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Supporting Information

Insight into the Lewis acid-catalyzed Intramolecular Aminocyanation and Oxycyanation of Alkenes: Concerted or Stepwise Mechanism

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COMPUTATIONAL DETAILS

All calculations are performed with the Gaussian09 program. The popular M06-2x functional is used in all DFT calculations. The LANL2DZ basis set[S1] is employed for the tin atom and the 6-311G(d,p) basis set[S2] is used for all other atoms in the reactants and catalysts. Geometry optimizations are conducted without any constraint in the gas phase and in toluene or tetrahydrofuran solutions (using the self-consistent reaction field (SCRF) method[S3] with the IEFPCM solvation model). We have performed vibrational frequency calculations to verify whether the optimized stationary points are minima or saddle points and to get relevant thermodynamic energy corrections. Further, intrinsic reaction coordinate (IRC)[S4] analysis has been carried out to confirm the connectivity between the transition state and its neighboring minima. Natural population analyses (NPA)[S5] are performed also at the same level of theory.

[S1] C. E. Check, T. O. Faust, J. M. Bailey, B. J. Wright, T. M. Gilbert and L. S. Sunderlin, *J. Phys. Chem. A.*, 2001,**105**, 8111-8116.

[S2] R. Krishnan, J. S. Binkley, R. Seeger and J. A. Pople. *J. Chem. Phys.*, 1980, **72**, 650-654.

[S3] M. Cossi, N. Rega, G. Scalmani and V. Barone, *J. Comput. Chem.*, 2003, **24**, 669-681.

[S4] (a) K. Fukui, *Acc. Chem. Res.*, 1981, **14**, 363-68; (b) H. P. Hratchian and H. B. Schlegel, *Theory and Applications of Computational Chemistry: The First 40 Years*, Elsevier, Amsterdam, 2005, PP. 195-249.

[S5] (a) A. E. Reed and F. Weinhold, *J. Chem. Phys.*, 1983, **78**, 4066-4073; (b) J. P. Foster and F. Weinhold, *J. Am. Chem. Soc.*, 1980, **102**, 7211-7218.

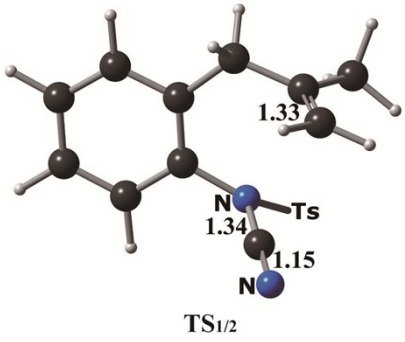

Figure S1. Optimized structure of the transition state $\mathbf{TS_{1/2}}$ in the intramolecular addition of the reactant **1** in toluene. All bond lengths are in Å.

The reaction pathway A of the intramolecular aminocyanation reaction of the reactant 1 catalyzed by the Lewis acid $B(C_6F_5)_3$.

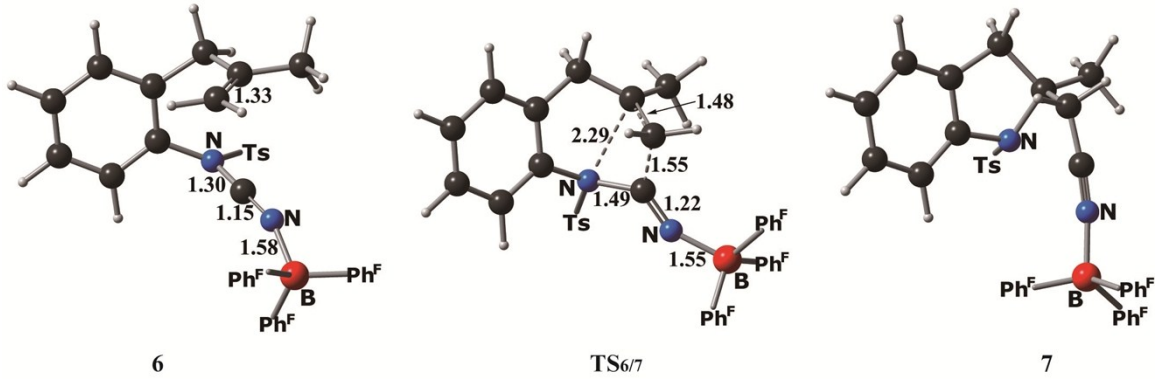

Figure S2. Optimized structures of intermediates, transition states and products in the pathway A of the intramolecular addition of the reactant **1** in toluene. All bond lengths are in Å.

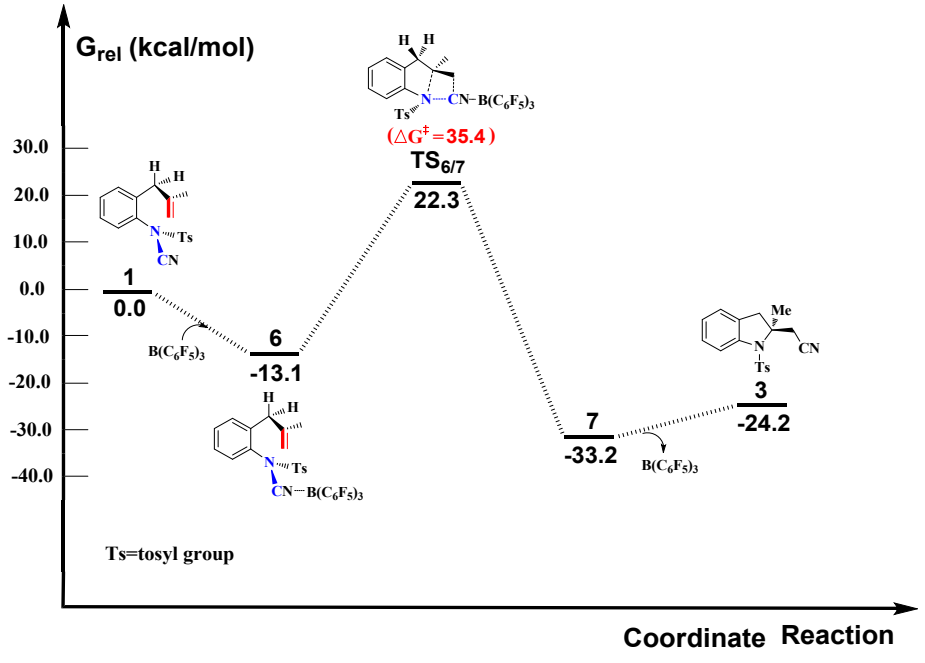

Figure S3. Gibbs free energy profiles of the pathway A of the intramolecular addition of the reactant **1**with $B(C_6F_5)_3$ as the catalyst in toluene. Relative free energies calculated at 298.15 K and 1 atm (with respect to that of the reactants) are given.

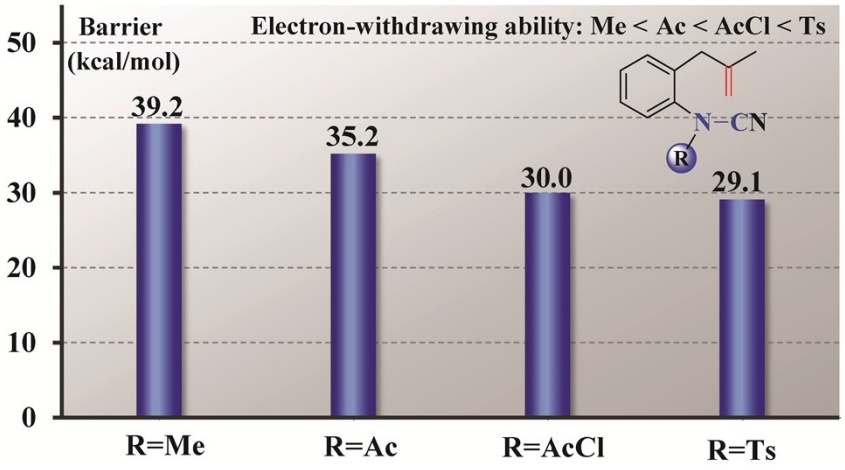

Figure S4. Gibbs free energy barriers of the intramolecular alkene addition reactions catalyzed by the Lewis acid $B(C_6F_5)_3$. Different reactants with various substituents at the N3 atom are used in different reactions.

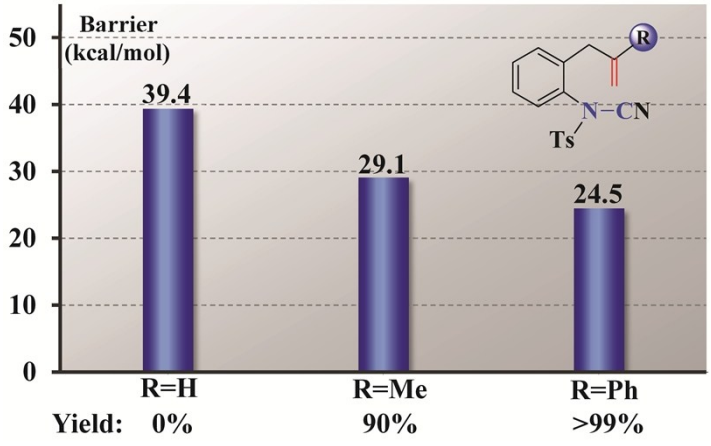

Figure S5. Gibbs free energy barriers of the intramolecular alkene addition reactions catalyzed by the Lewis acid $B(C_6F_5)_3$. Different reactants with various substituents on the alkene moiety are used in different reactions.

The intramolecular aminocyanation reaction of the reactant *a* catalyzed by the Lewis acid $B(C_6F_5)_3$.

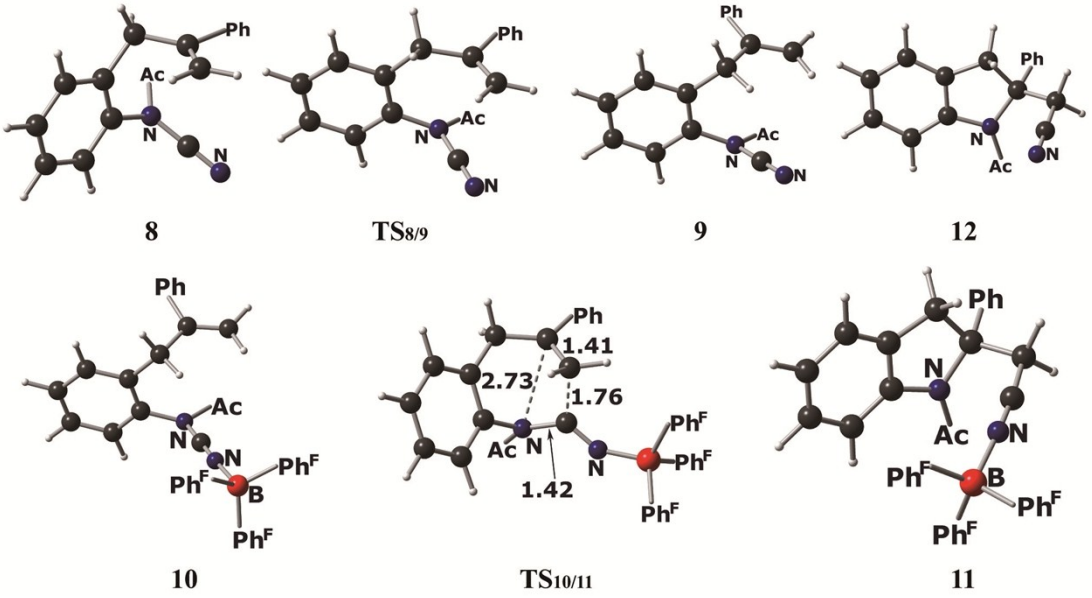

Figure S6. Optimized structures of intermediates, transition states and products in the intramolecular addition of the reactant ***a*** in toluene. All bond lengths are in Å.

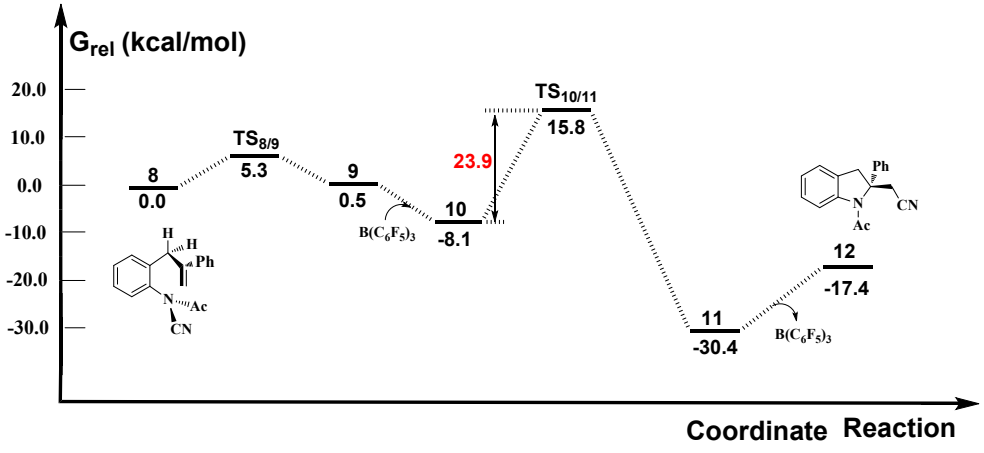

Figure S7. Gibbs free energy profiles of the intramolecular addition of the reactant ***a*** catalyzed by $B(C_6F_5)_3$ in toluene. Relative free energies calculated at 298.15 K and 1 atm (with respect to that of the reactants) are given.

The intramolecular oxycyanation of the substrate *b* catalyzed by $B(C_6F_5)_3$

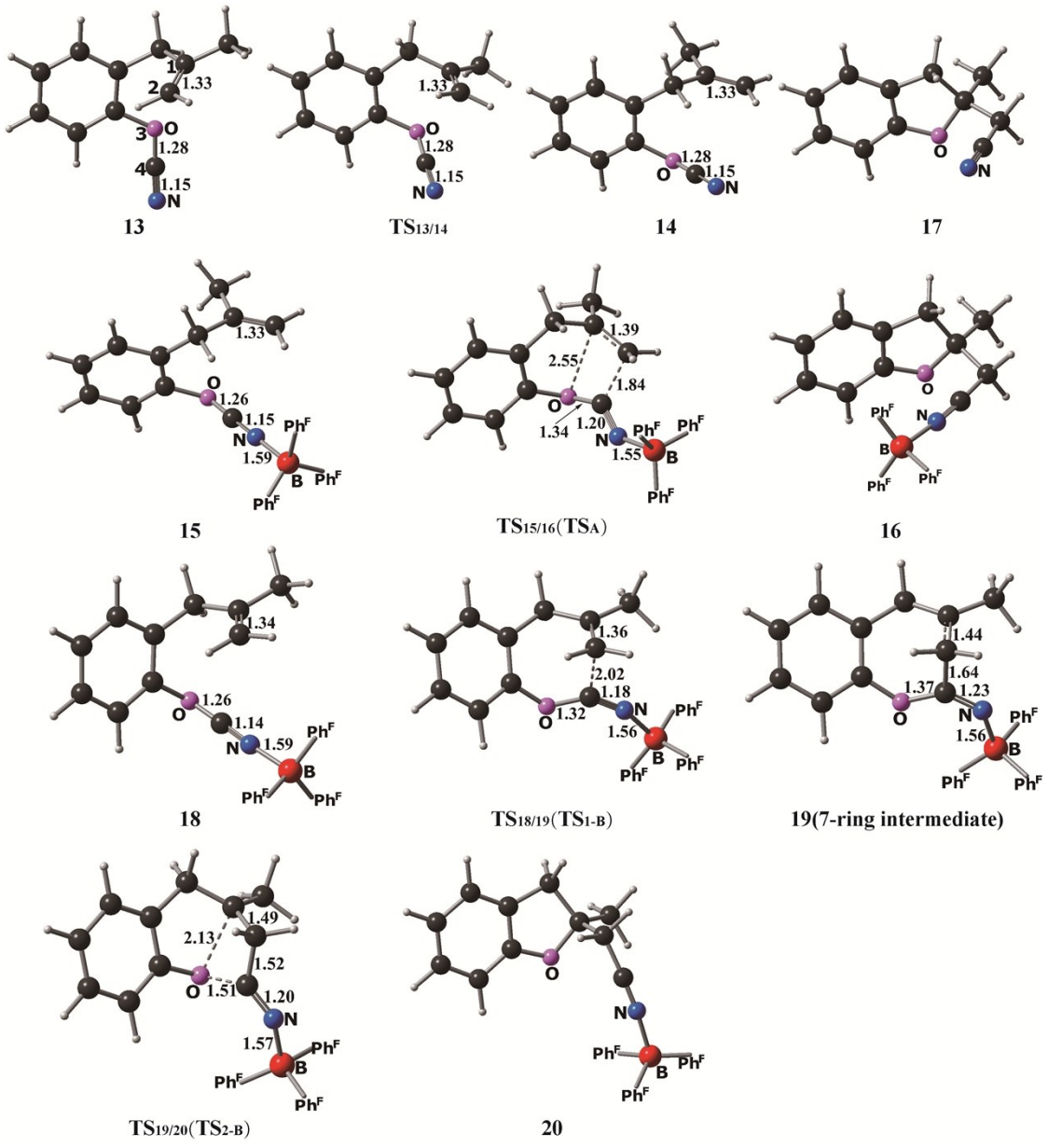

Figure S8. Optimized structures of intermediates, transition states and products in the intramolecular oxycyanation of the substrate ***b*** catalyzed by $B(C_6F_5)_3$ in tetrahydrofuran. All bond lengths are in Å.

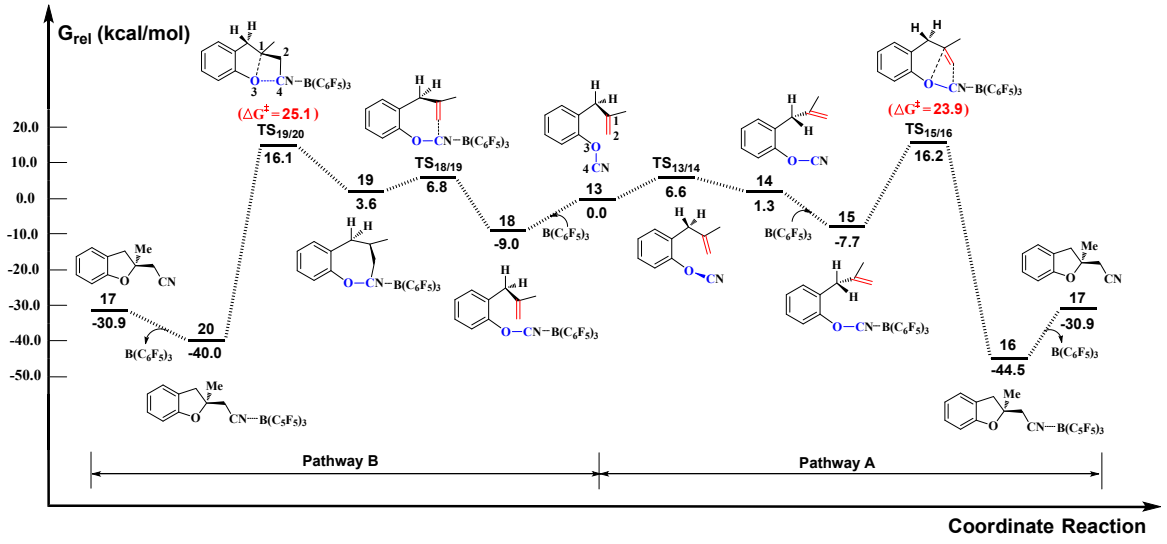

Figure S9. Gibbs free energy profiles of intramolecular oxycyanation of the substrate ***b*** catalyzed by $B(C_6F_5)_3$ in tetrahydrofuran. Relative free energies calculated at 298.15 K and 1 atm (with respect to that of the reactants) are given.

Table S1. Cartesian coordinates and energies of all species.

1

M06 free energy in solution: -1354.363901 a.u.

Symbol	X	Y	Z
C	2.4870390	2.5951360	-0.4947690
C	2.2048070	1.2348810	-0.4003250
C	1.0019030	0.8740210	0.2111070
C	0.1138580	1.8129140	0.7207200
C	0.4182640	3.1647940	0.6122150
C	1.6044730	3.5513870	-0.0002990
H	3.4173490	2.9066320	-0.9563230
H	-0.7989330	1.4802530	1.2038450
H	-0.2643910	3.9062300	1.0078040
H	1.8501120	4.6029870	-0.0866150
C	0.5927310	-1.0683810	1.5535560
N	0.4982860	-1.5316030	2.6048140
C	3.1647940	0.1829980	-0.8802440
H	3.9412180	0.6525150	-1.4934670
H	2.6396000	-0.5151080	-1.5394170
C	3.8351060	-0.6095040	0.2270950
C	3.8301050	-0.2371700	1.5037730
H	3.3276000	0.6627950	1.8412510
H	4.3286760	-0.8358450	2.2572700
C	4.5139780	-1.8642790	-0.2460650
H	5.0531590	-2.3570570	0.5628150
H	3.7727960	-2.5626080	-0.6477980
H	5.2178630	-1.6433290	-1.0543800
S	-0.2776170	-1.2731600	-0.9009290
O	0.1760000	-0.6663320	-2.1282380
O	-0.1814490	-2.6892060	-0.6495290
C	-1.9078470	-0.7097700	-0.5285740
C	-2.3896290	0.4384260	-1.1467840
C	-2.6397540	-1.3915730	0.4397470
C	-3.6458540	0.9048890	-0.7842380
H	-1.7938630	0.9440990	-1.8968790
C	-3.8896110	-0.9030710	0.7872200
H	-2.2384880	-2.2865780	0.8998080
C	-4.4085700	0.2460390	0.1829870
H	-4.0403630	1.7955340	-1.2596400
H	-4.4734900	-1.4226430	1.5383540
C	-5.7811050	0.7416570	0.5482510
H	-5.9903320	0.5713130	1.6049750
H	-5.8872360	1.8058430	0.3371430
H	-6.5395350	0.2074330	-0.0304230
N	0.6925130	-0.5366780	0.3261050

$TS_{1/2}$

M06 free energy in solution: -1354.351391 a.u.

Symbol	X	Y	Z
C	2.7868180	2.6784580	-0.1028010
C	2.5003390	1.3119330	0.0196390
C	1.1730670	0.9812510	0.2977290
C	0.1986680	1.9592430	0.5103590
C	0.5157110	3.3000770	0.3879000
C	1.8218760	3.6576360	0.0628610
H	3.8090530	2.9679590	-0.3240250
H	-0.8047690	1.6499760	0.7795620
H	-0.2422940	4.0561270	0.5490840
H	2.0909660	4.7016020	-0.0430440
C	0.6295670	-0.9671080	1.5927880
N	0.5126470	-1.4522540	2.6321360
C	3.6940600	0.3698270	-0.0822780
H	4.4028710	0.7088950	0.6790010
H	4.1713240	0.5601520	-1.0502650
C	3.4875820	-1.1183110	0.0774320
C	3.6544650	-1.7104830	1.2561830
H	3.9185350	-1.1438310	2.1431460
H	3.5068900	-2.7780520	1.3763450
C	3.1723800	-1.8788420	-1.1817340
H	2.7522270	-2.8613360	-0.9663780
H	2.4727520	-1.3277500	-1.8137750
H	4.0883810	-2.0101980	-1.7677000
S	-0.2060970	-1.0938950	-0.8751960
O	0.2249810	-0.4168240	-2.0741720
O	-0.0803460	-2.5183280	-0.6899510
C	-1.8615680	-0.6057410	-0.4971090
C	-2.4179430	0.4805410	-1.1622100
C	-2.5559250	-1.3050020	0.4861830
C	-3.7055580	0.8733960	-0.8242250

H	-1.8524360	0.9933310	-1.9307190
C	-3.8379280	-0.8883700	0.8110450
H	-2.1052110	-2.1613310	0.9733970
C	-4.4272660	0.2033780	0.1670440
H	-4.1600070	1.7106610	-1.3417390
H	-4.3937670	-1.4246310	1.5716640
C	-5.8097440	0.6577020	0.5485120
H	-5.7589970	1.3487170	1.3943980
H	-6.2971700	1.1752300	-0.2779990
H	-6.4313270	-0.1870270	0.8470930
N	0.7533290	-0.4038120	0.3841750

2

M06 free energy in solution: -1354.362918 a.u.

Symbol	X	Y	Z
C	2.9610090	2.4149780	0.2426900
C	2.4994410	1.1154840	0.4494880
C	1.1175350	0.9468200	0.5833580
C	0.2331030	2.0179470	0.5389450
C	0.7199190	3.2996000	0.3167370
C	2.0877120	3.4942070	0.1660640
H	4.0280140	2.5779160	0.1375270
H	-0.8253280	1.8389370	0.6874720
H	0.0364720	4.1382530	0.2757530
H	2.4792350	4.4903200	-0.0016270
N	0.5760780	-0.3772110	0.7834960
C	0.8197470	-1.0486800	1.9104440
N	1.0406950	-1.6102590	2.8937000
C	3.4621230	-0.0499880	0.5315020
H	3.3443900	-0.5669440	1.4877970
H	4.4777090	0.3578520	0.5101110
C	3.3071880	-1.0400570	-0.6045850
C	3.0477410	-2.3223140	-0.3667560
H	2.9163070	-2.6985470	0.6429740
H	2.9400500	-3.0328920	-1.1787320
C	3.4725840	-0.4778200	-1.9878870
H	2.7098080	0.2810080	-2.1826260
H	4.4521950	0.0003940	-2.0936590
H	3.3759860	-1.2573760	-2.7434280
S	-0.2324650	-1.1962140	-0.5040230
O	0.3386290	-0.6799000	-1.7226630
O	-0.1934550	-2.5905070	-0.1396530
C	-1.8941360	-0.6050160	-0.3665900
C	-2.3412850	0.3693720	-1.2484600
C	-2.7031580	-1.1121760	0.6459290
C	-3.6397230	0.8442220	-1.1082010
H	-1.6845320	0.7394570	-2.0260600
C	-3.9921440	-0.6198620	0.7693990
H	-2.3310380	-1.8808280	1.3132930
C	-4.4775550	0.3616770	-0.1021580
H	-4.0062600	1.6007830	-1.7925720
H	-4.6369600	-1.0039670	1.5517270
C	-5.8904550	0.8601550	0.0345490
H	-6.5901640	0.1283550	-0.3776960
H	-6.1505290	1.0107150	1.0834770
H	-6.0325980	1.8002290	-0.4980110

$TS_{2/3}$

M06 free energy in solution: -1354.282246 a.u.

Symbol	X	Y	Z
C	2.6113690	2.8224960	-0.2675000
C	2.3751070	1.4518310	-0.2382300
C	1.1084550	0.9856700	0.1216600
C	0.0917510	1.8662650	0.4831010
C	0.3352230	3.2321800	0.4263170
C	1.5880760	3.7085880	0.0465730
H	3.5930790	3.1942360	-0.5381610
H	-0.8641870	1.4849350	0.8208760
H	-0.4498400	3.9268890	0.6976140
H	1.7715090	4.7754790	0.0109760
N	0.9967110	-0.4406530	0.2048020
C	1.2429320	-0.9871910	1.6083660
N	0.4760880	-1.3658220	2.4368900
C	3.4033140	0.4024860	-0.5745880
H	4.3985910	0.7490830	-0.2697870
H	3.4261840	0.2287380	-1.6533280
C	3.1280610	-0.8819480	0.1510830
C	2.9239500	-0.9123120	1.5739840
H	3.2087040	-0.0029350	2.1013650
H	3.2607560	-1.8179720	2.0685750
C	3.2595810	-2.1619580	-0.5934780
H	2.8606360	-2.0804600	-1.6056260

H	4.3311860	-2.3906180	-0.6700020
H	2.7674760	-2.9804130	-0.0681370
S	-0.0949970	-1.2354270	-0.8323500
O	0.2553890	-0.7443100	-2.1535080
O	0.0371710	-2.6397770	-0.5159020
C	-1.7338740	-0.6819080	-0.4488860
C	-2.3143420	-1.0702430	0.7555470
C	-2.3870550	0.1459880	-1.3515020
C	-3.5881360	-0.6092510	1.0472340
H	-1.7528710	-1.6764220	1.4580970
C	-3.6654490	0.5919930	-1.0372110
H	-1.8989790	0.4308390	-2.2751290
C	-4.2802780	0.2225560	0.1592580
H	-4.0553150	-0.8938500	1.9836370
H	-4.1902280	1.2382380	-1.7316420
C	-5.6715900	0.6902040	0.4910930
H	-5.9655720	1.5349210	-0.1320340
H	-6.3908500	-0.1167920	0.3283380
H	-5.7429750	0.9882710	1.5384830

3

M06 free energy in solution: -1354.402382 a.u.

Symbol	X	Y	Z
C	3.4832280	1.5553790	1.1936240
C	2.6141750	0.5229890	0.8863980
C	1.8850820	0.5409230	-0.3008840
C	2.0206440	1.5879480	-1.2078400
C	2.8933820	2.6246120	-0.8809630
C	3.6205800	2.6188350	0.3037220
H	4.0468490	1.5336700	2.1196580
H	1.4865460	1.5927570	-2.1460110
H	3.0082390	3.4454370	-1.5786200
H	4.2951600	3.4344100	0.5318040
N	1.0842650	-0.6297200	-0.3781530
C	-0.6257850	-0.8055550	2.1039520
N	-1.1448390	0.0963560	2.5905340
C	2.2921580	-0.7076050	1.6864650
H	1.7964750	-0.4379720	2.6233070
H	3.1883390	-1.2784100	1.9375470
C	1.3605930	-1.5523480	0.7717570
C	0.0726150	-1.9515770	1.5199810
H	0.3519400	-2.6223860	2.3367480
H	-0.6071330	-2.4994910	0.8644590
C	2.0785840	-2.8066660	0.2775060
H	2.9786360	-2.5115270	-0.2655500
H	2.3743980	-3.4206940	1.1317830
H	1.4418540	-3.3911550	-0.3851930
S	-0.1011030	-0.9019820	-1.5093130
O	0.2933800	-0.2071740	-2.7159510
O	-0.3389220	-2.3332820	-1.5245800
C	-1.5599140	-0.1264120	-0.8599730
C	-1.5741180	1.2554030	-0.6902530
C	-2.6406920	-0.9147570	-0.4912090
C	-2.6857190	1.8421970	-0.1108140
H	-0.7282010	1.8605250	-0.9948420
C	-3.7514460	-0.3039010	0.0785510
H	-2.6094410	-1.9851670	-0.6543210
C	-3.7830430	1.0729940	0.2910590
H	-2.7038860	2.9157310	0.0398380
H	-4.6023700	-0.9096740	0.3689980
C	-4.9584000	1.7261670	0.9650340
H	-5.8391640	1.0843990	0.9376770
H	-4.7196120	1.9294350	2.0124750
H	-5.2041810	2.6772610	0.4901400

$B(C_6F_5)_3$

M06 free energy in solution: -2208.062144 a.u.

Symbol	X	Y	Z
B	-1.4801400	-0.3128700	-0.1263000
C	-1.7873800	-0.8232000	1.3896400
C	-1.6069200	0.0625600	2.4451100
C	-2.2382200	-2.0872000	1.7427600
C	-1.8401800	-0.2630100	3.7692500
C	-2.4860800	-2.4541100	3.0573600
C	-2.2842500	-1.5385500	4.0754900
C	-2.3948400	0.9648000	-0.5408600
C	-1.9323000	1.9960100	-1.3460100
C	-3.7098900	1.0905900	-0.1124100
C	-2.6903400	3.1077100	-1.6730400
C	-4.5074500	2.1791100	-0.4280700
C	-3.9902300	3.1996900	-1.2082000
C	-1.4184700	-1.4891400	-1.2471900

C	-0.4651200	-2.4928300	-1.1306900
C	-2.2476100	-1.5878000	-2.3549300
C	-0.3094300	-3.5200100	-2.0392100
C	-2.1324500	-2.6095600	-3.2903000
C	-1.1565600	-3.5769100	-3.1349300
F	-0.6890300	1.9563600	-1.8639700
F	-2.1803100	4.0791100	-2.4269200
F	-4.7372700	4.2530400	-1.5142100
F	-5.7606800	2.2530000	0.0076100
F	-4.2757500	0.1256600	0.6207900
F	-3.2169000	-0.6957300	-2.5771200
F	-2.9494600	-2.6614200	-4.3372600
F	-1.0318400	-4.5531000	-4.0249900
F	0.6337500	-4.4475000	-1.8705300
F	0.3540900	-2.5035200	-0.0614300
F	-1.1937900	1.3157900	2.1936200
F	-1.6479800	0.6264300	4.7375900
F	-2.4718600	-3.0228400	0.8153800
F	-2.9177300	-3.6781600	3.3478500
F	-2.5150100	-1.8814300	5.3361700

4

M06 free energy in solution: -3562.442218 a.u.

Symbol	X	Y	Z
C	-5.4962110	1.2531980	0.3569940
C	-4.3997310	0.5164570	-0.0912610
C	-3.7834010	-0.3198730	0.8447560
C	-4.2135680	-0.4154530	2.1627890
C	-5.3156040	0.3208250	2.5713570
C	-5.9564190	1.1562100	1.6640100
H	-5.9953560	1.9148470	-0.3416570
H	-3.6922440	-1.0677730	2.8502090
H	-5.6637240	0.2461120	3.5933990
H	-6.8152390	1.7388060	1.9743450
N	-2.6237620	-1.1049890	0.4546770
C	-1.5579790	-0.5068300	0.0146350
N	-0.5968860	0.0141600	-0.3418350
C	-3.9139890	0.6637450	-1.5180810
H	-2.9623090	1.2063250	-1.5332010
H	-4.6372620	1.2981130	-2.0399390
C	-3.7754970	-0.6379350	-2.2818310
C	-2.6863850	-0.8973490	-2.9996920
H	-1.8551070	-0.2025020	-3.0435390
H	-2.6007260	-1.8158050	-3.5695940
C	-4.9527720	-1.5699040	-2.2172670
H	-5.1704840	-1.8688140	-1.1869680
H	-5.8510120	-1.0715260	-2.5968750
H	-4.7704590	-2.4720210	-2.7995010
S	-2.6023770	-2.8969000	0.4610060
O	-3.5793140	-3.2090510	1.4696150
O	-2.7398370	-3.3535990	-0.8947190
C	-0.9510160	-3.1487100	1.0148480
C	-0.6195740	-2.7812190	2.3167730
C	-0.0142050	-3.6655470	0.1264960
C	0.6945900	-2.9243530	2.7256850
H	-1.3669130	-2.3762140	2.9884180
C	1.2905560	-3.8283050	0.5723380
H	-0.3063570	-3.9352580	-0.8812900
C	1.6653520	-3.4496020	1.8637270
H	0.9749250	-2.6239890	3.7294900
H	2.0343130	-4.2482760	-0.0955930
C	3.0821880	-3.6172790	2.3339050
H	3.7686470	-3.6973100	1.4921120
H	3.3847990	-2.7683090	2.9487280
H	3.1697100	-4.5217010	2.9420990
B	0.8279050	0.6763840	-0.3693340
C	0.6467710	2.1438280	-1.0530690
C	-0.3902270	2.9652840	-0.6299460
C	1.4928530	2.6949670	-2.0054920
C	-0.6084410	4.2395210	-1.1241670
C	1.3136310	3.9698720	-2.5209610
C	0.2554630	4.7449420	-2.0804540
C	1.3545010	0.8818300	1.1605490
C	0.6981910	0.5857920	2.3444680
C	2.6273620	1.4203320	1.3142420
C	1.2771390	0.7588260	3.5948980
C	3.2344600	1.6277680	2.5376720
C	2.5498500	1.2869770	3.6942660
C	1.6949940	-0.3996770	-1.2377940
C	1.3880910	-0.5873500	-2.5817340
C	2.6686350	-1.2493100	-0.7363170
C	1.9886310	-1.5386410	-3.3850050

C	3.2939670	-2.2193490	-1.5070860
C	2.9531320	-2.3695110	-2.8367860
F	-0.5538790	0.0891640	2.3609880
F	0.6109780	0.4131400	4.6966710
F	3.1131370	1.4648660	4.8838440
F	4.4617160	2.1335020	2.6184240
F	3.3416410	1.7137040	0.2195460
F	3.0427740	-1.2076580	0.5495650
F	4.1855460	-3.0448060	-0.9538170
F	3.5332900	-3.3046510	-3.5784500
F	1.6509290	-1.6688930	-4.6644310
F	0.4598480	0.1870220	-3.1609180
F	-1.2446460	2.5279110	0.3125360
F	-1.6276960	4.9775400	-0.6897670
F	2.5341150	2.0056040	-2.4810350
F	2.1463670	4.4539650	-3.4389130
F	0.0704960	5.9656430	-2.5695190

$TS_{4/5}$

M06 free energy in solution: -3562.395875 a.u.

Symbol	X	Y	Z
C	4.3990020	-3.4802410	1.2711920
C	3.6595300	-2.7059640	0.3786300
C	3.6450460	-1.3131310	0.5537790
C	4.3745720	-0.7289470	1.5875890
C	5.1198580	-1.5193890	2.4491110
C	5.1276970	-2.9007320	2.2988650
H	4.4045630	-4.5571640	1.1446750
H	4.3740710	0.3463100	1.7048340
H	5.6860260	-1.0501140	3.2437080
H	5.7026200	-3.5234780	2.9724050
N	2.8731030	-0.4933780	-0.3387040
C	1.5307330	-0.8441220	-0.6538770
N	0.5339070	-0.4213660	-0.1364590
C	2.8664480	-3.4311810	-0.7088260
H	1.9049130	-3.7632890	-0.3077700
H	3.4452020	-4.3063730	-1.0190500
C	2.6561080	-2.5393500	-1.8834030
C	1.4100470	-1.9287640	-2.0449690
H	0.5361870	-2.5035170	-1.7567570
H	1.2792700	-1.2712550	-2.8991080
C	3.8231900	-2.1606920	-2.6999730
H	4.7431510	-2.1346310	-2.1118670
H	3.9393360	-2.9600170	-3.4482230
H	3.6630110	-1.2225690	-3.2302750
S	3.3485730	0.9934640	-0.9769390
O	4.7624410	1.1204910	-0.7047560
O	2.8689240	0.9980980	-2.3470860
C	2.3929630	2.1910740	-0.0781190
C	1.9774070	1.9464090	1.2277490
C	2.0944380	3.3815750	-0.7289530
C	1.2587020	2.9293010	1.8885790
H	2.1569010	0.9902230	1.7038500
C	1.3825470	4.3576270	-0.0404250
H	2.3991380	3.5366900	-1.7571840
C	0.9557950	4.1475860	1.2709430
H	0.9068640	2.7420740	2.8973880
H	1.1359450	5.2877540	-0.5413230
C	0.1418010	5.1763410	2.0058540
H	0.0798780	6.1087540	1.4457930
H	-0.8733760	4.8020800	2.1574360
H	0.5760410	5.3818930	2.9863100
B	-0.9829090	-0.2268630	-0.0589110
C	-1.7867560	-1.4857210	-0.7455350
C	-1.4500180	-2.7754440	-0.3561410
C	-2.8464190	-1.3981260	-1.6368680
C	-2.0796210	-3.9150690	-0.8251870
C	-3.5132890	-2.5127460	-2.1259060
C	-3.1267700	-3.7783100	-1.7206000
C	-1.4402000	-0.1972310	1.5072590
C	-0.6455250	-0.4686870	2.6092260
C	-2.7748620	0.0669460	1.7868170
C	-1.1345380	-0.4550690	3.9099810
C	-3.3031220	0.0882840	3.0628220
C	-2.4688730	-0.1772550	4.1376280
C	-1.1572940	1.2086270	-0.8346910
C	-0.8404960	1.2746340	-2.1865150
C	-1.4712780	2.4276980	-0.2525730
C	-0.8356110	2.4392870	-2.9304940
C	-1.4842700	3.6200230	-0.9629150
C	-1.1609840	3.6306810	-2.3045250
F	0.6590250	-0.7657430	2.4837030

F	-0.3279870	-0.7155350	4.9393130
F	-2.9504310	-0.1646760	5.3770540
F	-4.5888500	0.3635570	3.2726450
F	-3.6054630	0.3518470	0.7733540
F	-1.7527940	2.5367090	1.0535660
F	-1.7433750	4.7721670	-0.3420400
F	-1.1278830	4.7778240	-2.9763720
F	-0.5185510	2.4297060	-4.2228650
F	-0.5208630	0.1443760	-2.8434070
F	-0.4316680	-2.9618430	0.5091830
F	-1.6885780	-5.1272960	-0.4324440
F	-3.2830140	-0.2130440	-2.0724730
F	-4.5218800	-2.3785420	-2.9834650
F	-3.7530320	-4.8527820	-2.1881480

5

M06 free energy in solution: -3562.482159 a.u.

Symbol	X	Y	Z
C	4.5247350	-2.9837950	0.1603640
C	4.0023930	-1.9737130	-0.6250430
C	4.2811780	-0.6377750	-0.3402160
C	5.0895180	-0.2844040	0.7320410
C	5.6059590	-1.3140970	1.5197420
C	5.3344310	-2.6486230	1.2453280
H	4.2993810	-4.0205110	-0.0631290
H	5.3358500	0.7456490	0.9438250
H	6.2380520	-1.0564290	2.3608730
H	5.7504110	-3.4266080	1.8726670
N	3.5866890	0.1837670	-1.2790680
C	0.7545700	-0.1653100	-1.9595580
N	-0.0431750	-0.1943370	-1.1461140
C	3.0463320	-2.0594500	-1.7818600
H	2.0369320	-2.2594240	-1.4064960
H	3.3022950	-2.8356220	-2.5047600
C	3.1391950	-0.6585150	-2.4317210
C	1.7787980	-0.1962900	-2.9904450
H	1.4434850	-0.9069540	-3.7516140
H	1.8480810	0.7938100	-3.4445780
C	4.1766090	-0.6487880	-3.5535270
H	5.1315690	-0.9973050	-3.1546850
H	3.8674230	-1.3271390	-4.3519970
H	4.3038920	0.3531130	-3.9611480
S	3.6976270	1.8447950	-1.3484900
O	4.9427440	2.2431490	-0.7292890
O	3.4091660	2.2276310	-2.7202370
C	2.3592330	2.4361610	-0.3397920
C	2.2971070	2.0671000	1.0030340
C	1.4746770	3.3587850	-0.8814600
C	1.3442460	2.6617580	1.8120840
H	2.9796480	1.3297070	1.4105920
C	0.5346020	3.9559640	-0.0462080
H	1.5453160	3.6272690	-1.9284560
C	0.4815470	3.6457910	1.3114260
H	1.2900050	2.3913720	2.8612540
H	-0.1397910	4.7023820	-0.4519860
C	-0.4304470	4.3882600	2.2481440
H	-1.1270850	5.0283330	1.7061860
H	-1.0022130	3.7034260	2.8761210
H	0.1649440	5.0231030	2.9095010
B	-1.2363030	-0.3132910	-0.1163400
C	-2.1744320	-1.5066790	-0.7239930
C	-1.5934660	-2.7289750	-1.0373130
C	-3.5495470	-1.4393250	-0.9028760
C	-2.3015870	-3.8168000	-1.5152700
C	-4.2973720	-2.5071800	-1.3771380
C	-3.6704430	-3.7003530	-1.6888110
C	-0.6508620	-0.8011780	1.3169000
C	0.6778500	-1.0054170	1.6496400
C	-1.5669080	-1.1217500	2.3119960
C	1.0882660	-1.4567120	2.8963600
C	-1.2047030	-1.5773960	3.5651950
C	0.1402020	-1.7451370	3.8595790
C	-1.9478720	1.1497880	-0.1378820
C	-2.3090870	1.6959360	-1.3647410
C	-2.2986230	1.9103000	0.9680230
C	-2.9614760	2.9059110	-1.5101350
C	-2.9995590	3.1044950	0.8687470
C	-3.3141630	3.6171020	-0.3751850
F	1.6588160	-0.7807140	0.7614660
F	2.3829810	-1.6186890	3.1602340
F	0.5113190	-2.1825820	5.0571350
F	-2.1230980	-1.8544840	4.4863180

F	-2.8739630	-0.9602470	2.0702890
F	-1.9779840	1.5333870	2.2117550
F	-3.3562900	3.7736820	1.9632700
F	-3.9498820	4.7774950	-0.4795310
F	-3.2692260	3.3787620	-2.7149760
F	-2.0527730	1.0143950	-2.4937970
F	-0.2678550	-2.8958380	-0.8706100
F	-1.6877180	-4.9618430	-1.8048830
F	-4.2319600	-0.3278850	-0.6107520
F	-5.6130110	-2.3939460	-1.5333520
F	-4.3753580	-4.7269210	-2.1475360

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M06 free energy in solution: -3562.446958 a.u.

Symbol	X	Y	Z
C	4.9945540	-3.2458120	0.1090370
C	4.0396600	-2.5523520	-0.6273880
C	3.5886330	-1.3414200	-0.0999820
C	4.0417970	-0.8220400	1.1025140
C	4.9959810	-1.5358240	1.8184970
C	5.4716800	-2.7418360	1.3168320
H	5.3622990	-4.1940350	-0.2661820
H	3.6406110	0.1147350	1.4712300
H	5.3620150	-1.1510220	2.7616910
H	6.2159660	-3.2996690	1.8719510
C	1.3383400	-0.6262740	-0.6367740
N	0.2025760	-0.5354650	-0.4849440
C	3.4299710	-3.0866800	-1.8943180
H	4.0133510	-3.9387160	-2.2551500
H	3.4781660	-2.3294190	-2.6836960
C	1.9801140	-3.5176990	-1.7091310
C	1.5296090	-4.0023820	-0.5533190
H	2.1688160	-4.0899140	0.3191410
H	0.5063180	-4.3463280	-0.4589930
C	1.1095370	-3.3670140	-2.9239580
H	0.1152520	-3.7791750	-2.7550110
H	1.0110920	-2.3069110	-3.1864120
H	1.5608920	-3.8658040	-3.7869870
B	-1.1564650	-0.1126110	0.1992090
C	-2.2984490	0.0232270	-0.9442830
C	-2.0642500	0.1255570	-2.3057280
C	-3.6355260	0.0173330	-0.5676900
C	-3.0821000	0.1999340	-3.2458710
C	-4.6801340	0.0898720	-1.4701990
C	-4.3981860	0.1769720	-2.8245900
C	-1.4721920	-1.3864430	1.1654100
C	-1.6800820	-1.3425190	2.5353230
C	-1.5385200	-2.6481830	0.5869020
C	-1.9166270	-2.4800040	3.2935730
C	-1.7598320	-3.8064210	1.3098450
C	-1.9480620	-3.7191720	2.6791760
C	-0.8099700	1.2767740	0.9900400
C	-1.5763630	2.4344570	0.9587410
C	0.3478540	1.3690700	1.7572380
C	-1.2306080	3.5900210	1.6477940
C	0.7442530	2.5080610	2.4310320
C	-0.0667840	3.6286200	2.3902920
F	-1.6680140	-0.1801940	3.1971780
F	-2.1071490	-2.3908760	4.6076110
F	-2.1600410	-4.8161020	3.3962210
F	-1.7809950	-4.9942200	0.7069540
F	-1.3775370	-2.7792290	-0.7383380
F	1.1524890	0.2975260	1.8943340
F	1.8942690	2.5398140	3.1019400
F	0.2910570	4.7385560	3.0271620
F	-1.9938940	4.6789930	1.5630720
F	-2.7076350	2.5062500	0.2494930
F	-0.8113760	0.1696380	-2.7925160
F	-2.8007840	0.2981530	-4.5433060
F	-3.9525820	-0.0235960	0.7329220
F	-5.9446110	0.0866900	-1.0568810
F	-5.3867600	0.2494350	-3.7087670
S	3.1233200	0.5985590	-2.0914320
O	4.5570460	0.5198840	-2.0380820
O	2.3575330	0.2680490	-3.2640100
C	2.5223980	2.0972140	-1.3914750
C	3.3003400	2.7673580	-0.4513130
C	1.2657620	2.5503520	-1.7817860
C	2.8033100	3.9432670	0.0894770
H	4.2783700	2.3915960	-0.1742660
C	0.7911610	3.7273370	-1.2207460
H	0.6872850	2.0000560	-2.5142900

C	1.5545800	4.4445120	-0.2956010
H	3.3961090	4.4878280	0.8152610
H	-0.1830130	4.1014910	-1.5170300
C	1.0592080	5.7578950	0.2437670
H	-0.0244010	5.7530220	0.3738600
H	1.5241630	5.9946270	1.2003470
H	1.3034100	6.5588790	-0.4592040
N	2.6190810	-0.5903470	-0.8713950

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M06 free energy in solution: -3562.390473 a.u.

Symbol	X	Y	Z
C	2.5725720	5.5946230	-0.6897000
C	1.9275140	4.5865270	0.0179010
C	2.3143880	3.2538460	-0.1566020
C	3.3761210	2.9405170	-1.0013540
C	4.0309930	3.9573720	-1.6832990
C	3.6264970	5.2802070	-1.5368430
H	2.2614390	6.6246750	-0.5611430
H	3.7025840	1.9169690	-1.1185290
H	4.8592460	3.7107500	-2.3353160
H	4.1384100	6.0678210	-2.0755330
C	0.2613180	1.7493060	0.0646120
N	0.0026820	0.5599110	0.0538560
C	0.8468010	4.8587140	1.0287840
H	0.2355580	5.7160380	0.7015650
H	1.2632680	5.1066490	2.0075250
C	-0.0999250	3.7310680	1.1240400
C	-0.5638000	3.0523740	-0.1056970
H	-0.2682750	3.5777660	-1.0147380
H	-1.6260490	2.8394860	-0.0986500
C	-0.7041250	3.3387060	2.4036650
H	-1.7499210	3.6799340	2.3758950
H	-0.7552610	2.2467300	2.4787860
H	-0.1926860	3.7628570	3.2635480
B	-1.0920330	-0.5090890	-0.2144560
C	-1.3142850	-1.2371330	1.2492660
C	-0.1967990	-1.6978960	1.9393570
C	-2.5138960	-1.4224010	1.9237070
C	-0.2323650	-2.2244160	3.2164810
C	-2.5991150	-1.9576740	3.2026670
C	-1.4503960	-2.3519700	3.8601640
C	-2.4804310	0.1578480	-0.8069050
C	-3.0688780	-0.1054740	-2.0365020
C	-3.1676370	1.0895720	-0.0398950
C	-4.2284910	0.5214080	-2.4792090
C	-4.3168410	1.7447830	-0.4361760
C	-4.8564130	1.4549090	-1.6783680
C	-0.3609430	-1.5062150	-1.3035790
C	-0.1346700	-2.8658510	-1.1573050
C	0.1834480	-0.9462490	-2.4531400
C	0.6108150	-3.6127170	-2.0624430
C	0.9148930	-1.6522180	-3.3883190
C	1.1378740	-3.0038880	-3.1834140
F	-2.5533410	-1.0039590	-2.8846390
F	-4.7406260	0.2288490	-3.6730530
F	-5.9603120	2.0682590	-2.0926400
F	-4.8997770	2.6482280	0.3537910
F	-2.7062160	1.4053390	1.1907210
F	0.0062090	0.3651240	-2.7023810
F	1.4416380	-1.0469070	-4.4551870
F	1.8869540	-3.6967390	-4.0394790
F	0.8360730	-4.9096120	-1.8516570
F	-0.6222780	-3.5486150	-0.1147090
F	1.0005170	-1.7010090	1.3447760
F	0.8870900	-2.6280160	3.8184240
F	-3.6929890	-1.0998260	1.3682300
F	-3.7845850	-2.0947640	3.8000560
F	-1.5158390	-2.8657070	5.0859140
S	2.4021240	1.3139480	1.7443780
O	3.4622250	2.1759000	2.2264560
O	1.3844130	0.8678720	2.6714050
C	3.1206970	-0.0745850	0.9012520
C	2.8814500	-0.3583210	-0.4360160
C	3.8741520	-0.9269320	1.7013840
C	3.4221120	-1.5155900	-0.9768000
H	2.2574880	0.2821550	-1.0449720
C	4.3778780	-2.0944970	1.1466960
H	4.0385230	-0.7010630	2.7483450
C	4.1545130	-2.4090940	-0.1950920
H	3.2556360	-1.7373570	-2.0244840
H	4.9420910	-2.7773420	1.7714860

C	4.6857180	-3.6798780	-0.8006260
H	4.8655750	-4.4354180	-0.0357880
H	3.9786050	-4.0845580	-1.5276400
H	5.6290700	-3.4927360	-1.3205170
N	1.5674090	2.2644120	0.5775490

7

M06 free energy in solution: -3562.478958 a.u.

Symbol	X	Y	Z
C	4.2155220	-2.9466360	-2.2442460
C	3.6275110	-1.7127990	-2.4717760
C	3.0682080	-1.0075630	-1.4073170
C	3.0426890	-1.5147590	-0.1184890
C	3.6397270	-2.7547860	0.1034570
C	4.2259470	-3.4581770	-0.9454620
H	4.6500180	-3.5114130	-3.0608130
H	2.5714660	-0.9620180	0.6869890
H	3.6310970	-3.1790940	1.1009600
H	4.6776450	-4.4240650	-0.7552400
C	-0.0312260	-0.5083280	-2.3441870
N	-0.7153200	-0.2712370	-1.4648990
C	3.3807280	-0.9462720	-3.7482860
H	3.1154990	-1.5813110	-4.5962690
H	4.2472550	-0.3376920	-4.0186560
C	2.2081710	-0.0321460	-3.3267470
C	0.9034800	-0.8886100	-3.3866670
H	1.1194630	-1.9463060	-3.2031540
H	0.4200790	-0.7979630	-4.3609630
C	2.0354500	1.2133170	-4.1821650
H	1.8210030	0.8920560	-5.2035370
H	1.2167880	1.8358010	-3.8182530
H	2.9441680	1.8140930	-4.2009040
B	-1.5314960	-0.1099460	-0.1281580
C	-1.8376680	1.4605680	0.1348880
C	-1.4441580	2.5348650	-0.6475160
C	-2.6413080	1.7742240	1.2247520
C	-1.8182440	3.8432420	-0.3679290
C	-3.0328390	3.0603260	1.5397150
C	-2.6172380	4.1056240	0.7286000
C	-2.9445710	-0.8834190	-0.3814720
C	-3.5344550	-1.7838780	0.4941760
C	-3.6755260	-0.5959730	-1.5274010
C	-4.7612390	-2.3801550	0.2426890
C	-4.8998830	-1.1718720	-1.8170040
C	-5.4450310	-2.0760210	-0.9210540
C	-0.5643670	-0.8410530	0.9682980
C	-0.0564370	-0.2702690	2.1259290
C	-0.1877440	-2.1634920	0.7516160
C	0.7570840	-0.9614730	3.0153140
C	0.6262390	-2.8837630	1.6048440
C	1.1130510	-2.2693590	2.7470230
F	-2.9403090	-2.1173160	1.6446520
F	-5.2880630	-3.2408030	1.1101160
F	-6.6180250	-2.6435960	-1.1761210
F	-5.5522510	-0.8682710	-2.9369770
F	-3.1934470	0.2875770	-2.4162020
F	-0.6262470	-2.8031380	-0.3435700
F	0.9773460	-4.1362730	1.3261270
F	1.9296150	-2.9255840	3.5648550
F	1.2097870	-0.3665660	4.1181850
F	-0.3218840	0.9999360	2.4553470
F	-0.6711670	2.3622820	-1.7279600
F	-1.4176970	4.8426380	-1.1492350
F	-3.0418500	0.7883160	2.0399880
F	-3.7940620	3.3076140	2.6025310
F	-2.9836190	5.3513330	1.0075500
S	3.3575900	1.6335970	-1.5034670
O	4.6534630	1.5414100	-2.1603580
O	2.4888360	2.7581770	-1.7800780
C	3.5792410	1.4785370	0.2398850
C	2.5166760	1.7979990	1.0765450
C	4.7863590	0.9944370	0.7285830
C	2.6768280	1.6164840	2.4435630
H	1.5906950	2.1858530	0.6647870
C	4.9188930	0.8075040	2.0962150
H	5.5913790	0.7602770	0.0426530
C	3.8659130	1.1010040	2.9680870
H	1.8637910	1.8678420	3.1132460
H	5.8511710	0.4233850	2.4952250
C	4.0109310	0.8473670	4.4436830
H	5.0002190	1.1442530	4.7949240
H	3.2557520	1.3878470	5.0135320

H	3.8855440	-0.2184380	4.6529670
N	2.4426310	0.2156440	-1.8554150

$B(C_6H_5)_3$

M06 free energy in solution: -719.449133 a.u.

Symbol	X	Y	Z
B	0.0009000	-0.0015900	-0.0045500
C	1.4714700	-0.5371800	-0.0042700
C	1.8089700	-1.7400400	0.6382800
C	2.5044800	0.1684900	-0.6430500
C	3.1169700	-2.2082500	0.6571500
C	3.8089800	-0.3093500	-0.6537800
C	4.1179200	-1.4959100	0.0040000
C	-1.1989800	-1.0057500	-0.0030000
C	-2.4069700	-0.6953000	0.6432600
C	-1.1092800	-2.2514600	-0.6459700
C	-3.4689700	-1.5911900	0.6621900
C	-2.1782600	-3.1390900	-0.6572400
C	-3.3576100	-2.8122100	0.0046200
C	-0.2704500	1.5398500	-0.0026400
C	0.6003500	2.4334000	0.6427200
C	-1.3959400	2.0818100	-0.6453200
C	0.3525200	3.8004400	0.6599300
C	-1.6332600	3.4506800	-0.6581300
C	-0.7618800	4.3114200	0.0019200
H	-4.1889500	-3.5079400	0.0076000
H	-2.0915200	-4.0873000	-1.1748100
H	-0.1896300	-2.5193500	-1.1558000
H	-4.3851600	-1.3367800	1.1821500
H	-2.5063800	0.2592800	1.1495800
H	-2.0870300	1.4168000	-1.1528900
H	-2.4993100	3.8471400	-1.1751400
H	-0.9513500	5.3787300	0.0038400
H	1.0297200	4.4686600	1.1790100
H	1.4775400	2.0449500	1.1496700
H	2.2745300	1.1001800	-1.1494700
H	4.5859800	0.2445000	-1.1676400
H	5.1371700	-1.8648300	0.0077400
H	3.3565500	-3.1304900	1.1735400
H	1.0328800	-2.3076000	1.1412300

TS

(Lewis acid =$B(C_6H_5)_3$)

M06 free energy in solution: -2073.756469 a.u.

Symbol	X	Y	Z
C	-4.4601890	0.3618530	1.8263060
C	-3.6543190	0.2975880	0.6912430
C	-2.7780880	-0.7881890	0.5523780
C	-2.7064330	-1.7660460	1.5390610
C	-3.5321810	-1.6955930	2.6506440
C	-4.4134210	-0.6305450	2.7954310
H	-5.1366320	1.2014380	1.9433440
H	-1.9988770	-2.5758090	1.4347470
H	-3.4741670	-2.4660230	3.4091390
H	-5.0588790	-0.5690040	3.6626450
N	-1.9491380	-0.8288290	-0.6159810
C	-1.0355130	0.2798150	-0.7625150
N	0.0248430	0.4021540	-0.2063140
C	-3.7022920	1.4722580	-0.2925700
H	-3.1831260	2.3212800	0.1645380
H	-4.7506610	1.7399310	-0.4525110
C	-3.0702300	1.1575170	-1.6078090
C	-1.7107400	1.4750650	-1.7968610
H	-1.3510130	2.3878060	-1.3239840
H	-1.3096370	1.2787710	-2.7889490
C	-3.8583640	0.4011040	-2.5972000
H	-4.5323000	-0.3090820	-2.1114890
H	-4.4885320	1.1401070	-3.1158690
H	-3.2269220	-0.0961190	-3.3317170
S	-1.5774310	-2.2219380	-1.4933880
O	-2.6026590	-3.1867690	-1.1625170
O	-1.4026060	-1.7320420	-2.8488520
C	-0.0010970	-2.7703350	-0.9100300
C	0.0848470	-3.6771150	0.1414670
C	1.1320840	-2.1821180	-1.4581940
C	1.3356420	-3.9519960	0.6777280
H	-0.8040690	-4.1710120	0.5153210
C	2.3708400	-2.4611820	-0.9038320
H	1.0451780	-1.5000370	-2.2931110
C	2.4853700	-3.3231020	0.1887990
H	1.4198300	-4.6554690	1.4985770
H	3.2503860	-1.9702940	-1.3083170

C	3.8159580	-3.5222710	0.8586260
H	4.6339430	-3.4451480	0.1415430
H	3.9584100	-2.7403130	1.6114000
H	3.8731480	-4.4895420	1.3592150
B	1.2148110	1.3384480	0.2030100
C	2.4455260	0.9813870	-0.8038790
C	2.2454550	0.8792090	-2.1877800
C	3.7459530	0.7530460	-0.3393900
C	3.2735240	0.5440680	-3.0638880
C	4.7900880	0.4307980	-1.2053080
C	4.5566600	0.3151210	-2.5716440
C	0.6600640	2.8668700	0.0703850
C	-0.3924690	3.2856600	0.9028670
C	1.0900880	3.7721970	-0.9046560
C	-0.9998230	4.5287910	0.7555460
C	0.4927690	5.0243570	-1.0603190
C	-0.5600600	5.4043340	-0.2371190
C	1.5691950	0.9115620	1.7319590
C	1.4522790	-0.4227010	2.1456150
C	2.0877410	1.8213660	2.6597130
C	1.8424680	-0.8346240	3.4161690
C	2.4833430	1.4213240	3.9355500
C	2.3629290	0.0897580	4.3191070
H	1.2507670	1.0541010	-2.5942520
H	3.0776840	0.4623080	-4.1276430
H	5.3636780	0.0545990	-3.2468560
H	5.7861060	0.2618860	-0.8099130
H	3.9455430	0.8155590	0.7256050
H	1.9082050	3.4938380	-1.5614100
H	0.8524970	5.7030470	-1.8261680
H	-1.0267070	6.3755690	-0.3569800
H	-1.8090690	4.8218040	1.4164230
H	-0.7419830	2.6119540	1.6828720
H	2.1849560	2.8664400	2.3783740
H	2.8842090	2.1504700	4.6317560
H	2.6676690	-0.2237680	5.3112010
H	1.0443310	-1.1525680	1.4507180
H	1.7374440	-1.8761200	3.7043130

Lewis Complex
(Lewis acid=$SnCl_4$)

M06 free energy in solution: -3198.728411 a.u.

Symbol	X	Y	Z
C	4.4162490	-1.6311890	1.8770550
C	3.5739730	-1.3325240	0.8051190
C	2.7334320	-0.2283360	0.9636060
C	2.7014270	0.5331570	2.1248180
C	3.5558940	0.2146070	3.1690140
C	4.4172800	-0.8693150	3.0391180
H	5.0834710	-2.4812870	1.7912650
H	2.0020300	1.3565210	2.2034480
H	3.5435000	0.8039260	4.0767840
H	5.0886920	-1.1273430	3.8488290
N	1.8417290	0.1508850	-0.1146750
C	0.8412440	-0.6106980	-0.4433180
N	-0.0801540	-1.2547070	-0.7345860
C	3.5578520	-2.2109640	-0.4294400
H	2.6431300	-2.8137160	-0.4355390
H	4.3916190	-2.9140760	-0.3350150
C	3.6860520	-1.4797890	-1.7500460
C	2.8639900	-1.7447820	-2.7609370
H	2.0596390	-2.4666110	-2.6632320
H	2.9655740	-1.2369450	-3.7129150
C	4.8103420	-0.4868830	-1.8504860
H	4.7202140	0.2976470	-1.0919750
H	5.7711980	-0.9820690	-1.6749880
H	4.8313970	-0.0148610	-2.8323880
S	2.0041000	1.6903950	-1.0067680
O	3.1346670	2.3097430	-0.3700880
O	1.9775010	1.3351610	-2.3987820
C	0.4984090	2.4816560	-0.5606860
C	0.4602640	3.2656460	0.5872380
C	-0.6367650	2.2205930	-1.3220440
C	-0.7610610	3.7884650	0.9841080
H	1.3680290	3.4742900	1.1410520
C	-1.8469970	2.7476280	-0.8971700
H	-0.5728850	1.6226560	-2.2235170
C	-1.9291030	3.5197510	0.2649740
H	-0.8106760	4.4054570	1.8737660
H	-2.7441230	2.5404320	-1.4700480
C	-3.2628120	4.0108700	0.7511620
H	-3.8963860	4.3180090	-0.0816140

H	-3.7765180	3.2017000	1.2791710
H	-3.1527550	4.8480130	1.4400410
Sn	-2.2712090	-1.1547880	0.0489380
Cl	-4.4898120	-0.9218610	0.7894470
Cl	-2.6958790	-0.5092100	-2.1433980
Cl	-1.9928140	-3.3999590	0.5103790
Cl	-1.3701240	0.3193530	1.6266020

TS

(Lewis acid=$SnCl_4$)

M06 free energy in solution: -3198.676240 a.u.

Symbol	X	Y	Z
C	4.3815460	-0.9696720	2.0630110
C	3.6228020	-0.8943160	0.8954790
C	2.6249200	0.0857930	0.8008730
C	2.4174390	0.9715710	1.8548240
C	3.1972680	0.8985320	2.9970150
C	4.1794620	-0.0795280	3.1067050
H	5.1464760	-1.7338730	2.1439910
H	1.6239990	1.7014560	1.7777890
H	3.0250750	1.5958840	3.8068240
H	4.7873110	-0.1481670	4.0000520
N	1.8270220	0.2018800	-0.3874440
C	1.1937020	-0.9602780	-0.9475780
N	0.0849290	-1.4311710	-0.8082850
C	3.8865470	-1.9373190	-0.1940860
H	3.3508870	-2.8596380	0.0437130
H	4.9613470	-2.1395990	-0.2103880
C	3.4680410	-1.4182400	-1.5206730
C	2.2019120	-1.8039510	-2.0266010
H	1.9151260	-2.8322080	-1.8339100
H	1.9470050	-1.4316750	-3.0158260
C	4.2917970	-0.3864140	-2.1583170
H	4.7474800	0.2844920	-1.4246570
H	5.1187110	-0.9407360	-2.6338750
H	3.7569280	0.1598430	-2.9321950
S	1.6578440	1.6503490	-1.2461450
O	2.7191230	2.5157490	-0.7854560
O	1.5689520	1.2245840	-2.6316420
C	0.0914190	2.3023070	-0.7660150
C	0.0100550	3.2058930	0.2842030
C	-1.0445450	1.8075170	-1.4001810
C	-1.2471450	3.5846830	0.7366770
H	0.9115390	3.6106020	0.7288020
C	-2.2902000	2.1929710	-0.9260160
H	-0.9543950	1.1477400	-2.2549170
C	-2.4086340	3.0646130	0.1630710
H	-1.3269580	4.2858630	1.5593050
H	-3.1834640	1.8036220	-1.4026530
C	-3.7634640	3.4030580	0.7147090
H	-4.5000160	3.5019460	-0.0836630
H	-4.0956770	2.5932350	1.3708230
H	-3.7393140	4.3269960	1.2925160
Sn	-1.8088510	-1.1507410	0.1308140
Cl	-3.9307120	-0.3716750	0.8896840
Cl	-2.6179770	-1.1593930	-2.1018270
Cl	-1.8906820	-3.3482870	0.8944360
Cl	-0.7453800	0.0843380	1.8535990

Lewis Complex

R^1=Me R^2=Me

M06 free energy in solution: -2782.956866 a.u.

Symbol	X	Y	Z
C	5.4338610	1.6165150	-0.5320170
C	4.2954340	0.8349690	-0.7298230
C	3.5963010	1.0231530	-1.9260270
C	4.0103140	1.9353270	-2.8889200
C	5.1549540	2.6902570	-2.6708520
C	5.8643200	2.5304030	-1.4862180
H	5.9918890	1.4962030	0.3896880
H	3.4280390	2.0519710	-3.7955290
H	5.4827420	3.4031210	-3.4167370
H	6.7549160	3.1186840	-1.3022610
N	2.4290540	0.2217910	-2.2260130
C	1.3794490	0.2605100	-1.4642770
N	0.4188370	0.2623900	-0.8292200
C	3.8628470	-0.1764380	0.3103190
H	2.8622150	0.0642550	0.6712480
H	4.5337400	-0.0788350	1.1697160
C	3.9012060	-1.6098940	-0.1793700
C	2.8309550	-2.3973660	-0.0967800
H	1.8884340	-2.0349100	0.3028290

H	2.8639280	-3.4319860	-0.4208970
C	5.2223880	-2.0778270	-0.7239840
H	5.5189760	-1.4866600	-1.5967650
H	6.0099520	-1.9457230	0.0247150
H	5.1859220	-3.1292290	-1.0093640
B	-0.8438150	0.0516940	0.1043610
C	-1.8686540	-0.8839500	-0.7518090
C	-1.4230080	-1.9517270	-1.5198040
C	-3.2469420	-0.7188450	-0.7203710
C	-2.2611080	-2.7857740	-2.2365720
C	-4.1238550	-1.5360600	-1.4186710
C	-3.6280180	-2.5727760	-2.1870920
C	-0.2432680	-0.6951390	1.4244160
C	0.7906410	-0.0785430	2.1198700
C	-0.5846880	-1.9603270	1.8788300
C	1.4865180	-0.6702210	3.1550070
C	0.0780650	-2.5874120	2.9283090
C	1.1234110	-1.9445180	3.5634390
C	-1.4367310	1.5443610	0.3596150
C	-1.6903770	2.3651630	-0.7315590
C	-1.7562420	2.0836880	1.5962090
C	-2.2157990	3.6405290	-0.6228070
C	-2.2849510	3.3569430	1.7490350
C	-2.5147080	4.1404740	0.6329470
F	1.1744950	1.1588090	1.7588100
F	2.4998470	-0.0426120	3.7479430
F	1.7721110	-2.5360740	4.5587520
F	-0.2826820	-3.8063690	3.3211150
F	-1.5779090	-2.6617250	1.3206050
F	-1.5786090	1.3809590	2.7216110
F	-2.5743710	3.8304890	2.9591580
F	-3.0213790	5.3617300	0.7636940
F	-2.4390810	4.3839600	-1.7049230
F	-1.4439320	1.9185890	-1.9738370
F	-0.1096110	-2.2516700	-1.5665280
F	-1.7698500	-3.7909110	-2.9590630
F	-3.8101850	0.2383810	0.0262850
F	-5.4370460	-1.3351740	-1.3481120
F	-4.4542640	-3.3649230	-2.8601000
C	2.5181900	-0.8346010	-3.2558890
H	1.5954620	-1.4117510	-3.2471400
H	2.6603950	-0.3715780	-4.2314450
H	3.3563990	-1.4876770	-3.0128470

TS

R^1=Me R^2=Me

M06 free energy in solution: -2782.894319 a.u.

Symbol	X	Y	Z
C	5.5496200	-0.2819680	-0.1717620
C	4.3831840	-0.9782880	-0.4752260
C	3.6703950	-0.6592070	-1.6455490
C	4.1631080	0.3509600	-2.4742770
C	5.3369110	1.0238960	-2.1642080
C	6.0377140	0.7120680	-1.0079770
H	6.0862400	-0.5351420	0.7362820
H	3.6197450	0.6327710	-3.3645100
H	5.6926380	1.8023500	-2.8277360
H	6.9536020	1.2322200	-0.7582850
N	2.4844290	-1.3879580	-2.0095490
C	1.4478070	-1.3149520	-1.0190450
N	0.5421230	-0.5201110	-0.9638180
C	3.9167190	-2.0227660	0.5418790
H	3.4765590	-1.5012940	1.3965590
H	4.7887220	-2.5922710	0.8741700
C	2.9193030	-2.9421270	-0.0611590
C	1.5551240	-2.6251760	0.0724240
H	1.2525010	-2.1806910	1.0156930
H	0.8480060	-3.3546900	-0.3136390
C	3.4085260	-4.0609980	-0.8837490
H	4.2924530	-3.7703170	-1.4561100
H	3.7287860	-4.8433320	-0.1782080
H	2.6362800	-4.4737540	-1.5291980
B	-0.6287160	0.0547110	-0.1626140
C	-0.5130370	-0.3366300	1.4410430
C	0.6909630	-0.1154160	2.0999780
C	-1.5438540	-0.7905560	2.2531450
C	0.8946090	-0.3576500	3.4476210
C	-1.3883890	-1.0353990	3.6109410
C	-0.1611550	-0.8221720	4.2129460
C	-0.5263380	1.6895850	-0.1878880
C	0.5271470	2.4436100	-0.6828110
C	-1.5392640	2.4172660	0.4250650

C	0.5658430	3.8299680	-0.5892480
C	-1.5427130	3.7942050	0.5332870
C	-0.4721940	4.5083410	0.0189770
C	-1.9647900	-0.5494070	-0.8936710
C	-2.2104570	-1.9129810	-0.8083280
C	-2.8733670	0.1568390	-1.6677140
C	-3.2835130	-2.5493280	-1.4015940
C	-3.9683890	-0.4388360	-2.2814070
C	-4.1772060	-1.7978570	-2.1464500
F	1.5881650	1.8796040	-1.2798340
F	1.6023300	4.5119590	-1.0790700
F	-0.4440900	5.8351850	0.1138800
F	-2.5512900	4.4392020	1.1181100
F	-2.5955280	1.7615660	0.9313340
F	-2.7409440	1.4720070	-1.8773290
F	-4.8149700	0.2882960	-3.0086900
F	-5.2201560	-2.3799070	-2.7305140
F	-3.4647670	-3.8632140	-1.2679340
F	-1.3748810	-2.6914570	-0.0911560
F	1.7602820	0.3272040	1.4087460
F	2.0902980	-0.1595170	4.0046370
F	-2.7647630	-1.0193980	1.7587910
F	-2.4094320	-1.4769340	4.3418540
F	0.0031240	-1.0608280	5.5098650
C	1.9560850	-1.1379170	-3.3552400
H	1.1286600	-1.8267080	-3.5213620
H	1.5907860	-0.1152860	-3.4809990
H	2.7420090	-1.3475090	-4.0802240

Lewis Complex

R^1=Ac R^2=Me

M06 free energy in solution: -2896.285476 a.u.

Symbol	X	Y	Z
C	5.2245700	1.1808830	-1.5821890
C	4.3064510	0.4714580	-0.8092580
C	3.7315580	-0.6561350	-1.3958990
C	4.0438570	-1.0841660	-2.6770250
C	4.9698240	-0.3638060	-3.4194890
C	5.5539520	0.7718890	-2.8694390
H	5.6887550	2.0650950	-1.1605000
H	3.5686610	-1.9718500	-3.0761030
H	5.2293190	-0.6861510	-4.4196180
H	6.2726200	1.3422190	-3.4451090
C	1.5710980	-0.9292840	-0.4679500
N	0.5255180	-0.4776910	-0.3347300
C	3.9885260	0.8787200	0.6126660
H	2.9182420	1.0695870	0.7321300
H	4.5004510	1.8256960	0.8095880
C	4.4522030	-0.1443650	1.6331510
C	3.6400640	-0.5745340	2.5971510
H	2.6234390	-0.2064210	2.6862130
H	3.9863560	-1.2766620	3.3481970
C	5.8769890	-0.6056280	1.5037750
H	6.0219690	-1.1577570	0.5707670
H	6.5535330	0.2547090	1.4801760
H	6.1584900	-1.2517910	2.3349190
B	-0.9408970	0.0589390	-0.1090840
C	-1.2017510	-0.1542640	1.4899460
C	-0.2832170	0.3759850	2.3873960
C	-2.2926460	-0.7895650	2.0654130
C	-0.3911240	0.2566960	3.7611970
C	-2.4458900	-0.9222520	3.4382820
C	-1.4870890	-0.4036170	4.2909570
C	-0.9754560	1.6516160	-0.4160100
C	0.0721750	2.4500960	-0.8432210
C	-2.1675560	2.3166820	-0.1557500
C	-0.0483790	3.8225920	-1.0124400
C	-2.3318470	3.6789190	-0.3136400
C	-1.2562950	4.4391720	-0.7467770
C	-1.8563670	-0.8680420	-1.0867890
C	-1.8169660	-2.2472650	-0.9171620
C	-2.6548870	-0.4280170	-2.1321450
C	-2.5120230	-3.1444240	-1.7030220
C	-3.3764610	-1.2946440	-2.9441860
C	-3.3043940	-2.6577960	-2.7306310
F	1.2820320	1.9290930	-1.1127290
F	0.9889410	4.5470080	-1.4271160
F	-1.3875150	5.7510330	-0.9056030
F	-3.4982550	4.2651700	-0.0589400
F	-3.2295280	1.6079450	0.2501010
F	-2.7686290	0.8711550	-2.4265690
F	-4.1275430	-0.8210660	-3.9347850

F	-3.9801230	-3.4961490	-3.5065740
F	-2.4269560	-4.4552800	-1.4888760
F	-1.0664180	-2.7664390	0.0735170
F	0.7862300	1.0499510	1.9232970
F	0.5400590	0.7638680	4.5658540
F	-3.2638330	-1.3093060	1.3100230
F	-3.5059850	-1.5473150	3.9425880
F	-1.6197530	-0.5325790	5.6051740
N	2.7698560	-1.4333170	-0.6281470
C	3.1749140	-2.6372760	0.0809750
C	2.0988740	-3.2529750	0.9216360
H	1.7438520	-2.5346460	1.6648450
H	1.2495500	-3.5469880	0.3007960
H	2.5145950	-4.1246060	1.4193120
O	4.2857870	-3.0314750	-0.0751810

TS

R^1=Ac R^2=Me

M06 free energy in solution: -2896.229401 a.u.

Symbol	X	Y	Z
C	5.3860700	0.9378610	0.0487690
C	4.3831290	0.0013900	0.2991000
C	3.8236250	-0.6919160	-0.7808800
C	4.2686420	-0.4471350	-2.0783430
C	5.2766340	0.4749860	-2.3061390
C	5.8361750	1.1734940	-1.2406000
H	5.8156460	1.4832820	0.8816900
H	3.8164210	-0.9882860	-2.8980590
H	5.6163940	0.6570330	-3.3178600
H	6.6202000	1.9002190	-1.4128460
C	1.6192870	-1.1470490	0.1332220
N	0.6571420	-0.6030850	-0.3505190
C	3.9100190	-0.1593190	1.7478250
H	3.2706280	0.6878350	2.0086650
H	4.7932370	-0.1587050	2.3929460
C	3.1723920	-1.4370780	1.9218330
C	1.7669850	-1.4287040	1.8291180
H	1.2598480	-0.5666440	2.2488900
H	1.2628590	-2.3707150	2.0273300
C	3.9498900	-2.6854910	1.9952210
H	4.8180850	-2.6538330	1.3310590
H	4.3407380	-2.7445400	3.0226060
H	3.3434950	-3.5712050	1.8120830
B	-0.7106890	0.0491590	-0.1019450
C	-0.8562960	0.6280290	1.4346040
C	0.1332170	1.4792300	1.9112120
C	-1.9319650	0.4427160	2.2904130
C	0.1040070	2.0817540	3.1558130
C	-2.0109690	1.0380350	3.5428960
C	-0.9860460	1.8580480	3.9807640
C	-0.8574680	1.3715130	-1.0477190
C	0.1594160	1.9822870	-1.7647780
C	-2.0798810	2.0306390	-1.0631660
C	-0.0313050	3.1599200	-2.4775070
C	-2.3119980	3.2003750	-1.7600910
C	-1.2710620	3.7694650	-2.4775420
C	-1.7363480	-1.1761520	-0.4701690
C	-1.7368950	-2.3075420	0.3350650
C	-2.5450780	-1.2653000	-1.5940610
C	-2.4840760	-3.4422430	0.0865360
C	-3.3214190	-2.3818110	-1.8811670
C	-3.2922590	-3.4762740	-1.0381910
F	1.3988560	1.4742170	-1.7977110
F	0.9753390	3.7100200	-3.1569640
F	-1.4644530	4.8973540	-3.1557260
F	-3.5091860	3.7843740	-1.7517970
F	-3.1070840	1.5084110	-0.3751510
F	-2.6162200	-0.2714460	-2.4852910
F	-4.0848580	-2.4104790	-2.9711450
F	-4.0219090	-4.5536510	-1.3055990
F	-2.4256840	-4.4951610	0.9012290
F	-0.9574100	-2.3360690	1.4367410
F	1.2220610	1.7179720	1.1512710
F	1.1077130	2.8566940	3.5666220
F	-2.9649840	-0.3297450	1.9412600
F	-3.0637150	0.8278370	4.3288080
F	-1.0436520	2.4247110	5.1808160
N	2.7613800	-1.6361320	-0.5690630
C	2.7259230	-2.8823900	-1.2002590
C	1.4233420	-3.6358810	-1.0625680
H	1.0797430	-3.6877640	-0.0259510
H	0.6459710	-3.1239780	-1.6357280

H	1.5715620	-4.6387400	-1.4534920
O	3.6814390	-3.3041670	-1.8020110

Lewis Complex

R^1=AcCl R^2=Me

M06 free energy in solution: -3316.604309 a.u.

Symbol	X	Y	Z
C	-4.4713750	-1.4656670	0.2581450
C	-3.6504950	-0.4726320	-0.2724140
C	-3.1053620	-0.7268620	-1.5324980
C	-3.3413200	-1.8881980	-2.2485300
C	-4.1714310	-2.8540710	-1.6952040
C	-4.7262480	-2.6420060	-0.4384660
H	-4.9098130	-1.3130930	1.2382550
H	-2.8772000	-2.0280020	-3.2171550
H	-4.3716550	-3.7689730	-2.2373960
H	-5.3609850	-3.3984310	0.0060890
C	-0.9895010	0.2708980	-1.5318480
N	-0.0232730	0.1434230	-0.9316910
C	-3.4117130	0.8316760	0.4586150
H	-2.3439460	0.9945270	0.6430740
H	-3.8901030	0.7527020	1.4402550
C	-3.9959220	2.0213630	-0.2815080
C	-3.2612520	3.0992150	-0.5476700
H	-2.2220030	3.1718320	-0.2467770
H	-3.6932560	3.9541180	-1.0567670
C	-5.4410420	1.9020140	-0.6787990
H	-5.5751140	1.1168840	-1.4292180
H	-6.0548610	1.6298450	0.1857310
H	-5.8127510	2.8391560	-1.0924240
B	1.0679240	-0.1135880	0.2209780
C	1.8370220	1.3070490	0.3833790
C	1.0970160	2.4714760	0.5417140
C	3.2129460	1.4818180	0.3627640
C	1.6509000	3.7314480	0.6509010
C	3.8137430	2.7292330	0.4724190
C	3.0302200	3.8593430	0.6119950
C	0.0965740	-0.5204550	1.4693960
C	-0.8366180	-1.5414940	1.3092840
C	0.0743210	0.1128740	2.7037420
C	-1.7417930	-1.9127460	2.2856350
C	-0.8274870	-0.2205710	3.7058980
C	-1.7436350	-1.2337550	3.4937400
C	1.9932630	-1.3177070	-0.3400260
C	2.5611300	-1.2005730	-1.6022820
C	2.2934730	-2.4840690	0.3458340
C	3.3702790	-2.1667060	-2.1684270
C	3.1013370	-3.4795020	-0.1861180
C	3.6392230	-3.3207840	-1.4500580
F	-0.8794840	-2.2269180	0.1550440
F	-2.6018940	-2.9082470	2.0851860
F	-2.6118370	-1.5646090	4.4418390
F	-0.8130310	0.4218710	4.8699090
F	0.9375560	1.0897100	2.9978000
F	1.8169340	-2.7038870	1.5769250
F	3.3596410	-4.5852430	0.5077070
F	4.4115220	-4.2660490	-1.9721550
F	3.8941170	-2.0015770	-3.3804170
F	2.3481740	-0.0835780	-2.3156920
F	-0.2448980	2.3906040	0.6282680
F	0.8835800	4.8081530	0.7979900
F	4.0435160	0.4411840	0.2414500
F	5.1383070	2.8438820	0.4414340
F	3.5925020	5.0570500	0.7119410
N	-2.1814130	0.2538250	-2.0993180
C	-2.6202140	1.2099580	-3.0379650
O	-3.6974070	1.2042190	-3.5081330
Cl	-1.3708500	2.3710810	-3.4347870

TS

R^1=AcCl R^2=Me

M06 free energy in solution: -3316.556485 a.u.

Symbol	X	Y	Z
C	5.1509210	1.1254090	0.1968510
C	4.2183950	0.0972770	0.3337840
C	3.7079520	-0.4857600	-0.8313190
C	4.1204000	-0.0639760	-2.0903820
C	5.0589970	0.9485070	-2.2020910
C	5.5714250	1.5475300	-1.0554310
H	5.5494850	1.5946240	1.0893660
H	3.6916250	-0.5294570	-2.9683280
H	5.3790640	1.2784800	-3.1819570

H	6.2996900	2.3446910	-1.1370080
C	1.5362270	-1.1862070	0.0051780
N	0.5841900	-0.5745000	-0.3915620
C	3.7750010	-0.2766660	1.7525340
H	3.1117300	0.5055590	2.1284940
H	4.6685410	-0.3200240	2.3820140
C	3.0917640	-1.6003420	1.7794590
C	1.6941470	-1.6593370	1.6938420
H	1.1325000	-0.8612980	2.1692740
H	1.2307520	-2.6392070	1.7641320
C	3.9363520	-2.8068330	1.6872470
H	4.7773930	-2.6541620	1.0038210
H	4.3729210	-2.9553160	2.6859660
H	3.3719110	-3.7016630	1.4288760
B	-0.7608790	0.1114480	-0.0995070
C	-0.8325570	0.6247250	1.4647990
C	0.2211790	1.3890710	1.9493800
C	-1.8900620	0.4577760	2.3473260
C	0.2723410	1.9196010	3.2256980
C	-1.8899630	0.9871320	3.6314500
C	-0.8014030	1.7164100	4.0765560
C	-0.8667600	1.4777080	-0.9865320
C	0.1637240	2.0795020	-1.6920220
C	-2.0636390	2.1819660	-0.9601160
C	0.0081460	3.2885920	-2.3587640
C	-2.2618460	3.3828400	-1.6135490
C	-1.2095530	3.9404140	-2.3232570
C	-1.8427540	-1.0534650	-0.4825990
C	-1.8871360	-2.2005610	0.2984800
C	-2.6892150	-1.0631870	-1.5817140
C	-2.7187530	-3.2756700	0.0534630
C	-3.5469450	-2.1183660	-1.8641050
C	-3.5636940	-3.2297420	-1.0429960
F	1.3860340	1.5313160	-1.7574880
F	1.0275810	3.8278090	-3.0278780
F	-1.3699720	5.0975020	-2.9589600
F	-3.4376530	4.0066320	-1.5705340
F	-3.0996180	1.6753360	-0.2746090
F	-2.7216490	-0.0444040	-2.4473830
F	-4.3472160	-2.0716750	-2.9269540
F	-4.3757960	-4.2477520	-1.3055880
F	-2.7140160	-4.3443280	0.8491260
F	-1.0824750	-2.2970650	1.3763460
F	1.2914020	1.6144410	1.1598270
F	1.3373110	2.6065430	3.6397130
F	-2.9799110	-0.2294440	1.9959580
F	-2.9281820	0.7998370	4.4415340
F	-0.7870530	2.2206700	5.3051680
N	2.7078540	-1.5223570	-0.7382290
C	2.8913030	-2.7324430	-1.3419220
O	3.8399450	-3.0843970	-1.9579180
Cl	1.5024630	-3.8262620	-1.0703060

Lewis Complex

R^1=Ts R^2=H

M06 free energy in solution: -3523.159320 a.u.

Symbol	X	Y	Z
C	-5.7060190	0.6512970	0.5127940
C	-4.5059950	0.1585100	-0.0055950
C	-3.8775150	-0.8496470	0.7332820
C	-4.3966050	-1.3369960	1.9288420
C	-5.5958500	-0.8331310	2.4067340
C	-6.2509760	0.1639670	1.6928420
H	-6.2182500	1.4373350	-0.0302380
H	-3.8637570	-2.1117130	2.4635100
H	-6.0092190	-1.2134840	3.3319620
H	-7.1873830	0.5675540	2.0583630
N	-2.6195590	-1.4231800	0.2834920
C	-1.5611670	-0.6760700	0.1378630
N	-0.5977540	-0.0587930	0.0552870
C	-3.9334990	0.7714880	-1.2676180
H	-3.1332530	1.4688260	-0.9978940
H	-4.7261240	1.3803600	-1.7126020
C	-3.4282570	-0.1976250	-2.3032990
C	-2.2734670	-0.0538460	-2.9408140
H	-1.6011880	0.7717550	-2.7203510
H	-1.9527950	-0.7599840	-3.6968580
S	-2.5141440	-3.1258770	-0.2511470
O	-3.4266700	-3.7862770	0.6445400
O	-2.6999170	-3.1829790	-1.6755120
C	-0.8284790	-3.4397700	0.1515680
C	-0.3920260	-3.2175230	1.4568140

C	0.0126320	-3.9214240	-0.8429120
C	0.9348450	-3.4682320	1.7557550
H	-1.0668280	-2.8323510	2.2132790
C	1.3303290	-4.2061430	-0.5036190
H	-0.3552900	-4.0648660	-1.8515840
C	1.8106660	-3.9747080	0.7854990
H	1.3012070	-3.2781700	2.7582880
H	1.9993550	-4.5965310	-1.2632700
C	3.2380600	-4.2783770	1.1482580
H	3.8539090	-4.4344950	0.2614590
H	3.6725590	-3.4660070	1.7342710
H	3.2835440	-5.1859520	1.7558910
B	0.7367250	0.7690510	-0.0035030
C	0.3935220	1.9739950	-1.0509420
C	-0.7375060	2.7424190	-0.8073950
C	1.0962740	2.2995640	-2.2012670
C	-1.1879900	3.7385100	-1.6548050
C	0.6855930	3.2976810	-3.0738680
C	-0.4662150	4.0162590	-2.8036030
C	1.0315110	1.3760570	1.4740820
C	0.4567610	0.9646470	2.6660610
C	1.9582940	2.4053620	1.5839430
C	0.7539920	1.5501460	3.8884580
C	2.2855650	3.0139120	2.7811240
C	1.6696190	2.5839180	3.9454790
C	1.8532670	-0.3008920	-0.5181720
C	1.6308390	-0.9967800	-1.7006640
C	3.0407550	-0.6093690	0.1330780
C	2.5048040	-1.9317460	-2.2191320
C	3.9518640	-1.5326160	-0.3627850
C	3.6776100	-2.2043810	-1.5375860
F	-0.4238870	-0.0525240	2.7056930
F	0.1681790	1.1203910	5.0047680
F	1.9677550	3.1514760	5.1086700
F	3.1872730	3.9904710	2.8305520
F	2.6188550	2.8124960	0.4917210
F	3.3774660	-0.0354870	1.2929350
F	5.0647660	-1.8127300	0.3130320
F	4.4982920	-3.1555000	-1.9742390
F	2.1985540	-2.6236820	-3.3149010
F	0.5035440	-0.7778630	-2.3930010
F	-1.4755980	2.5066370	0.2928840
F	-2.3020700	4.4142910	-1.3836660
F	2.2217990	1.6551260	-2.5246540
F	1.3885720	3.5702010	-4.1694920
F	-0.8712570	4.9685680	-3.6346330
H	-4.0715330	-1.0431920	-2.5334430

TS

R^1=Ts R^2=H

M06 free energy in solution: -3523.096467 a.u.

Symbol	X	Y	Z
C	-4.9660740	-2.3501300	0.1091640
C	-3.7241040	-2.3249050	-0.5167360
C	-2.6008890	-2.7804180	0.1855260
C	-2.7280630	-3.2762780	1.4780200
C	-3.9777330	-3.3212820	2.0778300
C	-5.0956310	-2.8505730	1.3979080
H	-5.8371610	-1.9860000	-0.4238580
H	-1.8503290	-3.6335360	1.9994140
H	-4.0749540	-3.7137050	3.0819490
H	-6.0709710	-2.8792940	1.8671930
N	-1.3254720	-2.6944350	-0.4673690
C	-0.8876470	-1.3915660	-0.9020490
N	-0.3819740	-0.5749690	-0.1702130
C	-3.6247430	-1.7245450	-1.9276130
H	-3.7540570	-0.6412850	-1.8557950
H	-4.4295240	-2.1528980	-2.5321700
C	-2.3286650	-2.0477020	-2.5555740
C	-1.2332710	-1.1570650	-2.5318960
H	-1.4596840	-0.0964530	-2.6011630
H	-0.3538050	-1.4669530	-3.0890520
S	-0.2486820	-3.9696940	-0.6947820
O	-0.7877260	-5.0845370	0.0493370
O	-0.0340560	-4.0849860	-2.1277460
C	1.2497980	-3.3485680	0.0161480
C	1.2345350	-2.8118350	1.2998150
C	2.4142680	-3.4148690	-0.7382700
C	2.4254270	-2.3578340	1.8417330
H	0.3051280	-2.7052880	1.8475890
C	3.5989280	-2.9607840	-0.1716030
H	2.3873790	-3.8068580	-1.7470740

C	3.6242140	-2.4421620	1.1237370
H	2.4270850	-1.9210840	2.8342000
H	4.5168320	-3.0055100	-0.7485480
C	4.9199370	-2.0050110	1.7503400
H	5.6204820	-1.6289200	1.0023920
H	4.7570970	-1.2255790	2.4953970
H	5.3937890	-2.8538020	2.2510330
B	0.1334470	0.8613880	-0.0109400
C	-0.5782990	1.8544470	-1.1164130
C	-1.9640010	1.8381240	-1.2163380
C	0.0572740	2.7741390	-1.9381160
C	-2.6874930	2.6331950	-2.0877480
C	-0.6287230	3.6022860	-2.8164850
C	-2.0081310	3.5285810	-2.8966870
C	-0.3246020	1.4288030	1.4520450
C	-1.1191870	0.7769770	2.3820740
C	0.0500730	2.7227730	1.7926130
C	-1.5067500	1.3644030	3.5805750
C	-0.3105730	3.3426210	2.9729710
C	-1.1014400	2.6512610	3.8775040
C	1.7551680	0.7095330	-0.1936480
C	2.2416700	0.2434260	-1.4073940
C	2.7276470	0.9595460	0.7649250
C	3.5797930	0.0347220	-1.6817770
C	4.0851540	0.8079620	0.5186120
C	4.5131500	0.3277070	-0.7040240
F	-1.5700150	-0.4707720	2.1779460
F	-2.2710900	0.6968810	4.4458230
F	-1.4641540	3.2224250	5.0221870
F	0.0914810	4.5807880	3.2537300
F	0.8340590	3.4139040	0.9510980
F	2.4092220	1.3503780	2.0047500
F	4.9791780	1.0709370	1.4718870
F	5.8069370	0.1024720	-0.9199620
F	3.9725900	-0.4657930	-2.8518530
F	1.3783760	-0.0234400	-2.4064180
F	-2.6747840	0.9740350	-0.4620590
F	-4.0147740	2.5329780	-2.1640620
F	1.3860760	2.9108580	-1.9199880
F	0.0274920	4.4671290	-3.5853840
F	-2.6743250	4.3062550	-3.7423970
H	-2.1717620	-3.0638320	-2.9126540

Lewis Complex

R^1=Ts R^2=Ph

M06 free energy in solution: -3754.100205 a.u.

Symbol	X	Y	Z
C	-4.2393710	1.6611640	2.6426080
C	-3.4069380	0.9866380	1.7483460
C	-2.7437990	-0.1411310	2.2431930
C	-2.8879570	-0.5771890	3.5561030
C	-3.7414060	0.1039570	4.4101530
C	-4.4170730	1.2275590	3.9495040
H	-4.7551610	2.5508910	2.2996990
H	-2.3422680	-1.4481160	3.8928170
H	-3.8665060	-0.2373170	5.4295530
H	-5.0787140	1.7737900	4.6104770
N	-1.8237470	-0.8822480	1.3914820
C	-0.7843730	-0.2880010	0.8724850
N	0.1655490	0.1960560	0.4451890
C	-3.2116210	1.5198690	0.3436920
H	-2.1662750	1.7987170	0.1978290
H	-3.7729040	2.4548660	0.2652150
C	-3.6253170	0.5811410	-0.7728480
C	-2.7578980	0.2699670	-1.7377060
H	-1.7379690	0.6413050	-1.7213670
H	-3.0378300	-0.3561450	-2.5761550
S	-2.1282380	-2.5870110	0.9404850
O	-2.8150500	-3.0928760	2.0991670
O	-2.7386900	-2.6253900	-0.3596290
C	-0.4690010	-3.1754220	0.8217430
C	0.4489920	-2.8991240	1.8306750
C	-0.1492320	-3.9678890	-0.2757400
C	1.7340740	-3.4000840	1.7060450
H	0.1821300	-2.2795700	2.6797250
C	1.1308020	-4.4995200	-0.3488630
H	-0.8788130	-4.1473490	-1.0555570
C	2.0905840	-4.2116160	0.6237980
H	2.4737460	-3.1533720	2.4586680
H	1.3983400	-5.1170270	-1.1998730
C	3.4842220	-4.7679050	0.5221630
H	3.7257740	-5.0556540	-0.5015410

H	4.2218400	-4.0394250	0.8639400
H	3.5788760	-5.6566880	1.1518840
B	1.4587010	0.7825490	-0.2710400
C	0.8445820	1.8316460	-1.3580650
C	0.0011900	2.8344060	-0.8942910
C	1.0199870	1.8004930	-2.7327360
C	-0.6658970	3.7239530	-1.7134580
C	0.3770630	2.6809510	-3.5936670
C	-0.4734300	3.6441650	-3.0837870
C	2.3408010	1.4875100	0.8973150
C	2.5882450	0.8146930	2.0865430
C	2.9178230	2.7452950	0.8008750
C	3.3352700	1.3367050	3.1250250
C	3.6752530	3.3079540	1.8187880
C	3.8816170	2.6023900	2.9891450
C	2.1542550	-0.5391090	-0.9249210
C	1.4059110	-1.3521420	-1.7682140
C	3.4731200	-0.9330390	-0.7435280
C	1.9127190	-2.4584410	-2.4189940
C	4.0156060	-2.0511530	-1.3640350
C	3.2329770	-2.8138030	-2.2088820
F	2.1207370	-0.4363490	2.2504490
F	3.5409610	0.6377760	4.2399500
F	4.6039940	3.1272570	3.9714530
F	4.2057010	4.5196540	1.6767610
F	2.7808010	3.4870320	-0.3041390
F	4.3079610	-0.2444160	0.0421630
F	5.2751250	-2.4126870	-1.1271220
F	3.7220290	-3.9185860	-2.7653030
F	1.1316230	-3.2238280	-3.1786020
F	0.1144970	-1.0622890	-1.9945660
F	-0.2047730	2.9577130	0.4299510
F	-1.4829800	4.6427490	-1.2046540
F	1.8283320	0.9050110	-3.3113020
F	0.5730510	2.6018350	-4.9067230
F	-1.0970690	4.4872270	-3.8964320
C	-5.0242220	0.0765090	-0.7725220
C	-5.3335150	-1.1764080	-1.3137800
C	-6.0677360	0.8493040	-0.2520140
C	-6.6445880	-1.6330100	-1.3456400
H	-4.5333680	-1.8065280	-1.6789790
C	-7.3804570	0.3937080	-0.2871260
H	-5.8653120	1.8276390	0.1672360
C	-7.6744550	-0.8498210	-0.8341710
H	-6.8603210	-2.6097680	-1.7624510
H	-8.1739600	1.0135930	0.1129620
H	-8.6964210	-1.2088350	-0.8558550

TS

R^1=Ts R^2=Ph

M06 free energy in solution: -3754.061183 a.u.

Symbol	X	Y	Z
C	-4.3336720	0.9826820	4.0588550
C	-3.7198120	0.9222310	2.8041430
C	-2.9793010	-0.2212050	2.4920370
C	-2.8833500	-1.2738180	3.4043050
C	-3.5252660	-1.2050060	4.6279180
C	-4.2499010	-0.0641170	4.9608080
H	-4.8996420	1.8717160	4.3163590
H	-2.3208010	-2.1588390	3.1348820
H	-3.4540410	-2.0342080	5.3200290
H	-4.7495560	0.0075440	5.9188900
N	-2.2987810	-0.3552980	1.2287540
C	-1.2513530	0.4904690	0.8495530
N	-0.1121480	0.2695200	0.5813920
C	-3.9058260	2.1292960	1.8979980
H	-3.5123660	3.0017980	2.4284330
H	-4.9738590	2.3003340	1.7561950
C	-3.2090310	2.0663600	0.5690850
C	-1.8299190	2.2510530	0.5622440
H	-1.3819540	2.7565090	1.4130370
H	-1.3206050	2.3831710	-0.3856000
S	-2.6276710	-1.6399710	0.1526730
O	-3.8290190	-2.2593640	0.6663030
O	-2.6106390	-1.0799590	-1.1819040
C	-1.2284620	-2.7313060	0.2676470
C	-0.2846780	-2.6287140	1.2819890
C	-1.0993760	-3.6663590	-0.7545200
C	0.8247240	-3.4615140	1.2474350
H	-0.3758770	-1.8821280	2.0589600
C	0.0028180	-4.5099050	-0.7519790
H	-1.8358410	-3.7240790	-1.5480480

C	0.9916010	-4.4024830	0.2286620
H	1.5844300	-3.3599100	2.0153550
H	0.1174990	-5.2365810	-1.5485390
C	2.2422570	-5.2318600	0.1482210
H	2.0597660	-6.1743400	-0.3685360
H	3.0033430	-4.6815780	-0.4119240
H	2.6413370	-5.4441850	1.1407140
B	1.2392020	0.4818950	-0.1262460
C	1.4364280	2.0764380	-0.4641480
C	1.3109140	2.9810780	0.5823410
C	1.7586050	2.6339150	-1.6925020
C	1.4543010	4.3494770	0.4399230
C	1.9209800	4.0003650	-1.8787490
C	1.7643360	4.8629290	-0.8082920
C	2.4682320	0.0532020	0.8515960
C	2.3859220	-0.2970530	2.1885980
C	3.7540270	0.0952350	0.3268550
C	3.4996040	-0.6215070	2.9530960
C	4.8887530	-0.2168200	1.0504410
C	4.7565140	-0.5816700	2.3814600
C	1.0539680	-0.4914230	-1.4336520
C	0.0135720	-0.2093090	-2.3093760
C	1.7180800	-1.6842830	-1.6844900
C	-0.3765190	-1.0330540	-3.3468750
C	1.3736140	-2.5317590	-2.7271830
C	0.3154590	-2.2133350	-3.5565680
F	1.2074330	-0.3446630	2.8318190
F	3.3635160	-0.9699470	4.2332070
F	5.8314540	-0.8896820	3.1009430
F	6.0960030	-0.1803230	0.4900550
F	3.9183140	0.4269580	-0.9614420
F	2.7228400	-2.1135830	-0.9059200
F	2.0169010	-3.6901230	-2.8916340
F	-0.0540360	-3.0505370	-4.5228200
F	-1.4121230	-0.7190760	-4.1210320
F	-0.6950130	0.9228340	-2.1457900
F	1.0071960	2.5299450	1.8135940
F	1.2950850	5.1687860	1.4785020
F	1.9296660	1.8681570	-2.7741780
F	2.2253930	4.4903530	-3.0787950
F	1.9110910	6.1733500	-0.9748270
C	-3.9354090	1.6241100	-0.5990490
C	-3.4617190	1.8896460	-1.8962560
C	-5.0781170	0.8171250	-0.4391070
C	-4.1022650	1.3520170	-2.9965950
H	-2.6003360	2.5285460	-2.0391540
C	-5.6994580	0.2620020	-1.5436430
H	-5.4425570	0.5735490	0.5523850
C	-5.2127550	0.5292700	-2.8205440
H	-3.7298360	1.5590920	-3.9915350
H	-6.5530790	-0.3902190	-1.4108890
H	-5.7001280	0.0924610	-3.6839950

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M06 free energy in solution: -879.867255 a.u.

Symbol	X	Y	Z
C	3.1567920	-1.4789150	-0.5344260
C	1.9173670	-0.8488940	-0.4475780
C	1.9009810	0.4737270	0.0034900
C	3.0608530	1.1411600	0.3663610
C	4.2849930	0.4876470	0.2828780
C	4.3299910	-0.8232100	-0.1730980
H	3.1981910	-2.5037720	-0.8862740
H	2.9971490	2.1662160	0.7127850
H	5.1932490	1.0037220	0.5670450
H	5.2788340	-1.3408410	-0.2457690
C	0.2115380	1.4805020	1.3557290
N	-0.1522870	1.7464150	2.4168860
C	0.6425440	-1.5647500	-0.8213210
H	0.8942800	-2.5698830	-1.1667220
H	0.1960380	-1.0414510	-1.6672620
C	-0.3429680	-1.6578430	0.3411270
C	0.0397930	-2.2165650	1.4899940
H	1.0530360	-2.5822870	1.6188840
H	-0.6404480	-2.3355840	2.3241210
N	0.6390110	1.1748200	0.1232860
C	-0.0885230	1.5864090	-1.0264280
O	0.3339420	1.3160410	-2.1166440
C	-1.3570310	2.3409430	-0.7485990
H	-2.0343210	1.7344730	-0.1421420
H	-1.1410140	3.2595510	-0.1989170
H	-1.8209940	2.5761800	-1.7025570

C	-1.7130480	-1.1091750	0.1584740
C	-2.3305530	-1.0992930	-1.0973890
C	-2.4172090	-0.5732770	1.2455960
C	-3.6130890	-0.5850950	-1.2598710
H	-1.8195460	-1.5136710	-1.9582920
C	-3.6979380	-0.0600770	1.0833650
H	-1.9396990	-0.5199630	2.2165320
C	-4.3021030	-0.0631360	-0.1710730
H	-4.0727410	-0.5948530	-2.2409990
H	-4.2171700	0.3597000	1.9368040
H	-5.2977750	0.3445330	-0.2986650

C	-1.7036240	-0.7392020	0.7048550
C	-1.3802430	-1.3395270	-0.5156570
C	-3.0395590	-0.3700100	0.9216840
C	-2.3413510	-1.5164130	-1.5068910
H	-0.3588400	-1.6377240	-0.7233620
C	-4.0007290	-0.5546050	-0.0608770
H	-3.3356380	0.0508980	1.8745460
C	-3.6539110	-1.1203330	-1.2869440
H	-2.0542080	-1.9570420	-2.4538680
H	-5.0264700	-0.2625140	0.1314710
H	-4.4039850	-1.2585720	-2.0564650

$TS_{8/9}$

M06 free energy in solution: -879.858731 a.u.

Symbol	X	Y	Z
C	2.8056390	-1.7674120	0.5341550
C	1.7198490	-0.8860870	0.6321340
C	1.7737780	0.2587290	-0.1648460
C	2.8490880	0.5128270	-1.0142550
C	3.9050120	-0.3772190	-1.0913910
C	3.8785810	-1.5280780	-0.3076360
H	2.7943290	-2.6657290	1.1429630
H	2.8324790	1.4117840	-1.6180770
H	4.7362770	-0.1789730	-1.7559030
H	4.6946680	-2.2389430	-0.3546370
C	0.6831490	2.1597850	0.7832230
N	0.6920760	2.9703540	1.6033540
C	0.6383950	-1.2772680	1.6359000
H	1.1119160	-1.2482460	2.6208600
H	0.3996200	-2.3292050	1.4453520
C	-0.6547260	-0.4951300	1.7307640
C	-0.8278320	0.3600450	2.7406560
H	-0.0492720	0.5138020	3.4784840
H	-1.7193130	0.9649210	2.8481040
N	0.6922680	1.2230230	-0.1724480
C	-0.1475700	1.3204000	-1.3216320
O	0.1230610	0.6871520	-2.3028000
C	-1.3743260	2.1764300	-1.1862260
H	-1.4350430	2.8336830	-2.0530130
H	-2.2273600	1.4918210	-1.2147050
H	-1.4117690	2.7575940	-0.2678000

9

M06 free energy in solution: -879.866497 a.u.

Symbol	X	Y	Z
C	0.2465960	2.5124740	0.7774390
C	-0.4356810	1.2965020	0.7989780
C	-1.3509390	1.0581910	-0.2282930
C	-1.5700780	1.9733190	-1.2482360
C	-0.8662420	3.1696990	-1.2559410
C	0.0388020	3.4401220	-0.2355980
H	0.9616370	2.7243290	1.5645760
H	-2.2860220	1.7377860	-2.0260110
H	-1.0272340	3.8865730	-2.0511950
H	0.5891010	4.3730640	-0.2313280
C	-2.9806370	-0.4091290	0.7311840
N	-3.7330980	-0.6132810	1.5812250
C	-0.1540190	0.2651790	1.8704640
H	-1.0704370	-0.0218670	2.3915210
H	0.4983040	0.7216600	2.6194380
C	0.5065210	-0.9777730	1.3030980
C	-0.0452640	-2.1822240	1.4564420
H	-0.9848190	-2.3008480	1.9878250
H	0.4396770	-3.0777970	1.0842420
N	-2.0976630	-0.1817930	-0.2478050
C	-1.7728040	-1.2074620	-1.1790320
C	-2.5690580	-2.4741270	-1.0343920
H	-2.3877670	-2.9240280	-0.0560900
H	-3.6381670	-2.2682160	-1.1139200
H	-2.2605220	-3.1571680	-1.8209050
O	-0.9241410	-1.0135860	-2.0023000

C	1.7865950	-0.7892630	0.5689100
C	2.7711940	0.0731900	1.0616250
C	2.0274570	-1.4638650	-0.6310380
C	3.9738430	0.2380780	0.3866430
H	2.6084390	0.6044560	1.9923750
C	3.2287260	-1.2947730	-1.3093160
H	1.2511730	-2.0925720	-1.0503520
C	4.2066230	-0.4458130	-0.8023490
H	4.7296130	0.9023960	0.7887720
H	3.3947490	-1.8169070	-2.2440990
H	5.1409230	-0.3106020	-1.3339150

10

M06 free energy in solution: -3087.942339 a.u.

Symbol	X	Y	Z
C	4.3148740	0.9077450	2.5468650
C	3.5132700	0.7003230	1.4251980
C	2.8976930	1.8243460	0.8756780
C	3.0665450	3.1032740	1.3847500
C	3.8840170	3.2826050	2.4922470
C	4.5013030	2.1800470	3.0740950
H	4.8118620	0.0566270	2.9978730
H	2.5682930	3.9389760	0.9085690
H	4.0323910	4.2746500	2.8992280
H	5.1371910	2.3121940	3.9408720
C	0.8808400	1.1263780	-0.1541560
N	-0.1546120	0.6548160	-0.0110280
C	3.3744950	-0.6692230	0.8008020
H	2.3215160	-0.9337730	0.6734270
H	3.8024730	-1.3987260	1.4941360
C	4.0878880	-0.7983760	-0.5351320
C	3.4412680	-1.2046940	-1.6272160
H	2.3854200	-1.4552340	-1.5948040
H	3.9614200	-1.3313280	-2.5702930
B	-1.5937830	0.0166190	0.0754620
C	-1.6752790	-0.9554850	-1.2367660
C	-0.6741790	-1.9007540	-1.4245510
C	-2.6915480	-0.9753160	-2.1810150
C	-0.6400130	-2.7878630	-2.4854210
C	-2.7016210	-1.8540740	-3.2550650
C	-1.6687450	-2.7611340	-3.4121940
C	-1.6882100	-0.9243740	1.3940880
C	-0.7092690	-1.1460370	2.3477720
C	-2.8585050	-1.6556100	1.5576430
C	-0.8727990	-2.0334910	3.4027020
C	-3.0660920	-2.5431230	2.5950060
C	-2.0575360	-2.7337210	3.5274640
C	-2.6064080	1.2904730	0.0473650
C	-2.5446720	2.1620910	-1.0339490
C	-3.5339110	1.6287200	1.0214670
C	-3.3426930	3.2796760	-1.1741650
C	-4.3621790	2.7393160	0.9185160
C	-4.2664480	3.5687390	-0.1820980
F	0.4725530	-0.5071960	2.2951240
F	0.1020430	-2.2139910	4.2915740
F	-2.2308660	-3.5834200	4.5332050
F	-4.2106130	-3.2102970	2.7111600
F	-3.8577940	-1.4841510	0.6818510
F	-3.6836030	0.8972280	2.1304380
F	-5.2407200	3.0162770	1.8780770
F	-5.0483110	4.6357750	-0.2893470
F	-3.2367950	4.0718100	-2.2383150
F	-1.6723200	1.9101600	-2.0294730
F	0.3369850	-1.9813620	-0.5380860
F	0.3602980	-3.6558120	-2.6185360
F	-3.7291940	-0.1384600	-2.0974170
F	-3.6954380	-1.8309220	-4.1382800
F	-1.6661320	-3.6030550	-4.4382260
N	2.0658480	1.6639310	-0.3068580
C	2.5782700	1.9892060	-1.6289950
C	1.6460020	1.6584440	-2.7534290
H	1.4682880	0.5802810	-2.7785130
H	0.6845880	2.1596240	-2.6212970
H	2.1086060	1.9753480	-3.6838560
O	3.6564400	2.4841890	-1.7047270
C	5.5629790	-0.5701460	-0.5528890
C	6.1290600	0.6903960	-0.3335280
C	6.4077520	-1.6582000	-0.7889520
C	7.5102090	0.8502190	-0.3519180
H	5.4907700	1.5525190	-0.1814650
C	7.7886810	-1.4962030	-0.8008120
H	5.9711560	-2.6366770	-0.9563770

C	8.3431760	-0.2406020	-0.5791800
H	7.9361710	1.8341670	-0.1942920
H	8.4296930	-2.3505450	-0.9835530
H	9.4188000	-0.1106230	-0.5890440

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M06 free energy in solution: -3087.904211 a.u.

Symbol	X	Y	Z
C	4.2043940	4.2348270	0.0586090
C	3.7420610	2.9667670	-0.2801100
C	2.6944690	2.8592000	-1.1956950
C	2.1031140	3.9827700	-1.7540970
C	2.5826370	5.2430560	-1.4165520
C	3.6321690	5.3666370	-0.5125970
H	5.0148720	4.3373610	0.7716460
H	1.2758160	3.8549770	-2.4411640
H	2.1319150	6.1257360	-1.8522710
H	4.0021920	6.3482610	-0.2435140
C	1.2785830	1.0165040	-0.5477650
N	0.1534950	0.6191020	-0.6957080
C	4.3479460	1.7133870	0.2871060
H	4.9579370	1.9510060	1.1708880
H	5.0511200	1.2829680	-0.4317270
C	3.3788840	0.6768620	0.7634170
C	2.0386590	1.0319380	1.0340680
H	1.8640430	2.0695760	1.3220850
H	1.4511420	0.2992520	1.5735780
B	-1.0763850	-0.1137770	-0.1390430
C	-1.0563860	-0.1876460	1.5095860
C	-0.9081760	0.9994300	2.2166800
C	-1.2473990	-1.3168350	2.2928850
C	-0.9105840	1.0838350	3.5976250
C	-1.2620740	-1.2790820	3.6811010
C	-1.0909110	-0.0732690	4.3373260
C	-2.4299390	0.7133390	-0.5196110
C	-2.4905220	1.9785220	-1.0823440
C	-3.6547870	0.1527790	-0.1800380
C	-3.6910480	2.6382500	-1.3160550
C	-4.8699460	0.7733830	-0.3960760
C	-4.8848110	2.0332330	-0.9737130
C	-0.9521250	-1.5777220	-0.8703910
C	0.1524770	-2.3623990	-0.5709280
C	-1.7664370	-2.0838250	-1.8731350
C	0.4564240	-3.5569660	-1.1922150
C	-1.5100970	-3.2886400	-2.5176510
C	-0.3922710	-4.0286050	-2.1798960
F	-1.3828930	2.6498620	-1.4278320
F	-3.6995710	3.8532200	-1.8657450
F	-6.0403370	2.6543010	-1.1940790
F	-6.0168460	0.1831660	-0.0626150
F	-3.6784810	-1.0696460	0.3732440
F	-2.8517280	-1.4251150	-2.2934400
F	-2.3268470	-3.7308080	-3.4715640
F	-0.1299280	-5.1744570	-2.7997330
F	1.5597670	-4.2340870	-0.8703220
F	1.0279550	-1.9402770	0.3649240
F	-0.7120950	2.1474160	1.5438440
F	-0.7369050	2.2503920	4.2170130
F	-1.4318460	-2.5205250	1.7396050
F	-1.4428850	-2.3925530	4.3891040
F	-1.0993550	-0.0251100	5.6654950
N	2.1695190	1.5601720	-1.5065550
C	2.8291040	0.7308940	-2.4224760
C	2.2410100	-0.6451170	-2.6145180
H	2.3222760	-1.2213530	-1.6877260
H	1.1838130	-0.5873400	-2.8776440
H	2.8052470	-1.1413770	-3.3999030
O	3.8190900	1.1245030	-2.9905790
C	3.8116340	-0.7042370	0.8510770
C	4.6994940	-1.2441500	-0.1008000
C	3.3045590	-1.5405460	1.8633190
C	5.0322990	-2.5874060	-0.0577250
H	5.0646680	-0.6368130	-0.9206170
C	3.6769650	-2.8708510	1.9238600
H	2.6377630	-1.1354090	2.6148750
C	4.5272240	-3.3989210	0.9552820
H	5.6805010	-3.0048350	-0.8175220
H	3.2910960	-3.5035220	2.7125300
H	4.7920650	-4.4489130	0.9857630

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M06 free energy in solution: -3087.977890 a.u.

Symbol	X	Y	Z
C	-2.1422120	3.5195540	-0.0758590
C	-2.5316980	2.2211530	-0.3531190
C	-2.4322090	1.2193780	0.6080750
C	-1.9370970	1.5031030	1.8794460
C	-1.5315740	2.8101920	2.1435820
C	-1.6305160	3.8140750	1.1857570
H	-2.2104990	4.2853580	-0.8399850
H	-1.8715760	0.7420430	2.6387860
H	-1.1284050	3.0369920	3.1231790
H	-1.3035310	4.8212290	1.4155340
N	-2.8444680	-0.0269130	0.0550800
C	-0.9279200	-0.5128430	-1.7720800
N	0.0584270	-0.3615790	-1.2232510
C	-3.0395820	1.6617490	-1.6473960
H	-2.3178050	1.8289140	-2.4514530
H	-3.9846590	2.1136220	-1.9517170
C	-3.2348910	0.1337860	-1.3709890
C	-2.2710740	-0.6695220	-2.3001080
H	-2.3023340	-0.2845490	-3.3207880
H	-2.4983740	-1.7364500	-2.3284420
B	1.2732830	-0.2231780	-0.2119150
C	2.5608090	-0.9033360	-0.9326610
C	2.8930360	-0.5062420	-2.2212830
C	3.4248060	-1.8133480	-0.3412870
C	3.9957590	-0.9831870	-2.9065060
C	4.5434860	-2.3123640	-0.9930130
C	4.8274130	-1.8981710	-2.2823070
C	1.5577800	1.3570210	0.0148390
C	0.9793850	2.4202720	-0.6600180
C	2.5267850	1.7017340	0.9495610
C	1.2729620	3.7449940	-0.3683530
C	2.8507310	3.0060980	1.2682150
C	2.2031860	4.0400640	0.6081670
C	0.6956070	-1.0416990	1.0795040
C	0.2927590	-2.3604240	0.8861270
C	0.5032000	-0.5650570	2.3692550
C	-0.2590510	-3.1582140	1.8683710
C	-0.0396510	-1.3380380	3.3869350
C	-0.4276140	-2.6383640	3.1396260
F	0.1051420	2.2270730	-1.6614210
F	0.6528040	4.7315680	-1.0153040
F	2.4829270	5.3041270	0.9071860
F	3.7666290	3.2815630	2.1929020
F	3.1758060	0.7265950	1.5991720
F	0.7994700	0.6925030	2.7139860
F	-0.2454890	-0.8037650	4.5885480
F	-0.9867130	-3.3693500	4.0935320
F	-0.6657840	-4.3968550	1.5906030
F	0.4144080	-2.9172590	-0.3356320
F	2.1188230	0.3910900	-2.8533810
F	4.2646970	-0.5753150	-4.1448470
F	3.2179650	-2.2510360	0.9040650
F	5.3461470	-3.1851680	-0.3896470
F	5.8928660	-2.3721410	-2.9175150
C	-2.9362310	-1.1920690	0.8010140
C	-3.1557490	-2.5044440	0.0783620
H	-3.9174540	-2.4570970	-0.6987540
H	-2.2100880	-2.8414500	-0.3595490
H	-3.4506370	-3.2318570	0.8314880
O	-2.7874900	-1.1735130	2.0046520
C	-4.6882850	-0.2605480	-1.6057950
C	-5.6250210	-0.0003090	-0.6029320
C	-5.1203270	-0.7999970	-2.8157330
C	-6.9678090	-0.2902800	-0.8054110
H	-5.3011540	0.4240460	0.3412480
C	-6.4676860	-1.0903780	-3.0154320
H	-4.4221250	-1.0033980	-3.6193250
C	-7.3932920	-0.8395620	-2.0114440
H	-7.6828880	-0.0906040	-0.0166360
H	-6.7890470	-1.5149290	-3.9587710
H	-8.4401900	-1.0697810	-2.1661550

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M06 free energy in solution: -879.895026 a.u.

Symbol	X	Y	Z
C	-2.4031730	-1.7734620	-1.5168320
C	-1.5174330	-0.8156190	-1.0603830
C	-1.6280870	-0.2872810	0.2259510
C	-2.6516030	-0.6989210	1.0764730
C	-3.5410690	-1.6644370	0.6027450
C	-3.4247330	-2.2054620	-0.6720360

H	-2.3030350	-2.1769260	-2.5181120
H	-2.7514260	-0.2868640	2.0663270
H	-4.3399560	-1.9969230	1.2548780
H	-4.1270320	-2.9571680	-1.0105140
C	-0.2512810	2.8884080	-1.2253020
N	-1.1286740	3.6274310	-1.2706990
C	-0.3939730	-0.1412090	-1.7860770
H	-0.7982850	0.6069280	-2.4768230
H	0.2423790	-0.8220180	-2.3522100
C	0.4140730	0.5569460	-0.6537300
C	0.8653310	1.9482010	-1.1631030
H	1.2607550	1.8365010	-2.1750570
H	1.6584030	2.3818570	-0.5551970
N	-0.5672050	0.6304980	0.4612350
C	-0.3499930	1.2254510	1.6921120
C	0.8986020	2.0594050	1.8799750
H	1.7944100	1.5862440	1.4784820
H	0.7619950	3.0393710	1.4162510
H	1.0144480	2.2042970	2.9511220
O	-1.1466540	1.1047930	2.5989090
C	1.6159830	-0.3084680	-0.2689460
C	1.4985150	-1.2734520	0.7331260
C	2.8267000	-0.1991710	-0.9564510
C	2.5703810	-2.1034110	1.0434400
H	0.5680460	-1.3825970	1.2780140
C	3.8987240	-1.0274040	-0.6420160
H	2.9516900	0.5314120	-1.7471900
C	3.7746580	-1.9823950	0.3602530
H	2.4599270	-2.8456120	1.8248620
H	4.8322160	-0.9224530	-1.1817440
H	4.6101140	-2.6262150	0.6066820

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M06 free energy in solution: -555.470479 a.u.

Symbol	X	Y	Z
C	0.3208710	-2.1530290	-0.3137810
C	-0.0740580	-0.8284860	-0.4841550
C	0.8834620	0.1445180	-0.2201830
C	2.1741360	-0.1382760	0.1844050
C	2.5355810	-1.4733330	0.3426980
C	1.6104650	-2.4794680	0.0951960
H	-0.4040620	-2.9369470	-0.5034930
H	2.8837330	0.6584660	0.3740530
H	3.5420160	-1.7164630	0.6588090
H	1.8910450	-3.5177630	0.2189700
C	1.2368270	2.4363580	-0.1200340
N	1.9268190	3.3274530	0.1171300
C	-1.4734310	-0.4563130	-0.8861560
H	-1.9352150	-1.3066270	-1.3984590
H	-1.4492040	0.3612660	-1.6142870
C	-2.3761960	-0.0421830	0.2608930
C	-1.9999650	-0.0601630	1.5363400
H	-1.0076480	-0.3739410	1.8398900
H	-2.6865180	0.2406970	2.3195940
C	-3.7521140	0.3852200	-0.1707340
H	-4.2488330	-0.4195310	-0.7213780
H	-4.3718710	0.6560090	0.6839960
H	-3.6924270	1.2442690	-0.8457670
O	0.4347240	1.4761650	-0.3973460

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M06 free energy in solution: -555.459900 a.u.

Symbol	X	Y	Z
C	-1.8740490	-1.4895170	-0.3542340
C	-0.6483810	-0.8812910	-0.0496800
C	-0.7227770	0.4491660	0.3366890
C	-1.9082950	1.1639900	0.4223460
C	-3.0999900	0.5311220	0.1069820
C	-3.0778610	-0.8066010	-0.2805110
H	-1.8650360	-2.5292740	-0.6642740
H	-1.8801110	2.2000160	0.7385850
H	-4.0337930	1.0751740	0.1668830
H	-4.0005580	-1.3165000	-0.5281220
C	0.9216200	1.9943880	-0.1043500
N	1.3627480	2.7882540	-0.8130060
C	0.6107410	-1.7249960	-0.1798680
H	0.5364200	-2.2437260	-1.1389910
H	0.5637250	-2.4999740	0.5932720
C	1.9509620	-1.0258730	-0.1015120
C	2.5423530	-0.5594930	-1.1980630
H	2.0800280	-0.6576100	-2.1750320
H	3.5013320	-0.0554690	-1.1500060

C	2.5782180	-0.9417990	1.2626820
H	1.8748460	-0.5304080	1.9907670
H	2.8520700	-1.9434920	1.6088600
H	3.4756240	-0.3220950	1.2529390
O	0.4651220	1.1313740	0.7291600

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M06 free energy in solution: -555.468345 a.u.

Symbol	X	Y	Z
C	-1.6766840	-1.1477520	-0.9177420
C	-0.5317270	-0.4391160	-0.5481240
C	-0.7344970	0.6389090	0.3077910
C	-1.9701500	1.0128210	0.7996860
C	-3.0880240	0.2820090	0.4139410
C	-2.9381990	-0.7965930	-0.4500050
H	-1.5658010	-1.9972900	-1.5823210
H	-2.0398170	1.8601410	1.4698350
H	-4.0659040	0.5588870	0.7865880
H	-3.8035580	-1.3716570	-0.7555020
C	1.0868270	1.9986690	-0.0881770
N	1.7485530	2.5676630	-0.8402260
C	0.8402530	-0.8513000	-1.0371850
H	1.2480190	-0.0949610	-1.7136450
H	0.7112140	-1.7662230	-1.6239980
C	1.8338830	-1.1315480	0.0736760
C	3.0599330	-0.6164490	0.0466890
H	3.3725560	0.0571730	-0.7438110
H	3.7837740	-0.8503610	0.8198070
C	1.3584990	-2.0514950	1.1640950
H	0.5506780	-1.5875710	1.7383000
H	0.9544290	-2.9756320	0.7387590
H	2.1681400	-2.3034650	1.8487470
O	0.3757140	1.3885490	0.7888690

15

M06 free energy in solution: -2763.547582 a.u.

Symbol	X	Y	Z
C	5.4858430	1.0911440	-0.8550530
C	4.3068910	0.3793290	-1.0900000
C	3.5027960	0.8908790	-2.0986290
C	3.7904900	2.0028970	-2.8613820
C	4.9730240	2.6825590	-2.5946940
C	5.8159700	2.2249060	-1.5881590
H	6.1546240	0.7356670	-0.0797050
H	3.1048560	2.3182400	-3.6370120
H	5.2289240	3.5608190	-3.1729770
H	6.7396530	2.7483880	-1.3762290
C	1.3495760	0.1573970	-1.6286930
N	0.4529940	0.1110650	-0.9199890
C	3.9591740	-0.8492470	-0.2769060
H	3.1885700	-0.5956190	0.4560430
H	4.8525500	-1.1152090	0.2965360
C	3.5251240	-2.0585550	-1.0803690
C	2.4474570	-2.7561260	-0.7307610
H	1.8252650	-2.4606590	0.1085150
H	2.1509070	-3.6465990	-1.2735790
C	4.4046900	-2.4365870	-2.2393380
H	4.3857140	-1.6641990	-3.0145240
H	5.4448850	-2.5338830	-1.9135380
H	4.0850200	-3.3783890	-2.6843500
B	-0.7691780	0.0294750	0.1079150
C	-1.9619530	-0.7048400	-0.7187170
C	-1.7027660	-1.8987360	-1.3814680
C	-3.2634510	-0.2377790	-0.8317780
C	-2.6429770	-2.5855630	-2.1245150
C	-4.2381970	-0.8963020	-1.5695070
C	-3.9261180	-2.0726730	-2.2227270
C	-0.1528880	-0.8403910	1.3395750
C	1.0250610	-0.4025810	1.9329410
C	-0.6522210	-2.0349740	1.8347320
C	1.6983980	-1.0982910	2.9183330
C	-0.0125350	-2.7632310	2.8302460
C	1.1706900	-2.2969130	3.3716410
C	-1.1043410	1.5731360	0.4896890
C	-1.2488920	2.5176040	-0.5185230
C	-1.3042860	2.0454930	1.7776540
C	-1.5535370	3.8457510	-0.2853750
C	-1.6120000	3.3695490	2.0552990
C	-1.7338150	4.2757310	1.0185940
F	1.5778590	0.7550030	1.5276130
F	2.8410660	-0.6375210	3.4224960
F	1.7928960	-2.9873490	4.3192570

F	-0.5317830	-3.9082150	3.2662010
F	-1.7913840	-2.5590310	1.3694570
F	-1.2230240	1.2272760	2.8350730
F	-1.7928210	3.7730220	3.3115840
F	-2.0282470	5.5468050	1.2693890
F	-1.6821910	4.7068510	-1.2933090
F	-1.1233260	2.1426940	-1.8019000
F	-0.4849820	-2.4540900	-1.2822620
F	-2.3356950	-3.7291130	-2.7336900
F	-3.6603210	0.8839430	-0.2180260
F	-5.4718450	-0.4011170	-1.6509090
F	-4.8480770	-2.7113980	-2.9340960
O	2.2874480	0.1919040	-2.4629240

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M06 free energy in solution: -2763.509359 a.u.

Symbol	X	Y	Z
C	-5.7027170	-0.0569450	-0.5499250
C	-4.5169170	0.6523910	-0.7431040
C	-3.7412830	0.3092190	-1.8505180
C	-4.1116670	-0.6916930	-2.7332750
C	-5.2981010	-1.3799770	-2.5194180
C	-6.0945930	-1.0609200	-1.4240240
H	-6.3220990	0.1902160	0.3051390
H	-3.4629280	-0.9125150	-3.5712670
H	-5.5953050	-2.1637300	-3.2044640
H	-7.0219060	-1.5920160	-1.2505360
C	-1.5724440	0.9419140	-1.2670610
N	-0.6237650	0.2201340	-1.1551960
C	-4.1171280	1.6957730	0.2939660
H	-3.7758810	1.1789660	1.1935780
H	-4.9995850	2.2912230	0.5414020
C	-3.0464010	2.5907920	-0.2342690
C	-1.7174920	2.2762430	-0.0039590
H	-1.4723410	1.7033060	0.8866460
H	-0.9620020	2.9855630	-0.3326070
C	-3.4537660	3.6749410	-1.1508340
H	-4.2434710	3.3402000	-1.8281900
H	-3.8933000	4.4642000	-0.5246730
H	-2.6164150	4.0941720	-1.7044000
B	0.5446690	-0.0267660	-0.1629130
C	-0.0161980	-0.6162500	1.2635070
C	-1.3130570	-0.9856640	1.5823250
C	0.9235230	-0.8853050	2.2540260
C	-1.6680240	-1.5576260	2.7973870
C	0.6184300	-1.4581600	3.4728910
C	-0.6968240	-1.7993880	3.7476820
C	1.4754950	-1.2265770	-0.7848900
C	2.8589050	-1.2359310	-0.8853720
C	0.8457780	-2.3921920	-1.2059650
C	3.5733090	-2.3091710	-1.3967520
C	1.5209350	-3.4844470	-1.7230250
C	2.9005160	-3.4391780	-1.8223790
C	1.3245250	1.4107800	-0.0356560
C	1.3728130	2.2271840	1.0843230
C	1.9429780	1.9349760	-1.1657810
C	2.0088340	3.4609120	1.1031550
C	2.5882570	3.1574300	-1.1927740
C	2.6232220	3.9284080	-0.0421850
F	3.5919510	-0.1873790	-0.4857260
F	4.9033590	-2.2609440	-1.4814400
F	3.5731490	-4.4760520	-2.3151120
F	0.8627120	-4.5758740	-2.1154810
F	-0.4864860	-2.5083600	-1.0971820
F	1.9402150	1.2342520	-2.3083650
F	3.1744260	3.6003500	-2.3039730
F	3.2324930	5.1095540	-0.0440950
F	2.0169150	4.2027330	2.2103500
F	0.7561120	1.8798900	2.2260820
F	-2.3338290	-0.7958210	0.7233620
F	-2.9386660	-1.8734940	3.0475430
F	2.2066760	-0.5588610	2.0407280
F	1.5639100	-1.6827240	4.3836890
F	-1.0173320	-2.3498730	4.9146030
O	-2.5584540	1.0134360	-2.1716380

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M06 free energy in solution: -2763.606193 a.u.

Symbol	X	Y	Z
C	-3.9285420	-0.7873770	-0.3764350
C	-3.6444680	-0.3084920	0.8916890
C	-3.3351290	1.0342160	1.0705730

C	-3.2557490	1.9270730	0.0148460
C	-3.5286220	1.4306580	-1.2597070
C	-3.8726600	0.0950360	-1.4568630
H	-4.1877630	-1.8296770	-0.5281990
H	-2.9907360	2.9629060	0.1843880
H	-3.4697890	2.0991100	-2.1101200
H	-4.0809450	-0.2641770	-2.4574880
C	-0.8086800	-0.0736800	2.5160870
N	-0.1847450	-0.0531380	1.5627550
C	-3.6229860	-0.9839590	2.2371700
H	-2.9467980	-1.8434080	2.2631510
H	-4.6134840	-1.3368450	2.5326300
C	-3.1479610	0.1584940	3.1767670
C	-1.6956470	-0.0511270	3.6657490
H	-1.5863770	-0.9871020	4.2178910
H	-1.3873470	0.7816280	4.3023280
C	-4.0608680	0.3887510	4.3643450
H	-5.0739850	0.5711380	4.0039080
H	-4.0709430	-0.4911380	5.0108850
H	-3.7302680	1.2536710	4.9413680
B	0.5879330	-0.0774630	0.1898740
C	0.6646370	1.4316020	-0.4043490
C	0.1036400	2.5817910	0.1272900
C	1.3932110	1.6105500	-1.5738600
C	0.2247690	3.8256100	-0.4776830
C	1.5448420	2.8304880	-2.2031800
C	0.9500290	3.9519010	-1.6464500
C	2.0974410	-0.5820090	0.5442120
C	2.7940350	-1.5735700	-0.1313560
C	2.7997330	0.0557930	1.5588930
C	4.0968440	-1.9255270	0.1879660
C	4.0978550	-0.2687180	1.9112670
C	4.7509950	-1.2724160	1.2171490
C	-0.2821990	-1.1259080	-0.7049490
C	-0.8695170	-0.8818950	-1.9366630
C	-0.5025500	-2.4002580	-0.1905540
C	-1.6091740	-1.8383050	-2.6194970
C	-1.2479390	-3.3720180	-0.8280950
C	-1.8073030	-3.0852880	-2.0628300
F	2.2355000	-2.2392170	-1.1481360
F	4.7253730	-2.8836900	-0.4907160
F	5.9987380	-1.6020440	1.5332700
F	4.7208150	0.3720050	2.8987640
F	2.2147380	1.0498380	2.2463580
F	0.0371680	-2.7344920	0.9941830
F	-1.4347020	-4.5690460	-0.2742520
F	-2.5462400	-3.9937600	-2.6909430
F	-2.1779810	-1.5379560	-3.7869900
F	-0.7799390	0.3082350	-2.5395970
F	-0.6032780	2.5566820	1.2667690
F	-0.3556260	4.8967040	0.0638280
F	1.9489250	0.5416740	-2.1636820
F	2.2383330	2.9396780	-3.3345220
F	1.0736730	5.1367540	-2.2354280
O	-3.1194620	1.3652980	2.3789050

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M06 free energy in solution: -555.519646 a.u.

Symbol	X	Y	Z
C	2.0847030	-0.0379870	1.3792350
C	0.8612600	-0.1992880	0.7509190
C	0.7662880	-0.0480880	-0.6278900
C	1.8601350	0.2630530	-1.4178890
C	3.0871280	0.4259050	-0.7742220
C	3.2045620	0.2751070	0.6055300
H	2.1718990	-0.1506000	2.4539970
H	1.7558150	0.3742000	-2.4895930
H	3.9633090	0.6711640	-1.3627410
H	4.1692850	0.4036580	1.0804840
C	-2.4485390	1.4448600	0.0592900
N	-2.2718750	2.5723890	0.1862420
C	-0.5158630	-0.4908960	1.2852080
H	-0.9087370	0.3666100	1.8399910
H	-0.5469160	-1.3616120	1.9422420
C	-1.3150470	-0.7514850	-0.0177430
C	-2.6459590	0.0034450	-0.0859840
H	-3.3142360	-0.3425550	0.7057330
H	-3.1281350	-0.1852340	-1.0477230
C	-1.5294260	-2.2359310	-0.2646620
H	-0.5679860	-2.7526350	-0.2274780
H	-2.1824370	-2.6594930	0.5012160
H	-1.9772460	-2.3964970	-1.2466950

O	-0.4983670	-0.2332380	-1.1004850

18

M06 free energy in solution: -2763.549647 a.u.

Symbol	X	Y	Z
C	5.6404410	0.8741850	-1.5693230
C	4.4822600	0.1953980	-1.9484860
C	3.3965580	0.9945760	-2.2621590
C	3.3810340	2.3722750	-2.2319440
C	4.5534370	3.0147660	-1.8468150
C	5.6777180	2.2639700	-1.5189150
H	6.5181160	0.2956330	-1.3043140
H	2.4874530	2.9205750	-2.5033890
H	4.5826120	4.0957740	-1.8078720
H	6.5903130	2.7644930	-1.2205510
C	1.2669430	0.2213970	-1.8523000
N	0.3843340	0.1464220	-1.1305950
C	4.3769570	-1.3024700	-1.9507950
H	5.3811780	-1.7344100	-1.9970350
H	3.8569330	-1.6409440	-2.8534990
C	3.6627370	-1.8736080	-0.7384150
C	3.3025820	-1.1386720	0.3121820
H	3.4926840	-0.0730260	0.3713830
H	2.8102720	-1.5967330	1.1639860
C	3.4043480	-3.3529530	-0.8180340
H	4.2956850	-3.8819270	-1.1662770
H	3.1191640	-3.7605450	0.1515080
H	2.6020230	-3.5637660	-1.5327000
O	2.1931830	0.3114000	-2.6969270
B	-0.7268200	0.0099920	-0.0066440
C	-0.2128380	-1.2309280	0.9108760
C	0.0858250	-2.4448190	0.3023800
C	-0.0236250	-1.1929950	2.2835360
C	0.5296950	-3.5569090	0.9901540
C	0.4413960	-2.2821600	3.0097830
C	0.7230160	-3.4687770	2.3598510
C	-0.7458310	1.4428170	0.7661340
C	-1.9085850	2.0743590	1.1846850
C	0.4331630	2.1039400	1.0871670
C	-1.9101940	3.2909020	1.8508540
C	0.4757560	3.3183060	1.7474020
C	-0.7110960	3.9199460	2.1287380
C	-2.1081240	-0.2821080	-0.8151110
C	-3.0136660	-1.2867450	-0.5091850
C	-2.4726570	0.5467980	-1.8683850
C	-4.1995450	-1.4686710	-1.2046020
C	-3.6451450	0.3993110	-2.5873800
C	-4.5166430	-0.6223020	-2.2508230
F	-3.1096060	1.5172750	0.9812280
F	-3.0557850	3.8558750	2.2266170
F	-0.6967140	5.0874610	2.7622810
F	1.6381270	3.9058610	2.0252910
F	1.6192090	1.5478570	0.7821730
F	-1.6759650	1.5711240	-2.2141540
F	-3.9453540	1.2283950	-3.5855940
F	-5.6504290	-0.7842460	-2.9243890
F	-5.0385520	-2.4475200	-0.8700810
F	-2.7945020	-2.1329750	0.5056300
F	-0.0711420	-2.5754230	-1.0242030
F	0.7876430	-4.7011340	0.3577540
F	-0.2909010	-0.0905330	2.9946980
F	0.6104650	-2.1928110	4.3272330
F	1.1697710	-4.5185630	3.0394210

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M06 free energy in solution: -2763.524541 a.u.

Symbol	X	Y	Z
C	6.0445910	1.2798240	-1.3786070
C	4.7050590	1.1535650	-1.0185190
C	4.2001590	-0.1375960	-0.8875990
C	4.9690570	-1.2705710	-1.0867670
C	6.3071370	-1.1162520	-1.4286380
C	6.8434170	0.1587630	-1.5754810
H	6.4627760	2.2726110	-1.4998350
H	4.5123850	-2.2447250	-0.9647350
H	6.9242780	-1.9918320	-1.5845290
H	7.8843590	0.2819420	-1.8461090
C	1.7913040	0.2035540	-0.9324600
N	0.6347010	0.2064070	-0.7254300
C	3.8053620	2.3344380	-0.8003530
H	4.3200360	3.2716850	-1.0351260
H	3.5190340	2.4068870	0.2568440

C	2.5350310	2.2742580	-1.5984840
C	2.3180300	1.3065230	-2.5407320
H	3.1275090	0.6986190	-2.9306380
H	1.3832080	1.3035250	-3.0880120
C	1.4578140	3.2525580	-1.2760890
H	1.4412960	4.0265820	-2.0493950
H	0.4849070	2.7498930	-1.2991870
H	1.6104040	3.7274430	-0.3071840
O	2.8865460	-0.3644950	-0.4645680
B	-0.6661140	-0.1437740	0.0539590
C	-1.1447010	1.2607500	0.7444100
C	-0.2216490	2.1185670	1.3286260
C	-2.4611230	1.6963410	0.8000540
C	-0.5522100	3.3421250	1.8832890
C	-2.8384730	2.9080820	1.3597370
C	-1.8761980	3.7428080	1.8976350
C	-1.7175540	-0.6647950	-1.0811280
C	-2.4454080	-1.8434560	-1.0309320
C	-1.9222020	0.1069870	-2.2180530
C	-3.3089580	-2.2426560	-2.0413960
C	-2.7730170	-0.2529340	-3.2472410
C	-3.4728090	-1.4440700	-3.1570930
C	-0.2602740	-1.2800240	1.1573270
C	-0.5690080	-1.2405200	2.5081660
C	0.4864960	-2.3810850	0.7547780
C	-0.1508290	-2.2114930	3.4083320
C	0.9251730	-3.3679640	1.6169230
C	0.6047700	-3.2782210	2.9615740
F	-2.3584080	-2.6689030	0.0215620
F	-3.9813890	-3.3893540	-1.9448350
F	-4.2973190	-1.8131190	-4.1331950
F	-2.9293790	0.5301030	-4.3146480
F	-1.2917430	1.2880180	-2.3528540
F	0.7969200	-2.5353280	-0.5433730
F	1.6436500	-4.3994250	1.1726180
F	1.0150490	-4.2147420	3.8122470
F	-0.4701270	-2.1218680	4.6996120
F	-1.3130950	-0.2503330	3.0225260
F	1.0830590	1.7864690	1.3832150
F	0.3922450	4.1350350	2.3916850
F	-3.4569170	0.9382200	0.3206850
F	-4.1189020	3.2748750	1.3845450
F	-2.2190630	4.9117200	2.4296540

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M06 free energy in solution: -2763.529535 a.u.

Symbol	X	Y	Z
C	5.5721970	1.1645690	-1.9020500
C	4.2086500	1.0998410	-1.6217590
C	3.6863340	-0.1167680	-1.1782090
C	4.4867100	-1.2382690	-1.0096080
C	5.8454590	-1.1460120	-1.2784390
C	6.3891760	0.0547010	-1.7275140
H	5.9929990	2.0997240	-2.2544490
H	4.0285180	-2.1584300	-0.6663630
H	6.4780060	-2.0142660	-1.1431100
H	7.4477150	0.1259000	-1.9423490
C	1.3178620	0.1900310	-1.5969340
N	0.1328200	0.2309380	-1.2941690
C	3.3114900	2.2955940	-1.7689310
H	3.8099650	3.1096450	-2.3156390
H	3.0589920	2.7370760	-0.7947280
C	2.0370720	2.0578750	-2.4816010
C	1.7648010	0.7690830	-3.0349960
H	2.6331510	0.2064200	-3.3749430
H	0.8964370	0.7087240	-3.6793260
C	0.9900810	3.0866260	-2.4882710
H	0.8259840	3.4032200	-3.5252030
H	0.0514460	2.6062610	-2.1711500
H	1.2254830	3.9426010	-1.8594800
O	2.3607340	-0.2403070	-0.8206290
B	-0.6703810	-0.1485830	-0.0177150
C	-1.0970390	1.3148650	0.6125140
C	-0.1656600	2.3394770	0.7098690
C	-2.3680320	1.6542250	1.0557550
C	-0.4553770	3.6169270	1.1561030
C	-2.7028070	2.9163020	1.5232250
C	-1.7423210	3.9102590	1.5669300
C	-1.9816760	-0.9550410	-0.5950410
C	-2.3898270	-2.2335630	-0.2468770
C	-2.7708400	-0.3372720	-1.5614850
C	-3.4852580	-2.8682500	-0.8192510

C	-3.8704540	-0.9310820	-2.1527040
C	-4.2301710	-2.2148730	-1.7797420
C	0.2217630	-1.0231630	1.0462460
C	0.4226970	-0.7227770	2.3831550
C	0.9118120	-2.1412230	0.5929400
C	1.2691170	-1.4530060	3.2103810
C	1.7721760	-2.8862020	1.3717640
C	1.9551170	-2.5358950	2.7005480
F	-1.7434390	-2.9483290	0.6869820
F	-3.8227090	-4.1041370	-0.4460120
F	-5.2857020	-2.8058710	-2.3355410
F	-4.5950480	-0.2802410	-3.0653450
F	-2.5134880	0.9254180	-1.9396050
F	0.7620690	-2.5352720	-0.6823690
F	2.4418580	-3.9237510	0.8604320
F	2.7816300	-3.2377340	3.4728290
F	1.4273090	-1.1106460	4.4908700
F	-0.1997320	0.3117670	2.9712880
F	1.1265850	2.1229610	0.3779980
F	0.4913680	4.5570310	1.1919980
F	-3.3589340	0.7510720	1.0680400
F	-3.9433310	3.1815460	1.9324780
F	-2.0496250	5.1273030	2.0074480

$TS_{19/20}$

M06 free energy in solution: -2763.509632 a.u.

Symbol	X	Y	Z
C	5.7315650	0.1623870	-2.3430070
C	4.5429720	0.7464530	-1.9227920
C	3.6569510	0.0248370	-1.1237740
C	3.9431680	-1.2770640	-0.7380650
C	5.1377110	-1.8510530	-1.1589230
C	6.0307500	-1.1378140	-1.9540120
H	6.4167230	0.7232250	-2.9678660
H	3.2464330	-1.8372790	-0.1349550
H	5.3669890	-2.8677200	-0.8645570
H	6.9579460	-1.5962070	-2.2738960
C	1.2840770	0.5511720	-1.6075930
N	0.1762650	0.2391310	-1.2504400
C	4.1177970	2.1550670	-2.2429610
H	4.3622070	2.3892980	-3.2903940
H	4.6033510	2.8967960	-1.6064360
C	2.6461010	2.2541630	-2.1597330
C	1.7846860	1.2561500	-2.8637060
H	2.3591350	0.5913520	-3.5095850
H	0.9512250	1.7119210	-3.3939700
C	2.0133800	3.4591590	-1.6104910
H	2.2231480	4.2389140	-2.3609950
H	0.9336380	3.3625160	-1.5107060
H	2.4806900	3.7752810	-0.6784740
O	2.5048160	0.6899880	-0.7273630
B	-0.7034110	-0.0951520	-0.0149510
C	-1.3671240	1.3672040	0.3621610
C	-0.5140650	2.4250350	0.6543490
C	-2.7142850	1.6949680	0.3835320
C	-0.9308570	3.7176120	0.9056750
C	-3.1811530	2.9785460	0.6425520
C	-2.2867060	3.9990680	0.8979090
C	-1.8233860	-1.1737250	-0.5509200
C	-2.1430460	-2.3893450	0.0355760
C	-2.5233880	-0.8958290	-1.7222400
C	-3.0618500	-3.2816030	-0.5034510
C	-3.4438800	-1.7550620	-2.2926130
C	-3.7126820	-2.9666120	-1.6784830
C	0.1930540	-0.6977450	1.2206800
C	0.2428870	-0.2318630	2.5248760
C	0.9975800	-1.8006940	0.9746910
C	1.0512370	-0.7926340	3.5061900
C	1.8149490	-2.3932360	1.9172150
C	1.8495760	-1.8769310	3.2012550
F	-1.5809070	-2.7845520	1.1892470
F	-3.3192250	-4.4402780	0.1064880
F	-4.5954880	-3.8087100	-2.2105510
F	-4.0846820	-1.4255880	-3.4162000
F	-2.3676430	0.2860450	-2.3360380
F	0.9900410	-2.3666160	-0.2466530
F	2.5814310	-3.4398300	1.5961070
F	2.6350290	-2.4221660	4.1261390
F	1.0630810	-0.2884840	4.7411020
F	-0.5089660	0.8034270	2.9300050
F	0.8116280	2.2076600	0.7262120
F	-0.0463050	4.6856220	1.1559780

F	-3.6656540	0.7778760	0.1595990
F	-4.4898670	3.2342860	0.6416530
F	-2.7194630	5.2335490	1.1386000

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M06 free energy in solution: -2763.599045 a.u.

Symbol	X	Y	Z
C	-6.2445320	0.3304740	-2.3115790
C	-5.0897980	-0.3486750	-1.9597320
C	-4.3670950	0.0552790	-0.8416650
C	-4.7461620	1.1219240	-0.0474760
C	-5.9129780	1.7953490	-0.4106960
C	-6.6528350	1.4115320	-1.5269580
H	-6.8218010	0.0291760	-3.1781420
H	-4.1566850	1.4102070	0.8123010
H	-6.2419020	2.6378250	0.1858180
H	-7.5511160	1.9564810	-1.7890340
C	-0.8946370	-0.3171860	-1.9153840
N	-0.0351900	-0.0939470	-1.1992600
C	-4.4020820	-1.5614610	-2.5364360
H	-4.2991050	-1.5402410	-3.6225230
H	-4.9281880	-2.4797520	-2.2611050
C	-3.0340450	-1.4960460	-1.8240560
C	-2.0597430	-0.6651280	-2.7068570
H	-2.5385920	0.2643460	-3.0291530
H	-1.7426280	-1.2252100	-3.5887610
C	-2.4420400	-2.8265690	-1.4129200
H	-2.2175730	-3.4334930	-2.2919510
H	-1.5226750	-2.6807640	-0.8398770
H	-3.1579270	-3.3597240	-0.7869880
O	-3.2576460	-0.7208880	-0.6274800
B	0.9755900	0.0829700	0.0291100
C	2.3120640	-0.7412580	-0.3934980
C	2.1977340	-2.0425850	-0.8677700
C	3.6078990	-0.2514520	-0.3231900
C	3.2725550	-2.8152170	-1.2621960
C	4.7158140	-0.9926150	-0.7119800
C	4.5475840	-2.2788740	-1.1871530
C	1.2076880	1.6834290	0.1562650
C	1.0726480	2.4215700	1.3210890
C	1.5940340	2.4038740	-0.9662280
C	1.2990610	3.7893830	1.3736010
C	1.8292630	3.7658230	-0.9574220
C	1.6770460	4.4649320	0.2282670
C	0.1040550	-0.5921710	1.2324680
C	0.4686030	-1.7013850	1.9820320
C	-1.1768620	-0.1084090	1.4781910
C	-0.3870850	-2.3124800	2.8884030
C	-2.0638840	-0.6974900	2.3568510
C	-1.6635770	-1.8147230	3.0702590
F	0.7208760	1.8378210	2.4732070
F	1.1536290	4.4573540	2.5167780
F	1.8967690	5.7747980	0.2651000
F	2.2032620	4.4060190	-2.0637670
F	1.7853160	1.7589010	-2.1282470
F	-1.6017350	0.9911580	0.8391980
F	-3.2898050	-0.2051460	2.5253900
F	-2.4957030	-2.3975520	3.9261510
F	0.0123980	-3.3788710	3.5797290
F	1.6833530	-2.2526230	1.8674080
F	0.9857790	-2.6218170	-0.9224870
F	3.0995170	-4.0600990	-1.7023540
F	3.8648220	0.9773850	0.1417670
F	5.9385070	-0.4715340	-0.6304440
F	5.5980800	-2.9989100	-1.5637490