	-1.391108
H	1.274720	-5.364985	4.169713
H	1.839232	-1.661521	2.035398
C	-1.156661	-2.652801	-2.190855
H	-1.450301	-2.532930	-0.041783
C	3.054514	-2.069521	-1.150428
C	3.976036	-2.500782	-0.185024
C	3.274632	-0.831828	-1.774948
C	5.071921	-1.710809	0.168064
H	3.831134	-3.463208	0.309781
C	4.366978	-0.030565	-1.437229
H	2.575964	-0.483713	-2.541410
C	5.255917	-0.470490	-0.451198
H	5.783471	-2.048719	0.922605
H	4.534552	0.930260	-1.925524
H	1.410382	-2.579579	-2.425372
Cl	6.600724	0.537080	0.006363
H	-0.562688	-2.131354	-2.966008
O	-1.002819	-4.059111	-2.277697
H	-1.351817	-4.368587	-3.123999

MeOH

H = -115.650145

G = -115.677113

Esol = -115.705428

Cartesian coordinates

O	0.745331	-0.122467	0.000006
---	----------	-----------	----------

C	-0.654460	0.019563	0.000007
H	-1.040845	0.546796	-0.896021
H	-1.091534	-0.991017	0.000103
H	-1.040823	0.547045	0.895881
H	1.137313	0.759533	-0.000052

O2

H = -150.3092841

G = -150.3325471

Esol = -150.316457

Cartesian coordinates

O	0.000000	0.000000	0.599973
O	0.000000	0.000000	-0.599973

OTf

H = -961.654326

G = -961.695045

Esol = -961.689788

Cartesian coordinates

S	-0.935014	0.000001	-0.000000
C	0.945271	-0.000007	0.000003
F	1.450219	0.851907	-0.914006
F	1.450216	0.365610	1.194780
F	1.450215	-1.217524	-0.280762
O	-1.244461	1.408758	0.324785
O	-1.244489	-0.985656	1.057615
O	-1.244456	-0.423092	-1.382415

P1

H = -1153.605112

G = -1153.667756

Esol = -1153.889422

Cartesian coordinates

H	-1.243195	-1.544109	1.152887
C	3.356410	-0.189381	-0.000662
C	2.549191	0.438013	-0.952004
C	1.296567	-0.101333	-1.246010
C	0.833538	-1.261031	-0.607949
C	1.666714	-1.871014	0.340981
C	2.923024	-1.347035	0.649797
H	2.900930	1.342110	-1.450742
H	0.658992	0.399717	-1.977771
H	1.327919	-2.776758	0.851899
H	3.567388	-1.828691	1.386636
C	-4.144672	-1.425166	0.314870
H	-5.060994	-1.990094	0.116618
C	-2.950720	-1.886936	-0.094240
C	-1.601672	-1.246245	0.149556
C	-0.553647	-1.789505	-0.863665
H	-0.556103	-2.889674	-0.798819
O	-4.412205	-0.281752	0.980317
H	-3.602048	0.247934	1.057239
C	-1.609952	0.275131	0.119542
C	-2.217092	0.971690	-0.938896
C	-0.931262	1.011501	1.101378
C	-2.143614	2.363360	-1.013347
H	-2.758577	0.410026	-1.703951
C	-0.856881	2.405382	1.030892
H	-0.441076	0.481104	1.921530
C	-1.461052	3.085511	-0.028648

H	-2.624540	2.888701	-1.842073
H	-0.319864	2.959737	1.804119
H	-0.882374	-1.526808	-1.881712
Cl	4.927241	0.479833	0.379485
H	-1.404655	4.175038	-0.086371
H	-2.956529	-2.849037	-0.612852

P2

H = -1153.624965

G = -1153.688752

Esol = -1153.908232

Cartesian coordinates

H	-1.366662	-1.508588	0.817324
C	3.339419	-0.224693	0.057573
C	2.603684	0.541023	-0.849302
C	1.350644	0.089689	-1.265243
C	0.817625	-1.117763	-0.792203
C	1.578492	-1.865735	0.117638
C	2.833884	-1.431716	0.545705
H	3.010873	1.482654	-1.219932
H	0.770276	0.697510	-1.962414
H	1.183118	-2.810158	0.502321
H	3.421801	-2.020662	1.251052
C	-4.035281	-1.545311	0.598248
H	-5.084196	-1.824067	0.310056
C	-3.022397	-1.669687	-0.516322
C	-1.643293	-1.101560	-0.167299
C	-0.568539	-1.567518	-1.180648
H	-0.598401	-2.668096	-1.241657
O	-3.777293	-1.205547	1.724809

C	-1.664026	0.411691	-0.039549
C	-2.040947	1.221657	-1.121206
C	-1.259713	1.032430	1.148226
C	-2.010663	2.614367	-1.020545
H	-2.355332	0.763227	-2.063081
C	-1.224879	2.424644	1.254239
H	-0.970988	0.412629	1.999686
C	-1.599237	3.221325	0.169459
H	-2.307332	3.227950	-1.874913
H	-0.904183	2.888956	2.189913
H	-0.821753	-1.187492	-2.183632
Cl	4.911070	0.331838	0.586555
H	-1.572591	4.310584	0.250676
H	-3.446796	-1.208215	-1.425515
H	-2.956316	-2.750160	-0.752413

TS1

H = -2574.900834

G = -2575.021827

Esol = -2575.541357

Cartesian coordinates

Pd	-0.624707	-0.798520	0.201929
C	-0.703053	2.211701	0.518891
C	-1.105783	3.541460	0.618100
C	-2.460347	3.837725	0.440382
C	-3.344304	2.794093	0.170384
C	-2.855857	1.484300	0.095844
N	-1.567402	1.204094	0.270184
H	-2.823430	4.864094	0.515240
H	-0.368925	4.316613	0.830173

H	-3.525664	0.649570	-0.101416
C	-4.816834	3.042237	-0.083957
F	-5.223187	4.173421	0.500331
F	-5.055609	3.143721	-1.398038
F	-5.557247	2.029555	0.387938
C	0.691263	1.772921	0.666537
O	1.644312	2.657976	0.907760
N	1.024349	0.534913	0.544658
C	2.871848	1.887750	1.163699
H	2.975000	1.851352	2.258428
C	2.489225	0.453033	0.631763
H	2.767873	-0.294804	1.384576
C	-5.224482	-1.438945	-0.445368
C	-4.716333	-1.557198	0.854075
C	-3.339873	-1.696929	1.045189
C	-2.462367	-1.707358	-0.051614
C	-2.991669	-1.636741	-1.351775
C	-4.365839	-1.487569	-1.551461
H	-5.397395	-1.532370	1.705830
H	-2.953317	-1.782834	2.063572
H	-2.331041	-1.685970	-2.220943
H	-4.776829	-1.410886	-2.559123
C	1.414433	-4.235957	-1.631975
H	0.487895	-4.843871	-1.681592
H	2.050982	-4.690678	-0.848109
C	1.060965	-2.796258	-1.249160
H	1.971592	-2.190600	-1.306890
H	0.387158	-2.405733	-2.027448
C	0.402943	-2.673245	0.114688
C	-0.955121	-3.110834	0.195586

H	-1.362857	-3.616558	-0.679079
O	2.069903	-4.170189	-2.874612
H	2.314783	-5.062201	-3.151072
C	1.267326	-2.704834	1.333888
C	2.658735	-2.876649	1.225136
C	0.723118	-2.542039	2.624958
C	3.473860	-2.885299	2.360374
H	3.122130	-2.997894	0.248058
C	1.536381	-2.538926	3.755538
H	-0.351092	-2.393230	2.751004
C	2.920058	-2.711235	3.629633
H	4.550541	-3.031090	2.246683
H	1.088932	-2.404072	4.742666
H	-1.334855	-3.494096	1.142644
C	4.071681	2.537424	0.550161
C	5.302035	2.447054	1.211941
C	4.005815	3.150729	-0.707529
C	6.460688	2.951128	0.616576
H	5.356209	1.979819	2.199170
C	5.161230	3.663527	-1.296504
H	3.048417	3.229183	-1.224213
C	6.391343	3.558894	-0.639183
H	7.416955	2.877321	1.138773
H	5.103372	4.144875	-2.275078
H	7.295270	3.958406	-1.104045
C	3.105803	0.066457	-0.693403
C	4.356984	-0.562941	-0.702026
C	2.476543	0.351744	-1.910868
C	4.965361	-0.911213	-1.908338
H	4.857525	-0.781395	0.243999

C	3.081413	-0.001262	-3.119108
H	1.497506	0.834150	-1.920301
C	4.325049	-0.636482	-3.120538
H	5.940364	-1.403184	-1.903423
H	2.576210	0.214258	-4.062945
H	4.794681	-0.919659	-4.064672
Cl	-6.930594	-1.233397	-0.687650
H	3.557237	-2.716055	4.516451

TS2

H = -2574.909574

G = -2575.029798

Esol = -2575.548065

Cartesian coordinates

Pd	0.904735	-1.367030	-0.244793
C	3.339464	0.278451	-0.764741
C	4.657009	0.705882	-0.904925
C	5.681347	-0.222376	-0.707026
C	5.342222	-1.535558	-0.383559
C	3.992510	-1.884587	-0.257741
N	3.014012	-0.995461	-0.444339
H	6.728512	0.070894	-0.798999
H	4.861539	1.745317	-1.162833
H	3.699534	-2.901210	0.004667
C	6.408492	-2.599237	-0.209148
F	7.551925	-2.061510	0.224505
F	6.013338	-3.528134	0.671195
F	6.651832	-3.212554	-1.373234
C	2.184655	1.167261	-0.958494
O	2.381352	2.429566	-1.296841

N	0.976960	0.748645	-0.809330
C	1.057384	2.997658	-1.593534
H	0.984170	3.016149	-2.690701
C	0.076990	1.891740	-1.024291
H	-0.645729	1.636269	-1.811025
C	-6.211524	-1.718058	-1.492826
C	-5.368244	-2.721573	-1.010108
C	-4.008351	-2.459747	-0.830477
C	-3.478865	-1.197213	-1.127562
C	-4.344885	-0.200820	-1.602844
C	-5.703634	-0.450458	-1.791798
H	-5.778812	-3.703718	-0.771933
H	-3.377220	-3.253164	-0.428321
H	-3.952562	0.795221	-1.826341
H	-6.371320	0.328262	-2.162713
C	-0.750713	-4.016955	0.867404
H	0.042857	-4.735304	0.586293
C	-0.742988	-2.849510	-0.103838
H	1.084993	-2.858721	0.048754
H	-0.834176	-3.185086	-1.143510
C	-1.276977	-1.564944	0.156861
C	-2.000799	-0.862798	-0.982292
H	-1.917703	0.220233	-0.840498
C	-1.533675	-1.084103	1.547208
C	-0.602195	-1.286865	2.586795
C	-2.727444	-0.407529	1.857587
C	-0.869995	-0.868754	3.888903
H	0.359379	-1.756402	2.370825
C	-2.998223	0.001787	3.163094
H	-3.467185	-0.218037	1.082994

C	-2.078565	-0.233470	4.186346
H	-0.129570	-1.037917	4.673884
H	-3.938390	0.513571	3.377596
H	-1.487139	-1.107605	-1.927305
C	0.913243	4.381570	-1.043835
C	0.175715	5.323926	-1.770446
C	1.424796	4.724221	0.214447
C	-0.063830	6.593004	-1.238615
H	-0.214844	5.065867	-2.758698
C	1.194039	5.994881	0.740402
H	2.007111	3.996947	0.781678
C	0.443823	6.928891	0.018485
H	-0.640008	7.322801	-1.811218
H	1.598632	6.258209	1.719981
H	0.261803	7.922313	0.434100
C	-0.674627	2.282466	0.226728
C	-1.892675	2.961215	0.098075
C	-0.143623	2.063535	1.502612
C	-2.559945	3.436538	1.227798
H	-2.314283	3.136349	-0.895307
C	-0.809944	2.537797	2.632691
H	0.793557	1.517191	1.619278
C	-2.014744	3.230894	2.497551
H	-3.505719	3.970869	1.115891
H	-2.535132	3.601675	3.383117
Cl	-7.908391	-2.042673	-1.714751
H	-2.294802	0.088506	5.207314
O	-2.032994	-4.590774	0.736329
H	-2.135656	-5.302070	1.382116
H	-0.555143	-3.681036	1.896838

H -0.390702 2.356628 3.623567

TS3-R

H = -2574.911711

G = -2575.033823

Esol = -2575.549842

Cartesian coordinates

Pd	-0.566022	-0.796236	0.425869
C	-3.540171	-0.652603	0.334145
C	-4.888386	-0.943463	0.149085
C	-5.235146	-2.208022	-0.333300
C	-4.219489	-3.122001	-0.608951
C	-2.885157	-2.747279	-0.406729
N	-2.553972	-1.540343	0.054906
H	-6.279745	-2.477501	-0.497872
H	-5.640678	-0.188921	0.381006
H	-2.069161	-3.434843	-0.630964
C	-4.535851	-4.525908	-1.085704
F	-5.697518	-4.556634	-1.744646
F	-3.572605	-4.979686	-1.898131
F	-4.624668	-5.363614	-0.045684
C	-3.054948	0.641237	0.837651
O	-3.892158	1.643990	1.046823
N	-1.804785	0.837970	1.056963
C	-3.078866	2.830294	1.345959
H	-3.443108	3.220991	2.304670
C	-1.625251	2.222053	1.524003
H	-1.386686	2.183263	2.598285
H	0.201032	-2.012732	-0.131208
C	-3.236007	3.862542	0.262655

C	-2.795714	5.167657	0.520613
C	-3.740299	3.542380	-1.002401
C	-2.840151	6.135882	-0.481862
H	-2.403132	5.426767	1.507254
C	-3.790392	4.515467	-2.004316
H	-4.104262	2.534332	-1.206371
C	-3.335161	5.810601	-1.748729
H	-2.491083	7.149295	-0.273173
H	-4.190401	4.259967	-2.987982
H	-3.373556	6.569691	-2.532849
C	-0.484747	2.905669	0.810979
C	0.522285	3.534473	1.549266
C	-0.384711	2.862610	-0.588040
C	1.620711	4.110875	0.904933
H	0.463819	3.554837	2.640440
C	0.706787	3.441525	-1.233508
H	-1.159809	2.369410	-1.175989
C	1.713870	4.065828	-0.487023
H	2.408470	4.584569	1.493630
H	0.775923	3.405004	-2.322802
H	2.571215	4.514409	-0.993521
C	1.482131	0.217290	2.383650
C	1.306711	0.056127	0.893896
H	1.277863	1.008225	0.357951
C	1.754612	-1.058905	0.148759
C	2.101416	-0.832290	-1.325359
C	2.459949	-2.222058	0.779494
C	2.134840	-3.552627	0.477817
C	3.596079	-1.960577	1.564077
C	2.912607	-4.603984	0.962310

H	1.257855	-3.769451	-0.138431
C	4.377189	-3.014586	2.043567
H	3.871307	-0.927926	1.781533
C	4.038663	-4.336336	1.747367
H	2.639653	-5.635007	0.727322
H	5.261029	-2.797311	2.647326
H	4.650291	-5.158433	2.125315
H	1.451866	-0.046638	-1.737341
C	3.557224	-0.426318	-1.420413
C	3.942321	0.897720	-1.166812
C	4.550983	-1.378761	-1.681512
C	5.286469	1.268107	-1.178581
H	3.186283	1.655592	-0.951305
C	5.899709	-1.024282	-1.698097
H	4.269917	-2.418357	-1.865361
C	6.261577	0.301545	-1.443045
H	5.585393	2.298791	-0.983747
H	6.671498	-1.766921	-1.903756
Cl	7.943361	0.755174	-1.453927
H	1.928093	-1.754202	-1.896938
H	1.515157	-0.769019	2.878175
O	2.679767	0.951892	2.570733
H	2.866880	1.010296	3.517273
H	0.617381	0.770378	2.793752

TS4-S

H = -2574.908854

G = -2575.030310

Esol = -2575.547048

Cartesian coordinates

Pd	-0.073297	0.703937	-0.074234
C	-2.763022	1.673731	-0.878334
C	-3.866536	2.478941	-1.146515
C	-3.773603	3.845846	-0.876259
C	-2.582474	4.345347	-0.351123
C	-1.518732	3.468932	-0.107627
N	-1.607292	2.162714	-0.369291
H	-4.616853	4.512566	-1.064393
H	-4.773133	2.032089	-1.555402
H	-0.580563	3.829985	0.313252
C	-2.406245	5.827108	-0.084132
F	-3.573929	6.399082	0.222245
F	-1.552856	6.030650	0.927723
F	-1.913856	6.441425	-1.166891
C	-2.754320	0.221691	-1.107713
O	-3.821409	-0.369056	-1.618231
N	-1.733466	-0.500499	-0.810822
C	-3.542828	-1.806800	-1.674248
H	-3.574972	-2.084306	-2.736542
C	-2.048578	-1.900748	-1.137196
H	-1.389677	-2.213800	-1.961185
H	0.942908	1.753567	0.351528
C	-4.576118	-2.578005	-0.901272
C	-4.685933	-3.956251	-1.127359
C	-5.372191	-1.974183	0.077668
C	-5.567941	-4.725231	-0.368426
H	-4.071883	-4.435031	-1.894677
C	-6.262170	-2.743825	0.830841
H	-5.303039	-0.899084	0.249538
C	-6.357009	-4.120236	0.614677

H	-5.644156	-5.799614	-0.548304
H	-6.884495	-2.264706	1.589777
H	-7.050924	-4.721360	1.206017
C	-1.830879	-2.828388	0.030888
C	-1.176401	-4.049739	-0.161924
C	-2.297087	-2.491874	1.308869
C	-0.990284	-4.928778	0.908881
H	-0.807763	-4.317376	-1.156087
C	-2.112567	-3.367139	2.378267
H	-2.794033	-1.535083	1.475167
C	-1.459527	-4.588303	2.179889
H	-0.477091	-5.879570	0.749840
H	-2.471581	-3.092698	3.371985
H	-1.313161	-5.272378	3.018465
C	1.092804	-1.581166	1.571319
H	1.955226	-2.241751	1.793228
C	1.353629	-0.889403	0.245168
H	1.194904	-1.521442	-0.636745
C	2.193545	0.223372	0.083886
C	2.774146	0.540977	-1.297241
H	2.859990	1.630206	-1.415134
C	3.018378	0.750687	1.228057
C	3.947490	-0.132651	1.806909
C	3.025309	2.090874	1.639132
C	4.837697	0.309953	2.787765
H	3.997013	-1.166811	1.463098
C	3.913291	2.534790	2.619994
C	4.820745	1.643886	3.200467
H	5.553006	-0.391437	3.222243
H	3.894193	3.580509	2.934068

H	5.514149	1.990453	3.969541
H	2.320285	2.796986	1.193236
O	0.804959	-0.714555	2.639342
H	0.227191	-2.240230	1.454241
H	1.612531	-0.241049	2.884493
C	4.138494	-0.100814	-1.436861
C	5.304177	0.622002	-1.151248
C	4.255247	-1.456577	-1.773125
C	6.558041	0.013316	-1.197140
H	5.233123	1.676881	-0.876177
C	5.500946	-2.082236	-1.822964
H	3.359729	-2.039233	-2.005723
C	6.650266	-1.341473	-1.529078
H	7.463514	0.579332	-0.975195
H	5.590540	-3.135551	-2.091725
Cl	8.209415	-2.113905	-1.581438
H	2.090769	0.172410	-2.076366

TS5

H = -2574.91567

G = -2575.039566

Esol = -2575.553221

Cartesian coordinates

Pd	0.479388	-0.637398	-0.390726
C	1.549253	2.090994	0.241138
C	1.768435	3.463237	0.327656
C	0.858763	4.323023	-0.293249
C	-0.217584	3.770067	-0.984726
C	-0.368031	2.378418	-1.016765
N	0.484020	1.557338	-0.404573

H	0.986063	5.405717	-0.242191
H	2.638425	3.837095	0.868373
H	-1.207655	1.925101	-1.542105
C	-1.207890	4.639316	-1.732928
F	-0.833332	4.784533	-3.010094
F	-2.426708	4.081080	-1.724696
F	-1.292076	5.853168	-1.183265
C	2.473942	1.095081	0.803731
O	3.587900	1.473866	1.403504
N	2.248237	-0.164553	0.674863
C	4.231399	0.247471	1.912335
H	4.011427	0.225928	2.989463
C	3.410838	-0.898196	1.188765
H	3.078076	-1.625703	1.942493
H	-2.207204	-1.346634	0.624808
C	5.710109	0.270851	1.685628
C	6.552800	-0.284642	2.655658
C	6.256479	0.755192	0.489833
C	7.928226	-0.371135	2.427723
H	6.133137	-0.653494	3.595624
C	7.630767	0.678140	0.267398
H	5.606075	1.195415	-0.267203
C	8.468154	0.108895	1.232479
H	8.579195	-0.806349	3.188830
H	8.051785	1.060722	-0.664796
H	9.543834	0.046291	1.054288
C	4.146065	-1.634718	0.090905
C	4.944274	-2.734285	0.430691
C	4.106960	-1.203457	-1.241101
C	5.703937	-3.384394	-0.542351

H	4.981954	-3.078077	1.467480
C	4.860038	-1.859451	-2.217910
H	3.487444	-0.349725	-1.522470
C	5.663559	-2.947768	-1.869860
H	6.327451	-4.236755	-0.264414
H	4.822113	-1.516077	-3.254137
H	6.255913	-3.458007	-2.632389
C	-6.596946	0.386685	2.157357
C	-6.764626	0.207284	0.781452
C	-5.644210	0.201370	-0.049188
C	-4.355169	0.375596	0.471659
C	-4.212987	0.559932	1.854021
C	-5.321619	0.567101	2.701012
H	-7.765999	0.070744	0.371366
H	-5.777462	0.045040	-1.122094
H	-3.216086	0.701113	2.282529
H	-5.207637	0.714292	3.775795
C	-0.587387	-2.510648	-1.349071
H	0.635541	-2.214823	-0.534952
H	-0.000687	-2.742055	-2.246203
C	-1.293025	-1.252633	-1.307412
C	-2.525377	-1.145026	-0.412623
C	-3.137309	0.276968	-0.410799
H	-2.372317	0.979736	-0.050756
O	-1.009449	-3.624884	-0.724460
H	-1.901571	-3.494456	-0.352025
C	-3.575448	-2.194519	-0.760053
C	-3.973359	-2.410943	-2.088641
C	-4.203824	-2.922584	0.261546
C	-4.977194	-3.332952	-2.387313

H	-3.500700	-1.850744	-2.899293
C	-5.207957	-3.848696	-0.036517
H	-3.922389	-2.742621	1.302490
C	-5.596728	-4.054799	-1.361358
H	-5.278708	-3.490622	-3.425235
H	-5.691311	-4.403082	0.770674
H	-3.391968	0.560811	-1.445259
Cl	-7.988825	0.388821	3.205072
H	-6.381712	-4.776566	-1.596721
H	-1.325205	-0.710859	-2.261414

TS6

H = -2270.223182

G = -2270.333531

Esol = -2270.809659

Cartesian coordinates

Pd	-0.268669	-0.425841	-0.070572
C	0.886285	2.248683	-0.728240
C	1.738271	3.271466	-1.134074
C	3.119180	3.072229	-1.024592
C	3.576846	1.866590	-0.501329
C	2.650182	0.886328	-0.124898
N	1.341008	1.063649	-0.253056
H	3.824454	3.844186	-1.336068
H	1.320671	4.201338	-1.521015
H	2.982566	-0.064376	0.293917
C	5.047182	1.554965	-0.323397
F	5.346020	1.418324	0.975768
F	5.350777	0.394126	-0.928225
F	5.819938	2.513350	-0.836621

C	-0.577980	2.369956	-0.715847
O	-1.175410	3.432619	-1.236738
N	-1.317724	1.469784	-0.169728
C	-2.608025	3.139192	-1.172014
H	-2.921248	2.829967	-2.180220
C	-2.697666	1.998073	-0.132657
H	-3.392709	1.211353	-0.456241
C	-4.809101	-1.546454	-0.544098
C	-4.238552	-1.752052	0.715923
C	-2.849187	-1.736783	0.854400
C	-2.023939	-1.515672	-0.255595
C	-2.610261	-1.375501	-1.527008
C	-3.997450	-1.369795	-1.672607
H	-4.881982	-1.912848	1.582154
H	-2.416951	-1.884172	1.846474
H	-1.983787	-1.257696	-2.414646
H	-4.454935	-1.239577	-2.654480
C	-0.380766	-2.772914	-0.187299
H	-0.719458	-3.229427	-1.117256
C	0.927160	-2.198997	-0.187241
C	1.651798	-2.188084	-1.523598
H	2.496241	-1.485220	-1.523418
H	0.968738	-1.847102	-2.316965
C	2.185053	-3.561399	-1.943332
H	2.846419	-3.969002	-1.154384
H	1.334770	-4.266580	-2.042097
O	2.861859	-3.370828	-3.159772
H	3.231238	-4.212368	-3.455834
C	-3.101551	2.472669	1.299188
Cl	-6.538199	-1.512889	-0.712061

H	-0.730233	-3.285110	0.708161
C	1.730359	-2.189449	1.070804
C	1.105686	-2.136448	2.335776
C	3.139294	-2.199249	1.036768
C	1.855001	-2.082448	3.508062
H	0.016826	-2.118440	2.407333
C	3.890662	-2.147773	2.214197
H	3.669014	-2.255519	0.086007
C	3.253750	-2.084768	3.453835
H	1.345054	-2.035576	4.472618
H	4.981030	-2.157186	2.155719
H	3.840204	-2.041642	4.373783
H	-3.125629	4.061670	-0.891308
C	-2.978327	1.309815	2.292739
H	-3.234939	1.655096	3.305489
H	-3.663293	0.494240	2.030509
H	-1.955771	0.905104	2.318746
C	-4.571435	2.922675	1.240962
H	-5.223012	2.105341	0.892231
H	-4.915388	3.222032	2.242333
H	-4.722289	3.786763	0.575152
C	-2.207937	3.629758	1.776075
H	-1.154478	3.318822	1.856990
H	-2.259212	4.510039	1.118036
H	-2.526151	3.955416	2.777511

TS7

H = -2270.242042

G = -2270.347797

Esol = -2270.82683

Cartesian coordinates

Pd	0.329502	-0.371174	0.854482
C	-0.718869	2.343515	0.060933
C	-1.499287	3.421467	-0.350323
C	-2.728677	3.156814	-0.960384
C	-3.115636	1.829383	-1.131778
C	-2.262876	0.805503	-0.701884
N	-1.094397	1.056350	-0.117252
H	-3.374657	3.970109	-1.295273
H	-1.147453	4.439725	-0.183323
H	-2.547942	-0.239270	-0.826179
C	-4.462868	1.461671	-1.717882
F	-4.373995	0.343701	-2.452516
F	-5.352621	1.235888	-0.740714
F	-4.937825	2.441205	-2.492028
C	0.573894	2.507096	0.741497
O	1.060025	3.717734	0.960053
N	1.264356	1.499532	1.148217
C	2.269595	3.534929	1.756020
H	2.052427	3.900812	2.769307
C	2.539888	2.006129	1.699883
H	2.665938	1.596002	2.712984
C	3.609089	-1.473813	-2.269099
C	2.520323	-0.650653	-2.566696
C	1.241923	-1.046422	-2.178143
C	1.024974	-2.262795	-1.510337
C	2.127933	-3.096400	-1.277790
C	3.419105	-2.706503	-1.641769
H	2.680128	0.290036	-3.093734
H	0.392157	-0.399340	-2.408853

H	1.983331	-4.074547	-0.811826
H	4.275021	-3.353030	-1.444335
C	0.212254	-2.544222	1.406333
H	1.383038	-1.167799	1.626100
C	-0.730148	-2.259885	0.390658
C	-0.369390	-2.627542	-1.060175
H	-0.533700	-3.712581	-1.179447
C	-2.186571	-2.081838	0.673229
C	-2.648989	-1.361537	1.795688
C	-3.147473	-2.580199	-0.230995
C	-4.009883	-1.119642	1.977779
C	-4.510017	-2.341124	-0.040471
H	-2.842343	-3.166785	-1.096812
C	-4.947045	-1.595594	1.055767
H	-4.339450	-0.545664	2.846550
H	-5.230582	-2.734258	-0.760432
H	-1.084647	-2.135037	-1.731546
C	3.782583	1.593015	0.856042
Cl	5.221244	-0.941684	-2.666654
H	-6.010389	-1.389675	1.192862
H	3.055292	4.150748	1.306203
C	5.028998	2.198897	1.523971
H	5.931416	1.897563	0.971642
H	5.011595	3.299674	1.538044
H	5.139324	1.845524	2.561891
C	3.925457	0.063658	0.851633
H	3.970338	-0.336767	1.877673
H	3.094619	-0.422578	0.326279
H	4.852525	-0.223678	0.335013
C	3.650115	2.101973	-0.586943

H	3.640122	3.201478	-0.645086
H	4.497115	1.746860	-1.191869
H	2.732700	1.720337	-1.057899
C	-0.125905	-2.816349	2.875389
H	-1.099133	-3.329072	2.914457
H	1.124397	-3.037457	1.060518
H	-1.937880	-0.963974	2.519732
O	-0.247774	-1.683607	3.707472
H	0.631749	-3.516081	3.268561
H	0.634014	-1.337163	3.895214

TS8-R-2

H = -2270.239738

G = -2270.350049

Esol = -2270.823934

Cartesian coordinates

Pd	-0.702705	0.100313	0.187962
C	-3.623819	0.546527	0.132313
C	-5.001900	0.355416	0.088027
C	-5.487910	-0.893543	-0.304876
C	-4.575605	-1.896153	-0.631427
C	-3.204334	-1.625675	-0.557647
N	-2.741038	-0.430956	-0.184394
H	-6.560958	-1.083882	-0.362598
H	-5.668662	1.175984	0.353957
H	-2.468025	-2.388008	-0.812789
C	-5.042423	-3.285412	-1.017639
F	-4.184299	-3.854453	-1.874413
F	-5.121695	-4.069627	0.064813
F	-6.249125	-3.243351	-1.588723

C	-2.998220	1.826279	0.496270
O	-3.749759	2.856070	0.857035
N	-1.724005	1.990461	0.458013
C	-2.811006	3.895555	1.277620
H	-2.833031	3.926075	2.376584
C	-1.449872	3.421043	0.712346
H	-0.655780	3.482634	1.467050
H	-0.153231	-1.305466	-0.082562
C	-0.988880	4.172946	-0.574071
C	1.280882	0.821652	2.359948
C	1.242363	0.667448	0.861853
H	1.421847	1.592699	0.309999
C	1.532242	-0.542651	0.200325
C	2.019360	-0.490984	-1.252417
C	1.987527	-1.753545	0.967669
C	1.372238	-3.009423	0.879933
C	3.182133	-1.638764	1.698909
C	1.921295	-4.120757	1.521553
H	0.446469	-3.120340	0.309260
C	3.734314	-2.749498	2.338937
H	3.701933	-0.680277	1.740428
C	3.104113	-3.993034	2.255047
H	1.422137	-5.089373	1.449500
H	4.665789	-2.641687	2.898628
H	3.533972	-4.862004	2.757682
H	-3.170650	4.848157	0.875758
C	-2.054517	4.094034	-1.678514
H	-3.015496	4.532608	-1.369076
H	-1.717779	4.646947	-2.568156
H	-2.234697	3.053127	-1.989553

C	-0.725585	5.639823	-0.192204
H	-0.342963	6.194171	-1.062256
H	-1.636370	6.157977	0.145135
H	0.025591	5.714287	0.610314
C	0.319470	3.559428	-1.094306
H	1.109290	3.600445	-0.327800
H	0.178501	2.512901	-1.401304
H	0.677182	4.120226	-1.970742
H	1.543344	0.354529	-1.769371
H	2.327569	1.044930	2.649509
O	0.423157	1.882291	2.740324
H	0.549388	2.052512	3.682775
H	1.004938	-0.128110	2.850134
C	3.525626	-0.347583	-1.284802
C	4.121370	0.915356	-1.159160
C	4.353451	-1.475207	-1.366053
C	5.508357	1.056097	-1.111347
H	3.495222	1.810173	-1.105947
C	5.741913	-1.352854	-1.321525
H	3.907926	-2.468546	-1.456224
C	6.314354	-0.084325	-1.188584
H	5.970561	2.039981	-1.021606
H	6.383568	-2.232337	-1.387063
H	1.716796	-1.413039	-1.767697
Cl	8.046036	0.079328	-1.124388

TS8-R

H = -2270.242184

G = -2270.353705

Esol = -2270.826085

Cartesian coordinates

Pd	-0.807176	-0.472141	-0.241141
C	-3.628819	0.478880	-0.516739
C	-4.790152	1.242823	-0.598631
C	-4.721178	2.594212	-0.251169
C	-3.495312	3.120533	0.153369
C	-2.376042	2.280852	0.211046
N	-2.443755	0.990071	-0.110265
H	-5.608046	3.228897	-0.292185
H	-5.720689	0.779992	-0.928130
H	-1.408453	2.668532	0.533625
C	-3.343034	4.590317	0.490942
F	-4.493545	5.100952	0.936843
F	-2.405404	4.764586	1.432594
F	-2.970705	5.283029	-0.591827
C	-3.581238	-0.949762	-0.862202
O	-4.678385	-1.573285	-1.257704
N	-2.492239	-1.632404	-0.787676
C	-4.265170	-2.923975	-1.627779
H	-4.319509	-2.993422	-2.723310
C	-2.818157	-3.045074	-1.077424
H	-2.133104	-3.408745	-1.857348
H	0.281785	-1.534289	-0.487260
C	-2.667049	-3.969916	0.167892
C	0.658711	1.095251	1.858366
C	0.780582	0.751911	0.392259
H	0.722782	1.628117	-0.266323
C	1.536541	-0.339992	-0.107825
C	2.128424	-0.223485	-1.516496
C	2.285489	-1.283720	0.788145

C	2.259542	-2.670968	0.583592
C	3.174328	-0.751974	1.737055
C	3.083424	-3.516701	1.325512
H	1.583734	-3.096076	-0.162270
C	4.003508	-1.600210	2.474524
H	3.227489	0.327953	1.879004
C	3.959511	-2.981511	2.275028
H	3.043504	-4.595644	1.161057
H	4.695473	-1.173882	3.204059
H	2.140193	-1.210275	-1.998953
H	4.608956	-3.641320	2.854334
H	-4.981957	-3.620961	-1.181445
C	-3.069848	-5.394264	-0.252997
H	-2.452924	-5.753372	-1.092420
H	-2.924538	-6.088540	0.587898
H	-4.127034	-5.466571	-0.551225
C	-1.200772	-3.990315	0.624141
H	-1.068734	-4.719964	1.437004
H	-0.531381	-4.284649	-0.199809
H	-0.871492	-3.011295	0.999214
C	-3.555736	-3.481939	1.321975
H	-3.261081	-2.475051	1.656415
H	-4.622917	-3.457709	1.051235
H	-3.456571	-4.156485	2.185333
C	3.541614	0.309474	-1.406191
C	4.635806	-0.565631	-1.422748
C	3.776043	1.675675	-1.199671
C	5.935798	-0.095034	-1.243149
H	4.471188	-1.635956	-1.566677
C	5.069742	2.163382	-1.017521

H	2.939262	2.377881	-1.174404
C	6.146431	1.271578	-1.037485
H	6.785820	-0.778169	-1.258222
H	5.250566	3.227412	-0.860762
H	1.499836	0.442397	-2.126046
Cl	7.764776	1.869468	-0.803833
H	0.758207	0.183460	2.472839
O	1.668335	2.047297	2.135353
H	1.634756	2.283315	3.072439
H	-0.344897	1.516603	2.060967

TS9-S-2

H = -2270.233574

G = -2270.345562

Esol = -2270.817462

Cartesian coordinates

Pd	0.687708	0.261921	0.268130
C	3.395025	0.077909	-0.927931
C	4.588247	-0.402348	-1.461680
C	4.893318	-1.754725	-1.294392
C	3.992062	-2.565741	-0.605355
C	2.810062	-2.006647	-0.106727
N	2.519538	-0.714061	-0.268763
H	5.822310	-2.171663	-1.687077
H	5.257639	0.278481	-1.987804
H	2.089116	-2.614860	0.440056
C	4.247157	-4.050062	-0.434196
F	3.690927	-4.501393	0.697313
F	3.715103	-4.735128	-1.454602
F	5.556674	-4.309349	-0.398498

C	2.995482	1.490888	-0.999711
O	3.728554	2.335341	-1.711167
N	1.964232	1.950861	-0.379714
C	2.994253	3.595297	-1.704231
H	2.504017	3.693765	-2.684083
C	1.995647	3.425781	-0.535106
H	0.992636	3.779228	-0.815206
H	-0.018932	-1.057831	0.543562
C	2.423897	4.150915	0.777345
C	-1.309077	1.589459	2.187654
C	-1.211342	1.168405	0.731243
H	-1.271979	1.987767	0.004890
C	-1.594470	-0.111970	0.277872
C	-1.946871	-0.317259	-1.200043
C	-2.264718	-1.097684	1.202223
C	-3.495946	-0.716608	1.764749
C	-1.811524	-2.408034	1.408586
C	-4.235744	-1.616530	2.534724
H	-3.894517	0.280330	1.571788
C	-2.548770	-3.308402	2.179232
C	-3.762921	-2.913276	2.747914
H	-5.190621	-1.302261	2.961032
H	-2.172217	-4.321096	2.337489
H	-4.339613	-3.616104	3.352704
H	-0.864471	-2.729878	0.966726
H	3.719519	4.404569	-1.573799
C	3.829003	3.713752	1.221419
H	4.111377	4.246549	2.141472
H	3.863606	2.636632	1.446926
H	4.600253	3.936063	0.468328

C	2.398089	5.666007	0.511836
H	3.130574	5.976190	-0.249227
H	1.400927	5.998186	0.180753
H	2.641498	6.212589	1.435040
C	1.419864	3.823513	1.887736
H	1.676458	4.370106	2.807368
H	0.401858	4.126408	1.596260
H	1.414986	2.750675	2.126095
H	-1.399475	0.414704	-1.812052
C	-3.440069	-0.168918	-1.401196
C	-4.279028	-1.290951	-1.400202
C	-4.019745	1.102711	-1.509375
C	-5.663028	-1.154648	-1.501991
H	-3.847061	-2.289954	-1.305836
C	-5.402254	1.258123	-1.610442
H	-3.384521	1.992621	-1.519809
C	-6.220369	0.123663	-1.601477
H	-6.313231	-2.030279	-1.501807
H	-5.851319	2.247988	-1.701090
H	-1.626490	-1.321385	-1.511991
Cl	-7.946787	0.306166	-1.719869
H	-0.768895	2.533167	2.318364
O	-0.755446	0.671819	3.096095
H	-1.345316	-0.091939	3.167442
H	-2.370255	1.810269	2.418397

TS9-S

H = -2270.242227

G = -2270.354051

Esol = -2270.826228

Cartesian coordinates

Pd	0.805948	-0.522258	0.241699
C	3.714768	0.170091	0.131966
C	4.945875	0.819466	0.097477
C	4.957796	2.214001	0.009422
C	3.741688	2.893125	-0.043478
C	2.547631	2.162603	0.008733
N	2.536020	0.834286	0.099082
H	5.899214	2.765473	-0.014300
H	5.867038	0.237604	0.138051
H	1.583321	2.672866	-0.015171
C	3.685294	4.400483	-0.191806
F	4.788667	4.972178	0.296857
F	3.574236	4.740508	-1.481229
F	2.623439	4.898618	0.457065
C	3.577981	-1.293336	0.188662
O	4.651647	-2.062044	0.256220
N	2.426330	-1.867836	0.158273
C	4.163560	-3.431219	0.399091
H	4.390608	-3.753032	1.424936
C	2.639816	-3.328579	0.111725
H	2.058268	-3.790205	0.923511
H	-0.291762	-1.584793	0.341162
C	2.181463	-3.968478	-1.232875
C	-0.645081	1.700797	1.691256
C	-0.729984	0.920268	0.401061
H	-0.592254	1.538660	-0.495562
C	-1.523581	-0.238717	0.231322
C	-2.048647	-0.568401	-1.168623
H	-2.077401	-1.657707	-1.307867

C	-2.346669	-0.823945	1.342101
C	-3.272622	0.006814	1.994755
C	-2.348837	-2.197746	1.624261
C	-4.170738	-0.532375	2.918493
H	-3.295242	1.072079	1.762661
C	-3.242807	-2.733283	2.551248
C	-4.158735	-1.899759	3.200691
H	-4.889867	0.123248	3.414273
H	-3.225421	-3.803663	2.767346
H	-4.862092	-2.317866	3.924015
H	-1.639698	-2.857192	1.115922
H	4.719186	-4.053568	-0.310168
C	2.923741	-3.335766	-2.419673
H	2.598383	-3.803213	-3.360903
H	2.710742	-2.258147	-2.496693
H	4.014889	-3.468477	-2.353744
C	2.477085	-5.476720	-1.157186
H	1.954543	-5.944881	-0.307540
H	2.131988	-5.973881	-2.075842
H	3.551829	-5.693448	-1.057624
C	0.668033	-3.773553	-1.416796
H	0.322707	-4.334246	-2.298276
H	0.105598	-4.142934	-0.544043
H	0.409482	-2.716718	-1.570139
C	-3.444285	0.001805	-1.312223
C	-4.568812	-0.812146	-1.123183
C	-3.635696	1.369712	-1.549365
C	-5.857125	-0.281467	-1.173226
H	-4.438218	-1.877732	-0.920692
C	-4.917118	1.917280	-1.601754

H	-2.774603	2.027446	-1.690491
C	-6.024988	1.086023	-1.409853
H	-6.730969	-0.917452	-1.027057
H	-5.064526	2.981411	-1.789731
H	-1.369692	-0.148785	-1.925887
Cl	-7.628680	1.761381	-1.465848
H	-0.811630	1.030065	2.552240
O	-1.619325	2.723735	1.606337
H	-1.615065	3.235517	2.426654
H	0.368442	2.131674	1.802683

TS-S10

H = -2403.401368

G = -2403.512448

Esol = -2403.917831

Cartesian coordinates

C	0.352928	-1.724199	-0.090000
C	0.691179	-3.071512	-0.127389
C	1.933290	-3.428918	-0.663286
C	2.762778	-2.425758	-1.158576
C	2.342297	-1.090785	-1.099098
N	1.178356	-0.748117	-0.552692
H	2.246017	-4.473418	-0.704292
H	-0.006158	-3.815656	0.259010
H	2.956357	-0.286028	-1.498360
C	-0.917607	-1.201612	0.420564
N	-1.140552	0.070567	0.401320
C	-2.903435	-1.087517	1.451417
C	-2.520364	0.317794	0.834129
Pd	0.466992	1.200641	-0.153130

O	-0.249270	2.919618	0.391014
B	2.199891	3.411207	-0.563966
O	2.141999	4.748538	-0.379110
O	1.839720	2.888851	-1.788150
H	1.531450	3.564867	-2.410644
C	2.762734	2.332612	0.448645
C	3.845038	1.521019	0.031896
C	2.280488	2.148869	1.767872
C	4.397422	0.551346	0.861966
H	4.260437	1.659294	-0.970071
C	2.819617	1.171870	2.610836
H	1.462638	2.774839	2.129779
C	3.862089	0.367132	2.145867
H	5.223765	-0.076476	0.526636
H	2.431350	1.027974	3.619900
O	-1.871292	-1.983580	0.879890
H	-2.704661	-1.072334	2.533064
H	-2.523399	1.077334	1.627319
C	-4.282432	-1.593876	1.178911
C	-4.623280	-2.154392	-0.059387
C	-5.270341	-1.417922	2.155584
C	-5.941272	-2.529193	-0.316576
H	-3.856747	-2.299332	-0.821514
C	-6.592404	-1.783608	1.892404
H	-5.007037	-0.992013	3.127676
C	-6.928998	-2.338014	0.655362
H	-6.201307	-2.969747	-1.281341
H	-7.358071	-1.643312	2.658191
H	-7.961376	-2.628885	0.449631
C	-3.399205	0.778273	-0.307000

C	-4.567888	1.490978	-0.011068
C	-3.110518	0.455546	-1.638293
C	-5.441791	1.867762	-1.031008
H	-4.800066	1.746960	1.025577
C	-3.980428	0.840710	-2.661111
H	-2.198798	-0.091219	-1.886283
C	-5.149182	1.543704	-2.359354
H	-6.352463	2.419736	-0.789254
H	-3.744332	0.589898	-3.697519
H	-5.830529	1.842761	-3.158662
C	4.137469	-2.725685	-1.720638
F	5.084453	-2.399882	-0.824975
F	4.362476	-2.005246	-2.826120
F	4.272343	-4.018676	-2.016015
Cl	4.501533	-0.888126	3.161503
H	2.421336	5.052819	0.492536
C	-1.135348	3.541767	-0.494975
H	-0.691477	3.725293	-1.492915
H	-2.078401	2.982944	-0.629047
H	-1.390017	4.527651	-0.062887

TS-S11

H = -1497.654336

G = -1497.740606

Esol = -1498.029738

Cartesian coordinates

Pd	-0.889964	1.891900	-0.428175
C	-1.511276	-0.965331	-0.421502
C	-2.160867	-2.186536	-0.296167
C	-3.517347	-2.184495	0.043994

C	-4.160952	-0.963641	0.239919
C	-3.435833	0.227119	0.105021
N	-2.141482	0.223614	-0.218524
H	-4.065751	-3.121121	0.159522
H	-1.608639	-3.112398	-0.462519
H	-3.910205	1.196015	0.268332
C	-5.644458	-0.903358	0.559461
F	-6.025140	-1.987751	1.238103
F	-5.925363	0.181754	1.289849
F	-6.358092	-0.841883	-0.568800
C	-0.095791	-0.805694	-0.777967
O	0.720816	-1.815873	-0.948526
N	0.381984	0.385420	-0.907309
C	2.033679	-1.246655	-1.354319
H	2.124007	-1.473863	-2.424946
C	1.822350	0.317596	-1.165660
H	2.037430	0.821805	-2.118146
C	3.152680	-1.875687	-0.588486
C	4.372733	-2.097113	-1.239229
C	3.030817	-2.171078	0.775773
C	5.467034	-2.596409	-0.529726
H	4.470103	-1.879639	-2.306305
C	4.120642	-2.681509	1.480151
H	2.080207	-2.012084	1.287257
C	5.341882	-2.888421	0.830518
H	6.415538	-2.766755	-1.043072
H	4.018848	-2.917579	2.541441
H	6.194979	-3.285077	1.385027
C	2.626389	0.984404	-0.073007
C	3.870279	1.543181	-0.389970

C	2.175403	1.023906	1.253540
C	4.657426	2.125664	0.604883
H	4.227604	1.523225	-1.422575
C	2.957206	1.616715	2.247838
H	1.210975	0.586835	1.521067
C	4.201273	2.165844	1.925512
H	5.626844	2.556644	0.346506
H	2.596415	1.644353	3.278284
H	4.814130	2.626996	2.702797
O	0.294088	3.475436	-0.686389
H	-1.940919	3.199623	0.025011
H	-1.143687	3.601136	-0.134695
H	0.945447	3.444658	0.037415

TS-S12

H = -2364.151492

G = -2364.257020

Esol = -2364.637821

Cartesian coordinates

C	-0.400567	-2.007532	-0.733519
C	-0.771440	-3.295259	-0.368059
C	-2.125099	-3.552492	-0.124934
C	-3.045951	-2.515599	-0.267639
C	-2.601138	-1.243401	-0.645670
N	-1.308604	-1.001802	-0.863888
H	-2.458625	-4.545817	0.179692
H	-0.009722	-4.069412	-0.267548
H	-3.285859	-0.402020	-0.751282
C	0.968575	-1.551563	-0.975510
N	1.165748	-0.321934	-1.330032

C	3.195384	-1.508157	-1.209163
C	2.606781	-0.041422	-1.263993
Pd	-0.524888	0.829164	-1.290049
O	0.152669	2.695919	-1.553661
B	-1.438468	3.186187	-1.486272
O	-2.085753	2.325758	-2.466232
H	-2.091403	2.715091	-3.352741
O	-1.512951	4.542383	-1.794687
H	-1.389650	5.130804	-1.042591
C	-1.848368	2.554282	-0.037159
C	-0.959312	2.465010	1.065327
C	-3.164306	2.064968	0.157286
C	-1.350203	1.903764	2.281521
H	0.062461	2.835686	0.959311
C	-3.571193	1.498972	1.361699
H	-3.869987	2.127111	-0.674598
C	-2.651564	1.409282	2.418095
H	-0.656104	1.837626	3.120486
H	-4.584285	1.116720	1.495712
H	0.501950	2.867417	-2.442505
O	2.023325	-2.311395	-0.786037
H	3.418511	-1.842057	-2.233080
H	2.937539	0.438736	-2.194589
C	4.370230	-1.733374	-0.314269
C	4.218101	-1.894419	1.069286
C	5.654780	-1.696034	-0.871430
C	5.342509	-2.013063	1.885423
H	3.220232	-1.933892	1.507273
C	6.779766	-1.802632	-0.050993
H	5.778755	-1.584262	-1.952090

C	6.624307	-1.960106	1.328329
H	5.219251	-2.145190	2.962360
H	7.778474	-1.772752	-0.491399
H	7.503109	-2.049653	1.970470
C	2.947872	0.848526	-0.089971
C	4.058299	1.695849	-0.181685
C	2.222110	0.797489	1.107004
C	4.445231	2.474936	0.909818
H	4.631358	1.741785	-1.111206
C	2.604542	1.580731	2.197218
H	1.345799	0.153358	1.198664
C	3.718133	2.419476	2.102123
H	5.314919	3.130092	0.827979
H	2.032443	1.533741	3.126535
H	4.018122	3.031097	2.955581
C	-4.531809	-2.732095	-0.047150
F	-4.750759	-3.805918	0.713560
F	-5.156497	-2.907387	-1.215587
F	-5.074193	-1.663513	0.553862
Cl	-3.134082	0.661921	3.909832

TS-S13

H = -2270.239899

G = -2270.346666

Esol = -2270.824502

Cartesian coordinates

Pd	0.345249	0.497964	-0.970926
C	-0.710092	-2.315539	-0.519033
C	-1.485915	-3.444564	-0.264660
C	-2.712315	-3.274215	0.382313

C	-3.102284	-1.985764	0.743495
C	-2.255993	-0.907673	0.456826
N	-1.088337	-1.067968	-0.160987
H	-3.352725	-4.129818	0.603299
H	-1.130021	-4.427387	-0.574381
H	-2.540360	0.107828	0.734054
C	-4.445378	-1.721805	1.391378
F	-4.376526	-0.678250	2.230053
F	-5.368162	-1.436097	0.460754
F	-4.868322	-2.788021	2.076171
C	0.589632	-2.380567	-1.200804
O	1.089520	-3.547069	-1.574094
N	1.283202	-1.325002	-1.448831
C	2.307356	-3.244096	-2.321968
H	2.091135	-3.426470	-3.384289
C	2.586243	-1.752321	-2.001989
H	2.782173	-1.182742	-2.921997
C	3.100276	0.647934	2.706168
C	1.823782	0.082229	2.636818
C	0.781400	0.818275	2.074645
C	0.990175	2.112668	1.568958
C	2.269460	2.669808	1.691971
C	3.324939	1.948729	2.253564
H	1.652614	-0.919966	3.031456
H	-0.219868	0.384841	2.052227
H	2.453207	3.693481	1.357812
H	4.318531	2.390103	2.339198
C	0.119805	2.639584	-1.558753
H	1.352241	1.344738	-1.747554
C	-0.671626	2.396129	-0.410242

C	-0.165607	2.882521	0.959883
H	0.111571	3.945126	0.878121
C	-2.139336	2.134232	-0.576833
C	-2.636199	1.513872	-1.745397
C	-3.074086	2.464851	0.422616
C	-3.985724	1.206991	-1.886421
H	-1.952026	1.226606	-2.545028
C	-4.432902	2.163685	0.277743
H	-2.763513	2.974712	1.333070
C	-4.894925	1.521476	-0.869142
H	-4.332152	0.711562	-2.795953
H	-5.127579	2.429584	1.076832
H	-0.988612	2.848652	1.680204
C	3.764535	-1.506309	-1.012401
Cl	4.423372	-0.278945	3.359003
H	-5.951310	1.268162	-0.974040
C	1.283556	3.620042	-1.602932
H	-0.394560	2.584855	-2.522458
H	1.922086	3.529751	-0.711887
O	0.786991	4.922464	-1.793589
H	1.914606	3.399571	-2.476191
H	3.084347	-3.936181	-1.981859
C	5.058571	-1.987839	-1.690240
H	5.918574	-1.796214	-1.031517
H	5.049564	-3.068117	-1.902912
H	5.237403	-1.454421	-2.637657
C	3.890705	-0.003757	-0.719647
H	4.014568	0.577088	-1.648020
H	3.014838	0.383922	-0.184190
H	4.770612	0.180341	-0.085997

C	3.536209	-2.267572	0.301943
H	4.353501	-2.061494	1.007011
H	2.605181	-1.945486	0.791527
H	3.493955	-3.357797	0.154884
H	0.388616	5.243802	-0.973990

TS-S14-R

H = -2270.241620

G = -2270.352850

Esol = -2270.825700

Cartesian coordinates

Pd	0.763452	0.380941	-0.428147
C	3.717324	-0.078016	-0.400630
C	4.992605	-0.631718	-0.317400
C	5.112220	-1.965603	0.079204
C	3.953996	-2.683738	0.375340
C	2.710942	-2.050287	0.263419
N	2.595433	-0.780652	-0.122227
H	6.092453	-2.437758	0.165990
H	5.864286	-0.021078	-0.554038
H	1.792062	-2.587063	0.501317
C	4.017329	-4.146202	0.767711
F	3.975304	-4.924120	-0.320710
F	5.145095	-4.416096	1.428720
F	2.976351	-4.474128	1.546605
C	3.471075	1.325205	-0.764323
O	4.480349	2.111031	-1.101708
N	2.288171	1.832262	-0.747473
C	3.883949	3.381008	-1.507324
H	3.980084	3.452063	-2.599940

C	2.411566	3.278526	-1.027512
H	1.716387	3.538377	-1.839317
H	-0.496100	1.250671	-0.682084
C	2.063064	4.159905	0.208399
C	-0.690235	-1.123109	-0.267524
C	-1.555463	0.014363	-0.285007
C	-2.454871	0.342684	-1.489061
C	-0.560287	-2.129366	-1.396105
H	-0.504331	-1.545121	0.729878
H	4.462049	4.182894	-1.036487
C	2.216550	5.633127	-0.206668
H	1.558971	5.880577	-1.055464
H	1.941261	6.290446	0.631481
H	3.249466	5.887580	-0.490601
C	0.606414	3.907012	0.621063
H	-0.080941	4.060435	-0.226676
H	0.461939	2.886713	1.001200
H	0.312439	4.603869	1.420288
C	2.988652	3.838201	1.391761
H	4.049391	4.021959	1.160825
H	2.731487	4.472251	2.253230
H	2.880165	2.790490	1.712832
H	-2.445377	1.426479	-1.666047
H	-0.660069	-1.640845	-2.374394
O	-1.553907	-3.132453	-1.348754
H	-1.447479	-3.658860	-0.544644
H	0.450607	-2.576725	-1.373701
C	-3.883105	-0.087554	-1.214149
C	-4.841429	0.865904	-0.842968
C	-4.263151	-1.435304	-1.278039

C	-6.150611	0.493411	-0.541397
H	-4.564828	1.921096	-0.785056
C	-5.569964	-1.822757	-0.979163
H	-3.527749	-2.194808	-1.548395
C	-6.508678	-0.855984	-0.608026
H	-6.893943	1.238826	-0.256266
H	-5.866980	-2.870979	-1.034237
Cl	-8.138956	-1.335506	-0.226720
H	-2.060085	-0.132839	-2.396399
C	-2.074085	0.542551	1.022459
C	-2.481062	-0.349341	2.024880
C	-2.275138	1.917430	1.218570
C	-3.058891	0.125345	3.204943
H	-2.386697	-1.425166	1.868068
C	-2.842818	2.392995	2.398759
H	-1.979331	2.624473	0.441559
C	-3.235929	1.496405	3.398035
H	-3.382601	-0.582820	3.970580
H	-2.983130	3.466899	2.539307
H	-3.687300	1.866910	4.320773

TS-S15-S

H = -2270.241095

G = -2270.352041

Esol = -2270.825324

Cartesian coordinates

Pd	0.717312	-0.512510	0.146732
C	3.598354	0.298327	0.185702
C	4.800820	0.998546	0.239643
C	4.759516	2.393930	0.186893

C	3.519877	3.023652	0.087950
C	2.357944	2.242792	0.049231
N	2.396280	0.913103	0.090573
H	5.676676	2.983689	0.230688
H	5.741278	0.453401	0.323611
H	1.375654	2.713444	-0.009062
C	3.407127	4.530396	-0.023054
F	4.452995	5.135046	0.544849
F	3.357810	4.902024	-1.308977
F	2.287219	4.966706	0.570853
C	3.521050	-1.169131	0.230050
O	4.624564	-1.895186	0.304836
N	2.394220	-1.788851	0.187585
C	4.187544	-3.282319	0.438129
H	4.404296	-3.595359	1.469093
C	2.667718	-3.238209	0.118980
H	2.088531	-3.740076	0.908108
H	-0.327910	-1.626273	0.274231
C	2.265743	-3.868033	-1.249065
C	-0.917034	0.835949	-0.012802
C	-1.596784	-0.348602	0.362380
C	-2.440090	-1.154776	-0.634267
H	-2.561043	-2.177992	-0.251305
C	-1.981879	-0.520064	1.803687
C	-2.516832	0.565124	2.514243
C	-1.925739	-1.775368	2.431115
C	-2.974658	0.401402	3.824335
H	-2.613754	1.538066	2.029381
C	-2.377796	-1.939023	3.739205
C	-2.904649	-0.848735	4.441057

H	-3.398093	1.254361	4.358950
H	-2.318328	-2.919936	4.215656
H	-3.262575	-0.977143	5.464755
H	-1.510681	-2.631409	1.893077
C	-0.980887	1.497321	-1.369854
H	-0.747383	1.550838	0.800822
H	4.781941	-3.882470	-0.258586
C	2.625534	-5.363338	-1.197483
H	2.321820	-5.854938	-2.133585
H	3.706224	-5.536416	-1.078478
H	2.105394	-5.871631	-0.369663
C	0.749674	-3.735136	-1.465810
H	0.183085	-4.135725	-0.609626
H	0.448355	-2.689501	-1.618986
H	0.449606	-4.303259	-2.359129
C	3.005558	-3.177538	-2.404942
H	2.741948	-2.110201	-2.466192
H	4.099991	-3.260376	-2.314982
H	2.724140	-3.640612	-3.362389
C	-3.797685	-0.503689	-0.807821
C	-4.790166	-0.612412	0.178923
C	-4.083520	0.239457	-1.962957
C	-6.026795	0.013674	0.026937
H	-4.600559	-1.199094	1.079715
C	-5.317057	0.870275	-2.131080
H	-3.330453	0.310179	-2.750447
C	-6.283528	0.759603	-1.127893
H	-6.796617	-0.076540	0.794370
H	-5.537852	1.439795	-3.034823
H	-1.924424	-1.205084	-1.597647

Cl	-7.824149	1.546773	-1.322704
H	-1.992163	1.935702	-1.487095
O	-0.695712	0.578160	-2.404922
H	-0.801689	1.021208	-3.257342
H	-0.265945	2.341667	-1.382376

TS-S1

H = -2574.898564

G = -2575.018478

Esol = -2575.538478

Cartesian coordinates

Pd	-0.643428	-0.889642	0.365427
C	-0.565657	2.119686	0.543168
C	-0.914317	3.463777	0.648685
C	-2.229453	3.831736	0.345665
C	-3.127167	2.843299	-0.053839
C	-2.690947	1.515242	-0.139809
N	-1.443528	1.167126	0.158139
H	-2.549387	4.872710	0.414003
H	-0.168439	4.195817	0.959739
H	-3.365363	0.723744	-0.463755
C	-4.580465	3.148170	-0.352216
F	-5.349724	2.811093	0.692633
F	-4.764073	4.447185	-0.603014
F	-5.003577	2.444694	-1.410838
C	0.788237	1.604398	0.793850
O	1.784465	2.435187	1.046857
N	1.056761	0.345311	0.710383
C	2.945515	1.584860	1.368262
H	2.943529	1.482398	2.464862

C	2.522139	0.212424	0.724627
H	2.827565	-0.615287	1.378184
C	-5.171157	-1.278373	-0.742437
C	-4.812184	-1.314336	0.611230
C	-3.482813	-1.550993	0.964721
C	-2.498232	-1.730727	-0.022419
C	-2.882872	-1.737617	-1.373721
C	-4.211092	-1.501901	-1.737315
H	-5.572593	-1.154253	1.376878
H	-3.213686	-1.579187	2.022731
H	-2.144005	-1.913541	-2.159149
H	-4.506660	-1.488903	-2.787321
C	-0.507144	-2.306831	3.304908
H	-1.351224	-3.024501	3.303022
H	-0.916888	-1.322314	2.993032
C	0.573071	-2.745605	2.323517
H	1.435042	-2.081200	2.482138
H	0.912456	-3.751385	2.627074
C	0.216377	-2.772717	0.845053
C	-1.107607	-3.167860	0.459434
H	-1.771189	-3.537317	1.239790
O	0.111636	-2.238166	4.566254
H	-0.558378	-2.089618	5.244865
C	4.224163	2.202425	0.901059
C	5.385933	2.003667	1.656793
C	4.299123	2.890621	-0.317160
C	6.617107	2.470975	1.190771
H	5.330315	1.478674	2.614522
C	5.526765	3.366261	-0.775745
H	3.396248	3.048160	-0.907934

C	6.688693	3.151132	-0.027219
H	7.519506	2.311640	1.784777
H	5.579208	3.903757	-1.724903
H	7.649719	3.521472	-0.390727
C	3.081591	-0.003047	-0.667695
C	4.396754	-0.467196	-0.794623
C	2.375888	0.363351	-1.819446
C	5.007162	-0.535111	-2.045880
H	4.956238	-0.758081	0.096808
C	2.982017	0.284341	-3.075844
H	1.344302	0.710126	-1.743917
C	4.301915	-0.155850	-3.191343
H	6.037744	-0.886904	-2.127391
H	2.420362	0.572427	-3.967298
H	4.779498	-0.207870	-4.172180
Cl	-6.816724	-0.956074	-1.188877
H	-1.224033	-3.684704	-0.492856
C	1.342321	-3.026770	-0.106511
C	1.163597	-2.901379	-1.497997
C	2.606364	-3.428425	0.361640
C	2.203848	-3.163164	-2.384688
H	0.203077	-2.568554	-1.896085
C	3.644097	-3.707809	-0.529156
H	2.787000	-3.551378	1.428820
C	3.450488	-3.572901	-1.903796
H	2.044603	-3.038224	-3.457289
H	4.612794	-4.030517	-0.141478
H	4.267233	-3.776918	-2.598420

TS-S2

H = -2574.891791

G = -2575.011771

Esol = -2575.531603

Cartesian coordinates

Pd	0.251650	-0.218028	-0.589991
C	-0.646703	2.659625	-0.628618
C	-0.716019	4.049974	-0.568751
C	0.449532	4.756100	-0.257282
C	1.627094	4.044365	-0.026299
C	1.605889	2.646215	-0.097754
N	0.493664	1.976042	-0.385089
H	0.441340	5.845531	-0.191997
H	-1.661478	4.557705	-0.762180
H	2.503004	2.057336	0.094719
C	2.932959	4.754005	0.264926
F	3.581906	5.032521	-0.872579
F	2.720060	5.904819	0.911624
F	3.734909	3.986623	1.016725
C	-1.794967	1.795102	-0.949378
O	-3.018467	2.293280	-1.029171
N	-1.648688	0.524954	-1.111112
C	-3.903453	1.187163	-1.425465
H	-4.101399	1.331964	-2.497585
C	-2.978109	-0.081586	-1.236523
H	-3.018914	-0.694277	-2.147700
C	4.609790	0.348054	0.648832
C	4.315221	-0.082866	-0.653590
C	3.083071	-0.680022	-0.909087
C	2.116179	-0.809938	0.108341
C	2.440102	-0.385667	1.410043

C	3.680672	0.190188	1.686783
H	5.057435	0.036890	-1.443891
H	2.876282	-1.067478	-1.909456
H	1.715585	-0.490377	2.219689
H	3.933467	0.526625	2.693262
C	-0.107368	-4.206081	1.616681
H	-0.240216	-4.396944	2.698417
H	0.520624	-5.019301	1.221586
C	0.639570	-2.864512	1.467371
H	-0.015937	-2.052369	1.818076
C	1.062968	-2.605853	0.029542
C	-0.014088	-2.210320	-0.857994
H	-1.020225	-2.429626	-0.492072
O	-1.331860	-4.264480	0.925183
H	-1.993965	-3.741622	1.400064
C	-5.185512	1.205135	-0.651877
C	-6.351340	0.732390	-1.266698
C	-5.223619	1.602069	0.690647
C	-7.542115	0.642325	-0.542590
H	-6.330946	0.434177	-2.318590
C	-6.416358	1.522379	1.409913
H	-4.321121	1.983753	1.170099
C	-7.575568	1.036436	0.797288
H	-8.447524	0.273543	-1.029146
H	-6.442240	1.840702	2.454306
H	-8.507691	0.973189	1.362847
C	-3.298188	-0.963246	-0.046446
C	-4.135499	-2.071671	-0.218578
C	-2.797589	-0.679405	1.231247
C	-4.478431	-2.879418	0.867728

H	-4.525762	-2.307392	-1.211573
C	-3.130617	-1.489900	2.318683
H	-2.134937	0.174339	1.382431
C	-3.976934	-2.590279	2.141219
H	-5.132701	-3.740649	0.719113
H	-2.736764	-1.256773	3.310563
H	-4.247243	-3.219086	2.992460
Cl	6.142797	1.085959	0.980616
H	0.123794	-2.403323	-1.928041
C	2.171534	-3.487070	-0.464832
C	3.345216	-3.655558	0.295012
C	2.041934	-4.210999	-1.660540
C	4.358195	-4.507210	-0.133095
H	3.483246	-3.083032	1.213856
C	3.058963	-5.068903	-2.090463
H	1.129758	-4.133312	-2.252132
C	4.220069	-5.217670	-1.332285
H	5.264838	-4.615242	0.466108
H	2.934416	-5.628906	-3.019769
H	1.513535	-2.895027	2.131392
H	5.015304	-5.886170	-1.669032

TS-S3

H = -2574.889965

G = -2575.011633

Esol = -2575.530035

Cartesian coordinates

Pd	-0.270244	0.253048	-0.841948
C	0.375549	-2.679242	-0.559387
C	0.320235	-4.059765	-0.380810

C	-0.905694	-4.631412	-0.026998
C	-2.014177	-3.800196	0.131711
C	-1.870893	-2.422218	-0.072492
N	-0.703740	-1.879710	-0.405899
H	-0.998865	-5.709274	0.116422
H	1.217224	-4.663906	-0.520417
H	-2.719382	-1.747414	0.032929
C	-3.358667	-4.345818	0.565835
F	-4.357735	-3.618848	0.047618
F	-3.511548	-5.615779	0.178052
F	-3.472920	-4.303313	1.900267
C	1.601099	-1.949325	-0.921023
O	2.774037	-2.561837	-0.944518
N	1.576186	-0.685607	-1.169741
C	3.767442	-1.568936	-1.373372
H	3.991057	-1.803787	-2.424750
C	2.960292	-0.210789	-1.307801
H	3.069990	0.322743	-2.261711
C	-4.679789	-0.003303	0.319650
C	-4.353162	0.159826	-1.033614
C	-3.104857	0.680989	-1.375796
C	-2.165450	1.018801	-0.382409
C	-2.526668	0.873175	0.969867
C	-3.771158	0.356057	1.326054
H	-5.074785	-0.118871	-1.802625
H	-2.863287	0.813246	-2.432268
H	-1.829177	1.169166	1.755617
H	-4.047864	0.231664	2.373888
C	-1.442135	4.808371	-2.131738
H	-0.396891	4.720687	-2.492542

H	-1.423971	5.479923	-1.252737
C	-1.955961	3.424060	-1.724977
H	-2.975873	3.524296	-1.332845
H	-2.026338	2.830762	-2.646269
C	-1.023889	2.734422	-0.743720
C	0.177621	2.169312	-1.334352
H	0.216431	2.199792	-2.431275
O	-2.312423	5.270312	-3.135624
H	-2.070297	6.173971	-3.373516
Cl	-6.221145	-0.665613	0.755166
C	5.014768	-1.650168	-0.544297
C	6.196127	-1.103586	-1.062320
C	5.011288	-2.191558	0.745835
C	7.359167	-1.084642	-0.291353
H	6.209445	-0.690117	-2.074671
C	6.178651	-2.181145	1.512194
H	4.097723	-2.632782	1.146275
C	7.351934	-1.623123	0.998633
H	8.276095	-0.656712	-0.702044
H	6.171642	-2.612682	2.515464
H	8.263515	-1.614929	1.599938
C	3.313224	0.731415	-0.177923
C	3.988383	1.926657	-0.448524
C	2.974221	0.424403	1.147466
C	4.323197	2.803307	0.587303
H	4.253801	2.177174	-1.478949
C	3.314732	1.293587	2.184439
H	2.437904	-0.498078	1.377537
C	3.988075	2.487232	1.906054
H	4.847426	3.734577	0.362923

H	3.050712	1.039968	3.213402
H	4.250971	3.170473	2.716420
C	-0.928993	3.308897	0.636031
C	-1.946392	4.137386	1.142437
C	0.161733	3.012272	1.473685
C	-1.869093	4.663288	2.432082
H	-2.819334	4.370144	0.533031
C	0.239407	3.536505	2.763200
H	0.959519	2.353544	1.134074
C	-0.775045	4.366291	3.249249
H	-2.670189	5.307386	2.800776
H	1.100446	3.292655	3.389061
H	1.137306	2.399024	-0.864425
H	-0.715209	4.777259	4.259330

TS-S4

H = -2574.907377

G = -2575.028073

Esol = -2575.546327

Cartesian coordinates

Pd	0.891333	-1.352178	-0.043681
C	3.285314	0.268896	-0.795902
C	4.589514	0.694470	-1.032687
C	5.635251	-0.194882	-0.775944
C	5.329566	-1.468517	-0.298207
C	3.991076	-1.817646	-0.082370
N	2.992259	-0.966115	-0.326597
H	6.673437	0.098715	-0.940132
H	4.768068	1.702465	-1.407992
H	3.724854	-2.802368	0.302452

C	6.418754	-2.493901	-0.050040
F	7.570800	-1.897728	0.269309
F	6.075277	-3.320120	0.946087
F	6.622270	-3.233115	-1.146797
C	2.110437	1.121267	-1.027970
O	2.275276	2.363322	-1.449330
N	0.913942	0.696845	-0.814716
C	0.932129	2.888630	-1.737738
H	0.811656	2.808922	-2.828324
C	-0.002730	1.824878	-1.033332
H	-0.786322	1.530194	-1.744297
C	-6.257257	-1.754997	-1.253034
C	-5.362440	-2.822810	-1.360436
C	-3.994533	-2.592135	-1.207325
C	-3.493789	-1.311620	-0.933832
C	-4.413389	-0.254008	-0.859649
C	-5.783737	-0.462516	-1.012342
H	-5.737393	-3.824403	-1.574953
H	-3.319848	-3.436684	-1.341446
H	-4.053860	0.763110	-0.681474
H	-6.486678	0.368999	-0.947933
C	-0.649174	-2.947744	0.247380
H	1.085755	-2.795768	0.443126
C	-1.255078	-1.667085	0.370393
C	-2.004816	-1.023744	-0.799884
H	-1.889920	0.060476	-0.701317
C	-1.486362	-1.123337	1.745878
C	-0.699103	-1.541951	2.841781
C	-2.507087	-0.191099	1.997013
C	-0.935834	-1.060422	4.126832

H	0.122456	-2.244276	2.696807
C	-2.756681	0.275687	3.287495
H	-3.135390	0.168021	1.189814
C	-1.975114	-0.154036	4.359443
H	-0.308170	-1.400495	4.953366
H	-3.567981	0.987428	3.448772
H	-1.503635	-1.304462	-1.737354
C	0.787482	4.312663	-1.303390
C	-0.003585	5.175822	-2.071084
C	1.349358	4.770766	-0.104613
C	-0.246686	6.481065	-1.637192
H	-0.433193	4.827398	-3.014416
C	1.114285	6.077077	0.322819
H	1.973196	4.105182	0.493171
C	0.310465	6.932029	-0.438377
H	-0.864369	7.148880	-2.241314
H	1.558002	6.430478	1.255992
H	0.125591	7.953772	-0.099811
C	-0.645807	2.294305	0.252235
C	-1.856725	2.995165	0.185171
C	-0.013672	2.136636	1.490959
C	-2.413785	3.555223	1.335885
H	-2.354403	3.127649	-0.779222
C	-0.572152	2.691964	2.642709
H	0.919005	1.575011	1.562990
C	-1.767107	3.410500	2.566289
H	-3.351582	4.111093	1.270605
H	-0.075489	2.555602	3.605056
H	-2.201047	3.848987	3.467386
Cl	-7.964076	-2.032553	-1.435864

H	-2.168928	0.214948	5.368862
C	-0.779587	-3.895028	-0.932054
H	-0.529382	-3.512931	1.176287
H	-1.112683	-3.360820	-1.839306
O	-1.631952	-4.965090	-0.591529
H	0.191732	-4.350818	-1.167932
H	-2.455043	-4.620390	-0.219048

TS-S5-R

H = -2574.907051

G = -2575.027818

Esol = -2575.545284

Cartesian coordinates

Pd	0.235025	0.988745	0.598118
C	3.173568	1.291967	0.164885
C	4.433826	1.804171	-0.131485
C	4.523862	3.117178	-0.598088
C	3.351671	3.858351	-0.744939
C	2.122078	3.266094	-0.434525
N	2.036673	2.009280	0.007732
H	5.490455	3.557702	-0.848295
H	5.315875	1.177774	0.004211
H	1.188592	3.816319	-0.554215
C	3.391835	5.304250	-1.197713
F	3.481135	6.123375	-0.143194
F	4.445982	5.528413	-1.987669
F	2.279063	5.622762	-1.872610
C	2.954853	-0.075883	0.656012
O	3.960218	-0.935654	0.680990
N	1.788548	-0.482734	1.016631

C	3.438235	-2.167365	1.295658
H	3.782320	-2.147198	2.340290
C	1.881291	-1.929824	1.257925
H	1.438742	-2.157784	2.233479
H	-0.683753	2.109338	0.105937
C	3.952242	-3.389473	0.600867
C	4.211648	-4.539490	1.355856
C	4.090442	-3.431276	-0.792710
C	4.590581	-5.726409	0.723965
H	4.118485	-4.508613	2.444977
C	4.479797	-4.613417	-1.421831
H	3.897417	-2.535752	-1.385088
C	4.723782	-5.764721	-0.665901
H	4.791885	-6.619258	1.319672
H	4.591835	-4.638590	-2.507901
H	5.025917	-6.690072	-1.161097
C	1.124532	-2.708933	0.201779
C	0.656279	-3.992971	0.510405
C	0.882661	-2.187808	-1.074689
C	-0.052503	-4.736980	-0.433157
H	0.855606	-4.416840	1.498055
C	0.169026	-2.929071	-2.021873
H	1.238846	-1.189699	-1.334958
C	-0.304568	-4.203368	-1.702193
H	-0.409278	-5.737828	-0.180233
H	-0.015796	-2.508482	-3.012911
H	-0.861929	-4.783857	-2.440468
C	-1.554649	0.112232	1.388042
C	-2.094957	0.981800	0.412357
C	-2.420913	0.458331	-0.989526

C	-2.869251	2.192623	0.848303
C	-2.918479	3.357753	0.063586
C	-3.660202	2.126704	2.004789
C	-3.724345	4.432310	0.431587
H	-2.309944	3.429695	-0.841910
C	-4.472387	3.203110	2.373891
H	-3.669182	1.216909	2.606935
C	-4.506254	4.357375	1.591007
H	-3.743741	5.333596	-0.184826
H	-5.087202	3.131665	3.273572
H	-5.141179	5.198018	1.878623
C	-1.665821	-1.386398	1.331145
H	-1.565265	0.483477	2.420403
H	-1.627810	-0.222273	-1.325490
H	-2.740937	-1.634180	1.440262
C	-3.752442	-0.270555	-1.023888
C	-3.788056	-1.657538	-1.228224
C	-4.967994	0.410881	-0.852670
C	-4.996225	-2.355567	-1.249187
H	-2.856508	-2.207273	-1.385129
C	-6.182946	-0.273484	-0.867355
H	-4.973971	1.492605	-0.711614
C	-6.192287	-1.658442	-1.060394
H	-5.017502	-3.433575	-1.414172
H	-7.124899	0.260449	-0.735769
Cl	-7.705354	-2.519050	-1.075558
H	-2.436481	1.306188	-1.689533
O	-0.915823	-1.926072	2.399405
H	-1.103268	-2.871983	2.447065
H	-1.342367	-1.788801	0.358492

TS-S6-S

H = 1-2574.907021

G = -2575.026299

Esol = -2575.545167

Cartesian coordinates

Pd	0.121872	-0.319744	-0.970673
C	0.157910	2.640879	-0.719243
C	0.574799	3.951280	-0.509478
C	1.916713	4.179419	-0.182781
C	2.777067	3.089218	-0.075280
C	2.279524	1.798611	-0.294333
N	1.002096	1.585699	-0.608903
H	2.287555	5.191820	-0.016015
H	-0.140512	4.768969	-0.603674
H	2.926485	0.922094	-0.219401
C	4.241397	3.239356	0.287880
F	4.484658	2.690908	1.483537
F	5.010471	2.610920	-0.613597
F	4.603628	4.523649	0.329760
C	-1.223828	2.256860	-1.055444
O	-2.204650	3.142826	-0.992247
N	-1.519235	1.042025	-1.352690
C	-3.465551	2.402233	-1.136298
H	-3.997803	2.857192	-1.981536
C	-2.975683	0.941550	-1.519088
H	-3.187940	0.756162	-2.583277
H	1.412814	-1.018181	-0.577435
C	-4.282141	2.506208	0.122569
C	-5.640761	2.168693	0.063914

C	-3.710068	2.850957	1.351791
C	-6.413327	2.156806	1.224887
H	-6.096617	1.902040	-0.893155
C	-4.487020	2.846326	2.513104
H	-2.657700	3.133983	1.403988
C	-5.836769	2.493340	2.453580
H	-7.470480	1.888636	1.170389
H	-4.035071	3.122463	3.468309
H	-6.442609	2.488210	3.362151
C	-3.531674	-0.206364	-0.711127
C	-4.445734	-1.093873	-1.287798
C	-3.100692	-0.424456	0.605817
C	-4.924113	-2.188228	-0.560061
H	-4.780015	-0.937328	-2.317034
C	-3.568277	-1.519273	1.329481
H	-2.379758	0.252797	1.065342
C	-4.481958	-2.404125	0.746964
H	-5.635186	-2.877647	-1.020129
H	-3.205834	-1.692377	2.344073
H	-4.843502	-3.266052	1.311742
C	-0.745407	-2.207371	-1.491502
C	0.285773	-2.581185	-0.610714
C	1.563182	-3.291948	-1.086748
C	-0.094465	-2.813266	0.825839
C	-0.947555	-3.896798	1.089163
C	0.366034	-2.033906	1.896006
C	-1.333432	-4.193297	2.397725
H	-1.313106	-4.505281	0.258538
C	-0.029135	-2.324981	3.203783
C	-0.878208	-3.405791	3.458705

H	-1.997592	-5.039474	2.587077
H	0.331186	-1.705136	4.027821
H	1.451080	-4.339510	-0.764562
H	-1.182732	-3.634283	4.482399
H	1.031388	-1.191196	1.704080
C	-0.693696	-2.460523	-2.978717
H	-1.750084	-2.160699	-1.063704
C	2.832654	-2.691810	-0.531811
C	3.269743	-2.954359	0.774062
C	3.532547	-1.736027	-1.288884
C	4.333976	-2.244110	1.333334
H	2.757862	-3.707483	1.375891
C	4.600695	-1.019198	-0.746948
H	3.228137	-1.538382	-2.320108
C	4.980288	-1.260871	0.577507
H	4.659534	-2.440498	2.355713
H	5.137048	-0.274613	-1.336893
H	1.594105	-3.303024	-2.182448
Cl	6.262261	-0.319990	1.286282
H	0.256185	-2.086277	-3.407775
O	-0.834059	-3.856640	-3.154014
H	-0.884094	-4.054853	-4.098837
H	-1.513276	-1.896687	-3.462542

TS-S7

H = -3536.568271

G = -3536.710444

Esol = -3537.241908

Cartesian coordinates

Pd	0.895723	-1.470312	-1.040266
----	----------	-----------	-----------

C	1.313426	1.947710	-0.764541
C	0.956535	3.097953	-0.050741
C	-0.208081	3.761071	-0.423028
C	-0.941768	3.269913	-1.505290
C	-0.470459	2.138654	-2.184295
N	0.627244	1.486802	-1.816274
H	-0.558205	4.632324	0.133403
H	1.551548	3.412608	0.805590
C	-2.211797	3.962128	-1.930341
F	-2.948109	3.200944	-2.749081
F	-2.968841	4.275883	-0.862539
F	-1.946522	5.113023	-2.573765
C	2.412473	1.097662	-0.270677
O	3.360012	1.672099	0.474080
N	2.477990	-0.176246	-0.429560
C	4.079427	0.592444	1.135881
H	3.612697	0.485772	2.126007
C	3.685555	-0.655810	0.258830
H	3.411385	-1.485210	0.924749
H	-1.927831	-1.567882	0.308096
C	5.540302	0.894541	1.258484
C	6.237705	0.446956	2.386409
C	6.239217	1.533271	0.225863
C	7.621535	0.617531	2.475830
H	5.693419	-0.041523	3.199306
C	7.619176	1.711306	0.318604
H	5.696740	1.886789	-0.651780
C	8.314878	1.248292	1.440324
H	8.157312	0.262751	3.359295
H	8.156872	2.209536	-0.491355

H	9.396663	1.384802	1.508810
C	4.746055	-1.129311	-0.711332
C	5.770370	-1.965099	-0.246378
C	4.768513	-0.699674	-2.043423
C	6.811930	-2.347764	-1.091092
H	5.759165	-2.306511	0.791620
C	5.807687	-1.089389	-2.893325
H	3.966385	-0.062080	-2.418899
C	6.834539	-1.908014	-2.418485
H	7.608398	-2.993027	-0.713322
H	5.813169	-0.750235	-3.931940
H	7.648676	-2.208796	-3.082031
C	-6.000367	1.126600	0.058053
C	-6.256605	-0.094981	-0.569326
C	-5.197220	-0.811618	-1.127513
C	-3.881981	-0.327343	-1.070128
C	-3.656233	0.900338	-0.431853
C	-4.701761	1.632710	0.130020
H	-7.277259	-0.477194	-0.615760
H	-5.397230	-1.771250	-1.609040
H	-2.638976	1.283588	-0.356575
H	-4.511271	2.588946	0.617349
C	0.077276	-3.391172	-0.305586
H	-0.041138	-0.472588	-0.082773
H	0.764982	-4.119568	-0.751835
C	-0.849927	-2.738025	-1.128570
C	-2.144122	-2.135300	-0.602344
C	-2.726993	-1.124097	-1.620013
H	-1.913265	-0.445910	-1.917599
O	0.051393	-3.518060	1.031145

H	-0.409298	-2.779856	1.480309
C	-3.158615	-3.193345	-0.205759
C	-3.578540	-4.183842	-1.105333
C	-3.724919	-3.165100	1.075052
C	-4.546262	-5.119661	-0.735317
H	-3.146060	-4.223896	-2.108501
C	-4.693342	-4.100132	1.450007
H	-3.405184	-2.393589	1.780336
C	-5.108512	-5.079588	0.545034
H	-4.863688	-5.884960	-1.448204
H	-5.125984	-4.060897	2.452682
H	-3.035075	-1.670514	-2.526626
Cl	-7.323194	2.033238	0.760529
H	-5.866228	-5.811432	0.835208
H	-0.867065	-3.078908	-2.170895
S	-0.283072	0.124926	2.102770
C	-1.641229	1.162746	2.862937
F	-1.660161	2.366090	2.290290
F	-2.814045	0.572179	2.683863
F	-1.404119	1.299278	4.160331
O	-0.623774	0.354468	0.610595
O	-0.562644	-1.260347	2.511242
O	0.987705	0.736133	2.489348
H	-1.022665	1.739031	-3.038872

TS-S8

H = -2438.825491

G = -2438.936518

Esol = -2439.302568

Cartesian coordinates

C	0.297324	1.916807	-0.592728
C	0.500447	3.297324	-0.617164
C	1.800010	3.782191	-0.471826
C	2.840733	2.865498	-0.319393
C	2.549631	1.496471	-0.324157
N	1.310130	1.028763	-0.451680
H	2.004204	4.853911	-0.486627
H	-0.352442	3.963603	-0.748612
H	3.343341	0.756872	-0.239931
C	-1.033263	1.309584	-0.726767
N	-1.205748	0.059015	-0.529640
C	-3.183927	1.084171	-1.316796
C	-2.613047	-0.270120	-0.721026
Pd	0.566426	-1.159301	-0.422335
O	-0.505609	-2.783798	-0.716211
B	1.452699	-3.945758	-0.995841
O	1.313569	-3.873381	-2.344743
H	0.454071	-3.399417	-2.548610
O	1.234208	-5.132787	-0.335368
H	1.478503	-5.094772	0.595641
C	2.247434	-2.777697	-0.205542
C	2.009380	-2.438738	1.156643
C	3.401388	-2.210349	-0.817080
C	2.881486	-1.593491	1.872580
H	1.179364	-2.906822	1.694148
C	4.285184	-1.405749	-0.111792
H	3.596015	-2.451549	-1.864766
C	4.010780	-1.097487	1.235105
H	2.682583	-1.334513	2.913363
H	5.181428	-0.998524	-0.583382

O	-2.098398	2.042818	-1.064075
H	-3.256329	0.993658	-2.410734
H	-2.659402	-1.076598	-1.468540
C	-4.481103	1.575008	-0.751463
C	-4.535901	2.201946	0.500164
C	-5.670177	1.318446	-1.443343
C	-5.765067	2.559400	1.052954
H	-3.611654	2.404016	1.042847
C	-6.902532	1.669172	-0.886639
H	-5.632404	0.834226	-2.423001
C	-6.951859	2.288806	0.363952
H	-5.798820	3.045551	2.030618
H	-7.825029	1.461360	-1.433533
H	-7.914193	2.564528	0.801383
C	-3.268596	-0.736991	0.559519
C	-4.472810	-1.447899	0.485177
C	-2.739313	-0.423726	1.816202
C	-5.149767	-1.819146	1.646756
H	-4.885311	-1.708157	-0.492442
C	-3.411252	-0.802249	2.981288
H	-1.790191	0.110807	1.883897
C	-4.621517	-1.494465	2.899986
H	-6.090415	-2.369913	1.574212
H	-2.985598	-0.555939	3.957112
H	-5.148770	-1.788431	3.810591
C	4.264746	3.323681	-0.111676
F	4.547633	3.443899	1.193886
F	4.475953	4.522009	-0.680264
F	5.139295	2.455312	-0.638431
Cl	5.077694	-0.001303	2.085064

O	-0.885759	-2.584473	-1.985626
---	-----------	-----------	-----------

TS-S9

H = -1536.670497

G = -1536.788946

Esol = -1537.308549

Cartesian coordinates

Pd	0.503171	-0.887341	-0.611413
----	----------	-----------	-----------

C	0.927333	2.060614	-1.070085
---	----------	----------	-----------

C	1.410339	3.365974	-1.091493
---	----------	----------	-----------

C	2.684805	3.610271	-0.568502
---	----------	----------	-----------

C	3.413814	2.539980	-0.055238
---	----------	----------	-----------

C	2.850471	1.257111	-0.067043
---	----------	----------	-----------

N	1.635075	1.027401	-0.554006
---	----------	----------	-----------

H	3.107597	4.616145	-0.569956
---	----------	----------	-----------

H	0.800298	4.163367	-1.517093
---	----------	----------	-----------

H	3.406064	0.397260	0.312667
---	----------	----------	----------

C	4.790000	2.716678	0.551966
---	----------	----------	----------

F	5.312469	3.904774	0.240150
---	----------	----------	----------

F	4.724786	2.623725	1.887996
---	----------	----------	----------

F	5.621172	1.757941	0.119978
---	----------	----------	----------

C	-0.374410	1.664902	-1.626900
---	-----------	----------	-----------

O	-1.223211	2.564501	-2.097714
---	-----------	----------	-----------

N	-0.725673	0.428106	-1.673151
---	-----------	----------	-----------

C	-2.492845	1.855467	-2.329341
---	-----------	----------	-----------

H	-2.851270	2.166177	-3.317924
---	-----------	----------	-----------

C	-2.029669	0.344873	-2.353188
---	-----------	----------	-----------

H	-1.826111	0.056848	-3.397954
---	-----------	----------	-----------

C	-2.348130	-0.287977	3.112552
---	-----------	-----------	----------

C	-1.410168	0.650217	2.672458
---	-----------	----------	----------

C	-0.115953	0.228796	2.372041
---	-----------	----------	----------

C	0.264138	-1.116740	2.502018
C	-0.685224	-2.028069	2.984805
C	-1.988441	-1.626156	3.283977
H	-1.696802	1.696338	2.570129
H	0.618192	0.966260	2.041384
H	-0.406312	-3.073032	3.142035
H	-2.721087	-2.343254	3.656149
C	0.998745	-4.095948	-0.813460
H	1.436913	-4.928727	-0.234748
H	1.722261	-3.846696	-1.603363
C	0.806208	-2.959947	0.172763
H	-0.422152	-2.110322	-0.754331
H	-0.020909	-3.173457	0.856026
C	1.799549	-2.078765	0.663867
C	1.653853	-1.553731	2.105153
H	2.002985	-2.347314	2.787919
O	-0.224809	-4.561257	-1.319664
C	3.189611	-2.040719	0.103250
C	3.434022	-1.927774	-1.281218
C	4.301156	-2.042952	0.966858
C	4.730910	-1.814759	-1.778168
H	2.593324	-1.882364	-1.976835
C	5.602229	-1.933745	0.467839
H	4.161844	-2.138905	2.043687
C	5.823310	-1.813645	-0.904546
H	4.889383	-1.716591	-2.854288
H	6.445879	-1.939196	1.161103
H	2.345133	-0.710439	2.240597
C	-3.488463	2.204653	-1.256604
C	-4.840405	1.918067	-1.487065

C	-3.094993	2.710374	-0.012072
C	-5.782370	2.107025	-0.476244
H	-5.156307	1.522464	-2.455386
C	-4.040691	2.905302	0.997118
H	-2.049298	2.961251	0.171680
C	-5.382927	2.594731	0.771222
H	-6.832103	1.871469	-0.662801
H	-3.729518	3.298734	1.966872
H	-6.118480	2.738460	1.565185
C	-2.967707	-0.667260	-1.754491
C	-3.715745	-1.496353	-2.598687
C	-3.133803	-0.769122	-0.365746
C	-4.628616	-2.410812	-2.065311
H	-3.587213	-1.426475	-3.682527
C	-4.046115	-1.678991	0.166414
H	-2.560166	-0.128177	0.303069
C	-4.796297	-2.500315	-0.681707
H	-5.207905	-3.053173	-2.731951
H	-4.183695	-1.732038	1.247048
H	-5.512227	-3.210722	-0.262659
Cl	-3.983898	0.215949	3.444258
H	6.839181	-1.717248	-1.292877
H	-0.519721	-3.970086	-2.025396