Supporting Information

Suzuki–Miyaura Cross-Coupling of Aryl Carbamates and Sulfamates: Experimental and Computational Studies

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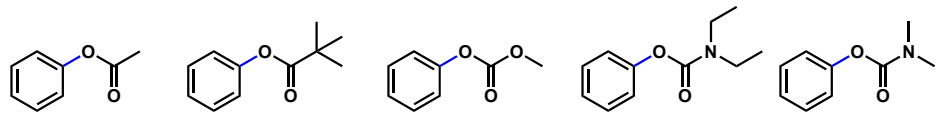
Complete Reference of Gaussian 03

Gaussian 03, Revision D.01: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A., Gaussian, Inc., Wallingford CT, **2004**.

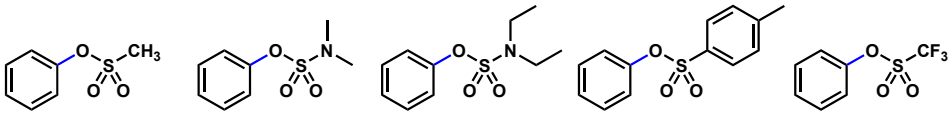
Bond Dissociation Enthalpies (BDEs) of C–O Bonds

Gas phase BDEs of various Ar–O bonds are calculated using B3LYP/6-31G(d). The results are shown below. The ArO–carbonyl bond is much weaker than the Ar–O bond in *N*,*N*-dimethyl phenyl *O*-carbamate.

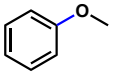
Aryl–O bonds



BDE ΔH(298K) 92.3 91.5 92.1 89.3 89.2

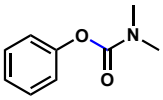


BDE ΔH(298K) 92.4 80.9 78.3 96.9 93.2



BDE ΔH(298K) 95.7

ArO–carbonyl bonds



66.8

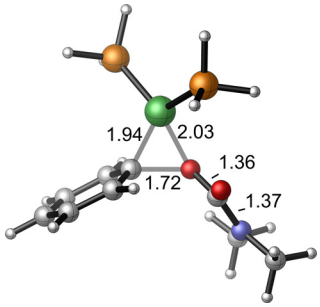
B3LYP/6-31G(d), gas phase calculations

Comparison of Mono- and Bis-ligated Oxidative Addition Transition States

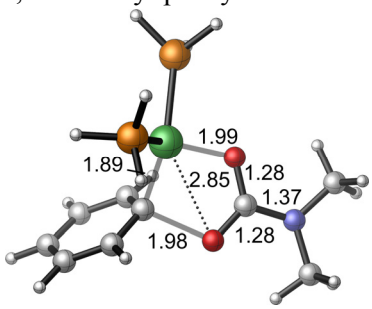
These calculations are performed using PH_3 as model ligand. Energies reported are Gibbs free energies with respect to $Ni(PH_3)_2$ at the B3LYP/LANL2DZ-6-31G(d) level. Geometries are optimized in gas phase. Single point CPCM solvation energy corrections are included.

The calculations suggest that the mono-ligated pathway is strongly favored for oxidative additions with both carbamates and sulfamates. It is postulated that bulkier ligands, such as PCy_3, may further increase the preference of mono-ligated pathway due to steric effects.

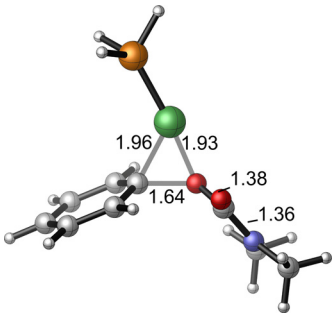
Oxidative addition transition states of the couplings with *N*,*N*-dimethyl phenyl *O*-carbamate.



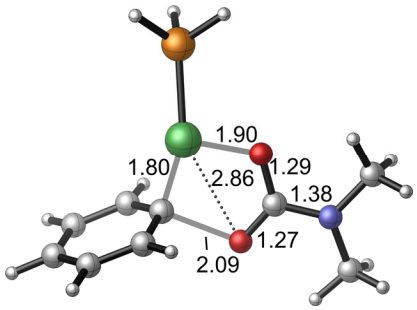
TS-S1
bis-ligated 3-centered TS
$\Delta G^{\ddagger}_{(sol)}$ = 28.8 kcal/mol



TS-S2
bis-ligated 5-centered TS
$\Delta G^{\ddagger}_{(sol)}$ = 22.6 kcal/mol

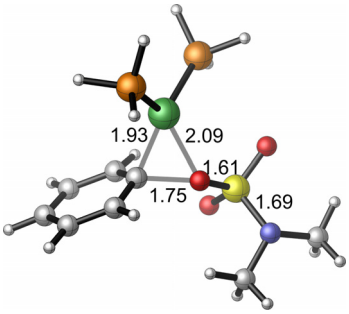


TS-S3
mono-ligated 3-centered TS
$\Delta G^{\ddagger}_{(sol)}$ = 27.6 kcal/mol

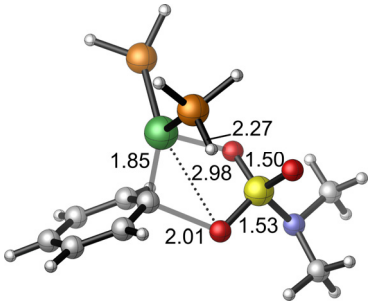


TS-S4
mono-ligated 5-centered TS
$\Delta G^{\ddagger}_{(sol)}$ = 16.5 kcal/mol

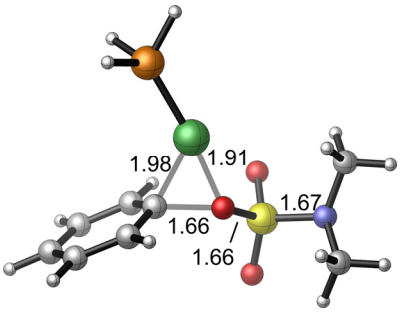
Oxidative addition transition states of the couplings with *N*,*N*-dimethyl phenyl *O*-sulfamate.



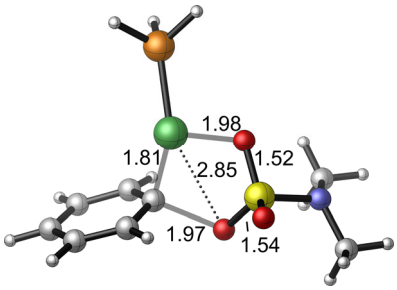
TS-S5
bis-ligated 3-centered TS
$\Delta G^{\ddagger}$ = 27.3 kcal/mol



TS-S6
bis-ligated 5-centered TS
$\Delta G^{\ddagger}$ = 21.0 kcal/mol



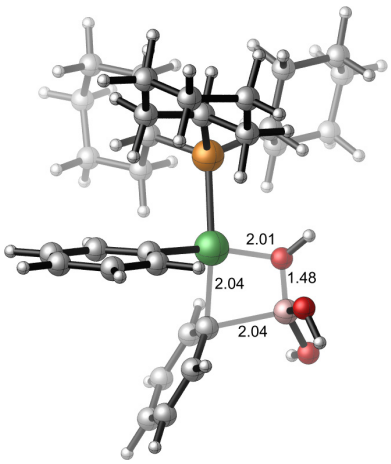
TS-S7
mono-ligated 3-centered TS
$\Delta G^{\ddagger}$ = 26.2 kcal/mol



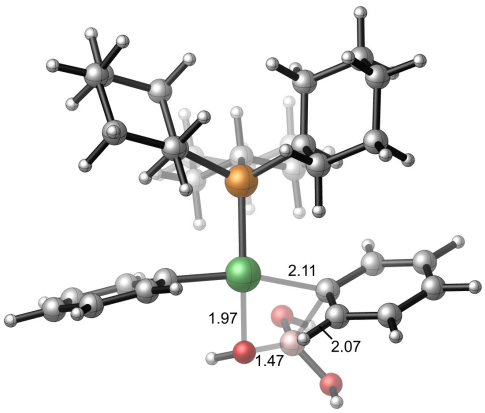
TS-S8
mono-ligated 5-centered TS
$\Delta G^{\ddagger}$ = 16.5 kcal/mol

Possible Isomers of the Transmetallation Transition States

Our calculations suggest that the transmetallation (**TS21**) occurs via a four-center transition state, in consistent with previous theoretical studies. In the most favorable transmetallation transition state (**TS21**), the two aryl groups on the Ni are *cis* to each other. The trans transmetallation transition state (**TS-S9**) is 3.5 kcal/mol higher in energy than **TS21**, presumably due to the repulsions between the PCy_3 ligand and the aryl groups that are adjacent to the ligand. The structures of these transition states are shown below.



TS21
two aryl groups are *cis*
$\Delta\Delta G^{\ddagger}$ = 0.0 kcal/mol



TS-S9
two aryl groups are *trans*
$\Delta\Delta G^{\ddagger}$ = 3.5 kcal/mol

Single Point Calculations using Larger Basis Sets and Other Density Functionals

We have performed single point calculations using higher level methods for the reaction energy profiles of the reactions shown in Figures 3 and 4 in the manuscript. The geometries were optimized using B3LYP and a mixed basis set of LANL2DZ for metal and 6-31G(d) for other atoms. Gas phase singlet point calculations were performed using B3LYP and wB97XD functionals. A considerably larger basis set of SDD for metal and 6-311+G(d,p) for other atoms was used for the single point calculations. wB97XD is one of the newest density functionals from Head-Gordon and coworkers, which includes empirical dispersion as well as long-range corrections.[1] The gas phase Gibbs free energies of the intermediates and transition states in the cross-couplings of phenyl *N,N*-dimethyl *O*-carbamate **15** and phenyl *N,N*-dimethyl *O*-sulfamate **6** are shown below.[2] These energies include zero-point energies and thermal corrections calculated at the B3LYP/LANL2DZ-6-31G(d) level. The single point calculations using xB97XD were calculated using Gaussian 09.

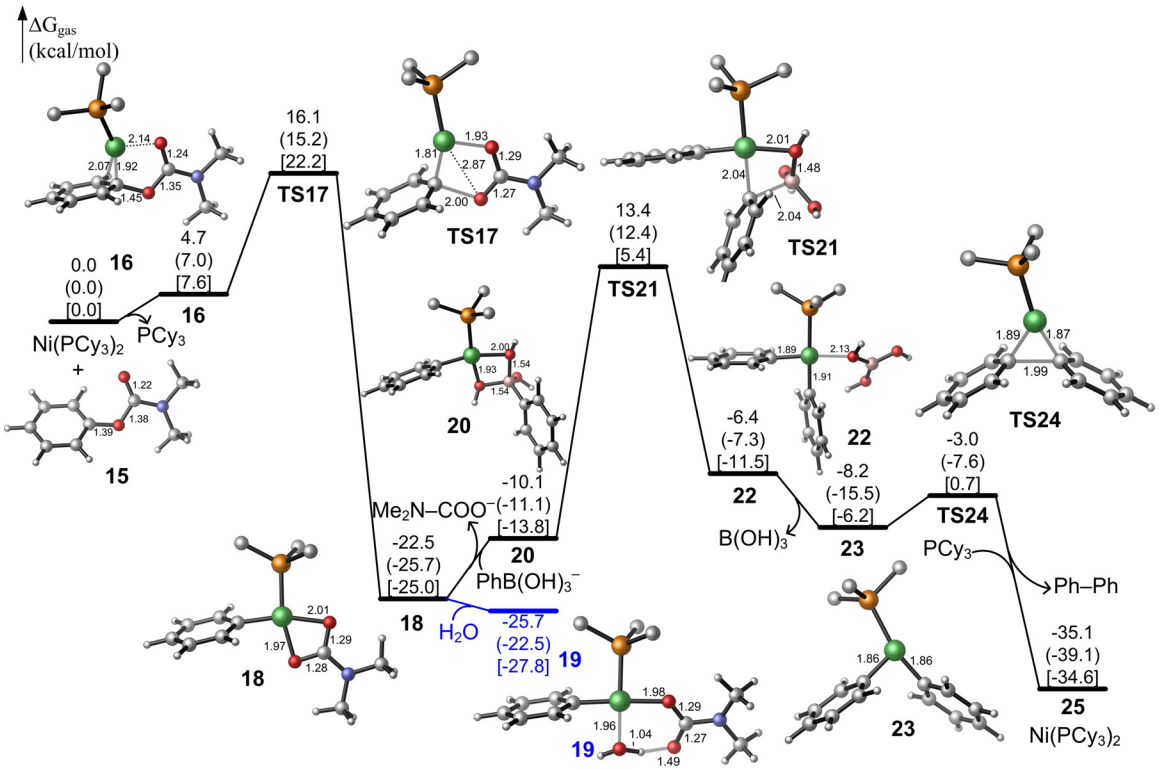


Figure S1. Gibbs free energy profile of Ni-catalyzed Suzuki-Miyaura cross-coupling of phenyl *N,N*-dimethyl *O*-carbamate **15** with phenylboronic acid. PCy_3 was used as ligand in the calculations. The cyclohexyal groups on the ligand are not shown for clarity. Energies reported are gas phase Gibbs free energies calculated using: a) B3LYP/LANL2DZ-6-31G(d); b) B3LYP/SDD-6-311+G(d,p) single point calculations (given in parentheses); c) wB97XD/SDD-6-311+G(d,p) single point calculations (given in brackets). Zero-point energies and thermal corrections calculated at the B3LYP/LANL2DZ-6-31G(d) level are included.

[1] J.-D. Chai and M. Head-Gordon, "Long-range corrected hybrid density functionals with damped atom-atom dispersion corrections," *Phys. Chem. Chem. Phys.*, **2008**, *10*, 6615-6620.

[2] See Figures 3 and 4 in the manuscript for Gibbs free energies in solution calculated at the B3LYP/LANL2DZ-6-31G(d) level.

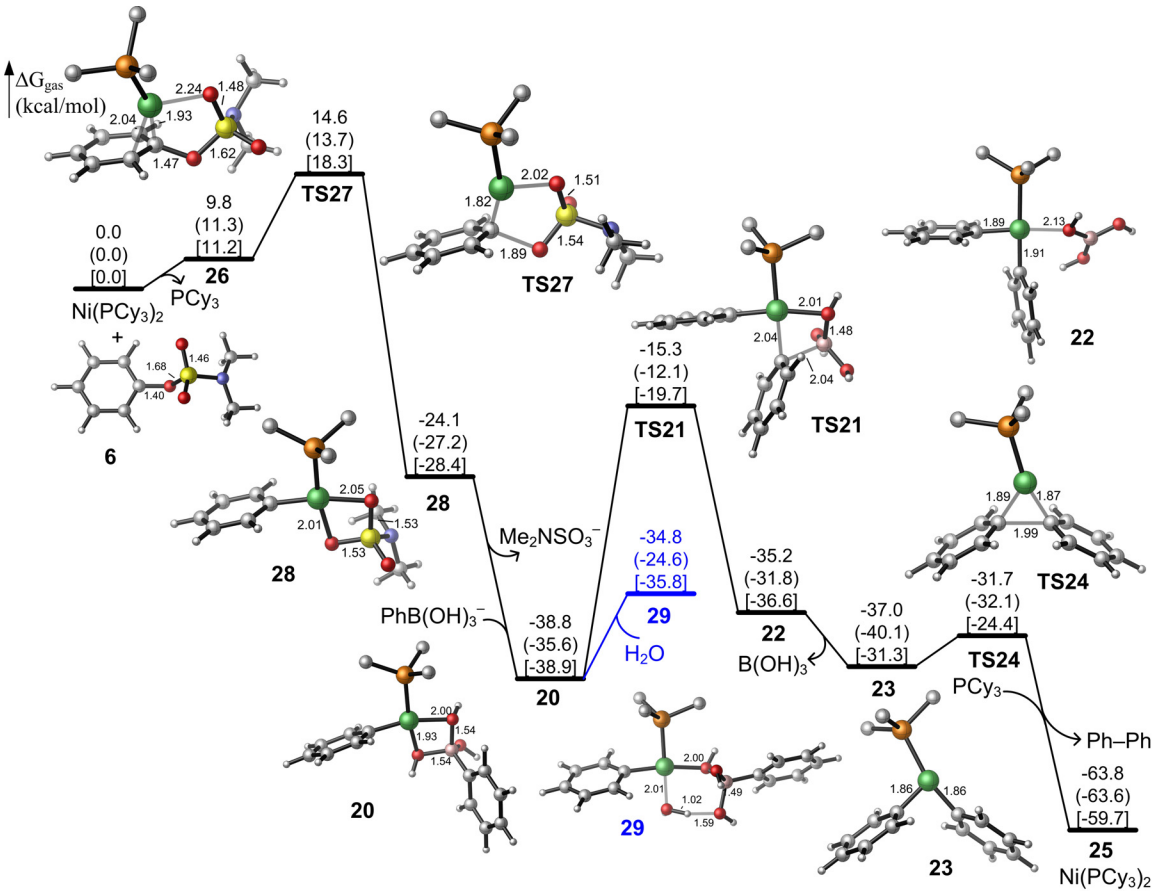


Figure S2. Gibbs free energy profile of Ni-catalyzed Suzuki-Miyaura cross-coupling of phenyl *N,N*-dimethyl *O*-sulfamate **6** with phenylboronic acid. PCy_3 was used as ligand in the calculations. The cyclohexyal groups on the ligand are not shown for clarity. Energies reported are gas phase Gibbs free energies calculated using: a) B3LYP/LANL2DZ-6-31G(d); b) B3LYP/SDD-6-311+G(d,p) single point calculations (given in parentheses); c) wB97XD/SDD-6-311+G(d,p) single point calculations (given in brackets). Zero-point energies and thermal corrections calculated at the B3LYP/LANL2DZ-6-31G(d) level are included.

B3LYP an wB97XD single point calculations with a larger basis set both predict slightly different energetics from B3LYP calculations with the small basis set (LANL2DZ-6-31G(d)). Nonetheless, the calculations at all theoretical levels lead to the same conclusions as discussed in the manuscript: transmetallation is rate-determining for both reactions; carbamates are more reactive than sulfamates in oxidative addition, etc. These benchmark calculations suggest that the theoretical method used in this manuscript (B3LYP with LANL2DZ and 6-31G(d) basis set) is adequate for the purpose of mechanistic studies of Ni-catalyed Suzuki-Miyaura coupling reactions.

Details of Conformational Searches of the PCy_3 ligand

Conformational searches of the PCy_3 ligand were performed to ensure that the optimized structures involve the lowest energy conformers of PCy_3. The conformational searches were performed in the following steps: a) the initial geometry of the PCy_3 ligand was taken from the crystal structure of $Ni(PCy_3)(C_2H_4)_2$ (Krüger and Tsay, *J. Organomet. Chem.* **1972**, *34*, 387); b) several rotamers around the P–Cy bonds and the Ni–P bond were tested as the initial geometry in the optimizations. The lowest energy conformation of the PCy_3 ligand agrees with the previous theoretical study of Liu *et al.* in a related system (ref. 8c).

The Cartesian coordinates (Å), total SCF energies, enthalpies at 298K, and Gibbs free energies at 298K for the optimized structures.

For transition state structures, one imaginary frequency was observed and given below. For all minimum structures, no imaginary frequency was observed.

6

Total SCF energy: -989.99311599 a.u.
Enthalpy at 298K: -989.790516 a.u.
Gibbs free energy at 298K: -989.845611 a.u.
Free energy in solution at 298K: -989.848304 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.896937	-1.191843	-0.333541
C	-3.280200	-1.193425	-0.147545
C	-1.231503	0.030138	-0.416515
C	-3.979686	0.011834	-0.047679
C	-3.294391	1.226516	-0.130063
C	-1.910894	1.242359	-0.312965
H	-5.056543	0.004495	0.095361
H	-3.835413	2.165157	-0.049688
H	-1.355544	2.172023	-0.374652
H	-1.332202	-2.114446	-0.410275
H	-3.810541	-2.139216	-0.080910
O	0.148631	0.047439	-0.674819
S	1.175284	-0.072937	0.646404
O	0.990617	1.115368	1.465502
O	1.034014	-1.410320	1.202919
N	2.630226	0.031446	-0.142424
C	3.002677	-1.123400	-0.969593
H	2.492326	-1.115740	-1.942675
H	4.084037	-1.082170	-1.130394
H	2.761629	-2.042606	-0.435962
C	2.965838	1.342384	-0.712315
H	4.047372	1.366591	-0.875406
H	2.452797	1.521243	-1.667533
H	2.700448	2.124278	-0.000890

15

Total SCF energy: -554.78391262 a.u.
Enthalpy at 298K: -554.582605 a.u.
Gibbs free energy at 298K: -554.634898 a.u.
Free energy in solution at 298K: -554.637193 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.784087	1.246185	-0.418686

C	-3.164118	1.050747	-0.482400
C	-0.971907	0.241588	0.106145
C	-3.725264	-0.144564	-0.028963
C	-2.897870	-1.141158	0.493760
C	-1.516560	-0.956553	0.570319
H	-4.799300	-0.298800	-0.081667
H	-3.327700	-2.073875	0.848880
H	-0.871706	-1.730171	0.966758
O	0.381462	0.549993	0.218465
C	1.333045	-0.372246	-0.161279
O	1.074348	-1.464880	-0.629101
H	-1.326259	2.166928	-0.766668
H	-3.797790	1.833940	-0.889536
N	2.590103	0.113225	0.064484
C	3.728506	-0.699848	-0.333297
H	4.291468	-0.210710	-1.140166
H	4.404994	-0.846976	0.518473
H	3.366634	-1.665938	-0.681797
C	2.890253	1.441890	0.575640
H	3.588555	1.364517	1.418921
H	3.361858	2.060681	-0.201012
H	1.980063	1.930667	0.914080

16

Total SCF energy: -1771.26923062 a.u.
Enthalpy at 298K: -1770.558417 a.u.
Gibbs free energy at 298K: -1770.664096 a.u.
Free energy in solution at 298K: -1770.653913 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	2.500581	1.761771	-0.177004
C	1.546548	3.904614	0.498993
C	0.994648	3.003001	-1.680921
C	1.763616	1.833505	-1.414414
H	0.514946	3.100092	-2.652940
C	0.877078	4.013960	-0.746255
H	0.282833	4.897096	-0.964318
H	2.052310	1.192198	-2.245523
C	2.361381	2.822641	0.771887
O	3.771213	1.055359	-0.136331
C	3.717307	-0.155058	0.448195
O	2.653228	-0.668965	0.830374
H	2.931987	2.772807	1.696192
H	1.443296	4.695416	1.238083
Ni	1.057640	0.504242	0.010312
P	-0.963170	-0.363091	-0.073380
C	-2.274938	0.877768	-0.646457
C	-1.482859	-1.122614	1.580480
C	-1.187336	-1.796470	-1.286495

C	-2.388382	2.072438	0.324156
C	-3.676655	0.373619	-1.050989
H	-1.795181	1.271154	-1.555702
C	-1.074040	-0.233330	2.776444
C	-2.932838	-1.617088	1.748350
H	-0.826661	-2.005090	1.626140
C	-0.263916	-2.983443	-0.932530
C	-0.899178	-1.321496	-2.728689
H	-2.228702	-2.147969	-1.239194
C	-3.228114	3.207497	-0.284962
H	-2.863245	1.744012	1.259398
H	-1.388176	2.439506	0.580771
C	-4.513574	1.511733	-1.665020
H	-3.604670	-0.451770	-1.768680
H	-4.204533	-0.020960	-0.174456
C	-1.260973	-0.974317	4.111428
H	-0.031148	0.085137	2.660467
H	-1.681038	0.681569	2.786989
C	-3.115499	-2.365058	3.081856
H	-3.616202	-0.757689	1.731109
H	-3.224126	-2.267199	0.913909
C	-0.371592	-4.126211	-1.957541
H	0.774597	-2.625732	-0.886701
H	-0.501783	-3.374187	0.063696
C	-1.009067	-2.465057	-3.751279
H	-1.580597	-0.511508	-3.013766
H	0.115202	-0.898945	-2.759854
C	-4.617380	2.716215	-0.717987
H	-3.323351	4.029893	0.436245
H	-2.695681	3.616072	-1.156197
H	-5.514749	1.140931	-1.921962
H	-4.048003	1.832239	-2.609102
C	-2.696297	-1.496160	4.277094
H	-0.560030	-1.821512	4.153752
H	-0.998830	-0.311095	4.946139
H	-2.506838	-3.281594	3.068006
H	-4.159974	-2.685871	3.190905
C	-0.091462	-3.638978	-3.385445
H	0.321952	-4.932622	-1.685051
H	-1.383112	-4.557397	-1.915255
H	-0.768571	-2.088963	-4.754351
H	-2.050605	-2.817798	-3.791689
H	-5.190963	2.423671	0.174541
H	-5.179365	3.528956	-1.196436
H	-2.791607	-2.063505	5.212048
H	-3.384255	-0.641163	4.358911
H	0.957427	-3.314809	-3.458307
H	-0.216348	-4.461179	-4.102010
N	4.927604	-0.759473	0.568284
C	6.179508	-0.152935	0.137974
H	6.664896	-0.783370	-0.618724
H	5.990880	0.830716	-0.285497

H	6.863553	-0.053105	0.991168
C	5.015132	-2.082282	1.167170
H	4.014677	-2.419712	1.432132
H	5.464291	-2.790793	0.459043
H	5.640185	-2.052779	2.069451

TS17

Total SCF energy: -1771.25063432 a.u.
Enthalpy at 298K: -1770.540967 a.u.
Gibbs free energy at 298K: -1770.645974 a.u.
Free energy in solution at 298K: -1770.636428 a.u.
Imaginary frequency: -157.6145 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.154166	-2.099396	0.093676
C	1.921133	-4.221465	-1.049070
C	1.338685	-4.053044	1.295637
C	1.704044	-2.695632	1.294963
H	0.997897	-4.514392	2.220292
C	1.443228	-4.812743	0.133011
H	1.169859	-5.864368	0.141339
H	1.707227	-2.130140	2.223300
C	2.299360	-2.882511	-1.074884
O	3.867566	-1.091699	0.332015
C	3.631782	0.128899	0.064540
O	2.456124	0.618508	-0.136390
H	2.700574	-2.434512	-1.979498
H	2.004479	-4.817982	-1.955146
Ni	1.040060	-0.680549	0.018829
P	-0.989370	0.433855	-0.034961
C	-1.992332	0.161338	1.544229
C	-2.005669	-0.027983	-1.556711
C	-0.839527	2.308073	-0.148911
C	-2.363592	-1.324139	1.744540
C	-3.215594	1.063786	1.812145
H	-1.241575	0.399962	2.313904
C	-1.975019	-1.544135	-1.855461
C	-3.445397	0.513197	-1.653452
H	-1.421535	0.449519	-2.358067
C	-0.108290	2.740944	-1.439710
C	-0.087902	2.857090	1.085568
H	-1.851445	2.739678	-0.164932
C	-2.928814	-1.569137	3.153968
H	-3.121210	-1.615881	1.004262
H	-1.488181	-1.961799	1.571193
C	-3.780520	0.817739	3.223837
H	-2.951932	2.121980	1.703962
H	-4.000623	0.859388	1.074403
C	-2.595902	-1.847669	-3.230644

H	-0.942926	-1.913123	-1.816508
H	-2.531646	-2.090126	-1.082483
C	-4.056788	0.216620	-3.034785
H	-4.067610	0.034096	-0.886239
H	-3.473585	1.591466	-1.455004
C	0.059041	4.269286	-1.509148
H	0.876783	2.257171	-1.466320
H	-0.655314	2.403841	-2.328065
C	0.077225	4.385068	1.017598
H	-0.614020	2.592143	2.010567
H	0.899636	2.379212	1.130774
C	-4.131913	-0.660534	3.446611
H	-3.211532	-2.624034	3.262995
H	-2.139064	-1.378339	3.895707
H	-4.664208	1.448909	3.384239
H	-3.034713	1.129973	3.969951
C	-4.020374	-1.285438	-3.352432
H	-1.963630	-1.405706	-4.015122
H	-2.597379	-2.931125	-3.405279
H	-3.494816	0.766060	-3.804493
H	-5.088065	0.590756	-3.073973
C	0.782073	4.822083	-0.273479
H	0.604417	4.537788	-2.423193
H	-0.932781	4.739509	-1.588652
H	0.636225	4.734509	1.895295
H	-0.913657	4.861146	1.068891
H	-4.963741	-0.937841	2.781858
H	-4.487611	-0.816388	4.473068
H	-4.418647	-1.471694	-4.357968
H	-4.680479	-1.817761	-2.651298
H	1.816956	4.450702	-0.262924
H	0.841844	5.916952	-0.324709
N	4.699643	0.990085	-0.037365
C	4.502137	2.421991	-0.171444
H	5.258054	2.835050	-0.850914
H	3.510657	2.612685	-0.577255
H	4.596546	2.940004	0.796347
C	6.036191	0.552853	0.329364
H	6.767574	0.982705	-0.366392
H	6.303618	0.875129	1.347916
H	6.082833	-0.533468	0.280609

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Total SCF energy: -1771.31568369 a.u.
Enthalpy at 298K: -1770.603372 a.u.
Gibbs free energy at 298K: -1770.707519 a.u.
Free energy in solution at 298K: -1770.698085 a.u.

Cartesian coordinates

ATOM	X	Y	Z

C	0.032383	2.473411	-0.106937
C	0.898919	4.377793	-1.372512
C	1.283156	4.256890	1.003255
C	0.586228	3.042925	1.050877
H	1.695572	4.679333	1.917744
C	1.448091	4.925882	-0.210641
H	1.992031	5.866551	-0.250807
H	0.471710	2.546671	2.012567
C	0.196919	3.168883	-1.317698
O	-2.604881	-0.353512	-0.266084
C	-3.354579	0.684503	-0.416430
O	-2.793713	1.839027	-0.405870
H	-0.237555	2.773195	-2.234309
H	1.011957	4.894671	-2.323656
Ni	-1.065205	0.936049	-0.121715
N	-4.699638	0.561613	-0.579999
C	-5.541331	1.732306	-0.754032
H	-6.055352	1.697794	-1.724596
H	-6.303013	1.779361	0.036241
H	-4.919180	2.624935	-0.707763
C	-5.339502	-0.740186	-0.600962
H	-5.849797	-0.905594	-1.560139
H	-4.581668	-1.509505	-0.460190
H	-6.086850	-0.816730	0.200952
P	0.560436	-0.553390	0.170852
C	2.344795	0.038742	0.094429
C	0.238906	-1.935611	-1.060966
C	0.402107	-1.375558	1.859077
C	2.770277	0.440183	-1.335907
C	3.422197	-0.858468	0.743632
H	2.292016	0.970216	0.674711
C	-0.008025	-1.419464	-2.496811
C	1.239912	-3.108850	-1.055869
H	-0.732132	-2.310953	-0.711314
C	-0.915114	-2.167991	2.020762
C	0.529054	-0.315768	2.977088
H	1.236356	-2.084727	1.957788
C	4.134627	1.149913	-1.325706
H	2.843896	-0.457782	-1.964835
H	2.016876	1.094927	-1.784636
C	4.790985	-0.151467	0.745015
H	3.153201	-1.115115	1.774092
H	3.507082	-1.805838	0.195452
C	-0.478920	-2.563094	-3.411770
H	-0.761212	-0.624213	-2.473975
H	0.909909	-0.983146	-2.909463
C	0.764510	-4.245364	-1.979183
H	2.220344	-2.756551	-1.402964
H	1.385805	-3.493165	-0.038612
C	-1.033705	-2.781179	3.427363
H	-1.767375	-1.506227	1.823607
H	-0.971634	-2.972652	1.279091

C	0.410662	-0.939794	4.377265
H	1.478847	0.226087	2.893840
H	-0.267921	0.429098	2.844487
C	5.215421	0.283316	-0.664750
H	4.424550	1.403606	-2.353387
H	4.037762	2.101128	-0.783909
H	5.546360	-0.815149	1.185489
H	4.734821	0.733815	1.395222
C	0.506168	-3.741511	-3.406669
H	-1.464571	-2.911349	-3.070046
H	-0.617104	-2.186419	-4.433270
H	-0.162491	-4.675702	-1.572375
H	1.507664	-5.053174	-1.986093
C	-0.899250	-1.723885	4.530741
H	-1.993456	-3.306190	3.515433
H	-0.249148	-3.541703	3.559205
H	0.478791	-0.151156	5.137374
H	1.262503	-1.614805	4.549277
H	5.390514	-0.611292	-1.281367
H	6.168991	0.824896	-0.623031
H	0.126784	-4.558358	-4.033753
H	1.458670	-3.420323	-3.854296
H	-1.747257	-1.025997	4.470822
H	-0.949212	-2.195732	5.520294

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Total SCF energy: -1847.74856255 a.u.
Enthalpy at 298K: -1847.008703 a.u.
Gibbs free energy at 298K: -1847.116221 a.u.
Free energy in solution at 298K: -1847.105799 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.358081	-2.210643	-0.650918
C	3.073118	-3.583913	0.430891
C	3.291677	-3.034459	-1.905354
C	2.087954	-2.323354	-1.848541
H	3.836221	-3.101295	-2.845141
C	3.791950	-3.664650	-0.762713
H	4.726164	-4.219083	-0.805618
H	1.710841	-1.858972	-2.758033
C	1.871636	-2.864749	0.483200
O	-2.195056	-0.632913	-0.739812
C	-3.264151	-1.352249	-0.633908
O	-3.281079	-2.613512	-0.526872
H	1.334418	-2.819382	1.428418
H	3.445011	-4.080403	1.325101
Ni	-0.365239	-1.397449	-0.672881
N	-4.470802	-0.679276	-0.623287
C	-5.722090	-1.415130	-0.622305

H	-6.396105	-1.016660	0.148287
H	-6.232154	-1.331784	-1.594474
H	-5.514651	-2.463460	-0.417267
C	-4.570897	0.744944	-0.864700
H	-5.188855	1.224285	-0.092385
H	-3.576010	1.183639	-0.852727
H	-5.036492	0.950042	-1.841566
H	-0.517056	-3.795435	-1.169213
H	-1.978081	-3.054957	-1.102596
O	-1.023075	-3.040299	-1.508131
P	0.365205	0.529659	0.240795
C	-0.392921	1.964442	-0.705589
C	2.235344	0.757174	0.392637
C	-0.259910	0.741578	2.007744
C	-0.275199	1.810308	-2.239115
C	0.021604	3.378815	-0.250572
H	-1.455921	1.829196	-0.473659
C	2.905637	1.040818	-0.970588
C	2.752375	1.752342	1.456470
H	2.560577	-0.246104	0.697529
C	0.154799	-0.474563	2.866878
C	-1.782945	0.973144	2.112532
H	0.238783	1.634186	2.409941
C	-1.088507	2.898731	-2.961237
H	0.773759	1.882861	-2.550442
H	-0.632853	0.818290	-2.534675
C	-0.795219	4.457673	-0.984867
H	-0.105740	3.493175	0.833265
H	1.087216	3.537429	-0.460305
C	4.437827	0.969078	-0.860491
H	2.557739	0.325445	-1.721601
H	2.623546	2.043272	-1.318868
C	4.288744	1.691806	1.559689
H	2.447261	2.775729	1.202232
H	2.326759	1.532158	2.441123
C	-0.293259	-0.321861	4.330034
H	-0.306206	-1.375762	2.439151
H	1.239650	-0.630506	2.825930
C	-2.226922	1.120100	3.578808
H	-2.072456	1.875855	1.562862
H	-2.312612	0.138874	1.640755
C	-0.684219	4.309794	-2.509115
H	-0.961514	2.794821	-4.046320
H	-2.157899	2.743846	-2.756289
H	-0.459570	5.454250	-0.670103
H	-1.851145	4.375033	-0.687608
C	4.969744	1.935659	0.206305
H	4.729808	-0.060330	-0.609809
H	4.887147	1.193425	-1.836483
H	4.580988	0.701394	1.938026
H	4.634627	2.423993	2.300852
C	-1.805706	-0.084597	4.430459

H	-0.005561	-1.215942	4.897728
H	0.240250	0.524601	4.787891
H	-3.315565	1.253443	3.617382
H	-1.785124	2.034582	4.002928
H	0.353903	4.506035	-2.816499
H	-1.305387	5.063556	-3.009459
H	6.058045	1.836085	0.306416
H	4.778312	2.970798	-0.114346
H	-2.337158	-0.981089	4.079268
H	-2.100250	0.065843	5.476856

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Total SCF energy: -1932.24103959 a.u.
Enthalpy at 298K: -1931.483413 a.u.
Gibbs free energy at 298K: -1931.593053 a.u.
Free energy in solution at 298K: -1931.581707 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-4.253637	-0.017193	-0.678303
B	-2.930670	-0.002674	-1.596523
C	-4.370914	-0.771127	0.501902
H	-3.533878	-1.390510	0.815152
O	-2.191640	1.346366	-1.481098
H	-2.676445	2.017195	-0.978021
O	-3.119656	-0.334704	-2.976375
H	-4.032801	-0.603657	-3.135597
O	-1.797258	-0.900254	-1.052731
H	-1.521029	-1.433203	-1.815489
C	-5.536255	-0.754064	1.272567
C	-6.625488	0.026699	0.879293
H	-5.597585	-1.352275	2.179407
H	-7.533546	0.042543	1.477264
C	-5.370026	0.756216	-1.053863
C	-6.539874	0.784004	-0.290919
H	-5.323838	1.347589	-1.968333
H	-7.383228	1.393145	-0.608682
C	0.057785	2.371357	-0.201503
C	0.415232	3.201842	-1.278251
C	0.084858	2.925710	1.089107
C	0.805409	4.529340	-1.071683
H	0.375729	2.816731	-2.295235
C	0.464386	4.257881	1.299223
H	-0.197950	2.323040	1.950078
C	0.833403	5.062128	0.219852
H	1.079984	5.150132	-1.922168
H	0.469300	4.665143	2.308417
H	1.131684	6.095064	0.381354
Ni	-0.631674	0.650602	-0.586505
P	1.132995	-0.495769	0.197182

C	2.654118	0.497230	0.701329
C	1.575014	-1.781883	-1.103452
C	0.684310	-1.497800	1.729793
C	3.392610	1.101042	-0.514616
C	3.658471	-0.177805	1.660968
H	2.200324	1.341269	1.237578
C	1.669580	-1.195802	-2.531709
C	2.786575	-2.687795	-0.798892
H	0.679342	-2.419776	-1.093487
C	-0.294119	-2.657816	1.437784
C	0.104650	-0.557682	2.811649
H	1.615185	-1.936068	2.115175
C	4.471847	2.100205	-0.064593
H	3.873896	0.298187	-1.088928
H	2.680864	1.599718	-1.179807
C	4.748242	0.818908	2.099958
H	3.151553	-0.559265	2.553565
H	4.131550	-1.039938	1.172566
C	1.800180	-2.316844	-3.576483
H	0.787543	-0.579950	-2.745967
H	2.537925	-0.531269	-2.609218
C	2.917658	-3.803406	-1.851601
H	3.704387	-2.085477	-0.799184
H	2.700847	-3.129575	0.201514
C	-0.679472	-3.406393	2.726403
H	-1.193355	-2.266483	0.947417
H	0.159057	-3.371654	0.739814
C	-0.279023	-1.319382	4.091049
H	0.819589	0.237984	3.054997
H	-0.787530	-0.062883	2.403439
C	5.470969	1.450880	0.902635
H	4.994111	2.496721	-0.944528
H	3.985279	2.956327	0.423195
H	5.465549	0.310328	2.756903
H	4.282386	1.613422	2.700976
C	2.994534	-3.235153	-3.276384
H	0.876044	-2.914028	-3.586578
H	1.896640	-1.878296	-4.577336
H	2.049564	-4.474656	-1.774076
H	3.803601	-4.413654	-1.634428
C	-1.257113	-2.462373	3.788424
H	-1.399681	-4.198114	2.484514
H	0.210686	-3.907877	3.135265
H	-0.715456	-0.620790	4.815984
H	0.628914	-1.729359	4.558218
H	6.039241	0.673363	0.370068
H	6.203833	2.189985	1.250125
H	3.040619	-4.051930	-4.007465
H	3.927628	-2.662906	-3.387343
H	-2.205034	-2.040507	3.423971
H	-1.491225	-3.017530	4.705495

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Total SCF energy: -1932.20428121 a.u.
Enthalpy at 298K: -1931.448490 a.u.
Gibbs free energy at 298K: -1931.555638 a.u.
Free energy in solution at 298K: -1931.542459 a.u.
Imaginary frequency: -236.1923 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-3.002195	-0.998940	-0.167811
B	-2.261210	-2.027182	-1.766959
C	-3.134223	-1.802695	0.989589
C	-4.329945	-1.876453	1.708375
H	-2.284903	-2.395720	1.329661
O	-2.213820	-1.224074	-2.918132
H	-3.000340	-1.399638	-3.454408
O	-3.124369	-3.124134	-1.845934
H	-3.189830	-3.581823	-0.997692
O	-0.917628	-2.226717	-1.181891
H	-0.278546	-2.231211	-1.913053
C	-5.440051	-1.143645	1.280697
H	-4.399164	-2.501335	2.596510
H	-6.375836	-1.199637	1.831800
C	-5.344090	-0.340876	0.139635
C	-4.140510	-0.265474	-0.559038
H	-6.207567	0.229442	-0.195666
H	-4.077109	0.369742	-1.439254
Ni	-1.058628	-0.409470	-0.345456
C	-1.557819	1.347095	0.164526
C	-1.660548	1.830971	1.478100
C	-1.894290	2.231504	-0.878379
C	-2.054216	3.148775	1.741823
H	-1.451937	1.174271	2.319959
C	-2.290500	3.548271	-0.621504
H	-1.861423	1.885812	-1.910539
C	-2.364679	4.016555	0.693349
H	-2.125084	3.494262	2.771602
H	-2.544735	4.207688	-1.449454
H	-2.671346	5.039512	0.897268
P	1.188628	0.022510	-0.059556
C	2.228139	-1.413953	-0.748620
C	1.553476	0.265583	1.768218
C	1.957599	1.526262	-0.896325
C	2.033483	-2.720030	0.055032
C	3.732088	-1.170298	-1.009425
H	1.768305	-1.573213	-1.738083
C	0.810900	-0.743735	2.673414
C	3.034328	0.382757	2.184515
H	1.077175	1.240241	1.946610
C	1.626261	2.883164	-0.235479

C	1.575430	1.536141	-2.394561
H	3.045297	1.394201	-0.824064
C	2.669753	-3.922237	-0.663134
H	2.509574	-2.609133	1.037895
H	0.969572	-2.907260	0.227879
C	4.375184	-2.378948	-1.716093
H	3.884319	-0.281474	-1.629925
H	4.251006	-0.985363	-0.060269
C	0.935229	-0.344499	4.153687
H	-0.243776	-0.801356	2.381247
H	1.227728	-1.749560	2.541290
C	3.157947	0.776923	3.667989
H	3.537993	-0.581371	2.031324
H	3.560326	1.115999	1.561302
C	2.295331	4.042382	-0.996398
H	0.543842	3.038491	-0.216563
H	1.968883	2.894509	0.805549
C	2.229876	2.709288	-3.143227
H	1.862983	0.591487	-2.874215
H	0.484395	1.610464	-2.480041
C	4.160075	-3.686721	-0.942820
H	2.531210	-4.827418	-0.058524
H	2.141877	-4.099563	-1.612170
H	5.446720	-2.190291	-1.860422
H	3.939109	-2.477211	-2.721425
C	2.404327	-0.202979	4.579347
H	0.415756	0.611399	4.315222
H	0.426168	-1.086706	4.781653
H	2.750627	1.789271	3.805891
H	4.217260	0.825068	3.951498
C	1.900861	4.053253	-2.479725
H	2.021564	4.992838	-0.521378
H	3.389475	3.953786	-0.913247
H	1.900575	2.705848	-4.190119
H	3.321335	2.568796	-3.158106
H	4.703501	-3.637702	0.012580
H	4.584266	-4.531380	-1.500174
H	2.469028	0.125009	5.624484
H	2.891304	-1.188582	4.530254
H	0.821781	4.245200	-2.564256
H	2.410066	4.871765	-3.004440

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Total SCF energy: -1932.23376920 a.u.
Enthalpy at 298K: -1931.475915 a.u.
Gibbs free energy at 298K: -1931.587224 a.u.
Free energy in solution at 298K: -1931.572276 a.u.

Cartesian coordinates

ATOM	X	Y	Z

Ni	-1.279582	0.064531	0.000764
C	-3.184040	0.227082	-0.064135
B	-2.084838	-2.968418	-0.592543
C	-3.934785	0.498152	-1.225128
C	-5.335870	0.438476	-1.231010
H	-3.423792	0.783025	-2.143038
O	-1.579557	-4.243098	-0.549065
H	-2.066638	-4.824077	-1.151389
O	-3.084374	-2.619299	-1.428875
H	-3.386387	-1.697015	-1.299455
O	-1.482156	-2.043124	0.268650
H	-0.810702	-2.472201	0.819647
C	-6.029587	0.131073	-0.060492
H	-5.881705	0.644583	-2.149668
H	-7.116120	0.093014	-0.058255
C	-5.310521	-0.121822	1.111196
C	-3.913439	-0.080043	1.103454
H	-5.840304	-0.356536	2.032701
H	-3.384033	-0.295520	2.030715
C	-1.254366	1.934587	-0.236568
C	-1.224641	2.818127	0.858112
C	-1.210484	2.507001	-1.521162
C	-1.120363	4.202308	0.680237
H	-1.297387	2.429210	1.871596
C	-1.105078	3.890213	-1.706222
H	-1.265532	1.869654	-2.402499
C	-1.053874	4.747028	-0.604259
H	-1.101283	4.857070	1.549675
H	-1.071406	4.298191	-2.714843
H	-0.977862	5.822487	-0.744502
P	1.091189	-0.177653	0.196571
C	2.128172	1.320086	-0.307649
C	1.700178	-1.714516	-0.720589
C	1.627216	-0.488047	1.983662
C	2.163266	1.525043	-1.838725
C	3.556174	1.441995	0.268198
H	1.528788	2.144804	0.102744
C	1.142251	-1.796907	-2.160883
C	3.210861	-2.023784	-0.706867
H	1.206161	-2.527926	-0.167085
C	1.059347	-1.796242	2.576996
C	1.216255	0.698320	2.885237
H	2.722964	-0.570179	1.995773
C	2.773491	2.890627	-2.198808
H	2.769475	0.733851	-2.300312
H	1.154231	1.449523	-2.254494
C	4.174605	2.806661	-0.091119
H	3.558539	1.330305	1.357338
H	4.193571	0.642176	-0.131131
C	1.420712	-3.177819	-2.778411
H	0.065759	-1.590568	-2.160338
H	1.605034	-1.024442	-2.786307

C	3.496202	-3.401544	-1.334360
H	3.747605	-1.252407	-1.274130
H	3.607033	-1.994525	0.315544
C	1.527954	-2.010256	4.028079
H	-0.040467	-1.745386	2.573883
H	1.355271	-2.664176	1.974611
C	1.685055	0.498156	4.336015
H	1.609206	1.643492	2.495546
H	0.122046	0.791314	2.864460
C	4.179886	3.053146	-1.605923
H	2.805601	3.002744	-3.290357
H	2.114081	3.683744	-1.820561
H	5.194701	2.865504	0.310388
H	3.596487	3.600815	0.403348
C	2.919625	-3.512880	-2.753696
H	0.861185	-3.939586	-2.216472
H	1.042418	-3.205702	-3.808285
H	3.051838	-4.182951	-0.700112
H	4.578019	-3.586952	-1.345771
C	1.158443	-0.818885	4.922599
H	1.092668	-2.936755	4.423607
H	2.618876	-2.149113	4.034280
H	1.357293	1.346548	4.949845
H	2.784859	0.497311	4.365951
H	4.861582	2.334995	-2.086318
H	4.574787	4.053115	-1.826099
H	3.092756	-4.519985	-3.153637
H	3.455845	-2.817154	-3.416159
H	0.063696	-0.761492	5.013256
H	1.548736	-0.970657	5.936733

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Total SCF energy: -1679.74041839 a.u.
Enthalpy at 298K: -1679.039423 a.u.
Gibbs free energy at 298K: -1679.141538 a.u.
Free energy in solution at 298K: -1679.129937 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Ni	-1.305096	0.436096	-0.072545
C	-2.096689	-1.154744	0.488354
C	-2.676490	-2.054585	-0.421299
C	-3.086091	-3.326923	-0.008236
H	-2.815169	-1.766133	-1.460565
C	-2.948343	-3.715974	1.326555
H	-3.525045	-4.011405	-0.731515
H	-3.274212	-4.702004	1.647922
C	-2.404625	-2.817493	2.246606
C	-1.989998	-1.545937	1.833670
H	-2.306690	-3.101717	3.292615

H	-1.582050	-0.860178	2.573542
C	-3.001637	1.201577	-0.028759
C	-3.667321	1.434392	-1.248174
C	-3.524273	1.808025	1.129114
C	-4.775527	2.284965	-1.318190
H	-3.321191	0.949142	-2.159985
C	-4.631500	2.658488	1.063668
H	-3.065187	1.614043	2.096834
C	-5.258429	2.901406	-0.161618
H	-5.267754	2.458539	-2.273178
H	-5.012561	3.124833	1.970117
H	-6.125513	3.555698	-0.212042
P	0.992879	0.041413	-0.237175
C	1.713216	-0.524012	1.408034
C	1.824407	1.634586	-0.817791
C	1.568956	-1.249147	-1.480575
C	1.491209	0.525869	2.518944
C	3.165838	-1.045221	1.440991
H	1.051863	-1.371220	1.646177
C	1.130194	2.884988	-0.228744
C	3.355756	1.748700	-0.684658
H	1.589506	1.634308	-1.892882
C	1.043307	-0.925195	-2.898037
C	1.114401	-2.668248	-1.066400
H	2.668787	-1.229009	-1.508466
C	1.835092	-0.049828	3.903463
H	2.127016	1.402339	2.331592
H	0.452464	0.879012	2.502544
C	3.504076	-1.626490	2.826650
H	3.325414	-1.811202	0.673972
H	3.862841	-0.228851	1.217726
C	1.655860	4.174193	-0.882741
H	0.042148	2.817355	-0.368462
H	1.300319	2.932790	0.854654
C	3.875422	3.037510	-1.347432
H	3.629926	1.763805	0.378367
H	3.850631	0.875078	-1.126381
C	1.476351	-1.986049	-3.924669
H	-0.054389	-0.873684	-2.865727
H	1.393474	0.058583	-3.231914
C	1.552993	-3.726526	-2.093627
H	1.513820	-2.932808	-0.080914
H	0.021407	-2.681978	-0.971852
C	3.267854	-0.601511	3.945633
H	1.700876	0.723531	4.670557
H	1.126192	-0.855594	4.142991
H	4.546138	-1.971128	2.838842
H	2.879157	-2.513314	3.007572
C	3.184064	4.283848	-0.774767
H	1.365182	4.182231	-1.943670
H	1.175870	5.046188	-0.421273
H	3.693629	2.985332	-2.431104

H	4.962804	3.109581	-1.216648
C	1.042212	-3.395425	-3.502575
H	1.060942	-1.734601	-4.908880
H	2.571082	-1.959237	-4.031253
H	1.191048	-4.713014	-1.777712
H	2.651780	-3.786666	-2.110396
H	3.978955	0.229981	3.829086
H	3.473342	-1.052833	4.924477
H	3.537654	5.185180	-1.291020
H	3.465168	4.398867	0.282662
H	-0.055803	-3.455261	-3.512602
H	1.403942	-4.137883	-4.225261

TS24

Total SCF energy: -1679.73338946 a.u.
Enthalpy at 298K: -1679.033395 a.u.
Gibbs free energy at 298K: -1679.133182 a.u.
Free energy in solution at 298K: -1679.125421 a.u.
Imaginary frequency: -244.4653 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.652040	-1.603029	0.149505
C	-2.986331	-2.296102	-1.032997
C	-2.975760	-2.206385	1.382529
C	-3.571045	-3.562690	-0.982467
H	-2.788346	-1.844301	-2.001683
C	-3.561120	-3.473115	1.430270
H	-2.769964	-1.683702	2.313163
C	-3.859749	-4.157565	0.248907
H	-3.807401	-4.084586	-1.907287
H	-3.790277	-3.924964	2.392958
C	-2.754156	0.384774	0.078488
C	-3.213099	0.923372	-1.142993
C	-3.163704	1.025855	1.267751
C	-3.987614	2.084467	-1.175201
H	-2.957521	0.435737	-2.080109
C	-3.937885	2.187213	1.232396
H	-2.869050	0.619810	2.231922
C	-4.350717	2.728184	0.011335
H	-4.313196	2.485354	-2.132858
H	-4.223871	2.669294	2.164919
H	-4.325887	-5.138687	0.287181
H	-4.962371	3.626098	-0.014352
Ni	-1.109108	-0.540889	0.092413
P	1.022889	0.200853	-0.019529
C	1.898499	-0.481139	-1.546645
C	2.013570	-0.162609	1.548152
C	1.164757	2.072557	-0.209776
C	1.646739	-1.993922	-1.736761

C	3.389063	-0.152302	-1.763397
H	1.334308	0.020629	-2.347622
C	2.074186	-1.674336	1.857731
C	3.406132	0.480064	1.709059
H	1.360357	0.282852	2.314404
C	0.573071	2.784855	1.028417
C	0.458028	2.561650	-1.493746
H	2.231043	2.332509	-0.284799
C	2.117449	-2.460949	-3.124381
H	2.184315	-2.562817	-0.966599
H	0.580414	-2.214732	-1.603615
C	3.857303	-0.614168	-3.155830
H	3.575716	0.922105	-1.645377
H	3.993470	-0.663715	-1.002865
C	2.641352	-1.930539	3.264650
H	1.075073	-2.118218	1.763350
H	2.715600	-2.177090	1.120992
C	3.971714	0.222983	3.118517
H	4.098216	0.063042	0.967807
H	3.361931	1.559455	1.524029
C	0.614192	4.316120	0.887042
H	-0.467792	2.460007	1.160645
H	1.113800	2.491563	1.936155
C	0.501618	4.094076	-1.624372
H	0.918948	2.113348	-2.382050
H	-0.588081	2.228788	-1.473644
C	3.592652	-2.112008	-3.372681
H	1.959343	-3.542173	-3.226305
H	1.496226	-1.980339	-3.894807
H	4.925227	-0.393133	-3.281157
H	3.325983	-0.034980	-3.925498
C	4.018959	-1.276812	3.446024
H	1.944177	-1.524873	4.012610
H	2.703787	-3.010599	3.449251
H	3.340923	0.736531	3.859289
H	4.973227	0.664409	3.202617
C	-0.094679	4.784054	-0.390448
H	0.155525	4.776754	1.771419
H	1.661750	4.652946	0.866233
H	-0.037063	4.397911	-2.531125
H	1.544397	4.420489	-1.755839
H	4.222205	-2.692332	-2.681615
H	3.889385	-2.407247	-4.387168
H	4.382387	-1.431342	4.469931
H	4.743027	-1.769137	2.779658
H	-1.164782	4.541358	-0.321079
H	-0.021766	5.874721	-0.490170

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Total SCF energy: -2206.47138322 a.u.

Enthalpy at 298K: -2205.759407 a.u.
Gibbs free energy at 298K: -2205.866773 a.u.
Free energy in solution at 298K: -2205.864654 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	2.317244	1.506834	-0.802649
C	1.779867	3.742867	-0.005315
C	0.656369	2.891187	-1.979763
C	1.332119	1.639079	-1.849105
H	-0.009968	3.037095	-2.827477
C	0.859007	3.911656	-1.074235
H	0.331017	4.854947	-1.184235
H	1.380490	0.973590	-2.709026
C	2.524070	2.587560	0.112966
O	3.479864	0.651539	-1.078247
O	2.342037	-0.983931	0.473606
H	3.282246	2.483250	0.883629
H	1.927073	4.548593	0.709639
Ni	0.795345	0.438903	-0.292661
P	-1.270315	-0.313476	-0.026804
C	-2.575786	0.955119	-0.539281
C	-1.608454	-0.907062	1.737122
C	-1.699166	-1.825501	-1.075219
C	-2.519444	2.216054	0.349400
C	-4.036520	0.497791	-0.737067
H	-2.191623	1.257802	-1.525218
C	-1.003323	0.040847	2.797210
C	-3.050877	-1.292527	2.119549
H	-1.003154	-1.825182	1.774973
C	-0.795258	-3.029284	-0.727331
C	-1.566272	-1.489335	-2.578298
H	-2.742809	-2.110551	-0.875833
C	-3.378335	3.349922	-0.235140
H	-2.891359	1.973423	1.354729
H	-1.480545	2.547390	0.459814
C	-4.891247	1.634755	-1.328519
H	-4.088615	-0.376696	-1.395763
H	-4.469347	0.191758	0.223008
C	-1.059666	-0.587421	4.200363
H	0.032230	0.283773	2.529973
H	-1.553282	0.991028	2.808769
C	-3.104703	-1.925681	3.522073
H	-3.681262	-0.393690	2.114136
H	-3.480001	-1.983325	1.383301
C	-1.086458	-4.244995	-1.624385
H	0.256132	-2.730366	-0.838632
H	-0.925533	-3.322041	0.320940
C	-1.863368	-2.705466	-3.471493
H	-2.232541	-0.662887	-2.852800
H	-0.541516	-1.140127	-2.768993
C	-4.829418	2.901825	-0.463029

H	-3.348503	4.221719	0.431476
H	-2.940795	3.672390	-1.191373
H	-5.930569	1.299084	-1.440532
H	-4.527946	1.869352	-2.340255
C	-2.489343	-1.000140	4.581980
H	-0.408211	-1.473925	4.224323
H	-0.656509	0.116187	4.940433
H	-2.555859	-2.879151	3.508663
H	-4.143373	-2.167385	3.783089
C	-0.966208	-3.897814	-3.114164
H	-0.402324	-5.063550	-1.366315
H	-2.103808	-4.611145	-1.419228
H	-1.732336	-2.429475	-4.525916
H	-2.918520	-2.994757	-3.353147
H	-5.301249	2.697108	0.509837
H	-5.410907	3.708711	-0.927513
H	-2.496303	-1.489193	5.564625
H	-3.112402	-0.098153	4.677353
H	0.079448	-3.645656	-3.343760
H	-1.222363	-4.768438	-3.731572
S	3.643888	-0.655406	-0.142495
O	4.341432	-1.658773	-0.938303
N	4.618113	-0.037706	1.100648
C	4.631592	-0.896263	2.298291
H	5.172762	-1.840001	2.136543
H	5.129117	-0.335262	3.094567
H	3.607026	-1.108584	2.604045
C	5.965032	0.337265	0.636534
H	5.879980	1.003092	-0.223931
H	6.452888	0.880032	1.451346
H	6.573811	-0.535785	0.364846

TS27

Total SCF energy: -2206.46074180 a.u.
Enthalpy at 298K: -2205.750160 a.u.
Gibbs free energy at 298K: -2205.858977 a.u.
Free energy in solution at 298K: -2205.852475 a.u.
Imaginary frequency: -242.0483 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.103472	1.937207	0.220486
C	-1.790536	4.239685	-0.408116
C	-1.217229	3.528931	1.839502
C	-1.624819	2.208456	1.529266
H	-0.883292	3.759352	2.848897
C	-1.286245	4.526614	0.880556
H	-0.975779	5.539186	1.122656
H	-1.732974	1.473542	2.323186
C	-2.234939	2.969854	-0.739200

O	-3.662518	0.869558	0.156163
O	-1.987869	-0.781904	-0.645404
H	-2.654239	2.750207	-1.715999
H	-1.837435	5.029992	-1.153768
Ni	-0.808562	0.668508	0.126633
S	-3.406283	-0.289276	-0.832657
O	-3.795104	0.021338	-2.207564
N	-4.365687	-1.579518	-0.310527
C	-4.071210	-2.045514	1.047808
H	-4.401214	-1.333648	1.819456
H	-4.593936	-2.996183	1.193239
H	-2.999013	-2.219367	1.145232
C	-5.798899	-1.389787	-0.571455
H	-5.934459	-1.046268	-1.597231
H	-6.289277	-2.361632	-0.456666
H	-6.261771	-0.670556	0.120998
P	1.265041	-0.289591	0.164194
C	2.660177	0.976326	0.220704
C	1.429613	-1.410636	-1.343902
C	1.623759	-1.431524	1.619304
C	2.361311	2.211932	-0.658478
C	4.098350	0.473406	-0.016219
H	2.600447	1.327058	1.262328
C	1.336037	-0.612480	-2.662871
C	2.595714	-2.419585	-1.404381
H	0.495574	-1.987702	-1.270717
C	0.584204	-2.574852	1.661717
C	1.621207	-0.668302	2.962267
H	2.621076	-1.873206	1.480070
C	3.391725	3.326973	-0.410866
H	2.384825	1.931067	-1.719440
H	1.349319	2.580071	-0.451945
C	5.125401	1.592166	0.236813
H	4.321899	-0.390005	0.622842
H	4.197834	0.131022	-1.054607
C	1.181162	-1.553457	-3.869413
H	0.491237	0.085514	-2.622304
H	2.245967	-0.010586	-2.795349
C	2.434624	-3.363439	-2.610996
H	3.551132	-1.887778	-1.492651
H	2.651508	-3.012114	-0.483710
C	0.809519	-3.515225	2.857666
H	-0.420695	-2.133729	1.726336
H	0.606010	-3.153734	0.731844
C	1.842896	-1.610693	4.158607
H	2.395026	0.107722	2.969575
H	0.657512	-0.151329	3.077369
C	4.830711	2.831783	-0.620586
H	3.181819	4.178816	-1.070125
H	3.281169	3.695227	0.619982
H	6.138322	1.220048	0.035529
H	5.100448	1.871014	1.300787

C	2.316513	-2.586215	-3.930289
H	0.215345	-2.072878	-3.794775
H	1.149314	-0.965982	-4.795855
H	1.532301	-3.976274	-2.469187
H	3.282182	-4.060007	-2.652202
C	0.813734	-2.748550	4.186770
H	0.035113	-4.292887	2.865655
H	1.771854	-4.034066	2.734970
H	1.803751	-1.034818	5.092140
H	2.854612	-2.038569	4.097944
H	4.975574	2.578762	-1.681521
H	5.546561	3.631274	-0.390603
H	2.157330	-3.279527	-4.765961
H	3.267076	-2.068913	-4.130210
H	-0.186895	-2.327866	4.366124
H	1.021388	-3.429967	5.021497

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Total SCF energy: -2206.52941939 a.u.
Enthalpy at 298K: -2205.815303 a.u.
Gibbs free energy at 298K: -2205.920704 a.u.
Free energy in solution at 298K: -2205.912019 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.086227	2.395842	-0.035276
C	0.547410	4.325576	-1.389165
C	0.818733	4.407474	1.005018
C	0.310876	3.106752	1.107028
H	1.113389	4.943127	1.905168
C	0.942997	5.019624	-0.243668
H	1.338729	6.029045	-0.323166
H	0.214186	2.658150	2.092905
C	0.039416	3.025535	-1.284009
O	-2.302546	-0.818115	0.055596
O	-2.835497	1.496423	0.177901
H	-0.269939	2.509335	-2.191517
H	0.631087	4.795275	-2.367118
Ni	-0.973051	0.739744	0.054000
S	-3.488382	0.116689	0.274886
O	-4.300134	-0.119232	1.462238
N	-4.497971	-0.134585	-1.052461
C	-5.840529	0.447279	-0.915909
H	-5.840341	1.540598	-1.042121
H	-6.475153	0.002603	-1.688832
H	-6.245074	0.194199	0.063535
C	-3.873081	0.117391	-2.354017
H	-2.922115	-0.414355	-2.406835
H	-4.536350	-0.283300	-3.126814
H	-3.706593	1.188323	-2.542769

P	0.867713	-0.499887	0.145332
C	2.533861	0.344042	-0.096873
C	0.640282	-1.942152	-1.034828
C	0.974178	-1.291393	1.852289
C	2.799002	0.729015	-1.569274
C	3.773750	-0.358602	0.499721
H	2.387167	1.284219	0.451888
C	0.279453	-1.507208	-2.472800
C	1.760475	-3.003284	-1.051874
H	-0.266573	-2.407323	-0.624594
C	-0.167013	-2.292693	2.140533
C	1.014034	-0.199011	2.945265
H	1.922129	-1.846591	1.883423
C	4.036289	1.634990	-1.686211
H	2.971214	-0.179613	-2.161918
H	1.927526	1.237413	-1.992134
C	5.019669	0.539266	0.373747
H	3.619490	-0.601333	1.556140
H	3.957369	-1.308491	-0.020041
C	-0.136698	-2.722920	-3.318515
H	-0.530489	-0.769496	-2.446196
H	1.137422	-1.017852	-2.948873
C	1.349942	-4.217077	-1.906415
H	2.676376	-2.564185	-1.469967
H	2.004964	-3.333133	-0.034858
C	-0.035290	-2.892044	3.552212
H	-1.135433	-1.790542	2.035706
H	-0.159531	-3.106524	1.406937
C	1.146962	-0.805623	4.351793
H	1.834653	0.505802	2.765056
H	0.084110	0.383480	2.891140
C	5.277853	0.969688	-1.076707
H	4.213767	1.879798	-2.741226
H	3.832622	2.585513	-1.173761
H	5.893024	0.012003	0.778568
H	4.877102	1.433802	0.997369
C	0.956482	-3.802308	-3.331752
H	-1.064240	-3.146913	-2.907313
H	-0.365161	-2.401077	-4.342626
H	0.499144	-4.721760	-1.425975
H	2.170825	-4.945060	-1.932878
C	0.019840	-1.807307	4.636105
H	-0.876048	-3.572474	3.735661
H	0.879083	-3.502612	3.604154
H	1.145256	-0.001969	5.098916
H	2.119423	-1.313082	4.439613
H	5.545104	0.085205	-1.674442
H	6.138418	1.648908	-1.122715
H	0.620299	-4.677744	-3.901340
H	1.843694	-3.411890	-3.852449
H	-0.940792	-1.273254	4.664078
H	0.155321	-2.263414	5.624914

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Total SCF energy: -2008.66370290 a.u.
Enthalpy at 298K: -2007.878008 a.u.
Gibbs free energy at 298K: -2007.990266 a.u.
Free energy in solution at 298K: -2007.975541 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-6.090153	-0.251948	0.871213
C	-4.787497	-0.753222	0.939695
C	-4.103916	-1.206028	-0.202499
C	-4.793455	-1.122580	-1.427895
C	-6.096379	-0.624072	-1.512471
C	-6.750446	-0.187043	-0.358306
B	-2.599574	-1.816626	-0.096600
O	-1.962496	-1.686627	1.203886
O	-1.690505	-1.055518	-1.083801
O	-2.543993	-3.249412	-0.507902
H	-2.195748	-2.457308	1.740293
H	-3.287217	-3.450171	-1.094497
H	-2.007726	-0.150111	-1.184703
H	-4.275921	-0.798000	1.898810
H	-4.299275	-1.451636	-2.342873
H	-6.600491	-0.574171	-2.475351
H	-7.764387	0.201561	-0.416786
H	-6.592201	0.086980	1.775141
C	2.101688	-1.858495	-0.884939
C	3.029739	-1.388579	-1.827080
C	2.507173	-2.914075	-0.047693
C	4.319477	-1.930965	-1.916654
H	2.757849	-0.595126	-2.519219
C	3.794609	-3.451984	-0.124617
H	1.805226	-3.338895	0.666063
C	4.710388	-2.957839	-1.058565
H	5.015284	-1.547379	-2.660380
H	4.080159	-4.265867	0.538859
H	5.711550	-3.376958	-1.121684
Ni	0.269804	-1.343320	-0.848931
H	-1.105957	-3.340597	-1.190130
H	-0.157461	-3.159283	-2.459536
O	-0.142947	-3.203025	-1.489707
P	0.766748	0.631896	0.140897
C	-0.839065	1.526685	0.625689
C	1.855295	1.768520	-0.887521
C	1.682606	0.467720	1.779514
C	-1.498546	2.275495	-0.557323
C	-0.795178	2.463135	1.855339
H	-1.481045	0.679123	0.896875
C	1.399619	1.916995	-2.357351

C	2.162485	3.153089	-0.277439
H	2.796332	1.202034	-0.914732
C	3.206356	0.233812	1.679553
C	1.021056	-0.623947	2.651490
H	1.546822	1.434292	2.282271
C	-2.917795	2.753480	-0.203795
H	-0.891484	3.152829	-0.816351
H	-1.523891	1.659665	-1.466014
C	-2.208030	2.965760	2.212008
H	-0.387920	1.942006	2.726395
H	-0.139380	3.323025	1.660139
C	2.472605	2.642970	-3.187214
H	1.182615	0.933405	-2.790230
H	0.468143	2.491823	-2.409327
C	3.228435	3.890117	-1.109622
H	1.246776	3.758415	-0.250429
H	2.505127	3.058065	0.759306
C	3.836341	0.176645	3.083552
H	3.408832	-0.702485	1.152162
H	3.686840	1.034211	1.105427
C	1.662253	-0.688420	4.047231
H	-0.059063	-0.463401	2.733855
H	1.140613	-1.590347	2.147694
C	-2.895469	3.663231	1.031362
H	-3.349972	3.283744	-1.062038
H	-3.561527	1.884924	-0.011229
H	-2.145426	3.642953	3.073683
H	-2.817871	2.108122	2.528754
C	2.816518	4.013548	-2.583972
H	3.380444	2.023182	-3.228563
H	2.125538	2.758820	-4.221872
H	4.178188	3.339427	-1.042690
H	3.412270	4.883310	-0.680328
C	3.180587	-0.898241	3.961876
H	4.913548	-0.011299	2.990276
H	3.731260	1.157751	3.571709
H	1.196057	-1.494114	4.628636
H	1.454545	0.246888	4.589367
H	-2.354848	4.591112	0.790487
H	-3.916039	3.957266	1.306090
H	3.616155	4.493997	-3.161655
H	1.937870	4.671452	-2.659827
H	3.385568	-1.888919	3.531142
H	3.625088	-0.892600	4.965443

TS30

Total SCF energy: -1771.23474880 a.u.
Enthalpy at 298K: -1770.525172 a.u.
Gibbs free energy at 298K: -1770.630553 a.u.
Free energy in solution at 298K: -1770.624593 a.u.

Imaginary frequency: -227.7525 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	1.019937	-0.245649	-0.294801
P	-1.139553	-0.152411	-0.101314
O	2.955840	-0.302109	-0.518703
O	3.243628	-1.149348	1.591116
C	2.400289	1.151567	-0.210549
C	2.592891	1.747020	1.058661
C	2.651251	3.137942	1.146274
C	2.573475	3.947057	0.007455
C	2.451870	3.341769	-1.251255
C	2.399234	1.957667	-1.376044
C	3.663032	-0.978011	0.457508
C	-1.869433	1.533887	-0.539073
C	-1.784362	-0.508322	1.647094
C	-2.041005	-1.355445	-1.241231
C	-3.405803	1.664447	-0.514346
C	-1.223108	2.658937	0.298136
C	-0.772375	-1.351658	2.456516
C	-3.199930	-1.113122	1.773459
C	-1.866272	-0.960127	-2.723945
C	-1.525312	-2.795205	-1.021541
C	-3.854503	3.049261	-1.016021
C	-1.674195	4.045879	-0.191127
C	-1.195612	-1.473885	3.929627
C	-3.624174	-1.230386	3.249482
C	-2.542426	-1.967912	-3.670230
C	-2.210655	-3.801803	-1.960427
C	-3.203886	4.179815	-0.205644
C	-2.613941	-2.046039	4.069091
C	-2.044889	-3.400129	-3.432264
H	2.659073	1.125022	1.941992
H	2.410141	3.955839	-2.148162
H	2.329111	1.485176	-2.350780
H	2.625854	5.028184	0.095086
H	2.759055	3.594619	2.127731
H	-1.533118	1.681824	-1.575828
H	-1.809372	0.490035	2.109711
H	-3.113260	-1.329216	-1.000937
H	-3.877638	0.880852	-1.119696
H	-3.767091	1.529484	0.514337
H	-0.132752	2.583435	0.256857
H	-1.510278	2.545289	1.354105
H	-0.701118	-2.357622	2.018409
H	0.229949	-0.916467	2.378539
H	-3.936806	-0.515492	1.226490
H	-3.213842	-2.114723	1.323074
H	-2.276036	0.039316	-2.910700
H	-0.791142	-0.906159	-2.949517
H	-0.439963	-2.808012	-1.198894

H	-1.669809	-3.104853	0.019729
H	-3.578708	3.154993	-2.075737
H	-4.948803	3.125440	-0.969384
H	-1.228224	4.823225	0.442128
H	-1.283300	4.210329	-1.205972
H	-1.158512	-0.479079	4.398759
H	-0.475686	-2.100275	4.471587
H	-3.710575	-0.221389	3.679738
H	-4.622662	-1.682728	3.312916
H	-3.631317	-1.932846	-3.515970
H	-2.366317	-1.669850	-4.712009
H	-3.282222	-3.857690	-1.716519
H	-1.799652	-4.805225	-1.789344
H	-3.499307	5.156375	-0.610629
H	-3.580009	4.143453	0.827858
H	-2.620224	-3.087895	3.715255
H	-2.914879	-2.073144	5.124386
H	-0.981462	-3.464709	-3.706416
H	-2.579828	-4.102799	-4.084078
N	4.865112	-1.426832	-0.007007
C	5.359312	-1.224110	-1.360654
H	4.708711	-0.537565	-1.896346
H	6.373487	-0.806228	-1.325525
H	5.401184	-2.178523	-1.904506
C	5.683542	-2.261443	0.859554
H	6.680591	-1.818808	0.980084
H	5.201092	-2.338462	1.832508
H	5.801109	-3.265214	0.428495

TS31

Total SCF energy: -1771.24090475 a.u.
Enthalpy at 298K: -1770.530749 a.u.
Gibbs free energy at 298K: -1770.635113 a.u.
Free energy in solution at 298K: -1770.630157 a.u.
Imaginary frequency: -58.5416 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.292708	-1.462048	0.742870
Ni	-0.919673	-0.344190	-0.541511
O	-2.809494	-0.900396	-0.519585
C	-3.839949	0.043942	-0.470077
C	-3.781378	1.107715	-1.370512
C	-4.932202	-0.122106	0.381841
C	-4.836975	2.019265	-1.419642
H	-2.916113	1.204252	-2.019374
C	-5.975383	0.802922	0.327178
H	-4.955150	-0.946708	1.084333
C	-5.935706	1.872563	-0.570368
H	-4.795159	2.846505	-2.123030

H	-6.825381	0.682490	0.993381
H	-6.753819	2.586301	-0.606144
O	-2.427230	-0.875868	1.809162
N	-2.127786	-2.832864	0.606138
C	-1.898782	-3.468488	-0.684265
C	-1.541159	-3.513365	1.752129
H	-2.508874	-2.991532	-1.449612
H	-0.842886	-3.415899	-0.990279
H	-2.189051	-4.521913	-0.605301
H	-0.439635	-3.503742	1.717338
H	-1.870170	-3.019260	2.665702
H	-1.877261	-4.555696	1.758108
P	1.122305	0.160133	-0.210896
C	1.803996	-0.584581	1.393380
C	1.369815	2.036505	-0.208793
C	2.354956	-0.430179	-1.517971
C	1.054041	-0.063132	2.639116
C	3.329189	-0.564946	1.633872
H	1.511980	-1.639636	1.275536
C	0.247010	2.773449	0.555737
C	2.750531	2.592711	0.192838
H	1.217795	2.276717	-1.272224
C	2.024227	0.148241	-2.911464
C	2.371239	-1.973517	-1.585261
H	3.360017	-0.083811	-1.235114
C	1.428544	-0.874482	3.891248
H	1.318721	0.989674	2.810819
H	-0.028398	-0.102037	2.475973
C	3.697618	-1.385065	2.884585
H	3.870948	-0.962390	0.768162
H	3.675801	0.466066	1.773207
C	0.323926	4.291996	0.324634
H	-0.729467	2.386331	0.241344
H	0.328107	2.568277	1.630805
C	2.826515	4.111820	-0.047832
H	2.926948	2.398063	1.258971
H	3.553727	2.087501	-0.357656
C	2.981095	-0.376447	-3.996203
H	0.990000	-0.123116	-3.169329
H	2.066031	1.243564	-2.896607
C	3.328281	-2.498779	-2.668692
H	2.649734	-2.402522	-0.615588
H	1.349711	-2.320734	-1.798405
C	2.945518	-0.891749	4.128962
H	0.908994	-0.464421	4.766703
H	1.067073	-1.906721	3.771155
H	4.782158	-1.341631	3.050205
H	3.451380	-2.442793	2.706761
C	1.704841	4.855886	0.692030
H	0.116041	4.506698	-0.734611
H	-0.459908	4.796180	0.904283
H	2.745919	4.310722	-1.126936

H	3.808082	4.490275	0.266497
C	2.999368	-1.910050	-4.046607
H	2.692412	0.034834	-4.972202
H	3.997743	-0.008670	-3.791220
H	3.284274	-3.595316	-2.700332
H	4.362175	-2.236128	-2.398436
H	3.284600	0.126040	4.374119
H	3.191229	-1.519162	4.995584
H	1.751102	5.930062	0.471014
H	1.859702	4.752951	1.776526
H	2.012355	-2.273277	-4.369351
H	3.722248	-2.259390	-4.795022

TS32

Total SCF energy: -2206.44676048 a.u.
Enthalpy at 298K: -2205.735507 a.u.
Gibbs free energy at 298K: -2205.841991 a.u.
Free energy in solution at 298K: -2205.831473 a.u.
Imaginary frequency: -293.1055 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.265011	1.184035	-0.030910
C	2.526332	2.890644	1.657593
H	2.605006	3.168048	2.706085
C	2.472238	3.504878	-0.678151
C	2.363270	2.165908	-1.041635
H	2.515580	4.262446	-1.457334
C	2.546581	3.881306	0.669918
H	2.645272	4.927544	0.943059
H	2.333598	1.866531	-2.084163
C	2.418000	1.540346	1.326998
H	2.422271	0.776415	2.096014
Ni	0.846488	-0.181300	-0.309409
O	2.753343	-0.253531	-0.544279
S	3.795233	-1.203943	0.347734
O	5.054897	-0.483756	0.442662
O	3.098624	-1.679063	1.538488
N	3.999612	-2.493615	-0.689041
C	4.720131	-2.203955	-1.934988
H	5.091056	-3.153154	-2.333327
H	4.072910	-1.726513	-2.684345
H	5.570316	-1.556800	-1.719453
C	2.856996	-3.402883	-0.831757
H	3.232191	-4.342220	-1.249701
H	2.425970	-3.599904	0.149483
H	2.082844	-2.993571	-1.497094
P	-1.303536	0.039789	-0.084678
C	-1.859712	-0.269203	1.693308
C	-2.259106	-1.081813	-1.278291

C	-1.982103	1.755664	-0.476597
C	-1.152861	-1.486320	2.332323
C	-3.374280	-0.308501	1.977567
H	-1.452338	0.616780	2.203021
C	-2.005254	-2.577972	-0.996261
C	-3.765945	-0.824429	-1.496852
H	-1.752159	-0.854942	-2.228655
C	-1.624453	2.149042	-1.927492
C	-1.463844	2.825046	0.510443
H	-3.077464	1.715421	-0.388351
C	-1.436172	-1.557707	3.842921
H	-1.502503	-2.413362	1.858833
H	-0.073047	-1.428517	2.150468
C	-3.651164	-0.373005	3.490839
H	-3.877424	0.564085	1.542761
H	-3.813026	-1.195989	1.502424
C	-2.552632	-3.461588	-2.129715
H	-0.931214	-2.756361	-0.858740
H	-2.496750	-2.863625	-0.056254
C	-4.312759	-1.708319	-2.633884
H	-4.323017	-1.040443	-0.577290
H	-3.952770	0.228314	-1.736202
C	-2.131800	3.556694	-2.284806
H	-0.532071	2.116089	-2.038271
H	-2.034840	1.421737	-2.638741
C	-1.972991	4.230801	0.145223
H	-1.778413	2.588331	1.533501
H	-0.366665	2.822653	0.507941
C	-2.942645	-1.569781	4.142344
H	-0.955104	-2.447509	4.268501
H	-0.975544	-0.688789	4.335901
H	-4.733073	-0.425224	3.669481
H	-3.300903	0.557746	3.961057
C	-4.045125	-3.198675	-2.378331
H	-1.987715	-3.256257	-3.051190
H	-2.386639	-4.519950	-1.890279
H	-3.835775	-1.411861	-3.579935
H	-5.388654	-1.529420	-2.757867
C	-1.611699	4.609412	-1.296838
H	-1.827607	3.807935	-3.309250
H	-3.232296	3.561333	-2.275987
H	-1.556514	4.963177	0.848409
H	-3.066258	4.266028	0.267080
H	-3.381732	-2.502036	3.756194
H	-3.116158	-1.569697	5.226029
H	-4.402909	-3.799653	-3.224075
H	-4.620554	-3.523908	-1.498689
H	-0.518399	4.680909	-1.385734
H	-2.016115	5.599203	-1.544949

TS33

Total SCF energy: -2206.45276698 a.u.
Enthalpy at 298K: -2205.741732 a.u.
Gibbs free energy at 298K: -2205.852213 a.u.
Free energy in solution at 298K: -2205.843384 a.u.
Imaginary frequency: -170.5468 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Ni	-0.429972	-1.141335	0.356184
O	-2.530205	0.045617	-0.843842
C	-3.394425	0.952612	-0.415278
C	-2.975033	2.071264	0.347452
C	-4.769591	0.852425	-0.746449
C	-3.879685	3.060826	0.719871
H	-1.928468	2.135469	0.633876
C	-5.664583	1.845884	-0.368545
H	-5.094935	-0.017385	-1.309084
C	-5.228602	2.958091	0.362976
H	-3.536016	3.915391	1.298588
H	-6.713816	1.756099	-0.640569
H	-5.933979	3.729459	0.659857
O	-1.268629	-2.719663	0.958303
S	-2.453511	-1.807208	0.422200
O	-3.503788	-1.537868	1.415441
N	-3.172863	-2.697476	-0.851864
C	-2.328007	-2.771598	-2.046013
C	-3.671826	-4.001378	-0.389026
H	-2.027820	-1.760060	-2.323116
H	-1.441294	-3.409448	-1.904607
H	-2.936593	-3.190965	-2.854026
H	-2.864241	-4.719913	-0.186367
H	-4.266716	-3.853861	0.514459
H	-4.321745	-4.400700	-1.174224
P	1.502077	0.099691	0.137979
C	1.210137	1.808186	-0.594792
C	2.809188	-0.877436	-0.805059
C	2.280079	0.416406	1.821401
C	0.403651	1.761973	-1.912791
C	2.425852	2.748770	-0.722553
H	0.535756	2.245082	0.157279
C	2.343173	-1.276955	-2.221607
C	4.245798	-0.316535	-0.842960
H	2.836695	-1.807710	-0.216934
C	2.615715	-0.921196	2.520282
C	1.343616	1.265132	2.711106
H	3.215273	0.974954	1.672835
C	-0.030292	3.177559	-2.332607
H	1.020524	1.325691	-2.709703
H	-0.479144	1.124059	-1.792339
C	1.976413	4.163642	-1.130230
H	2.992751	2.792832	0.215744

H	3.110991	2.362221	-1.488091
C	3.310911	-2.292970	-2.851993
H	1.328963	-1.692932	-2.180908
H	2.294803	-0.386364	-2.861696
C	5.213411	-1.334285	-1.475498
H	4.266998	0.608436	-1.432123
H	4.591674	-0.055926	0.164280
C	3.188923	-0.706703	3.931492
H	1.700015	-1.526585	2.587533
H	3.331172	-1.500145	1.924662
C	1.922688	1.470587	4.121577
H	1.157464	2.243178	2.252618
H	0.368831	0.761687	2.786582
C	1.161939	4.141335	-2.431959
H	-0.561151	3.128071	-3.291421
H	-0.754368	3.558825	-1.598654
H	2.854303	4.813578	-1.238240
H	1.365507	4.594713	-0.323459
C	4.751832	-1.761718	-2.876479
H	3.276775	-3.228390	-2.274325
H	2.977975	-2.540319	-3.867882
H	5.278695	-2.220481	-0.826980
H	6.222741	-0.905711	-1.519850
C	2.248170	0.135165	4.802908
H	3.376858	-1.681109	4.399560
H	4.164207	-0.202894	3.855563
H	1.211541	2.047093	4.726194
H	2.838308	2.076782	4.052134
H	1.816145	3.825942	-3.258812
H	0.814642	5.152657	-2.678277
H	5.430507	-2.521472	-3.283906
H	4.807334	-0.897245	-3.554785
H	1.315616	-0.421817	4.973760
H	2.695769	0.309710	5.789296

$Ni(PCy_3)_2$

Total SCF energy: -2263.65154064 a.u.
Enthalpy at 298K: -2262.633849 a.u.
Gibbs free energy at 298K: -2262.757735 a.u.
Free energy in solution at 298K: -2262.742771 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	0.000000	5.341592	-4.490750
C	-1.753386	-2.456973	-4.477159
C	-2.555467	-0.723279	-4.437513
C	-4.050171	-2.180222	-1.590145
C	-4.274309	-2.591308	-3.126233
C	-3.458759	4.705246	0.589300
C	-1.961799	4.385397	0.415664

C	0.980203	2.945847	-1.361898
C	0.757654	2.188187	-2.689928
C	1.754488	2.647061	-3.767522
C	1.701263	4.167343	-3.982143
C	1.898836	4.926233	-2.660863
C	0.890326	4.467493	-1.591178
C	0.799687	2.949730	1.588782
C	2.274662	2.512599	1.729515
C	2.925449	3.069669	3.007268
C	2.134267	2.681165	4.263435
C	0.667249	3.113191	4.140346
C	0.017759	2.556886	2.862149
H	-2.190622	2.319105	0.930165
H	-2.168656	3.037341	-2.034029
H	-2.412956	1.423985	-1.365294
H	-4.593958	2.555106	-1.913467
H	-4.466231	2.185901	-0.195564
H	-3.971578	4.917993	-1.500582
H	-5.341592	4.490750	-0.479783
H	-3.589862	5.776151	0.793524
H	-3.842161	4.170325	1.471124
H	-1.419996	4.673764	1.324061
H	-1.560848	5.003846	-0.395939
H	2.014940	2.724732	-1.058196
H	0.847839	1.109655	-2.512366
H	-0.265643	2.361179	-3.050992
H	2.771903	2.360330	-3.461414
H	1.553888	2.122799	-4.711165
H	2.456973	4.477159	-4.715621
H	0.723279	4.437513	-4.408142
H	2.920906	4.754547	-2.291529
H	1.804086	6.007833	-2.824961
H	-0.120697	4.727344	-1.932104
H	1.059437	5.017718	-0.657191
H	0.772967	4.044715	1.486945
H	2.312483	1.413681	1.741725
H	2.859494	2.834409	0.859849
H	3.960619	2.711209	3.080999
H	2.979435	4.166691	2.938416
H	2.180222	1.590145	4.397076
H	2.591308	3.126233	5.156843
H	0.096152	2.784380	5.018584
H	0.612915	4.212298	4.126822
H	-1.020411	2.903589	2.802354
H	-0.023564	1.459325	2.916420
Ni	0.000000	0.000000	0.036938
P	0.000000	-2.167724	0.061824
C	1.753386	-2.889863	0.096344
C	-0.980203	-2.945847	-1.361898
C	-0.799687	-2.949730	1.588782
C	2.555467	-2.492518	-1.161146
C	1.961799	-4.385397	0.415664

H	2.190622	-2.319105	0.930165
C	-0.757654	-2.188187	-2.689928
C	-0.890326	-4.467493	-1.591178
H	-2.014940	-2.724732	-1.058196
C	-2.274662	-2.512599	1.729515
C	-0.017759	-2.556886	2.862149
H	-0.772967	-4.044715	1.486945
C	4.050171	-2.815838	-0.995926
H	2.168656	-3.037341	-2.034029
H	2.412956	-1.423985	-1.365294
C	3.458759	-4.705246	0.589300
H	1.419996	-4.673764	1.324061
H	1.560848	-5.003846	-0.395939
C	-1.754488	-2.647061	-3.767522
H	-0.847839	-1.109655	-2.512366
H	0.265643	-2.361179	-3.050992
C	-1.898836	-4.926233	-2.660863
H	0.120697	-4.727344	-1.932104
H	-1.059437	-5.017718	-0.657191
C	-2.925449	-3.069669	3.007268
H	-2.312483	-1.413681	1.741725
H	-2.859494	-2.834409	0.859849
C	-0.667249	-3.113191	4.140346
H	1.020411	-2.903589	2.802354
H	0.023564	-1.459325	2.916420
C	4.274309	-4.294676	-0.645709
H	4.593958	-2.555106	-1.913467
H	4.466231	-2.185901	-0.195564
H	3.589862	-5.776151	0.793524
H	3.842161	-4.170325	1.471124
C	-1.701263	-4.167343	-3.982143
H	-2.771903	-2.360330	-3.461414
H	-1.553888	-2.122799	-4.711165
H	-2.920906	-4.754547	-2.291529
H	-1.804086	-6.007833	-2.824961
C	-2.134267	-2.681165	4.263435
H	-3.960619	-2.711209	3.080999
H	-2.979435	-4.166691	2.938416
H	-0.096152	-2.784380	5.018584
H	-0.612915	-4.212298	4.126822
H	3.971578	-4.917993	-1.500582
H	5.341592	-4.490750	6.685700
H	-2.456973	-4.477159	9.432000
H	-0.723279	-4.437513	18.867300
H	-2.180222	-1.590145	4.397076
H	-2.591308	-3.126233	5.156843

PCy_3

Total SCF energy: -1047.15889434 a.u.

Enthalpy at 298K: -1046.652794 a.u.

Gibbs free energy at 298K: -1046.720986 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	0.023253	-0.126660	-1.044031
C	-0.201009	1.611219	-0.291846
C	0.289175	1.859620	1.150578
C	-0.030695	3.291463	1.619100
C	0.552580	4.343638	0.665323
C	0.080274	4.105762	-0.776259
C	0.388661	2.674979	-1.247358
C	1.425404	-0.903615	-0.035769
C	1.465341	-2.435913	-0.225324
C	2.661782	-3.077065	0.499963
C	3.994704	-2.448458	0.072133
C	3.968411	-0.925363	0.259328
C	2.775196	-0.289847	-0.474006
C	-1.512802	-1.054008	-0.433016
C	-2.754781	-0.603509	-1.234488
C	-3.985345	-1.467842	-0.908365
C	-4.281736	-1.491647	0.598610
C	-3.048907	-1.931169	1.401520
C	-1.823042	-1.057604	1.076580
H	-1.293010	1.754282	-0.295505
H	1.376396	1.710240	1.202573
H	-0.156236	1.137619	1.843616
H	0.352977	3.444287	2.636631
H	-1.122318	3.418375	1.675384
H	1.651220	4.291878	0.699872
H	0.277345	5.353327	0.996677
H	0.544790	4.832710	-1.455382
H	-1.005548	4.276048	-0.832859
H	0.002037	2.518534	-2.261442
H	1.478880	2.543639	-1.313139
H	1.283957	-0.697825	1.034572
H	1.525798	-2.666600	-1.299593
H	0.539126	-2.893697	0.140393
H	2.671597	-4.158825	0.312468
H	2.534157	-2.950186	1.585421
H	4.180077	-2.678878	-0.987551
H	4.824597	-2.890381	0.638586
H	4.905509	-0.479972	-0.099635
H	3.902597	-0.691678	1.332517
H	2.776812	0.794290	-0.308999
H	2.896204	-0.435909	-1.557217
H	-1.310412	-2.093111	-0.734905
H	-2.540141	-0.640917	-2.309572
H	-2.986910	0.446015	-0.999419
H	-3.804055	-2.495168	-1.257788
H	-4.858717	-1.099902	-1.462611
H	-5.130861	-2.154559	0.809359
H	-4.583592	-0.484588	0.923752

H	-2.817060	-2.980529	1.165526
H	-3.261288	-1.893540	2.478167
H	-2.025285	-0.030085	1.409410
H	-0.956711	-1.408833	1.650922

$PhOCONMe_2$

Total SCF energy: -554.78391262 a.u.
Enthalpy at 298K: -554.582605 a.u.
Gibbs free energy at 298K: -554.634898 a.u.
Free energy in solution at 298K: -554.637193 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.784087	1.246185	-0.418686
C	-3.164118	1.050747	-0.482400
C	-0.971907	0.241588	0.106145
C	-3.725264	-0.144564	-0.028963
C	-2.897870	-1.141158	0.493760
C	-1.516560	-0.956553	0.570319
H	-4.799300	-0.298800	-0.081667
H	-3.327700	-2.073875	0.848880
H	-0.871706	-1.730171	0.966758
O	0.381462	0.549993	0.218465
C	1.333045	-0.372246	-0.161279
O	1.074348	-1.464880	-0.629101
H	-1.326259	2.166928	-0.766668
H	-3.797790	1.833940	-0.889536
N	2.590103	0.113225	0.064484
C	3.728506	-0.699848	-0.333297
H	4.291468	-0.210710	-1.140166
H	4.404994	-0.846976	0.518473
H	3.366634	-1.665938	-0.681797
C	2.890253	1.441890	0.575640
H	3.588555	1.364517	1.418921
H	3.361858	2.060681	-0.201012
H	1.980063	1.930667	0.914080

$PhOSO_2NMe_2$

Total SCF energy: -989.99311599 a.u.
Enthalpy at 298K: -989.790516 a.u.
Gibbs free energy at 298K: -989.845611 a.u.
Free energy in solution at 298K: -989.848304 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.896937	-1.191843	-0.333541
C	-3.280200	-1.193425	-0.147545
C	-1.231503	0.030138	-0.416515

C	-3.979686	0.011834	-0.047679
C	-3.294391	1.226516	-0.130063
C	-1.910894	1.242359	-0.312965
H	-5.056543	0.004495	0.095361
H	-3.835413	2.165157	-0.049688
H	-1.355544	2.172023	-0.374652
H	-1.332202	-2.114446	-0.410275
H	-3.810541	-2.139216	-0.080910
O	0.148631	0.047439	-0.674819
S	1.175284	-0.072937	0.646404
O	0.990617	1.115368	1.465502
O	1.034014	-1.410320	1.202919
N	2.630226	0.031446	-0.142424
C	3.002677	-1.123400	-0.969593
H	2.492326	-1.115740	-1.942675
H	4.084037	-1.082170	-1.130394
H	2.761629	-2.042606	-0.435962
C	2.965838	1.342384	-0.712315
H	4.047372	1.366591	-0.875406
H	2.452797	1.521243	-1.667533
H	2.700448	2.124278	-0.000890

NMe_2COO^-

Total SCF energy: -323.16571772 a.u.
Enthalpy at 298K: -323.065279 a.u.
Gibbs free energy at 298K: -323.101604 a.u.
Imaginary frequency: -112.3402 cm-1

Cartesian coordinates

ATOM	X	Y	Z
O	1.438517	1.139047	0.000045
C	0.911499	-0.000005	-0.000105
O	1.438754	-1.138965	0.000048
N	-0.561953	-0.000035	-0.000135
C	-1.299193	-1.224676	0.000031
H	-1.958425	-1.331461	0.888306
H	-1.958700	-1.331515	-0.888029
H	-0.564691	-2.033080	-0.000055
C	-1.299148	1.224629	0.000032
H	-1.958366	1.331452	0.888311
H	-0.564605	2.033008	-0.000058
H	-1.958654	1.331500	-0.888022

$NMe_2SO_3^-$

Total SCF energy: -758.42206327 a.u.
Enthalpy at 298K: -758.317761 a.u.
Gibbs free energy at 298K: -758.358095 a.u.
Free energy in solution at 298K: -758.408963 a.u.

Cartesian coordinates

ATOM	X	Y	Z
O	1.244809	-1.253371	-0.591691
O	1.244634	1.254110	-0.590451
S	0.736841	0.000029	0.016377
O	0.729299	-0.000789	1.506072
N	-0.967624	0.000041	-0.462848
C	-1.649065	-1.205763	-0.013579
H	-1.766596	-1.253787	1.085191
H	-2.649356	-1.248339	-0.470562
H	-1.071994	-2.073456	-0.340185
C	-1.649194	1.205738	-0.013533
H	-1.072326	2.073529	-0.340203
H	-2.649561	1.248087	-0.470376
H	-1.766641	1.253767	1.085259

$PhB(OH)_3^-$

Total SCF energy: -484.10770360 a.u.
Enthalpy at 298K: -483.960566 a.u.
Gibbs free energy at 298K: -484.006920 a.u.

Cartesian coordinates

ATOM	X	Y	Z
O	-2.073258	-0.090709	1.406553
B	-1.586619	-0.021694	0.009576
O	-2.037690	1.227586	-0.668761
H	-2.983583	1.261507	-0.456463
O	-2.127270	-1.230381	-0.648448
H	-2.007414	-1.061096	-1.593487
H	-1.634855	0.638490	1.867448
C	0.070548	0.005144	-0.035036
C	0.814134	-1.190608	-0.003301
C	0.821609	1.196014	-0.052210
C	2.211366	-1.205993	0.022154
H	0.260296	-2.128196	-0.012409
C	2.220891	1.202255	-0.027585
H	0.281427	2.140435	-0.101537
C	2.926739	-0.003509	0.012996
H	2.749308	-2.155069	0.046277
H	2.765348	2.147857	-0.045641
H	4.016593	-0.007236	0.031070

$B(OH)_3$

Total SCF energy: -252.47085225 a.u.
Enthalpy at 298K: -252.416847 a.u.
Gibbs free energy at 298K: -252.448568 a.u.
Free energy in solution at 298K: -252.450178 a.u.

Cartesian coordinates

ATOM	X	Y	Z
B	-0.000149	-0.000118	0.000267
O	-1.308782	-0.412095	-0.000129
H	-1.908661	0.347147	-0.000152
O	0.297516	1.339425	0.000149
H	1.254986	1.478927	-0.000905
O	1.011309	-0.927205	-0.000198
H	0.654077	-1.826493	0.001147

H_2O

Total SCF energy: -76.40702351 a.u.
Enthalpy at 298K: -76.382105 a.u.
Gibbs free energy at 298K: -76.403550 a.u.
Free energy in solution at 298K: -76.406020 a.u.

Cartesian coordinates

ATOM	X	Y	Z
O	0.000000	0.000000	0.119426
H	0.000000	0.762617	-0.477705
H	0.000000	-0.762617	-0.477705

Ph-Ph

Total SCF energy: -463.29643148 a.u.
Enthalpy at 298K: -463.104558 a.u.
Gibbs free energy at 298K: -463.147605 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.397370	1.138624	2.860624
C	-0.397704	1.137978	1.466146
C	0.000000	0.000000	0.743286
C	0.397704	-1.137978	1.466146
C	0.397370	-1.138624	2.860624
C	0.000000	0.000000	3.564548
H	-0.716937	2.027787	3.398212
H	-0.734276	2.020311	0.928639
H	0.734276	-2.020311	0.928639
H	0.716937	-2.027787	3.398212
H	0.000000	0.000000	4.651345
C	0.000000	0.000000	-0.743286
C	-0.397704	-1.137978	-1.466146
C	0.397704	1.137978	-1.466146
C	-0.397370	-1.138624	-2.860624
H	-0.734276	-2.020311	-0.928639
C	0.397370	1.138624	-2.860624
H	0.734276	2.020311	-0.928639

C	0.000000	0.000000	-3.564548
H	-0.716937	-2.027787	-3.398212
H	0.716937	2.027787	-3.398212
H	0.000000	0.000000	-4.651345