Supporting Information

Multiple Pathways for C-H Cleavage in Cationic Cp*Rh(III)-Catalyzed C-H Functionalizations without Carboxylate Assistance: A Computational Study

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Content:

1. Computational Details

All DFT calculations were carried out with the Gaussian 09 suite of computational programs.[1] The geometries of all stationary points were optimized using the B3LYP hybrid functional[2] at the basis set level of 6-31G(d) (Lanl2dz for Rh).[3] Frequencies were analytically computed at the same level of theory to obtain the Gibbs free energies and to confirm whether the structures are minima (no imaginary frequency) or transition states (only one imaginary frequency). The solvent effect was evaluated by using the PCM polarizable continuum model by carrying out single point calculations at the M06/6-311+G(d,p) (SDD for Rh) level.[4,5] All transition state structures were confirmed to connect the proposed reactants and products by intrinsic reaction coordinate (IRC) calculations. Solvation calculations were also done with TPSSh and B3PW91 functionals with the same basis set in M06 calculations, which lead to the same conclusion as given in the main text.

Excpet for the results in Scheme 2, all energies given in the text are the relative Gibbs free energies in solution (the solvent was used according to original experiments) under the temperature of 298.15 K and 1 atm. The computational method is validated as the same conclusions will be achieved when calculated by other methods.

[1] Gaussian 09, Revision A.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, **2009**.

[2] (a) Becke, A. D. J. *Chem. Phys.* **1993**, *98*, 5648. (b) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 1372. (c) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785. (d) Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. *J. Phys. Chem.* **1994**, *98*, 11623.

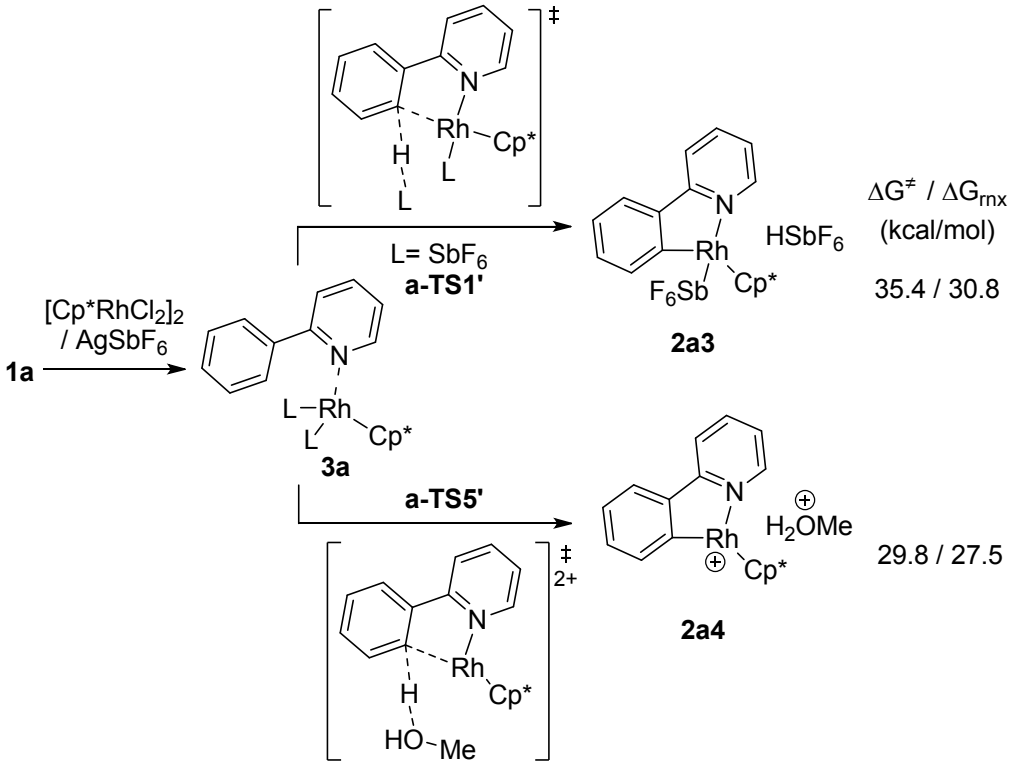
[3] (a) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 270. (b) Wadt, W. R.; Hay, P. J. *J. Chem. Phys.* **1985**, *82*, 284. (c) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 299.

[4] (a) Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215. (b) Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res.* **2008**, *41*, 157.

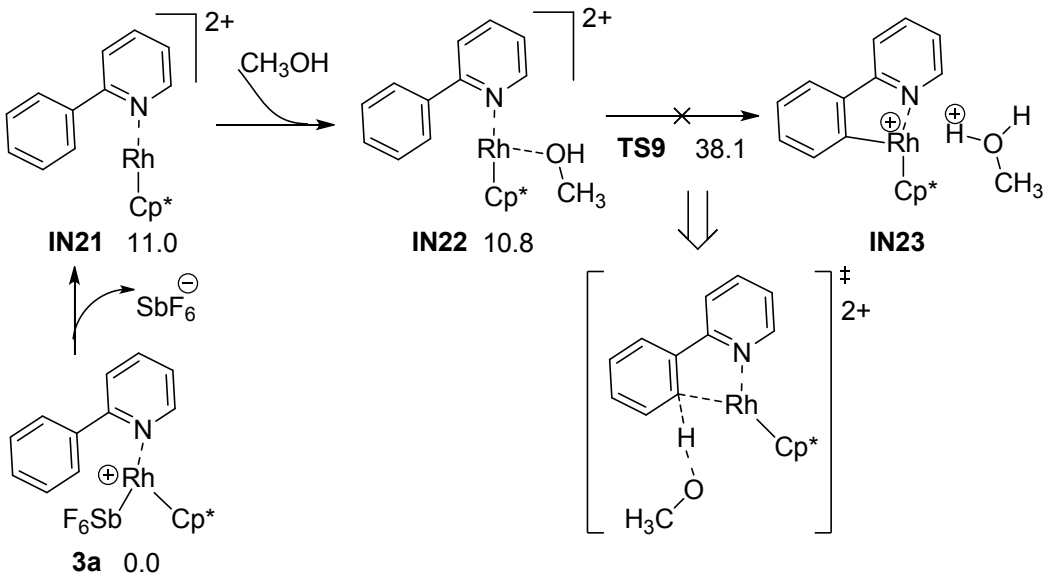
[5] (a) Szentpály, L.; Fuentealba, P.; Preuss, H.; Stoll, H. *Chem. Phys. Lett.* **1982**, *93*, 555. (b) Dolg, M.; Wedig, U.; Stoll, H.; Preuss, H. *J. Chem. Phys.* **1987**, *86*, 866. (c) Schwerdtfeger, P.; Dolg, M.; Schwarz, W. H. E.; Bowmaker, G. A.; Boyd, P. D. W. *J. Chem. Phys.* **1989**, *91*, 1762.

2. Determination of the Active Catalyst

To determine the catalytic active species in precatalytic system of $[Cp^*RhCl_2]_2/AgSbF_6$ or $[Cp^*Rh(SbF_6)_2(CH_3CN)_3]$, we compared the energies with thoese calculated with different possible Rh(III) catalysts, including $Cp^*Rh(SbF_6)_2$, $Cp^*Rh(SbF_6)^+$, and Cp^*Rh^{2+}. When using SbF_6 anion as a base, the cationic TS (**a-TS1**, Scheme 2) has almost the same activation energy of the neutral one (**a-TS1'**). If no SbF_6 anion is cationed, the +2 TS (**a-TS5'**) is obviously higher than the +1 TS (**a-TS5**, Scheme 2) when methanol is the proton acceptor. Thus, the using of cationic $Cp^*Rh(SbF_6)^+$ as a true catalyst is supported by the calculated energies.



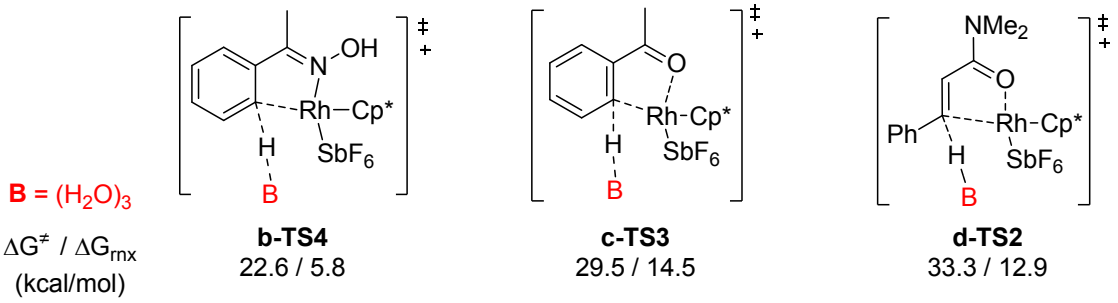
Scheme S1. Energies for Generation of Dicationic Rh Centre Calculated by Standard Method.



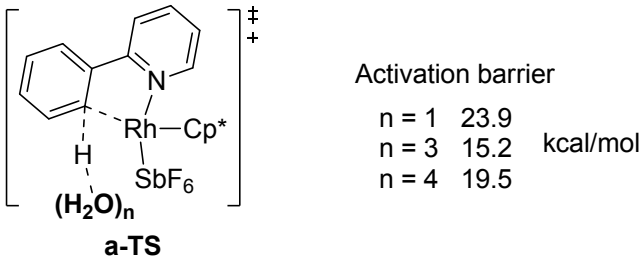
Scheme S2. Energies for Generation of Dicationic Rh Centre by Optimizations in Methanol Solution Calculated with (PCM)M06/6-31+G(D)-LANL2DZ Method.

3. Water-Assited C-H Activations

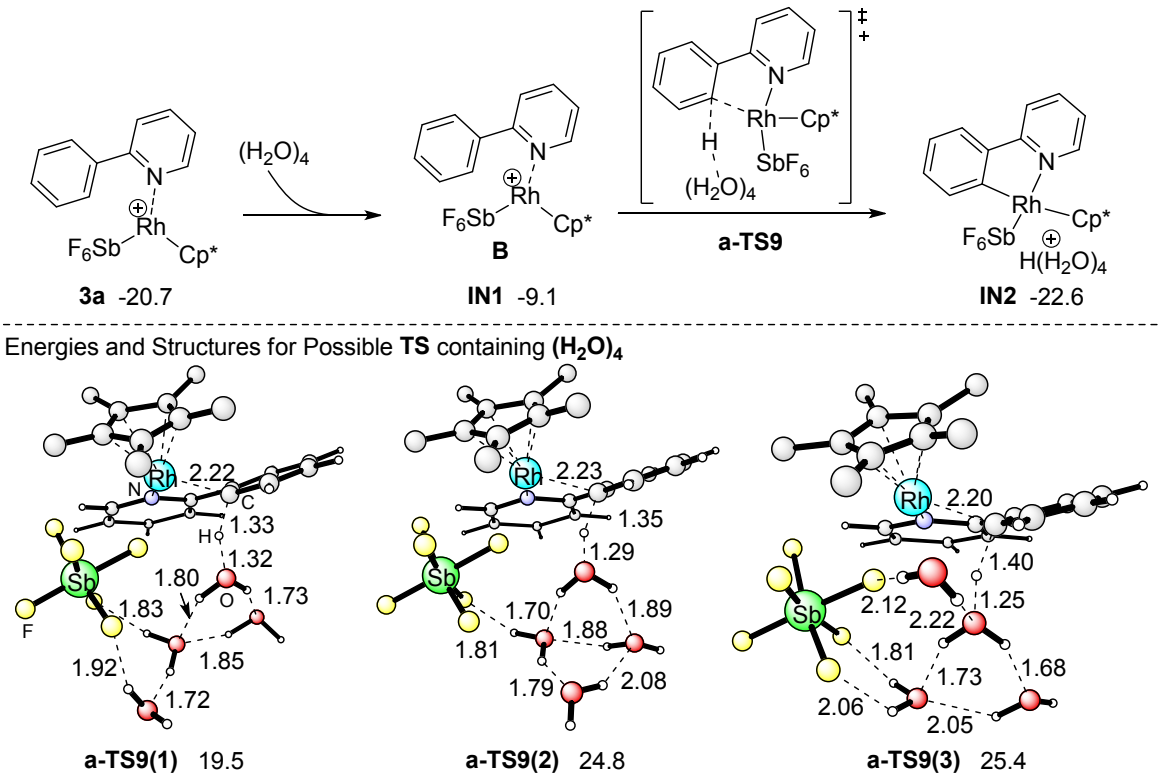
Calculations found that the water effect is mariginal in reactions of **1b**, **1c** and **1d** accrong to the energies above (Scheme S3). When considering different water-clusters, the involvement of a three-water cluster is found to be the most favorable. The energy is the lowest when n = 3 when **1a** is the substrate (Scheme S4). The different isomeris of the TS containing $(H_2O)_4$ are shown in Scheme S5.



Scheme S3.

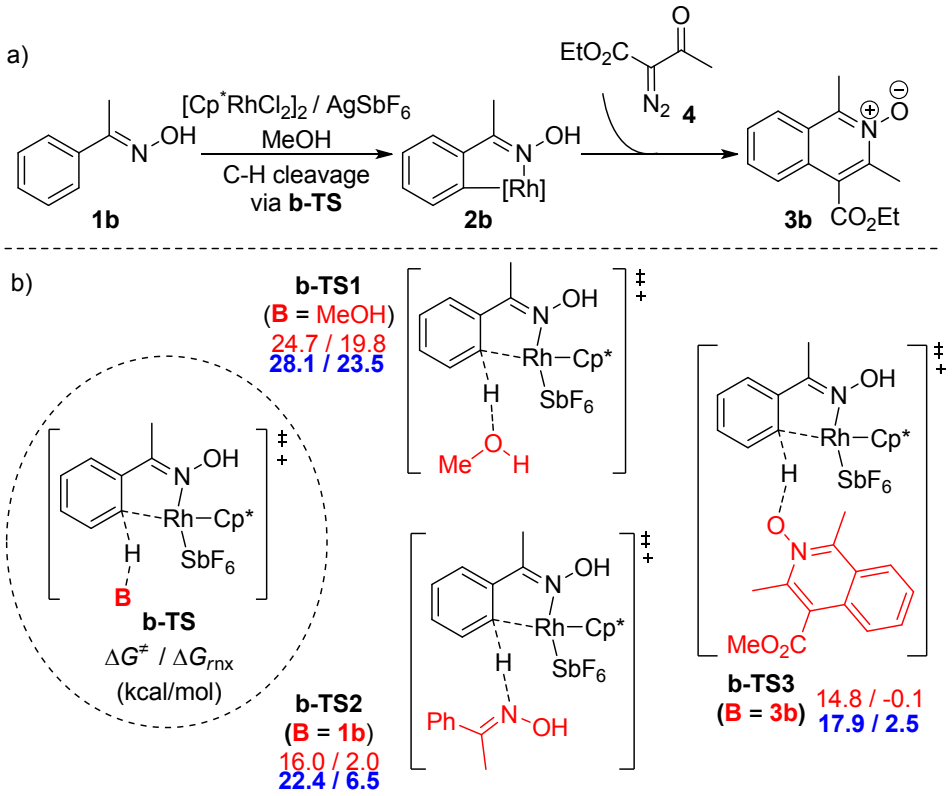


Scheme S4.



Scheme S5.

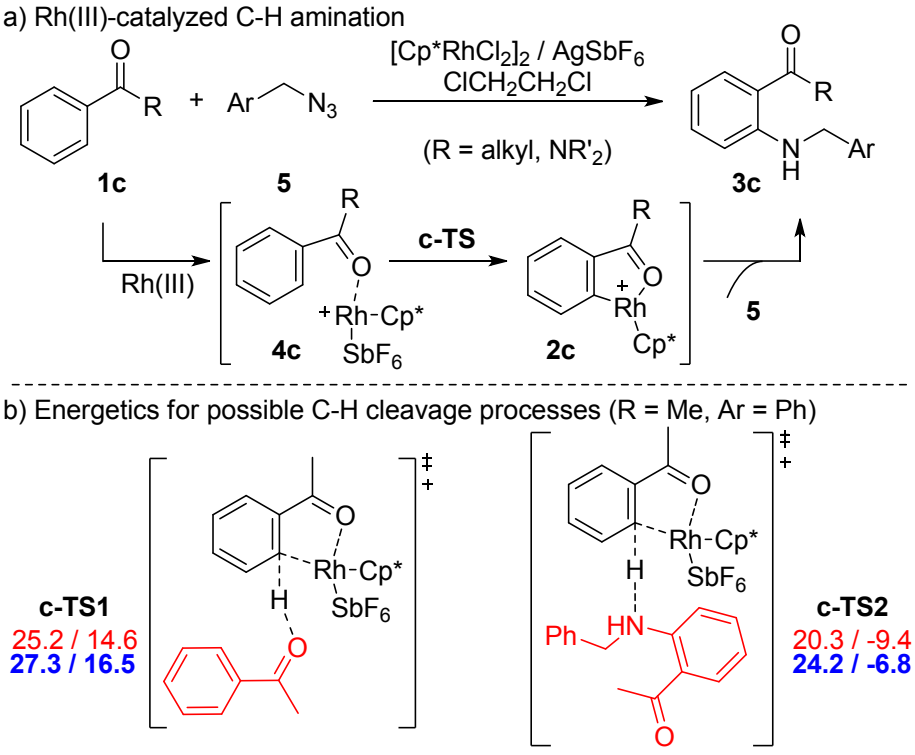
4. Validation of the Computational Method



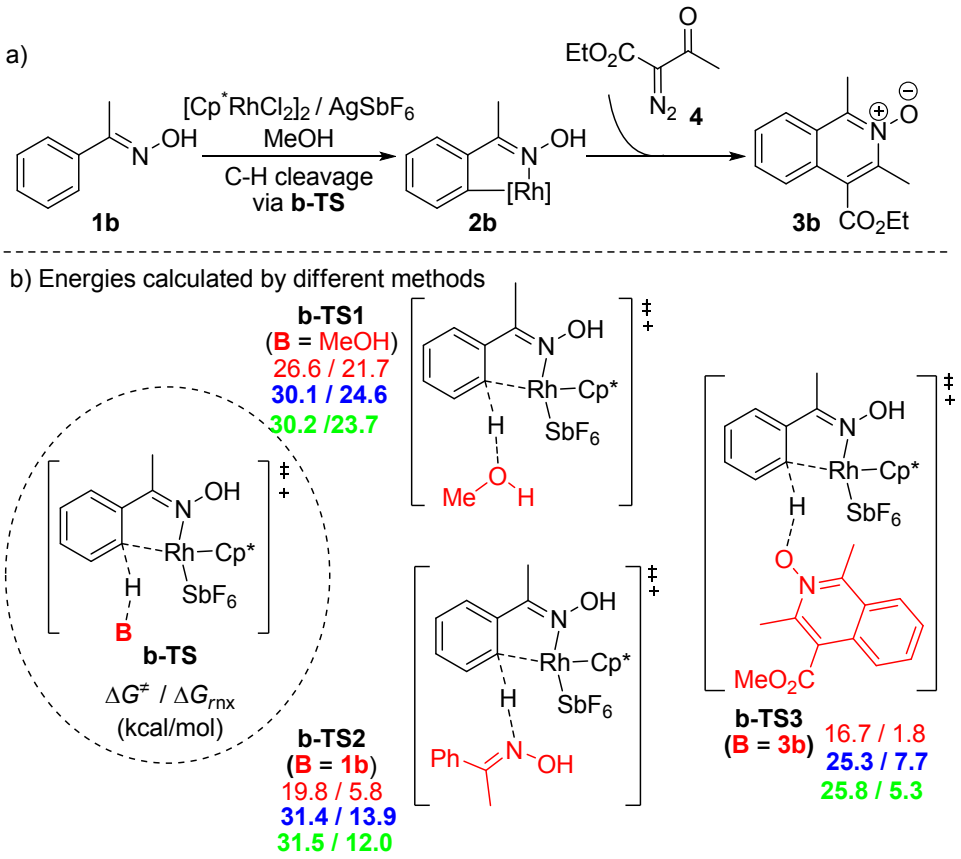
Scheme S6.

To validate the computational method, we also used the M06 for optimization and solvation calculations in studies of **1b** and **1c** (Schemes S6 and S7), which lead to the same conclusions as we obtained from the M06//B3LYP method. The energy values in red are from the M06//B3LYP calculations, while the energy values in blue are from (PCM)M06/6-311+G(d,p)(SDD)//M06/ 6-31G(d)(Lanl2dz) calculations (Schemes S6 and S7).

The same conclusions could be achieved by single point calculations with B3PW91 and TPSSh functional (Scheme S8).

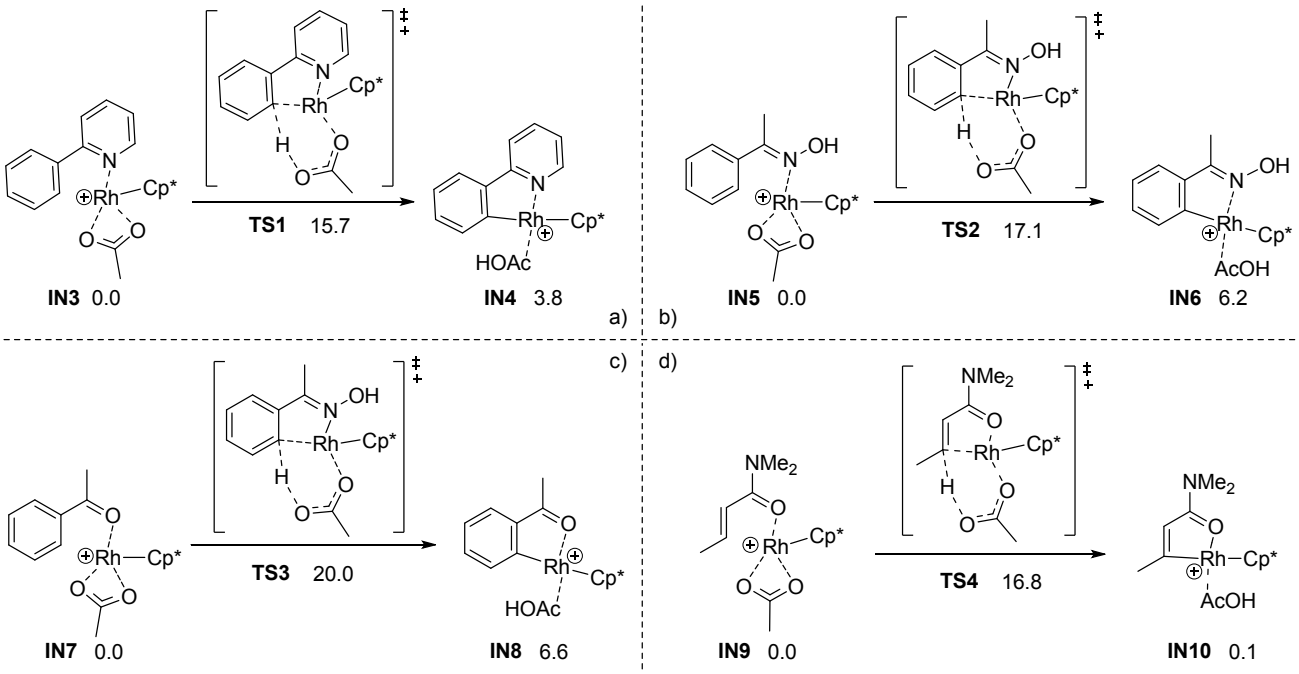


Scheme S7.



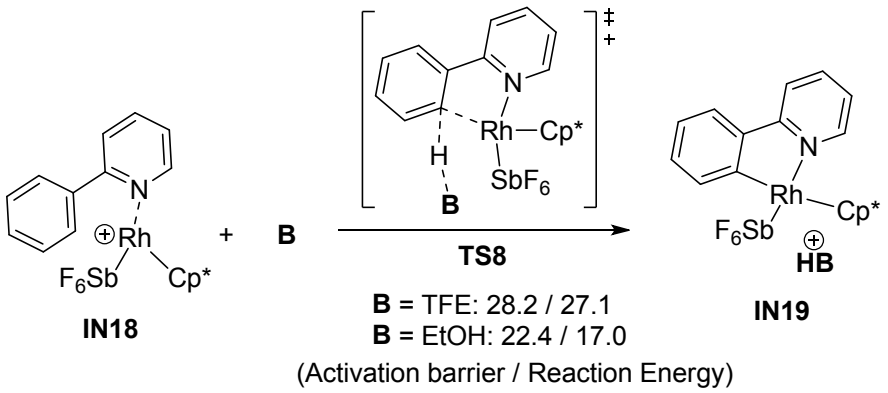
Scheme S8. Energies Calculated by Standard Method (in red), TPSSh//B3LYP (in blue), and B3PW91//B3LYP (in green).

5. Predicted Energies for Catalysis with Cp*Rh(OAc)$^+$



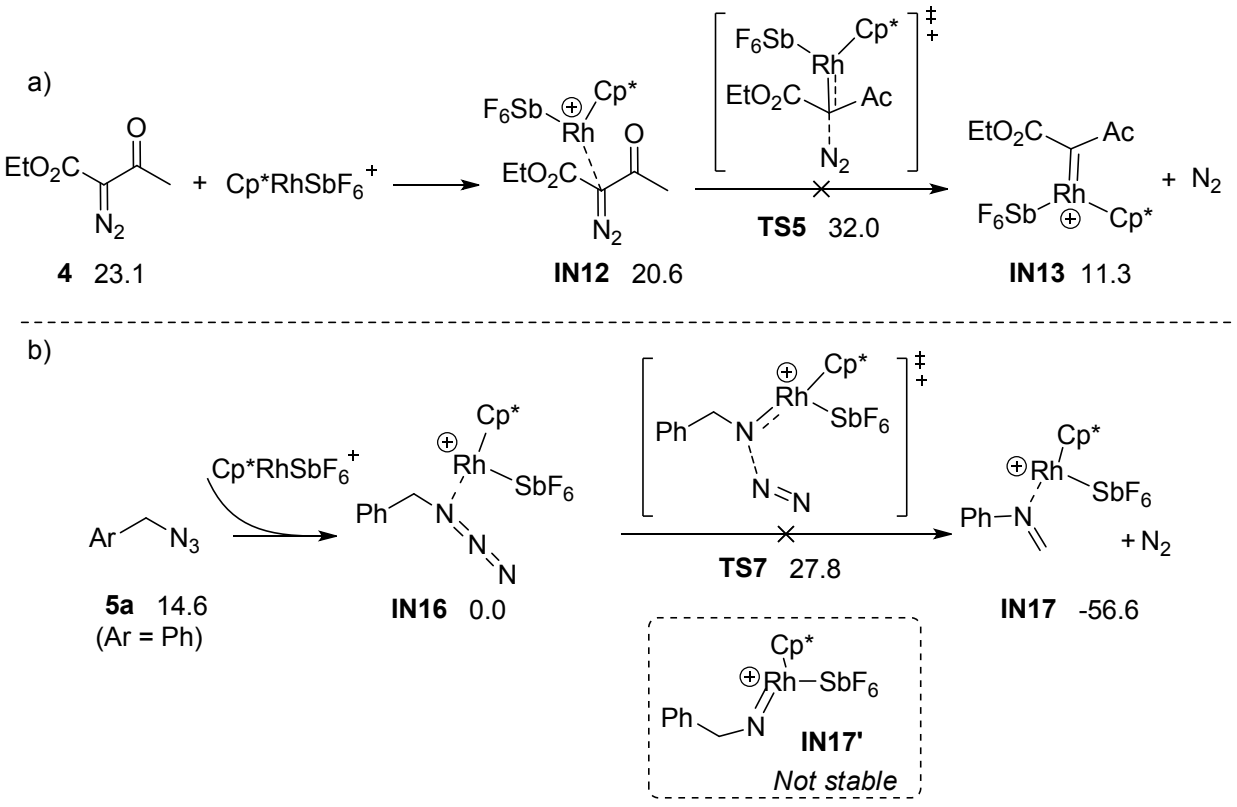
Scheme S9. Calculated Energies with Cp*Rh(OAc)$^+$ Catalyst.

6. Predicted Energies for Reactions in Other Alcoholic Solvents



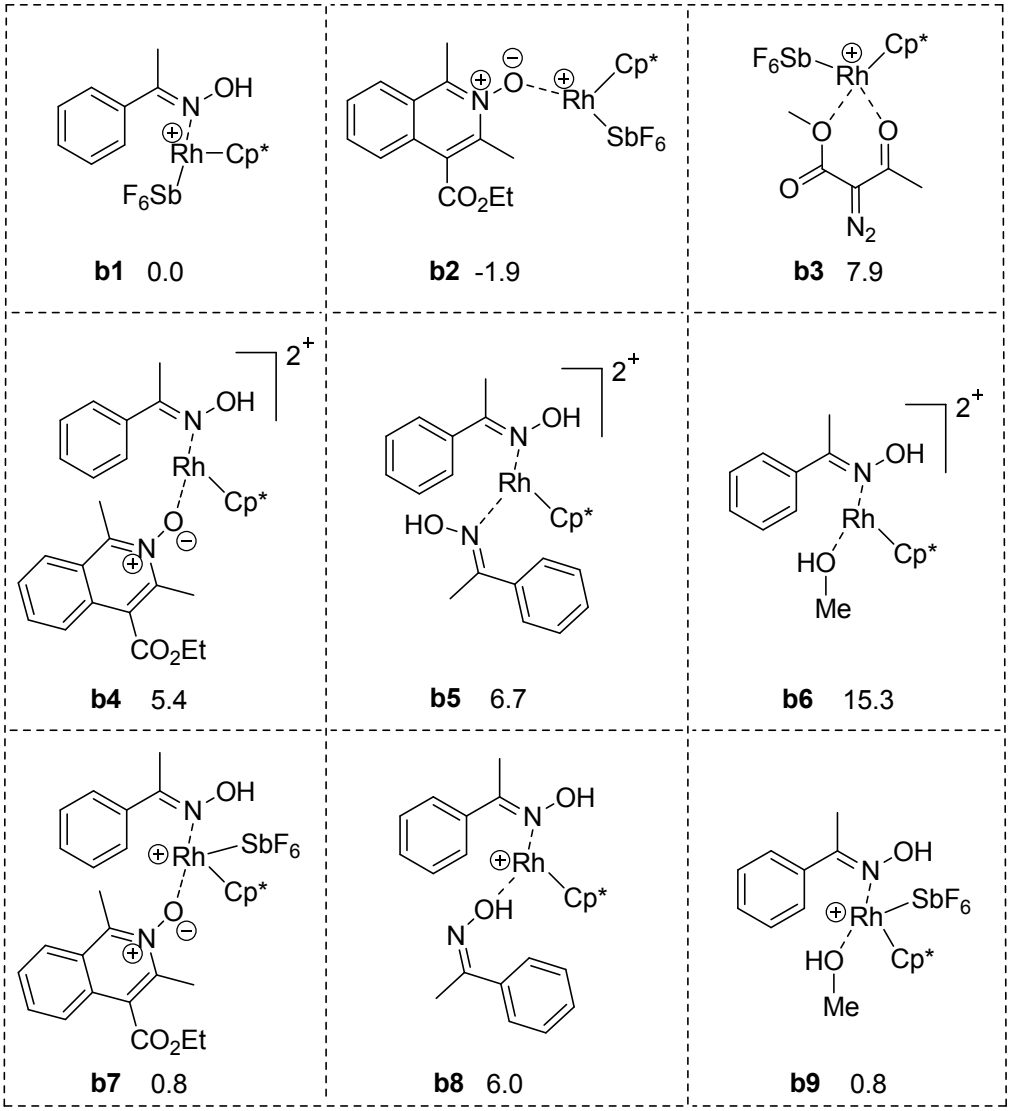
Scheme S10. Calculations with Other Alcohol Solvents.

7. Predicted Energies for Generation of Carbene and Nitrene Intermediates in Reactions with Substrates 4 and 5a

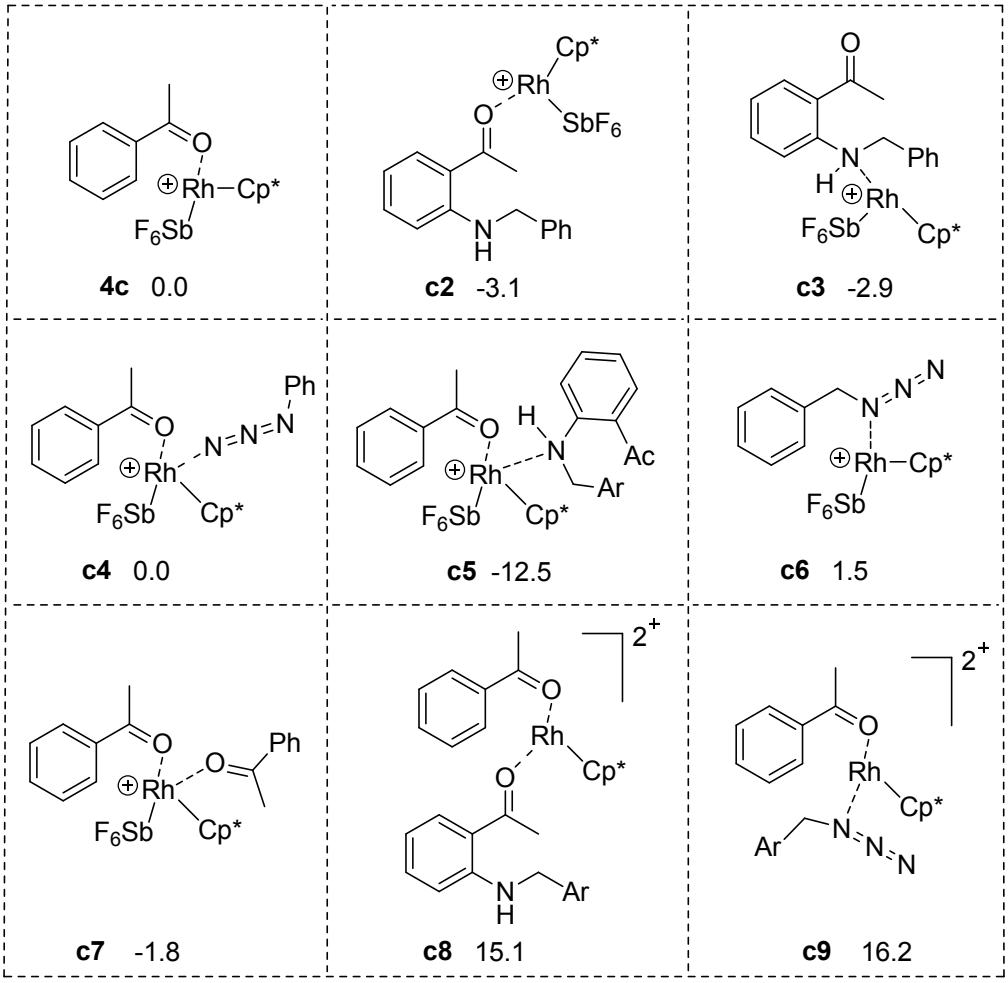


Scheme S11. Possible generations of Carbene and Nitrene Intermediates by First Reactions of Rh(III) with **4** and **5a**.

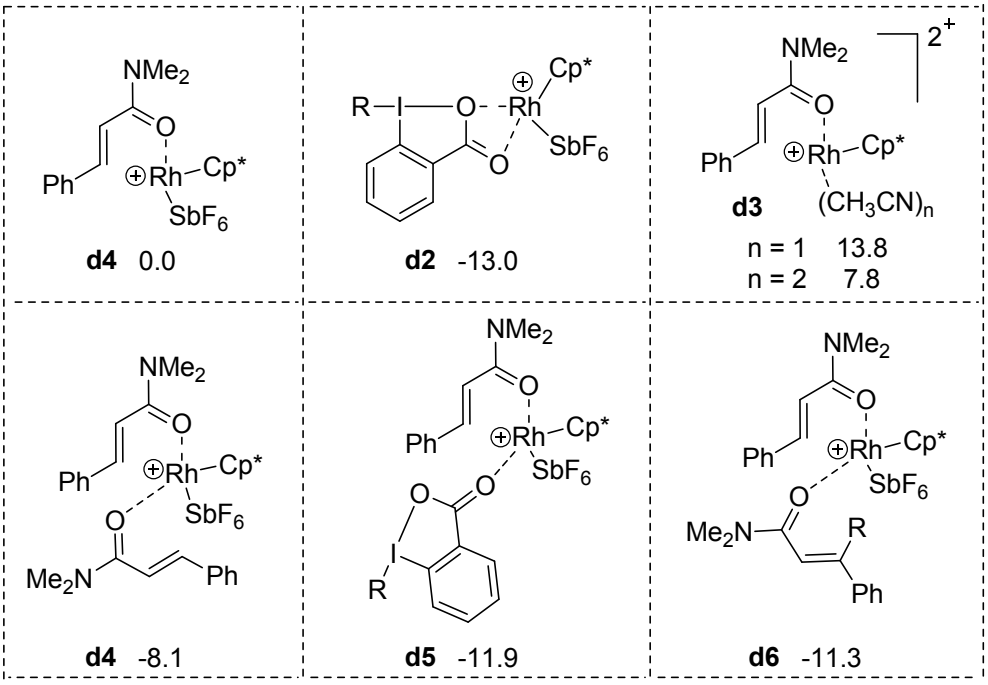
8. Relative Energies for Possible Reactant and Product Complexes Formed in the Reactions



Scheme S12.



Scheme S13.



Scheme S14.

9. Cartesian Coordinates and Energies for All Species

1a

C	-1.70486200	-1.41572900	-0.37821600
C	-0.46888100	-0.87881300	-0.74723200
C	-0.16931200	0.45278200	-0.46923800
C	-1.10319700	1.27960600	0.17804100
C	-2.33868300	0.72564100	0.55248900
C	-2.63674300	-0.60836900	0.27653300
H	-1.93772300	-2.45506700	-0.59414400
H	0.26466700	-1.50015500	-1.25446200
H	0.78978700	0.87619400	-0.74576300
H	-3.06840600	1.32748700	1.08595100
H	-3.59617100	-1.01847700	0.58071500
C	-0.76021300	2.70182000	0.45197100
C	-1.74230700	3.67073000	0.72391000
C	0.90484300	4.28707200	0.65008100
C	-1.35504600	4.98312900	0.97919500
H	-2.79457400	3.40824200	0.71487100
C	0.00057500	5.30759400	0.94844300
H	1.97323800	4.49506900	0.60397600
H	-2.10345700	5.74257400	1.18998700
H	0.34911500	6.31774900	1.14041500
N	0.54791300	3.02411100	0.40966400

Energy：

Sum of electronic and thermal Free Energies = -479.199747

3a

C	-3.99168500	4.28711900	2.78293900
C	-4.49108800	3.96231600	1.47034200
C	-5.71086500	3.20679200	1.63904700
C	-4.95503500	3.80150200	3.77049500
C	-6.01474500	3.15638900	3.07152100
C	-3.88284800	4.37212800	0.16812000
C	-6.59607900	2.69976400	0.54587100
C	-7.19679200	2.49566200	3.70190900
C	-4.84336800	3.94631500	5.25442800
C	-2.78261200	5.10275400	3.09899000
H	-2.06121300	5.10910300	2.28059300
H	-3.09409300	6.13961400	3.28882000
H	-2.27613400	4.73912400	3.99569500
H	-2.79982600	4.48520800	0.24553400
H	-4.10217200	3.65751300	-0.62880300
H	-4.30221800	5.34217900	-0.13140800
H	-7.11925800	1.78659800	0.84097800
H	-7.35774700	3.45537300	0.30991000
H	-6.03538600	2.49604600	-0.36949100
H	-6.89580200	1.89980500	4.56761000
H	-7.90168800	3.26478500	4.04515700
H	-7.72409400	1.84530100	3.00145800
H	-3.82340100	4.18987700	5.55834700
H	-5.50041500	4.75698800	5.59643700
H	-5.14071000	3.02594600	5.76283900
Rh	-4.12864100	2.11851400	2.60554700
C	0.90603300	3.97743500	2.72805900
C	0.66823700	4.13316400	1.35887000
C	-0.20623200	3.26890800	0.69874100
C	-0.87026400	2.25305800	1.40845400
C	-0.62272000	2.09845900	2.78250100
C	0.26365600	2.95793700	3.43455300
H	1.60267300	4.63752200	3.23655600
H	1.17543400	4.91592400	0.80238800
H	-0.37209700	3.37863000	-0.37016400
H	-1.09103200	1.28518400	3.32360600
H	0.46838700	2.81323800	4.49145700
C	-1.72137700	1.27105000	0.69068500
C	-1.19915100	0.58930100	-0.41840000
C	-3.68065100	0.00368900	0.53746200
C	-1.94221400	-0.39937100	-1.05299700
H	-0.19103500	0.82180900	-0.74274800
C	-3.20668000	-0.71000100	-0.55361900
H	-4.64968500	-0.21625300	0.96693400
H	-1.53259400	-0.93462800	-1.90420200
H	-3.81810900	-1.49229100	-0.98969300
N	-2.97411200	0.98945800	1.13604100
Sb	-4.01030900	-0.42457500	4.78695700
F	-4.97370200	0.12660400	3.16007300
F	-2.80572900	-1.22275200	3.63703400
F	-3.05369700	1.23456600	4.37972900
F	-2.99113600	-0.67132700	6.28969900
F	-5.22842000	0.69089300	5.65645500
F	-5.09396000	-1.89624500	4.92504300

Energy：

Sum of electronic and thermal Free Energies = -1583.027246

a-TS1

C	-4.45275400	4.18215600	3.75164600
C	-4.20703900	4.72834400	2.46476300
C	-4.99762600	3.95927700	1.51403500
C	-5.55260300	3.20216600	3.63743900

C	-5.90557500	3.09519700	2.28437900
C	-3.38865100	5.93656900	2.13028500
C	-5.12241800	4.24736500	0.05008400
C	-7.01071300	2.28040400	1.68540300
C	-6.13787300	2.47925900	4.80932200
C	-3.83965600	4.59266300	5.05553400
H	-2.99656800	5.27235700	4.91265000
H	-4.58293400	5.10796500	5.67785600
H	-3.48214000	3.72484600	5.61897200
H	-2.64057500	6.15583200	2.89572500
H	-2.88382800	5.84291200	1.16623600
H	-4.05533900	6.80737900	2.07056300
H	-5.42664100	3.36073400	-0.51244000
H	-5.88616200	5.02066600	-0.11312000
H	-4.18270100	4.61272200	-0.37109300
H	-7.37114700	1.50860800	2.37038700
H	-7.86340900	2.93023800	1.44858800
H	-6.70521200	1.79948600	0.75127500
H	-6.70210500	3.17735700	5.44136800
H	-6.81946700	1.68249000	4.50297800
H	-5.35140300	2.03865700	5.43010800
Rh	-3.66549400	2.55907800	2.44503600
C	0.30716700	3.81250900	0.88902500
C	0.59797400	2.74810400	0.04064000
C	-0.26835800	1.65312700	-0.02953700
C	-1.42856300	1.61805700	0.74763600
C	-1.75734700	2.70107800	1.61991700
C	-0.86554100	3.79086100	1.65718200
H	0.98069700	4.66191500	0.95521200
H	1.49840900	2.76140000	-0.56579200
H	-0.02781200	0.83652900	-0.70334700
H	-1.15666000	2.44420300	3.15823400
H	-1.06110500	4.62785900	2.32021400
C	-2.37842700	0.49683400	0.71293400
C	-2.16485600	-0.73052400	0.07681000
C	-4.46137200	-0.24830300	1.48132400
C	-3.13354800	-1.72653200	0.15123000
H	-1.23843700	-0.91177200	-0.45496000
C	-4.30459000	-1.48725700	0.87139000
H	-5.34579100	-0.01434900	2.06218000
H	-2.97103100	-2.68244100	-0.33697300
H	-5.07880200	-2.24032900	0.96737600
N	-3.53436800	0.71981700	1.39249200
Sb	-1.55294200	0.60762700	5.15322400
F	-3.17554900	1.11030300	4.28210900
F	-1.07981800	-0.13792000	3.52948600
F	-0.87162300	2.35295100	4.15340500
F	0.15649700	0.48844500	5.79030000
F	-2.03775600	1.84026100	6.43490400
F	-2.28452800	-0.88439400	5.90948500

Energy：

Sum of electronic and thermal Free Energies = -1582.970405

2a1

C	-4.19072200	4.66497400	2.79414200
C	-4.66252000	4.33527700	1.45753400
C	-5.82917700	3.44763100	1.59936800
C	-4.87930300	3.81582400	3.69979200
C	-5.93545000	3.10063400	2.95048400
C	-4.27693700	5.04835300	0.19798200
C	-6.73037600	3.03987700	0.47350700
C	-6.90258600	2.15781600	3.59542100
C	-4.72902900	3.74884200	5.18969900
C	-3.22943500	5.76570200	3.12119300
H	-2.39254600	5.81127500	2.41974600
H	-3.75829300	6.72658200	3.06725000
H	-2.82872800	5.67729900	4.13368000
H	-3.24579600	5.40797000	0.23673300
H	-4.38063900	4.40419900	-0.67954200
H	-4.93018300	5.91922000	0.04766600
H	-7.29469700	2.13228000	0.70491100
H	-7.46088400	3.83525300	0.27480900
H	-6.17772200	2.87746800	-0.45662200
H	-6.37839200	1.43692000	4.23183000
H	-7.60294100	2.70945400	4.23592300
H	-7.48861800	1.60272500	2.85937300
H	-3.81099500	4.23500100	5.52868200
H	-5.57197300	4.25464700	5.67892600
H	-4.71517900	2.71408600	5.54492700
Rh	-3.77506300	2.54249600	2.24259600
C	0.47504200	3.16849700	3.21188500
C	1.09406800	2.38006100	2.24959600
C	0.31520400	1.68339700	1.32063300
C	-1.08067200	1.76789400	1.34871600
C	-1.73573900	2.58721700	2.30747900
C	-0.93332100	3.26976300	3.24119400
H	1.06789300	3.71551400	3.93957900
H	2.17580500	2.29911100	2.21743100
H	0.81445800	1.06075900	0.58416900

H	-1.49572700	1.91070800	4.24141500
H	-1.38484200	3.95475600	3.95427700
C	-1.95698800	1.00842800	0.44631000
C	-1.53378300	0.11261900	-0.54168800
C	-4.19325500	0.52518500	-0.05527000
C	-2.47447200	-0.58143100	-1.29582100
H	-0.47573400	-0.04744800	-0.71219200
C	-3.83276500	-0.38039200	-1.04581400
H	-5.23363000	0.71305100	0.18270500
H	-2.15126000	-1.27771600	-2.06348600
H	-4.59905800	-0.91059300	-1.60026700
N	-3.28552700	1.21130500	0.65927000
Sb	-2.91835200	-0.41640300	4.79376800
F	-3.93602900	0.57682800	3.52532000
F	-1.64011500	-0.53906800	3.46773000
F	-1.91579700	1.47632200	5.05202800
F	-1.75082000	-1.00312900	6.07177900
F	-4.03912100	0.34332500	6.04386100
F	-3.82286900	-1.96626900	4.46574300

Energy：

Sum of electronic and thermal Free Energies = -1582.972610

a-TS2

C	-3.49216700	3.88635000	-0.55215800
C	-4.66868100	4.23597900	0.14475500
C	-4.28503200	4.75143200	1.45203000
C	-2.33871700	4.27113100	0.27105500
C	-2.84842500	4.91085300	1.46347800
C	-6.07344600	4.17971100	-0.34469600
C	-5.26001300	5.26462200	2.46415200
C	-2.06134400	5.76453500	2.40539700
C	-0.91472900	4.28287300	-0.18917600
C	-3.42152800	3.33120400	-1.93816800
H	-4.28164400	2.69275400	-2.15358300
H	-3.42508800	4.15274300	-2.66764000
H	-2.50719800	2.75562900	-2.10175900
H	-6.16114400	3.64496500	-1.28979600
H	-6.72328500	3.70177700	0.39086600
H	-6.43014900	5.20946100	-0.49196100
H	-4.78468200	5.47121700	3.42553100
H	-5.70866400	6.19927000	2.10119100
H	-6.06597000	4.54244300	2.61929900
H	-1.04638800	5.39492800	2.55895100
H	-1.98958900	6.76967700	1.96714400
H	-2.54845600	5.86835500	3.37708300
H	-0.67928200	3.40848500	-0.80077300
H	-0.73911500	5.17494700	-0.80606000
H	-0.21696000	4.31385500	0.65042000
Rh	-3.20639300	2.73703200	1.54427600
C	-0.17940900	2.76413500	4.82154700
C	0.68027700	1.75941400	4.38317600
C	0.37388600	1.04763500	3.22736800
C	-0.78817500	1.32764900	2.48979800
C	-1.63666500	2.37239900	2.92053400
C	-1.33244100	3.07159000	4.08951900
H	0.03387500	3.31207600	5.73454200
H	1.57992100	1.52262100	4.94206500
H	1.04946000	0.26595600	2.89505600
H	-3.37670000	2.98139600	3.06774200
H	-1.98454000	3.85395700	4.46235200
C	-1.17780100	0.55948100	1.30808600
C	-0.54537400	-0.60053900	0.84839300
C	-2.83654900	0.32200600	-0.34193600
C	-1.07416000	-1.29434800	-0.23570000
H	0.33614400	-0.97323000	1.35556700
C	-2.24704600	-0.83576100	-0.83436600
H	-3.77465500	0.69292400	-0.73099600
H	-0.58941600	-2.19850700	-0.59077300
H	-2.71729000	-1.36772000	-1.65356400
N	-2.29004900	1.01503200	0.67358400
Sb	-6.23581700	0.60565300	1.56598000
F	-6.62564000	-0.07575200	3.22670500
F	-7.85170700	0.22244100	0.78692300
F	-6.75233100	2.33328700	2.09060400
F	-5.59304300	1.42155700	-0.02682000
F	-4.48572800	1.14798300	2.30794200
F	-5.36271800	-0.92623400	1.00618100

Energy：

Sum of electronic and thermal Free Energies = -1582.946812

2a2

C	-3.54075800	3.85369300	-0.58129600
C	-4.69563300	4.24391300	0.11035900
C	-4.28745800	4.77385100	1.40145000
C	-2.36111500	4.17579400	0.25208400
C	-2.82904300	4.84327600	1.43266800
C	-6.11174800	4.19994500	-0.35756300
C	-5.23776500	5.38858000	2.37572000
C	-2.01227000	5.68096700	2.36570500
C	-0.94132600	4.12344800	-0.21853400

C	-3.48424500	3.28339100	-1.95895600
H	-4.37589700	2.69205000	-2.18037400
H	-3.43368000	4.09861300	-2.69452700
H	-2.60008800	2.65895000	-2.10818500
H	-6.21700900	3.64670700	-1.29070900
H	-6.75042000	3.73324700	0.39502200
H	-6.47143500	5.22518200	-0.52097200
H	-4.75940000	5.63817700	3.32488500
H	-5.64123000	6.31449400	1.94263500
H	-6.07753200	4.71494300	2.56613000
H	-1.00706100	5.28155700	2.50890800
H	-1.91925600	6.68652700	1.93324600
H	-2.48257300	5.78684700	3.34540200
H	-0.74986700	3.24614700	-0.84077700
H	-0.73026100	5.01340000	-0.82739100
H	-0.23772400	4.11418800	0.61660400
Rh	-3.24282300	2.70118400	1.60870800
C	-0.36541800	2.67033000	4.91841500
C	0.57892400	1.75694200	4.44999900
C	0.37130200	1.11104700	3.23538400
C	-0.77430300	1.38016500	2.46755200
C	-1.70039900	2.34057700	2.92751200
C	-1.50390500	2.96429800	4.15754300
H	-0.22650000	3.15855000	5.87862300
H	1.46487500	1.53546600	5.03640900
H	1.09888000	0.38283900	2.89063100
H	-3.73204400	3.25041900	2.97951000
H	-2.22235400	3.67576400	4.55039900
C	-1.11651900	0.64818400	1.24938600
C	-0.41431700	-0.44354100	0.72597300
C	-2.81089500	0.34219000	-0.35606700
C	-0.93044100	-1.14034100	-0.36154100
H	0.51073500	-0.76315900	1.19038600
C	-2.15889500	-0.75626000	-0.90155400
H	-3.78538700	0.66033900	-0.70098600
H	-0.39329400	-1.99343300	-0.76452800
H	-2.61940600	-1.30048100	-1.71831000
N	-2.27512400	1.04634600	0.65852700
Sb	-6.21630400	0.65029300	1.68351900
F	-6.61400100	0.00163400	3.35457900
F	-7.86955400	0.37631700	0.93750000
F	-6.61199800	2.41129800	2.20896100
F	-5.55672300	1.43708500	0.08073800
F	-4.41168200	1.07655000	2.38889800
F	-5.45191400	-0.92766000	1.10166800

Energy：

Sum of electronic and thermal Free Energies = -1582.948787

Pyridine

C	0.12480000	-0.98713900	4.29104500
C	0.52067900	-1.75532700	5.38827400
C	-0.18551900	0.86984900	5.58549900
C	0.55676800	-1.14947600	6.64394300
H	0.79233900	-2.79869900	5.25706400
C	0.19582200	0.19411500	6.74633500
H	-0.47358700	1.91927900	5.63037400
H	0.85960000	-1.71159700	7.52351100
H	0.20820900	0.71015300	7.70195700
N	-0.22483900	0.30256000	4.37295100
H	0.08579900	-1.42970800	3.29648500

Energy：

Sum of electronic and thermal Free Energies = -248.217974

a-TS3

C	-3.19977700	4.27387400	1.91704300
C	-4.52616100	3.68022200	2.02019100
C	-4.90774300	3.67580000	3.38977800
C	-2.82432800	4.73324000	3.25057300
C	-3.82135100	4.28387400	4.15745900
C	-5.35773000	3.20346100	0.87109600
C	-6.23353500	3.28869100	3.95766400
C	-3.84319300	4.47499500	5.64067700
C	-1.67646600	5.63408300	3.58473200
C	-2.50457100	4.63577900	0.64039600
H	-2.70985700	3.90878300	-0.14949500
H	-2.85627500	5.61551400	0.28951600
H	-1.42154300	4.69596000	0.77032700
H	-4.74187900	2.85359600	0.03882200
H	-6.03330100	2.39681800	1.16622000
H	-5.97518200	4.03181700	0.49834900
H	-6.13284700	2.80992400	4.93165900
H	-6.83526100	4.20017200	4.08597100
H	-6.78118500	2.61135500	3.30149800
H	-2.85002700	4.70335600	6.03438900
H	-4.50755900	5.31152800	5.89688100
H	-4.22226200	3.58262100	6.14532500
H	-0.87088800	5.56873200	2.85245200
H	-2.03872100	6.67132300	3.59185800
H	-1.26428000	5.42814600	4.57577600
Rh	-2.96012000	2.49079700	3.09694600

C	1.22598000	3.45186200	2.24020100
C	1.23462200	2.94700100	0.93352200
C	0.26531600	2.02719400	0.52539300
C	-0.72818400	1.61966800	1.42277300
C	-0.77470300	2.12432100	2.76080300
C	0.23223700	3.04659100	3.13020100
H	1.99611200	4.14959200	2.55729000
H	2.00139500	3.26568800	0.23314500
H	0.27429400	1.65755500	-0.49635300
H	-0.77190900	1.12977700	3.65485100
H	0.25627400	3.41534800	4.15304300
C	-1.78677100	0.66128100	1.06058000
C	-1.66470000	-0.32990600	0.08392700
C	-3.92825300	-0.10016400	1.61917200
C	-2.71509800	-1.22302600	-0.12159800
H	-0.74770700	-0.41275200	-0.48912900
C	-3.85961200	-1.11323100	0.66451200
H	-4.78572800	0.01700100	2.26836100
H	-2.63154000	-2.00216300	-0.87315600
H	-4.69113500	-1.80096700	0.55704900
N	-2.92416800	0.77344200	1.79837300
Sb	-4.46756800	0.00464600	5.60726300
F	-5.47067600	0.51163200	4.09744300
F	-3.62494600	-1.27232900	4.55080100
F	-3.06529100	1.20749400	4.93599000
F	-3.30623000	-0.33998800	7.01752700
F	-5.14028000	1.50798500	6.48818600
F	-5.77960300	-1.13170900	6.20619800
C	0.98141100	-0.35627200	3.75511400
C	1.74516100	-1.39469500	4.27254500
C	-0.62961000	-0.60279500	5.41391900
C	1.28566300	-2.05498400	5.41514900
H	2.67662400	-1.67523700	3.79252400
C	0.08310700	-1.65108100	5.99189500
H	-1.56742600	-0.26718400	5.82557400
H	1.85858200	-2.87028500	5.84666000
H	-0.31369400	-2.13379400	6.87835400
N	-0.17891900	0.02304200	4.31532900
H	1.29023000	0.19899300	2.87385400

Energy：

Sum of electronic and thermal Free Energies = -1831.214572

2a(B = Pyridine)

C	-3.64940900	4.36199300	1.66071900
C	-4.95335000	3.80114300	2.06753300
C	-5.04259400	3.88118600	3.45583700
C	-3.03851700	4.94870500	2.84306600
C	-3.80610100	4.51728600	3.95663500
C	-5.98447600	3.27301700	1.11765300
C	-6.19689600	3.48870800	4.32333300
C	-3.55326000	4.81392700	5.40344800
C	-1.88491300	5.90416500	2.84639800
C	-3.24249900	4.63771500	0.24360800
H	-3.52730500	3.81989900	-0.42440100
H	-3.73611000	5.54904500	-0.12130300
H	-2.16288400	4.78539600	0.15615500
H	-5.52972200	2.76057500	0.26453200
H	-6.67363200	2.58053600	1.60795700
H	-6.58162700	4.10107500	0.71257300
H	-5.86611900	2.98239900	5.23095700
H	-6.75015500	4.38869700	4.62551400
H	-6.89133200	2.82737000	3.80178000
H	-2.51187300	5.09253300	5.58438100
H	-4.18570700	5.64824900	5.73614600
H	-3.79215300	3.94891500	6.02853900
H	-1.11882700	5.63560400	2.11506600
H	-2.25242200	6.90726700	2.59116600
H	-1.41180800	5.97451300	3.82895100
Rh	-2.99788000	2.71843100	2.84601500
C	1.36541300	3.08218400	2.84002700
C	1.72091500	2.18081400	1.83191900
C	0.73141000	1.42846900	1.20031400
C	-0.61798300	1.59345000	1.55419900
C	-0.99468300	2.54041600	2.53983200
C	0.01874900	3.25255700	3.19226200
H	2.13245700	3.66383200	3.34563600
H	2.76085100	2.06348000	1.54134800
H	1.01788000	0.71552300	0.43191700
H	-1.25248500	-0.03446400	4.80555900
H	-0.22962100	3.96081300	3.97704700
C	-1.70752200	0.77841500	0.99847600
C	-1.57424000	-0.22959800	0.03671600
C	-3.99517500	0.30262400	1.20221700
C	-2.68697400	-0.97469700	-0.34251600
H	-0.60633400	-0.42919600	-0.40872200
C	-3.91892400	-0.71675900	0.25915100
H	-4.91797100	0.53438200	1.71811200
H	-2.59089900	-1.75475800	-1.09181300
H	-4.80564100	-1.28941400	0.01099400

N	-2.92694000	1.04249100	1.54329000
Sb	-4.06450700	0.12372700	5.43729200
F	-5.15836500	0.67129200	4.02593000
F	-3.36977400	-1.23814000	4.35056200
F	-2.62373200	1.18561500	4.62410800
F	-2.74896900	-0.34463600	6.67621500
F	-4.49663400	1.64769200	6.40972500
F	-5.36060300	-0.93732100	6.18712800
C	0.78857300	-0.10624600	4.63466800
C	1.92288600	-0.88311000	4.80875400
C	-0.59596800	-1.89013000	5.36609100
C	1.78294800	-2.19369100	5.27460000
H	2.89632900	-0.46345400	4.58339300
C	0.51125600	-2.70206000	5.55280600
H	-1.61878800	-2.18395300	5.55231300
H	2.66083900	-2.81563600	5.42051100
H	0.37416800	-3.71458200	5.91434400
N	-0.42084500	-0.62977700	4.91795700
H	0.80118900	0.91751000	4.27876800

Energy：

Sum of electronic and thermal Free Energies = -1831.258490

2-Phenylpyridine

C	-1.70486200	-1.41572900	-0.37821600
C	-0.46888100	-0.87881300	-0.74723200
C	-0.16931200	0.45278200	-0.46923800
C	-1.10319700	1.27960600	0.17804100
C	-2.33868300	0.72564100	0.55248900
C	-2.63674300	-0.60836900	0.27653300
H	-1.93772300	-2.45506700	-0.59414400
H	0.26466700	-1.50015500	-1.25446200
H	0.78978700	0.87619400	-0.74576300
H	-3.06840600	1.32748700	1.08595100
H	-3.59617100	-1.01847700	0.58071500
C	-0.76021300	2.70182000	0.45197100
C	-1.74230700	3.67073000	0.72391000
C	0.90484300	4.28707200	0.65008100
C	-1.35504600	4.98312900	0.97919500
H	-2.79457400	3.40824200	0.71487100
C	0.00057500	5.30759400	0.94844300
H	1.97323800	4.49506900	0.60397600
H	-2.10345700	5.74257400	1.18998700
H	0.34911500	6.31774900	1.14041500
N	0.54791300	3.02411100	0.40966400

Energy：

Sum of electronic and thermal Free Energies = -479.199747

a-TS4

C	-3.14252400	4.30804800	2.08641200
C	-4.44476300	3.65967400	2.14846500
C	-4.75469700	3.41184300	3.51469500
C	-2.71484400	4.55881300	3.45928500
C	-3.65279100	3.93416400	4.32325400
C	-5.31595400	3.34595100	0.97285600
C	-6.02891900	2.86943100	4.07458900
C	-3.61328400	3.87576900	5.81752300
C	-1.57420100	5.43404000	3.87695400
C	-2.51586100	4.89228000	0.85705100
H	-2.76249300	4.31133900	-0.03530400
H	-2.88520900	5.91482400	0.69952200
H	-1.42728200	4.93887300	0.94000200
H	-4.72976500	3.10900300	0.08131700
H	-5.98764300	2.50929800	1.17860300
H	-5.93807100	4.21946900	0.73583900
H	-5.85099100	2.22801900	4.93829100
H	-6.65507100	3.71317800	4.39871700
H	-6.59216800	2.29489800	3.33824500
H	-2.62025000	4.11270000	6.20684400
H	-4.31943500	4.60515700	6.23686700
H	-3.90689500	2.88593300	6.17839600
H	-0.78803000	5.47698600	3.12199000
H	-1.95178300	6.45533200	4.02373800
H	-1.13219900	5.11352500	4.82381000
Rh	-2.79860500	2.36397300	2.95147000
C	1.32734600	3.51102700	1.88230200
C	1.26707200	3.09031800	0.54827400
C	0.28121400	2.19113900	0.13978200
C	-0.65153500	1.70383200	1.06225000
C	-0.61753100	2.10703800	2.43384400
C	0.39241200	3.03125700	2.79625300
H	2.10324000	4.20158600	2.20088000
H	1.98651100	3.46544500	-0.17398800
H	0.22635400	1.89815900	-0.90464100
H	-0.55982800	1.12817600	3.33778300
H	0.47720800	3.34035400	3.83497500
C	-1.73731600	0.79544800	0.65923300
C	-1.68207300	-0.08036700	-0.42738000
C	-3.87741200	0.02479000	1.21483600
C	-2.76495100	-0.91612700	-0.69057300
H	-0.78684000	-0.12826700	-1.03543700

C	-3.87659000	-0.86950200	0.14733500
H	-4.70290200	0.08104300	1.91177500
H	-2.73135500	-1.60583200	-1.52833800
H	-4.73158000	-1.51923100	-0.00383700
N	-2.84178600	0.84757700	1.44862300
Sb	-4.11732500	-0.59674700	5.13850000
F	-5.29829800	0.05523200	3.82726800
F	-3.33970100	-1.67269000	3.83107500
F	-2.87063900	0.78086800	4.51997300
F	-2.81459600	-1.06874200	6.36340700
F	-4.76073800	0.73291600	6.28577600
F	-5.31868600	-1.87269500	5.68943700
C	0.55405500	-2.93672900	0.36797800
C	1.32795200	-1.82690500	0.71717600
C	1.13337100	-1.19730600	1.94726100
C	0.16788400	-1.68157500	2.84395300
C	-0.61353800	-2.79074800	2.48436500
C	-0.42222500	-3.40960100	1.24882900
H	0.71809300	-3.43723200	-0.58243500
H	2.09928000	-1.46483700	0.04275700
H	1.75775600	-0.35520700	2.23262000
H	-1.38299100	-3.14446900	3.16297600
H	-1.02972400	-4.26896600	0.97961500
C	0.05922500	-1.10130900	4.20722300
C	0.23984300	-1.91012200	5.33790300
C	-0.14884800	0.77502000	5.58110000
C	0.24093800	-1.34192200	6.60663200
H	0.40280000	-2.97343600	5.20186000
C	0.05815100	0.03555000	6.73480000
H	-0.34464100	1.84260200	5.62022300
H	0.38577000	-1.96376200	7.48455900
H	0.04898500	0.52045600	7.70455700
N	-0.14126100	0.22434600	4.35690400

Energy：

Sum of electronic and thermal Free Energies = -2062.188908

2a(B = 2-Phenylpyridine)

C	-3.89522100	5.09046900	2.30290000
C	-5.06746400	4.21544500	2.10343000
C	-5.32565100	3.55606600	3.30511800
C	-3.57708900	5.07630900	3.72144500
C	-4.34699100	4.03423300	4.30316700
C	-5.82830500	4.10222900	0.81802700
C	-6.42024100	2.57723300	3.60011000
C	-4.33271300	3.57822500	5.73054000
C	-2.67654100	6.04531700	4.42469900
C	-3.40539400	6.10330500	1.31071300
H	-3.43911500	5.71528600	0.28875000
H	-4.03495200	7.00335600	1.34330000
H	-2.37704200	6.40753700	1.52255100
H	-5.16471700	4.10686100	-0.05207500
H	-6.43781800	3.19560400	0.78255900
H	-6.50613300	4.95939300	0.70790800
H	-6.06789700	1.75182600	4.22155200
H	-7.23299400	3.07920100	4.14275700
H	-6.83977600	2.15084900	2.68645600
H	-3.42701800	3.89954300	6.25097100
H	-5.19507400	3.99271000	6.26999600
H	-4.39778400	2.48794200	5.79414900
H	-1.79507100	6.30050100	3.83146400
H	-3.22969300	6.97463200	4.61650700
H	-2.33826700	5.66470700	5.39164900
Rh	-3.03350600	3.17476600	2.68754600
C	1.12029100	3.98398800	3.77981000
C	1.78459500	3.73379800	2.57507600
C	1.06216800	3.28711900	1.46939400
C	-0.32864200	3.11330600	1.55823200
C	-1.01695900	3.42042600	2.75733200
C	-0.26880000	3.82663800	3.86635400
H	1.68051800	4.31562800	4.65052100
H	2.85738600	3.88723400	2.49778600
H	1.58798200	3.07277500	0.54274700
H	-0.84658600	-1.54122100	4.12094300
H	-0.76115900	4.03107200	4.81227200
C	-1.14611000	2.54518600	0.48010700
C	-0.68687000	2.14958900	-0.78205100
C	-3.29437400	1.76387800	-0.04256200
C	-1.56452300	1.55510500	-1.68278000
H	0.35101500	2.30566600	-1.05314900
C	-2.89143000	1.34422900	-1.30524000
H	-4.30453400	1.60827100	0.31298000
H	-1.21470300	1.25084200	-2.66479400
H	-3.60332100	0.86396200	-1.96734100
N	-2.45359400	2.36601100	0.81493700
Sb	-3.57524400	-0.47136100	3.57402100
F	-4.65825600	0.35975500	2.30638600
F	-2.29487600	-0.89996800	2.27578900
F	-2.58596200	1.16792000	3.77845900
F	-2.34313900	-1.18007700	4.83062800

F	-4.67276500	0.08545300	4.96360300
F	-4.38649700	-2.11434500	3.37739300
C	-1.25995500	-6.35513500	4.14852900
C	-1.93229500	-5.23676900	3.64966000
C	-1.25861700	-4.03008600	3.48320800
C	0.10609100	-3.93429200	3.81787300
C	0.77853500	-5.06684700	4.31290100
C	0.09562600	-6.26818200	4.47859100
H	-1.79038000	-7.29359200	4.27967400
H	-2.98304200	-5.29867000	3.38469700
H	-1.78631400	-3.18389000	3.05747300
H	1.82302500	-4.99919700	4.60266300
H	0.61796100	-7.13375300	4.87424700
C	0.82718200	-2.66459400	3.65390100
C	2.18310500	-2.55098300	3.31550300
C	0.66272100	-0.27312800	3.64801500
C	2.76189400	-1.29702400	3.15322400
H	2.76084700	-3.45260400	3.15259400
C	1.99452700	-0.13444700	3.31091300
H	-0.02159900	0.55485200	3.79336500
H	3.81150300	-1.22247600	2.88503900
H	2.41142000	0.85574800	3.17262000
N	0.13944200	-1.50498100	3.81994100

Energy：

Sum of electronic and thermal Free Energies = -2062.249440

MeOH

H	-1.45105	-0.24172	3.74091
O	-0.88989	0.53711	3.72968
C	-0.18734	0.63637	4.97124
H	0.41623	-0.23614	5.11026
H	0.43812	1.50444	4.95872
H	-0.89068	0.71508	5.77374

Energy：

Sum of electronic and thermal Free Energies = -115.683456

a-TS5

C	-4.07997300	4.61228900	2.87529500
C	-4.33422100	4.11188000	1.52891700
C	-5.45405700	3.17447500	1.61546600
C	-4.88979100	3.86070800	3.76863200
C	-5.78196800	3.00222300	2.98055700
C	-3.78494900	4.69661800	0.26319100
C	-6.13944400	2.54075800	0.44534800
C	-6.89942400	2.19186800	3.55441200
C	-4.93727700	3.96752100	5.26035800
C	-3.20878700	5.77799800	3.22620500
H	-2.36796600	5.88917600	2.53912300
H	-3.80931600	6.69613900	3.16853100
H	-2.81845600	5.70899900	4.24448000
H	-2.75955400	5.05078700	0.39431100
H	-3.79106200	3.96975000	-0.55342300
H	-4.39743400	5.55255900	-0.05136000
H	-6.63515500	1.60684500	0.72053900
H	-6.90980300	3.22148800	0.05901100
H	-5.44462800	2.33662400	-0.37349200
H	-6.60731100	1.69192200	4.47897800
H	-7.74229000	2.85868000	3.78459200
H	-7.25371700	1.43018300	2.85798400
H	-4.04080900	4.44608600	5.66157500
H	-5.80447600	4.56904100	5.56449700
H	-5.03929000	2.98160600	5.72208200
Rh	-3.57374700	2.43427300	2.63265800
C	0.40495100	4.30626500	2.35092300
C	0.71547200	3.90019800	1.04872400
C	-0.01370700	2.88228100	0.42690500
C	-1.06805500	2.27066200	1.10914700
C	-1.42233900	2.67591400	2.43453500
C	-0.66007600	3.70696600	3.02534900
H	0.99064500	5.08522100	2.83075500
H	1.53512700	4.37300300	0.51543400
H	0.24083000	2.58923800	-0.58762200
H	-1.26857200	1.52610200	3.21453100
H	-0.89236200	4.02612300	4.03871400
C	-1.86006800	1.15755000	0.55799300
C	-1.46405900	0.33461300	-0.49963800
C	-3.79963400	-0.12403200	0.86596600
C	-2.26936400	-0.73875500	-0.87543500
H	-0.52304300	0.51945500	-1.00528000
C	-3.45073900	-0.97990300	-0.17586000
H	-4.69317300	-0.27468600	1.45780100
H	-1.96775800	-1.38766000	-1.69192500
H	-4.09376100	-1.81884300	-0.41809900
N	-3.03343800	0.92423400	1.21100700
H	-1.54259300	-0.20142100	3.75289300
O	-0.80693500	0.46672500	3.68687700
Sb	-4.15215300	-0.50729700	5.03080800
F	-3.33027800	1.18128800	4.51991700
F	-5.24260300	-0.30076500	3.52040500
F	-2.82374000	-1.20682500	3.85219700

F	-4.84830600	-2.15730600	5.41630700
F	-2.88590700	-0.54141700	6.38076000
F	-5.35175200	0.49195800	6.03576800
C	-0.17631600	0.63202800	4.98839800
H	0.50846100	-0.20464900	5.13720800
H	0.38620400	1.56557200	4.94707100
H	-0.93342700	0.65688000	5.77209200

Energy：

Sum of electronic and thermal Free Energies = -1698.679129

2a(B = MeOH)

C	-4.30438700	4.69040700	2.70314200
C	-4.67090800	4.16142900	1.39783900
C	-5.78108200	3.21060800	1.60034800
C	-4.99083900	3.90858800	3.67009000
C	-5.95141300	3.02811400	2.97510400
C	-4.28025300	4.75021100	0.07553600
C	-6.56461300	2.58293600	0.48910800
C	-6.93706300	2.14224500	3.67352700
C	-4.90841600	4.02274000	5.16082900
C	-3.43033700	5.88133400	2.95182800
H	-2.59932700	5.93967800	2.24442600
H	-4.02539100	6.79764400	2.84158700
H	-3.01852400	5.88307700	3.96433700
H	-3.28115200	5.19201100	0.11124800
H	-4.29003800	3.99862100	-0.71883300
H	-4.98631400	5.54218600	-0.20987100
H	-7.11692400	1.70103900	0.82292900
H	-7.29714800	3.30254800	0.10002700
H	-5.92436300	2.29318400	-0.34942900
H	-6.46350500	1.55496800	4.46345300
H	-7.72496700	2.74862800	4.13968700
H	-7.41809400	1.44728000	2.98174900
H	-4.00100600	4.54019700	5.48154200
H	-5.76878800	4.58943900	5.54179600
H	-4.92972800	3.03690800	5.63409700
Rh	-3.68727800	2.56548700	2.42337700
C	0.50702700	3.81084900	2.81336000
C	1.09221000	3.15639000	1.72844000
C	0.31723400	2.31963000	0.92424500
C	-1.05058700	2.15269000	1.18629400
C	-1.67583600	2.86155200	2.24851700
C	-0.86691000	3.66007400	3.07114000
H	1.10843300	4.45172700	3.45302100
H	2.14941500	3.28325900	1.51680900
H	0.79207300	1.78755300	0.10492200
H	-0.69597000	1.47227900	3.66790000
H	-1.30532600	4.19738400	3.90769400
C	-1.90525600	1.19167000	0.47322900
C	-1.50797800	0.36233200	-0.58082700
C	-4.02252800	0.18596500	0.49116400
C	-2.40187200	-0.56990700	-1.10021800
H	-0.50583900	0.44196800	-0.98612700
C	-3.67871800	-0.67261200	-0.54727100
H	-4.99201600	0.14118700	0.96948600
H	-2.10073300	-1.21644200	-1.91882500
H	-4.39743400	-1.40133600	-0.90531600
N	-3.16882100	1.10455200	0.97335800
H	-1.13010700	-0.08753500	3.91870700
O	-0.34606000	0.58904300	3.97113700
Sb	-3.74561900	-0.40524100	4.86474000
F	-3.08787900	1.32972600	4.32733100
F	-4.82453300	-0.35321300	3.34918700
F	-2.26519700	-0.96683500	3.73769700
F	-4.20100500	-2.13604000	5.25064300
F	-2.45662600	-0.30042100	6.20129100
F	-5.02937400	0.43624400	5.89857300
C	0.26510700	0.66634100	5.31718200
H	0.67617300	-0.32285200	5.50792900
H	1.05455500	1.41115300	5.24281500
H	-0.50131500	0.92417200	6.04479400

Energy：

Sum of electronic and thermal Free Energies = -1698.691625

THF

C	-1.41035700	1.14873400	-2.63463300
O	-1.70244700	1.14599800	-1.23312200
C	-1.57097700	2.46773600	-0.70190100
C	-1.50892800	3.41283500	-1.90794700
C	-0.81390800	2.52661800	-2.95330300
H	-0.72468700	0.32189700	-2.85513700
H	-2.33942900	0.97924300	-3.20035300
H	-2.42193800	2.66560500	-0.03981200
H	-0.64987300	2.53465000	-0.10176800
H	-2.52059300	3.67329700	-2.24182700
H	-0.97126400	4.34177100	-1.69386000
H	-0.99752900	2.84042900	-3.98556200
H	0.27012900	2.52277500	-2.78706300

Energy：

Sum of electronic and thermal Free Energies = -232.356646

a-TS6

C	-3.91031	4.61709	3.5572
C	-3.9517	4.60468	2.10367
C	-5.0141	3.70885	1.69375
C	-4.96646	3.77159	4.02681
C	-5.60984	3.15352	2.88269
C	-3.19445	5.52076	1.19589
C	-5.47533	3.48056	0.28982
C	-6.78091	2.22192	2.94068
C	-5.32401	3.54926	5.456
C	-3.071	5.50443	4.42801
H	-2.13371	5.78404	3.94113
H	-3.61259	6.43301	4.65513
H	-2.83387	5.02133	5.37988
H	-2.23477	5.81698	1.62213
H	-3.01069	5.07496	0.21533
H	-3.7886	6.43227	1.04026
H	-5.83325	2.45866	0.1404
H	-6.31357	4.15717	0.07429
H	-4.68956	3.68306	-0.44153
H	-6.72741	1.56611	3.81449
H	-7.71816	2.79268	2.98758
H	-6.83001	1.58612	2.05165
H	-5.39525	4.51398	5.97283
H	-6.27678	3.02764	5.55636
H	-4.5795	2.93753	5.97667
Rh	-3.4696	2.56195	2.77919
C	0.37358	4.19317	1.15299
C	0.31882	3.5724	-0.09978
C	-0.56259	2.51266	-0.3274
C	-1.40273	2.067	0.69927
C	-1.37817	2.71629	1.96394
C	-0.47183	3.76513	2.17804
H	1.08043	4.99871	1.32967
H	0.97057	3.90825	-0.90079
H	-0.59872	2.0501	-1.30974
H	-1.35219	1.82004	3.07792
H	-0.41097	4.2325	3.15789
C	-2.33578	0.93327	0.5524
C	-2.21646	-0.09692	-0.38654
C	-4.18111	-0.14861	1.53763
C	-3.11205	-1.16406	-0.35303
H	-1.41043	-0.07658	-1.11174
C	-4.09934	-1.20281	0.633
H	-4.89791	-0.14393	2.3495
H	-3.02251	-1.97114	-1.0739
H	-4.78907	-2.0353	0.71702
N	-3.34236	0.90007	1.46739
Sb	-4.27654	-0.43947	5.61947
F	-3.90274	0.95607	4.29998
F	-5.93902	-0.55878	4.75492
F	-3.54851	-1.64344	4.37978
F	-4.62954	-1.75864	6.86258
F	-2.55921	-0.08363	6.24127
F	-4.94521	0.974	6.63748
C	0.12204	1.25137	5.04735
O	-0.65963	0.86642	3.86998
C	-0.45887	-0.55017	3.53302
C	0.29735	-1.11851	4.73062
C	1.10275	0.09525	5.23955
H	0.61005	2.20897	4.82596
H	-0.57649	1.35842	5.8877
H	-1.43758	-1.00249	3.37985
H	0.14388	-0.58833	2.61352
H	-0.42421	-1.44082	5.48691
H	0.93253	-1.96781	4.44944
H	1.41248	-0.0041	6.28593
H	2.00348	0.25396	4.62643

Energy：

Sum of electronic and thermal Free Energies = -1815.341169

2a(B = THF)

C	-4.38159100	4.42870500	3.77700500
C	-4.14381200	4.83251700	2.43797600
C	-5.03506600	4.04263300	1.60098600
C	-5.59237800	3.57990100	3.80704200
C	-5.99948900	3.36553000	2.49214000
C	-3.23640900	5.92317300	1.95693600
C	-5.20602400	4.20479900	0.12036300
C	-7.20011500	2.60637200	2.01621700
C	-6.25627700	3.11874300	5.06698300
C	-3.68319000	4.90543700	5.01422000
H	-2.71821800	5.36602600	4.78691000
H	-4.29709900	5.65444700	5.53248200
H	-3.51861800	4.07826700	5.71151800
H	-2.47292800	6.17804200	2.69598500
H	-2.73484300	5.66482700	1.02122400
H	-3.83070600	6.82934300	1.77838000
H	-5.61379400	3.30043200	-0.33977800
H	-5.90361300	5.02695600	-0.09198700

H	-4.25673400	4.43642900	-0.36950900
H	-7.59567300	1.94264000	2.78918300
H	-8.00083000	3.30447100	1.73773400
H	-6.97757400	2.00610000	1.12852100
H	-5.53495700	2.71450300	5.77970600
H	-6.76146000	3.96670900	5.54931300
H	-7.00450900	2.34782800	4.87344000
Rh	-3.74544400	2.64322300	2.55300200
C	0.28468100	3.48585400	1.07844600
C	0.45926300	2.47083400	0.13496200
C	-0.55355500	1.53538400	-0.06686900
C	-1.75092800	1.62075500	0.66181300
C	-1.95115200	2.66765700	1.59484600
C	-0.91191100	3.58003300	1.80073400
H	1.07430400	4.21467400	1.24455100
H	1.37941600	2.40638100	-0.43814200
H	-0.40304900	0.73984800	-0.79168600
H	-0.98581100	1.07260100	3.95365000
H	-1.02397400	4.38333900	2.52296800
C	-2.82603400	0.62500200	0.57298600
C	-2.84803700	-0.49034100	-0.27279900
C	-4.85061000	-0.05470100	1.54265300
C	-3.90308800	-1.39445000	-0.19864800
H	-2.04334200	-0.64735400	-0.98182700
C	-4.91884600	-1.18385600	0.73465700
H	-5.59923500	0.14953200	2.29711700
H	-3.92720500	-2.25891400	-0.85536900
H	-5.74709400	-1.87540300	0.84186300
N	-3.84744400	0.83444000	1.44909200
Sb	-3.32756700	0.14073700	5.48272500
F	-2.46874200	1.42102800	4.22120600
F	-4.92988000	0.44486000	4.58296500
F	-2.86378500	-1.11554700	4.18222000
F	-4.02425900	-1.07549400	6.66138000
F	-1.57537300	0.00942500	6.13649300
F	-3.62136400	1.63710000	6.54243800
C	0.82801700	1.47777100	4.92407500
O	-0.00249100	0.86267900	3.83453700
C	0.26635700	-0.62373000	3.74352200
C	1.20060100	-0.89620200	4.91356400
C	1.92574300	0.44686800	5.12884500
H	1.14816200	2.44268900	4.53361100
H	0.17224200	1.58337500	5.78789400
H	-0.70650700	-1.10837400	3.79424000
H	0.72793100	-0.74831200	2.76415200
H	0.61836800	-1.16338700	5.79841700
H	1.89307000	-1.71024300	4.68483100
H	2.35824400	0.53011700	6.12916800
H	2.72717400	0.58648300	4.39588100

Energy：

Sum of electronic and thermal Free Energies = -1815.366165

1,4-dioxane

C	-1.14398500	1.32285400	5.24429700
C	-2.68312500	-0.16435000	4.29145800
C	-2.83655900	-0.86727400	5.63712000
C	-1.29765400	0.61974500	6.58984400
H	-0.29599300	0.88225900	4.69369700
H	-3.62220200	-0.17765600	3.72853200
H	-3.02040600	-1.93867600	5.50622500
H	-2.07557300	1.12806600	7.18383000
O	-2.33841600	1.20374400	4.47930800
O	-1.64184200	-0.74849900	6.40177600
H	-0.96036600	2.39430900	5.37545200
H	-0.35885100	0.63318600	7.15313500
H	-3.68420700	-0.42616400	6.18781200
H	-1.90571200	-0.67294500	3.69703100

Energy：

Sum of electronic and thermal Free Energies = -307.558267

a-TS7

C	-4.59515700	4.25644800	3.76886000
C	-3.98082100	4.70100000	2.56725400
C	-4.54234900	3.91752500	1.47290900
C	-5.66827000	3.31807500	3.42493700
C	-5.64515500	3.12993800	2.02241200
C	-3.03041900	5.84869000	2.42449600
C	-4.27026300	4.13542900	0.01506800
C	-6.58991900	2.29298600	1.21803000
C	-6.65765100	2.77765800	4.40642500
C	-4.30742300	4.70856500	5.16626400
H	-3.35131400	5.23298200	5.23708000
H	-5.09323300	5.39607500	5.50662600
H	-4.29094400	3.85795500	5.85432400
H	-2.41652300	5.99132100	3.31740900
H	-2.37177500	5.73769700	1.56131300
H	-3.61260200	6.76930700	2.28093700
H	-4.51873000	3.25030000	-0.57644700
H	-4.88015100	4.96747700	-0.36228800
H	-3.22100500	4.38130700	-0.16758100

H	-7.06603200	1.52060700	1.82637300
H	-7.38555100	2.92824500	0.80648400
H	-6.08896200	1.80993300	0.37487400
H	-7.39399500	3.56101400	4.63525900
H	-7.19468600	1.91291300	4.01493500
H	-6.18127900	2.47945800	5.34171200
Rh	-3.60959600	2.49150300	2.78437400
C	0.23106400	3.85143800	1.06013500
C	0.26017200	3.01318800	-0.05902400
C	-0.59956700	1.91556700	-0.14029900
C	-1.49850900	1.65194700	0.89898000
C	-1.55737200	2.49113500	2.05620500
C	-0.67439300	3.59458400	2.09036200
H	0.90747900	4.69930000	1.12271600
H	0.95263900	3.21409600	-0.87124800
H	-0.57793700	1.29077600	-1.02853300
H	-1.18970600	1.71727800	3.21445100
H	-0.67982500	4.25057500	2.95731900
C	-2.44014200	0.51903400	0.87140400
C	-2.31323800	-0.61013900	0.05691600
C	-4.34861500	-0.38917300	1.88099100
C	-3.24293900	-1.64337600	0.16163800
H	-1.48496100	-0.68560300	-0.63851900
C	-4.27152200	-1.53678200	1.09498500
H	-5.10572400	-0.26877100	2.64412700
H	-3.15282000	-2.52470700	-0.46603200
H	-5.00158300	-2.32714900	1.23010800
N	-3.46897900	0.61812600	1.75742400
Sb	-3.79691000	0.18491300	5.82889400
F	-3.07666400	1.68467000	4.80989900
F	-2.91120900	-0.90585000	4.59145400
F	-2.25009100	0.28757900	6.85292800
F	-4.49930000	-1.22522200	6.77249000
F	-4.63940400	1.50711700	6.83602100
F	-5.25287300	0.21900900	4.63746000
C	0.82452800	1.03741600	6.02347300
C	0.44704200	-0.94331500	4.85525000
C	-0.06375700	-0.20284900	3.62750600
C	0.30763400	1.88254300	4.86493900
H	-0.00021800	0.81369700	6.71047000
H	0.93914200	-1.87027000	4.54799300
H	-0.89062200	-0.72860600	3.15269200
H	1.12109500	2.20534500	4.20552700
O	1.41431600	-0.15696300	5.53413800
O	-0.62657600	1.07253300	4.08100600
H	1.60458100	1.58998600	6.55494700
H	-0.27446700	2.73803100	5.21173800
H	0.74195900	0.00810600	2.91549100
H	-0.40117000	-1.17846200	5.51055200

Energy：

Sum of electronic and thermal Free Energies = -1890.536387

2a(B = 1,4-dioxane)

C	-4.71445400	4.38387000	3.57047300
C	-4.21223500	4.74560000	2.29396400
C	-4.88641600	3.89498900	1.32376100
C	-5.87745200	3.48927000	3.38549200
C	-5.99311700	3.21197300	2.02484800
C	-3.25091800	5.84772200	1.96962900
C	-4.75311500	4.00087700	-0.16586800
C	-7.04318100	2.38686900	1.34629500
C	-6.78705600	3.05191700	4.49032400
C	-4.30413100	4.94205800	4.89868800
H	-3.31878000	5.41324700	4.85508900
H	-5.02410400	5.70458000	5.22587600
H	-4.28404100	4.16037800	5.66314700
H	-2.64271000	6.13001400	2.83256200
H	-2.57918000	5.58533000	1.14883400
H	-3.81651000	6.73875500	1.66552200
H	-5.00694700	3.05979600	-0.66138000
H	-5.43415700	4.77179400	-0.55224000
H	-3.73666100	4.27564500	-0.45923200
H	-7.54179600	1.70827800	2.04296800
H	-7.81294600	3.03989500	0.91364400
H	-6.62812400	1.79440800	0.52529500
H	-7.43641400	3.88765800	4.78534700
H	-7.42862800	2.22290100	4.18437700
H	-6.22835600	2.73781800	5.37282000
Rh	-3.78409900	2.57320200	2.57307500
C	0.40284900	3.51217100	1.70896400
C	0.71542700	2.54056300	0.75322800
C	-0.23990800	1.58882800	0.39894200
C	-1.51581500	1.61505700	0.98682900
C	-1.86053300	2.62993900	1.91467200
C	-0.87630000	3.55478300	2.28037000
H	1.14852800	4.24897600	1.99695400
H	1.69806200	2.52197400	0.29151200
H	0.01803000	0.82565900	-0.33047900
H	-1.39847100	0.90902100	4.60570100

H	-1.10126000	4.33203900	3.00534000
C	-2.53268800	0.57768200	0.76546800
C	-2.40733400	-0.53560800	-0.07387300
C	-4.62250700	-0.19518600	1.50193600
C	-3.42251400	-1.48735200	-0.11665500
H	-1.52169100	-0.65482500	-0.68764000
C	-4.54590900	-1.32543600	0.69506800
H	-5.45900900	-0.02405100	2.16705400
H	-3.33254900	-2.35070400	-0.76907500
H	-5.34799900	-2.05492900	0.71034100
N	-3.65556500	0.73747300	1.51988900
Sb	-3.84899000	0.32396500	5.74734600
F	-2.77854600	1.52133900	4.54349100
F	-2.97442800	-0.98205400	4.74565600
F	-2.34476900	0.46910800	6.83635900
F	-4.75489700	-0.83808300	6.83373400
F	-4.51336600	1.89094100	6.49679400
F	-5.19075600	0.40310300	4.45188500
C	1.57519900	0.74558200	6.06179100
C	1.45833200	-0.77386600	4.28102900
C	0.21540000	-0.12343300	3.69594000
C	0.33670800	1.49775200	5.60786500
H	1.29344400	-0.03868200	6.77931800
H	2.06301700	-1.19235900	3.47207100
H	-0.51052700	-0.84087100	3.31229200
H	0.57193300	2.33130800	4.94100400
O	2.25632600	0.19173800	4.94650300
O	-0.47897800	0.53085700	4.83057400
H	2.26330500	1.44055100	6.55019400
H	-0.31437600	1.79859500	6.42792300
H	0.45095000	0.64756100	2.95927200
H	1.17115600	-1.58481000	4.96631500

Energy：

Sum of electronic and thermal Free Energies = -1890.555633

Three-water cluster

H	-3.17856900	0.71068800	-3.49146300
O	-2.42027000	0.43574400	-4.06389100
H	-1.82747000	-0.04488200	-3.46651800
O	-4.16306400	1.92603700	-2.56279600
H	-3.56496500	2.61266600	-2.94890800
H	-5.01431400	2.07132200	-3.00350800
H	-2.04859200	2.22436700	-4.23144200
O	-2.20445100	3.17607700	-4.01411700
H	-1.43042000	3.44372000	-3.49594800

Energy：

Sum of electronic and thermal Free Energies = -229.216804

a-TS8

C	-3.87791900	4.52550000	3.11672900
C	-4.23774500	4.23716300	1.73173800
C	-5.38751200	3.33669200	1.75946400
C	-4.66401700	3.68395400	3.94685800
C	-5.64874900	2.99356900	3.11054900
C	-3.74396700	4.97849300	0.52762900
C	-6.17588300	2.90024000	0.56474200
C	-6.81286900	2.22101700	3.63796800
C	-4.60774500	3.58140900	5.43801800
C	-2.95814700	5.60956200	3.58491000
H	-2.22363000	5.88717300	2.82821700
H	-3.56101100	6.50077000	3.80776100
H	-2.43048800	5.33834700	4.50269100
H	-2.69509700	5.26635200	0.63069900
H	-3.84415800	4.38015000	-0.38167900
H	-4.33288100	5.89532400	0.38835900
H	-6.66629500	1.93829500	0.73194300
H	-6.96042000	3.63909300	0.35281300
H	-5.55111300	2.82086200	-0.32859200
H	-6.54266500	1.61237200	4.50072200
H	-7.58364700	2.93724100	3.95776500
H	-7.25221900	1.56750200	2.88375300
H	-5.43096000	4.15763000	5.88201200
H	-4.71726600	2.54354800	5.76276000
H	-3.66987300	3.97450300	5.83677400
Rh	-3.49487500	2.38773400	2.51247600
C	0.34669300	4.43168400	1.66658300
C	0.45235800	4.05792300	0.32289000
C	-0.31231500	3.00097900	-0.17582400
C	-1.19612000	2.31641600	0.66544100
C	-1.33801800	2.68378500	2.03806100
C	-0.54230300	3.75549900	2.50128300
H	0.96168800	5.23707600	2.05803100
H	1.13436600	4.58585500	-0.33732800
H	-0.23348900	2.73734800	-1.22661600
H	-1.14009600	1.73607700	2.97082500
H	-0.58129400	4.01697700	3.55500700
C	-2.04320000	1.21523500	0.18045500
C	-1.75327600	0.41641000	-0.92992300
C	-3.98619700	-0.02416200	0.59961600
C	-2.61588900	-0.62125900	-1.27604700
H	-0.85087600	0.59719100	-1.50309900

C	-3.74738500	-0.85059800	-0.49548400
H	-4.83736300	-0.17331200	1.25045600
H	-2.39903700	-1.24884700	-2.13512600
H	-4.43624900	-1.65884700	-0.71482000
N	-3.16261900	0.98887500	0.91900400
H	0.35251800	0.72687400	3.59361000
O	-0.55547900	1.03121500	3.89027100
H	-1.01304500	0.16674500	4.05062600
O	1.56348400	-0.45705200	3.35486400
H	0.98561900	-1.21626500	3.57425700
H	2.00246200	-0.68025000	2.52087000
H	-1.15407700	-1.83126800	5.01278600
O	-0.85512900	-1.66273900	4.10153000
H	-1.62181000	-1.95273300	3.56852200
Sb	-4.36761500	-0.89478900	4.48800100
F	-3.24072700	0.60080300	3.95460200
F	-3.41757900	-1.84042000	3.16025500
F	-3.02813500	-1.31956000	5.71036100
F	-5.40954800	-2.33823100	4.92826000
F	-5.16737800	0.27456900	5.69436100
F	-5.55608200	-0.33272500	3.15175300

Energy：

Sum of electronic and thermal Free Energies = -1812.219800

2a(B = there-water cluster)

C	-4.03479200	4.65986400	2.83639800
C	-4.55492700	4.23787700	1.54410300
C	-5.72003300	3.36628800	1.79781000
C	-4.68233500	3.86409100	3.81618400
C	-5.78796400	3.12660300	3.16902400
C	-4.24420800	4.88513000	0.22764000
C	-6.65601900	2.87100100	0.73845800
C	-6.82570300	2.34394900	3.91051900
C	-4.45473100	3.88154200	5.29649400
C	-3.08697800	5.79627600	3.06721800
H	-2.31602600	5.86008900	2.29590200
H	-3.65185200	6.73812900	3.05076600
H	-2.59536300	5.73217700	4.04097400
H	-3.20842200	5.23125300	0.18235600
H	-4.41016000	4.19945100	-0.60790200
H	-4.89570800	5.75646900	0.07355600
H	-7.20471900	1.98269000	1.06171100
H	-7.39608700	3.64663900	0.49988000
H	-6.13180000	2.63277800	-0.19179700
H	-6.38445400	1.73212600	4.69802400
H	-7.53655300	3.03495000	4.38432000
H	-7.39039100	1.68644700	3.24672700
H	-5.23464700	4.47610300	5.79142100
H	-4.49990500	2.87063100	5.71086200
H	-3.48732600	4.31928800	5.55495000
Rh	-3.58173500	2.52596500	2.35012500
C	0.61079600	3.78839200	2.31885800
C	1.05846600	3.23396800	1.11259100
C	0.19859600	2.42389000	0.36524500
C	-1.11621100	2.19763800	0.80181900
C	-1.59837800	2.80859600	1.98775200
C	-0.70419600	3.56837400	2.75024500
H	1.28057400	4.40152100	2.91618500
H	2.06379900	3.43740000	0.75416200
H	0.55836100	1.98360600	-0.56085700
H	-1.23137900	0.42391700	4.28803600
H	-1.02637300	4.01646700	3.68532000
C	-2.05401500	1.29618000	0.11733800
C	-1.78149800	0.54282100	-1.02980100
C	-4.18744400	0.33346200	0.26192400
C	-2.74551100	-0.32742500	-1.53107600
H	-0.82110200	0.63418200	-1.52420900
C	-3.96761200	-0.44593000	-0.86898500
H	-5.10797500	0.27009600	0.82723300
H	-2.54087900	-0.91257700	-2.42256000
H	-4.73849900	-1.12654900	-1.21294900
N	-3.26543100	1.19168200	0.72988900
H	0.38893600	0.32160300	3.87243300
O	-0.36446200	-0.01099500	4.49204500
H	-0.49667600	-1.05969500	4.36751500
O	1.60665900	0.70786100	3.03213600
H	2.00845300	0.01063500	2.48999000
H	1.47735200	1.48007800	2.44681900
H	-0.89791600	-2.90070100	4.91828900
O	-0.73037600	-2.45687300	4.06835900
H	-1.61128200	-2.42485200	3.62967000
Sb	-4.08253700	-0.71340000	4.40392300
F	-2.87957300	0.74324100	3.86040600
F	-3.15214900	-1.71190200	3.09258200
F	-2.70623700	-1.17685200	5.57109400
F	-5.14932400	-2.12870600	4.87289100
F	-4.79331000	0.47551800	5.63792500
F	-5.24750500	-0.11649900	3.07743400

Energy：

Sum of electronic and thermal Free Energies = -1812.248483

1b

C	0.40685700	4.38395700	1.95174300
C	0.38033100	3.98503400	0.61646900
C	-0.35979500	2.86543000	0.23064700
C	-1.08796000	2.12260400	1.17385500
C	-1.05207700	2.53704500	2.51939000
C	-0.31461100	3.65223000	2.90134700
H	0.98235200	5.25520900	2.25265100
H	0.93575500	4.54372400	-0.13216400
H	-0.36501600	2.57473400	-0.81475800
H	-1.61117600	1.96975700	3.25491200
H	-0.30114300	3.95426100	3.94538900
C	-1.87594200	0.93041600	0.76147800
C	-1.90486900	0.51173200	-0.68772000
H	-0.89276800	0.29020800	-1.04616000
N	-2.50346600	0.31388300	1.70308000
H	-2.52409300	-0.37394700	-0.82119900
H	-2.30443000	1.31771400	-1.31435400
O	-3.22595600	-0.79818700	1.24916400
H	-3.62116800	-1.12766800	2.07106300

Energies:

Sum of electronic and zero-point Energies = -440.026023

Sum of electronic and thermal Enthalpies = -440.015956

Sum of electronic and thermal Free Energies = -440.061332

Electronic energies = -440.1810386

Single point energies in solution = -439.997467461

b-TS1

C	-4.09084300	4.64253900	3.01217500
C	-4.27646400	4.21390300	1.62942900
C	-5.37807800	3.25300000	1.61142800
C	-4.94795000	3.84781100	3.82104200
C	-5.77247000	3.00495500	2.95023600
C	-3.67035600	4.86570300	0.42458900
C	-5.98224300	2.64846800	0.38300800
C	-6.89744500	2.13605000	3.41666300
C	-5.07497600	3.88259800	5.31032800
C	-3.24376800	5.78808500	3.47409900
H	-2.40134000	5.97211000	2.80509200
H	-3.85500000	6.70038000	3.49700200
H	-2.85654400	5.63099400	4.48429000
H	-2.65302400	5.21300500	0.62058200
H	-3.63816700	4.18466900	-0.42952200
H	-4.27188900	5.73647100	0.13040400
H	-6.35096800	1.63683300	0.56556600
H	-6.83304600	3.26153300	0.05681400
H	-5.26979500	2.60651900	-0.44389500
H	-6.64274600	1.59478900	4.32932900
H	-7.77523900	2.76135600	3.63065800
H	-7.18563000	1.40438900	2.65955800
H	-4.21470300	4.36239000	5.78234900
H	-5.97256600	4.45064200	5.59052300
H	-5.18197600	2.87514200	5.72151500
Rh	-3.55669100	2.48572500	2.68785500
C	0.44162400	4.28581900	2.04331900
C	0.69979100	3.73876900	0.78410700
C	-0.07266600	2.67738700	0.29716300
C	-1.11704600	2.17211800	1.07265200
C	-1.40817900	2.71016600	2.36974800
C	-0.60653400	3.77923900	2.81814800
H	1.05889500	5.09635300	2.42017900
H	1.51153900	4.13123800	0.17865100
H	0.14113400	2.26679900	-0.68512700
H	-1.20906300	1.64207700	3.26023800
H	-0.78430200	4.20073100	3.80462800
C	-1.97302200	1.06038500	0.62418300
C	-1.63823700	0.14165900	-0.51025400
H	-0.55653300	0.03437100	-0.61765300
N	-3.06166400	0.94387700	1.32455900
H	-1.41384800	-0.07318500	3.82687500
O	-0.72268900	0.64158100	3.81035200
Sb	-4.08978200	-0.55361400	4.94096500
F	-3.33416700	1.19376300	4.55813300
F	-5.08539900	-0.32419600	3.33755100
F	-2.67079000	-1.12840600	3.80906500
F	-4.74410900	-2.24588000	5.17268700
F	-2.92427500	-0.59644400	6.37249200
F	-5.42617500	0.33469000	5.86670800
C	-0.21084300	0.87310000	5.15383200
H	0.51061800	0.08523800	5.37623000
H	0.29367300	1.83967400	5.13339300
H	-1.02782800	0.86583200	5.87521700
H	-2.08967800	-0.83897500	-0.34867900
H	-2.03817800	0.53545100	-1.45391700
O	-3.92550300	-0.05267600	0.94770600
H	-4.42223200	-0.26543100	1.77402100

Energies:

Sum of electronic and zero-point Energies = -1659.475147

Sum of electronic and thermal Enthalpies = -1659.437715

Sum of electronic and thermal Free Energies = -1659.541863

Electronic energies = -1659.9216692

Single point energies in solution = -1660.61014793

2b(B = MeOH)

C	-4.18038200	4.67599800	2.85127700
C	-4.57866000	4.19322200	1.53658400
C	-5.70386000	3.25721700	1.72685400
C	-4.87121700	3.88154100	3.80483800
C	-5.85933100	3.04108700	3.09940400
C	-4.20138900	4.81095800	0.22410000
C	-6.49331700	2.65851200	0.60425900
C	-6.85641600	2.16040100	3.78868600
C	-4.76456100	3.94640100	5.29685500
C	-3.27432700	5.83748400	3.12375300
H	-2.46471200	5.91038000	2.39340000
H	-3.85262800	6.76957800	3.07173900
H	-2.83176000	5.78673600	4.12210100
H	-3.18698500	5.21764200	0.24423400
H	-4.26328900	4.08564700	-0.59184800
H	-4.88709800	5.63572100	-0.01406300
H	-7.17721400	1.88314400	0.95622800
H	-7.09330500	3.43651100	0.11469000
H	-5.84351200	2.21483900	-0.15562200
H	-6.38402500	1.51520500	4.53334700
H	-7.60315200	2.77316300	4.31052000
H	-7.38673400	1.52007800	3.08080800
H	-3.84312800	4.43537800	5.62202000
H	-5.60859400	4.51592800	5.70885200
H	-4.79997200	2.94568500	5.73810400
Rh	-3.61553900	2.54982800	2.49881900
C	0.64421300	3.69275200	2.62385100
C	1.12236000	3.06431400	1.47570800
C	0.26430900	2.26607900	0.71268300
C	-1.07624300	2.11822300	1.09028500
C	-1.60119000	2.80883900	2.22207500
C	-0.70936600	3.56283700	2.99523000
H	1.31098100	4.30093600	3.22963200
H	2.16026600	3.17978400	1.17947300
H	0.64855700	1.75418300	-0.16472800
H	-0.60025200	1.36785000	3.48868100
H	-1.06225600	4.08672300	3.88018200
C	-2.00065600	1.18870400	0.42247100
C	-1.64152500	0.35766300	-0.76932800
H	-0.65846600	-0.10392500	-0.63433800
N	-3.15711100	1.14052700	1.01095200
H	-1.09637500	-0.18358800	3.62591700
O	-0.29862900	0.45462200	3.76258100
Sb	-3.72515900	-0.62726800	4.54822100
F	-3.06176700	1.16850700	4.30283400
F	-4.82685100	-0.32653700	3.04968600
F	-2.27933800	-1.00040400	3.31301900
F	-4.21201300	-2.38887900	4.61863900
F	-2.42829200	-0.76816900	5.86776700
F	-5.01112600	0.04729700	5.68627900
C	0.23546900	0.43096900	5.14418700
H	0.57593900	-0.58906500	5.30836900
H	1.06898600	1.12996100	5.15161600
H	-0.55577300	0.70058100	5.84013200
H	-2.38524900	-0.42017600	-0.93946400
H	-1.58678600	0.98970100	-1.66486300
O	-4.10319700	0.29243600	0.46774700
H	-4.58426700	-0.03176900	1.25963100

Energies:

Sum of electronic and zero-point Energies = -1659.484051

Sum of electronic and thermal Enthalpies = -1659.445825

Sum of electronic and thermal Free Energies = -1659.552988

Electronic energies = -1659.9348263

Single point energies in solution = -1660.61998019

b-TS2

C	-4.12137200	4.60769300	2.94639800
C	-4.15884800	4.21006000	1.54202500
C	-5.20574900	3.20655100	1.39580400
C	-5.04343100	3.78408500	3.64770900
C	-5.73424100	2.92319100	2.68725800
C	-3.45642900	4.91417600	0.42312400
C	-5.66020600	2.58871300	0.11093700
C	-6.88653800	2.02622300	3.00829900
C	-5.32531300	3.79661000	5.11522500
C	-3.35142900	5.75740600	3.52011800
H	-2.47817300	6.00791500	2.91560900
H	-3.99845700	6.64423100	3.55447100
H	-3.01703900	5.55654600	4.54145300
H	-2.45592000	5.24175700	0.71463700
H	-3.36340200	4.28166800	-0.46260100
H	-4.03085700	5.80514300	0.13464800
H	-5.89472100	1.52857100	0.23466700
H	-6.56964900	3.09638000	-0.23656400

H	-4.90710900	2.68143600	-0.67451000
H	-6.74934400	1.51128900	3.95989000
H	-7.80225500	2.62994700	3.07955500
H	-7.04290700	1.27319400	2.23346400
H	-6.26614800	4.33247100	5.30175000
H	-5.44374000	2.78164200	5.50379600
H	-4.53726200	4.30189100	5.67835200
Rh	-3.50956700	2.47070400	2.64281700
C	0.33303500	4.50761600	1.89047800
C	0.57109200	3.94053000	0.63292800
C	-0.10179400	2.77952200	0.23953600
C	-1.02959400	2.19045200	1.10310000
C	-1.29107900	2.74074700	2.39853600
C	-0.58943100	3.91451700	2.75307700
H	0.87853800	5.39572200	2.19709100
H	1.28916200	4.39854800	-0.04125300
H	0.08857000	2.35460300	-0.74161300
H	-1.12506100	1.88223800	3.38421200
H	-0.72573400	4.32532500	3.75032000
C	-1.80645600	1.00126800	0.71624100
C	-1.39080400	0.03993500	-0.35400000
H	-0.30210900	-0.02811800	-0.40536600
H	-4.24040300	-0.37546200	1.85329800
N	-2.90802200	0.87095500	1.39046400
Sb	-4.30100300	-0.58678100	4.97056400
F	-3.49657400	1.15966700	4.54324200
F	-2.82539000	-1.30417500	4.09578100
F	-3.35202700	-0.44788300	6.55558700
F	-5.07278400	-2.21090500	5.31575200
F	-5.71286400	0.41391700	5.65360200
F	-5.11816800	-0.44043900	3.25725300
H	-1.80978000	-0.94779500	-0.15524200
H	-1.76621200	0.36766000	-1.33250600
O	-3.71339700	-0.18093200	1.03921600
C	1.80479000	-1.80049200	1.30487400
C	0.93342600	-2.54841300	2.10329000
C	0.30470100	-1.95823300	3.19757600
C	0.52342800	-0.60021400	3.48544300
C	1.38658200	0.15127800	2.67250900
C	2.03172800	-0.45225100	1.59182300
H	2.31458800	-2.27207400	0.46953600
H	0.75319300	-3.59574200	1.88012200
H	-0.37698500	-2.53740500	3.81241500
H	2.72435600	0.12577500	0.98658800
C	-0.11115500	0.01761400	4.67315700
C	-0.03579700	-0.64604600	6.01963700
H	0.42924100	-1.62913400	5.94061200
H	-2.11350400	1.67095000	5.63655600
N	-0.69872900	1.15400800	4.50947600
H	0.55837500	-0.02790100	6.70158000
H	-1.03654900	-0.73367800	6.45093600
O	-1.14166700	1.78883500	5.67769200
H	1.58088800	1.19157300	2.91537900

Energies:

Sum of electronic and zero-point Energies = -1983.841720

Sum of electronic and thermal Enthalpies = -1983.797098

Sum of electronic and thermal Free Energies = -1983.918144

Electronic energies = -1984.3892349

Single point energies in solution = -1984.92520487

2b(B = 1b)

C	-4.51003900	4.92458600	2.66311000
C	-4.89715900	4.40616800	1.35753100
C	-5.96611700	3.40981700	1.56908200
C	-5.13047100	4.09619400	3.63156300
C	-6.08054800	3.19379800	2.94371000
C	-4.56886200	5.03426300	0.03687600
C	-6.73618400	2.75900400	0.46140400
C	-6.98707000	2.23942300	3.65828700
C	-5.02125600	4.19836900	5.12226900
C	-3.67586500	6.14527600	2.90233500
H	-2.85334200	6.22889200	2.18774400
H	-4.30396700	7.03966500	2.79396300
H	-3.25531400	6.16410900	3.91091600
H	-3.57198300	5.48293500	0.04022500
H	-4.61370100	4.30399500	-0.77572400
H	-5.29289000	5.82877000	-0.19159900
H	-7.36662200	1.94662800	0.82980500
H	-7.38795100	3.49478600	-0.02708400
H	-6.06925500	2.34780000	-0.30215400
H	-6.42930600	1.53807800	4.28579400
H	-7.67692200	2.78907600	4.31148000
H	-7.58421800	1.65161100	2.95849600
H	-5.90259900	4.70947000	5.53262600
H	-4.97572300	3.20736200	5.58426500
H	-4.13771700	4.76313400	5.43036400
Rh	-3.81808700	2.83371300	2.30707300
C	0.34477700	4.17856900	2.75376700
C	0.96861100	3.50235800	1.70359100

C	0.21942000	2.64771400	0.89164700
C	-1.15434400	2.48257300	1.13024700
C	-1.80689800	3.19132700	2.17492300
C	-1.03048400	4.02292000	2.98428700
H	0.92464700	4.83927400	3.39291800
H	2.02820900	3.64423800	1.51242400
H	0.70055500	2.12478900	0.06945500
H	-0.53667800	0.77139900	3.35028000
H	-1.48468700	4.56765100	3.80662600
C	-1.99577600	1.56521400	0.35136300
C	-1.49577100	0.73344000	-0.78844200
H	-0.56689400	0.22631800	-0.50812300
H	-4.62705000	0.31457000	0.81386200
N	-3.22078400	1.53826500	0.77527800
Sb	-3.87004800	-0.66244400	3.87799000
F	-3.39701900	1.24246400	4.06655400
F	-2.43649900	-0.65758500	2.67545100
F	-2.64991800	-0.93759100	5.25911800
F	-4.23686400	-2.44116200	3.63081500
F	-5.23408400	-0.32159100	5.07693600
F	-5.02053100	-0.14075500	2.47096000
H	-2.23740200	-0.00875100	-1.08082600
H	-1.27511600	1.37028400	-1.65412500
O	-4.10541500	0.72537000	0.08816600
C	2.45674000	-2.78479700	2.02544200
C	1.95509600	-3.34372000	3.20395600
C	1.28825200	-2.54444300	4.12739300
C	1.09277000	-1.17511500	3.86252600
C	1.60350800	-0.61757700	2.67202400
C	2.28642700	-1.42148100	1.76520400
H	2.99073900	-3.40885900	1.31518000
H	2.08653900	-4.40203900	3.40539500
H	0.88888300	-2.98984900	5.03249900
H	2.70145400	-0.98394600	0.86242900
C	0.34608200	-0.35512500	4.81667600
C	0.37147200	-0.56405300	6.29595200
H	1.02807300	-1.38921600	6.56635900
H	-1.94012300	1.48822000	4.91558200
N	-0.38129900	0.61545600	4.34725000
H	0.72332600	0.34644000	6.79269200
H	-0.64869300	-0.75149200	6.64778700
O	-0.98532000	1.51142200	5.18220900
H	1.51500400	0.44906700	2.48297400

Energies:

Sum of electronic and zero-point Energies = -1983.874506

Sum of electronic and thermal Enthalpies = -1983.829611

Sum of electronic and thermal Free Energies = -1983.953083

Electronic energies = -1984.4287337

Single point energies in solution = -1984.95204238

3b

C	-5.88183100	0.64318300	-0.27297500
C	-4.50596200	0.58925900	-0.28286000
C	-3.72467300	1.76694300	-0.15102000
C	-4.39221500	3.02793000	-0.01743500
C	-5.81663500	3.04517500	-0.00649500
C	-6.54205000	1.88328800	-0.13039300
H	-6.45992800	-0.27064400	-0.37557400
H	-4.00790900	-0.36678100	-0.38374200
C	-2.29181600	1.77016800	-0.18507200
C	-3.62803000	4.21879900	0.09335200
H	-6.34056400	3.98810500	0.09443000
H	-7.62773100	1.92124700	-0.12216500
C	-1.58131800	2.94665900	-0.10138400
C	-4.16130100	5.60603600	0.25823900
H	-3.82165700	6.23832000	-0.57028400
H	-5.24901500	5.63220900	0.31052000
H	-3.74250600	6.05821000	1.16452000
N	-2.27106000	4.16146100	0.04903800
O	-1.57986000	5.24012800	0.14652300
C	-0.09424300	3.10848400	-0.11711900
H	0.19828000	3.76116700	-0.94630600
H	0.23113500	3.61850000	0.79552100
H	0.41107600	2.15084400	-0.22153000
C	-1.51840100	0.49175700	-0.35648600
O	-0.68971600	0.28960300	-1.21829500
O	-1.83930900	-0.41966200	0.58855500
C	-1.12952200	-1.66938700	0.50041000
H	-0.05468400	-1.50459100	0.60972000
H	-1.51154000	-2.27704300	1.32076100
H	-1.31856100	-2.15291400	-0.46147500

Energies:

Sum of electronic and zero-point Energies = -783.361789

Sum of electronic and thermal Enthalpies = -783.345370

Sum of electronic and thermal Free Energies = -783.404488

Electronic energies = -783.6007537

Single point energies in solution = -783.289343448

b-TS3

C	-3.74084100	4.57760200	3.15270000

C	-3.68620100	4.18488000	1.74667100
C	-4.93044400	3.49598300	1.43667500
C	-4.92429100	4.02095600	3.70773800
C	-5.67923600	3.36404500	2.64097500
C	-2.67575800	4.65945400	0.74740700
C	-5.35485100	3.00842800	0.08642800
C	-7.05183200	2.79078100	2.79335400
C	-5.39117500	4.10411400	5.12589000
C	-2.78463100	5.49841500	3.84595500
H	-1.78556100	5.45792100	3.40870100
H	-3.14700100	6.53118200	3.75298000
H	-2.70492200	5.27623800	4.91332800
H	-1.68703100	4.77936200	1.19663900
H	-2.58182100	3.96514100	-0.09121300
H	-2.98106400	5.63301300	0.34066800
H	-5.84093900	2.03143300	0.14508900
H	-6.07269800	3.71617100	-0.34856400
H	-4.51012100	2.92708600	-0.60115800
H	-7.15349200	2.22280100	3.71968500
H	-7.78356200	3.61074600	2.81465200
H	-7.30996200	2.13154000	1.96278100
H	-4.59305700	4.42235200	5.80049400
H	-6.20782400	4.83460000	5.20305500
H	-5.77708900	3.13957100	5.46798900
Rh	-3.66540900	2.34694500	2.87950800
C	0.65996300	3.27865100	2.90646100
C	0.96798200	2.67947800	1.68201100
C	0.08858300	1.75614100	1.10519300
C	-1.10837400	1.43899600	1.75230600
C	-1.44984200	2.02665200	3.01492500
C	-0.53489500	2.95565400	3.55479500
H	1.35524800	3.98195900	3.35642900
H	1.89654000	2.92463700	1.17487200
H	0.33525100	1.30989500	0.14616200
H	-1.72947100	1.11104500	3.93564900
H	-0.74552800	3.40361100	4.52332900
C	-2.09458600	0.51601700	1.16627000
C	-1.78246400	-0.52220400	0.13166500
H	-0.71684800	-0.75863100	0.11771200
N	-3.29259900	0.68327900	1.63470100
Sb	-5.36849500	-0.44355800	4.82652800
F	-4.18644600	1.09058000	4.63332000
F	-5.98955200	0.01378700	3.06914300
F	-4.08256100	-1.44581600	3.94559700
F	-6.56183500	-1.83172500	4.95972100
F	-4.60377300	-0.69837900	6.49361200
F	-6.57925000	0.81855300	5.47874900
H	-2.35691400	-1.42963200	0.33473200
H	-2.07561400	-0.17515100	-0.86745500
O	-4.26623200	-0.11419000	1.10070500
H	-4.95461900	-0.17609000	1.81370700
C	2.86543400	0.47397300	9.05689900
C	2.81391400	-0.22609800	7.87154600
C	1.64787900	-0.20271100	7.06284000
C	0.52468700	0.57516800	7.50213600
C	0.61133800	1.28146200	8.73557300
C	1.75647300	1.23176500	9.49509200
H	3.76713900	0.44126600	9.66094900
H	3.66599300	-0.81326000	7.55683600
C	1.54216300	-0.90637400	5.81893700
C	-0.63938000	0.63813800	6.69045400
H	-0.22594500	1.87627100	9.07815700
H	1.80966200	1.77738900	10.43197600
C	0.40649000	-0.80220700	5.04407400
C	-1.91767300	1.32899700	7.05283400
H	-1.91351900	1.66353400	8.08854900
H	-2.09586200	2.19455700	6.40504700
H	-2.75926000	0.64829700	6.89488800
N	-0.63370200	0.00348800	5.49938300
O	-1.73196200	0.07649300	4.73783400
C	0.13435800	-1.53123100	3.76175700
H	-0.87557200	-1.94833900	3.78456500
H	0.18937600	-0.84556100	2.90991100
H	0.86759100	-2.31816400	3.59923200
C	2.68041400	-1.73396300	5.27534200
O	3.11321300	-1.61906000	4.14856800
O	3.13627800	-2.62004200	6.17389100
C	4.21341000	-3.47228600	5.72020100
H	5.07718100	-2.87044100	5.42883600
H	4.45040400	-4.11035900	6.57038500
H	3.88440600	-4.06914300	4.86674800

Energies:

Sum of electronic and zero-point Energies = -2327.170755

Sum of electronic and thermal Enthalpies = -2327.119888

Sum of electronic and thermal Free Energies = -2327.255984

Electronic energies = -2327.8028104

Single point energies in solution = -2328.22113465

2b(B = 3b)

C	-4.78040600	3.98047200	1.50404300
C	-4.56967100	2.80756300	0.66967000
C	-5.13164100	1.64288100	1.38217200
C	-5.20543100	3.50865600	2.77239100
C	-5.48644500	2.06022200	2.66492800
C	-4.21550100	2.82196100	-0.78697900
C	-5.24507200	0.27233700	0.78733500
C	-6.06914400	1.24070700	3.77546100
C	-5.51685000	4.32624000	3.98964700
C	-4.62890900	5.40292200	1.05927600
H	-3.75081400	5.54487800	0.42452600
H	-5.51387800	5.69704900	0.47909800
H	-4.55058700	6.09035000	1.90486000
H	-3.55054000	3.65449900	-1.03098000
H	-3.72312300	1.89257600	-1.08628500
H	-5.12369300	2.92785500	-1.39666200
H	-5.54145000	-0.46926300	1.53306900
H	-5.99989500	0.26557200	-0.00966100
H	-4.29649200	-0.05071200	0.34737100
H	-5.51578500	1.36694200	4.71056400
H	-7.10700200	1.54523000	3.96527800
H	-6.07030600	0.17592200	3.53348700
H	-5.03467900	5.30648600	3.95610000
H	-6.59995100	4.48819800	4.07568000
H	-5.18708600	3.81860200	4.90136700
Rh	-3.19615800	2.61782500	2.28858800
C	-0.33916200	5.92706200	2.06827400
C	0.76892500	5.30177000	1.49624500
C	0.71482300	3.94072200	1.19489800
C	-0.45669300	3.21551100	1.45344800
C	-1.60098500	3.85291100	1.99495300
C	-1.51706000	5.20552400	2.31623600
H	-0.29437900	6.98323500	2.32171200
H	1.67428600	5.86663300	1.29577700
H	1.58433600	3.44877600	0.76808400
H	0.24900100	0.83034500	7.12892800
H	-2.36140300	5.71910400	2.76648700
C	-0.56479500	1.76831700	1.25233700
C	0.53302300	0.91650700	0.69521300
H	1.48105700	1.15464300	1.18736900
N	-1.71393400	1.29747900	1.63075500
Sb	-2.18654200	0.66604500	5.33354200
F	-2.44030500	2.35347400	4.49988300
F	-3.11787800	-0.19845600	3.94191900
F	-0.60388400	0.46125900	4.37588700
F	-1.85485300	-0.93410000	6.21670100
F	-1.17533100	1.53688700	6.69363400
F	-3.75434400	0.95096700	6.27286100
H	0.30974100	-0.14134600	0.82762200
H	0.65941300	1.11808100	-0.37578400
O	-1.93325100	-0.06344800	1.45020200
H	-2.41286600	-0.31461900	2.26869100
C	-1.52808500	-4.45377200	10.78505000
C	-0.84262500	-4.44956200	9.59059600
C	-0.39002200	-3.23300400	9.01618800
C	-0.65474700	-2.00795500	9.72031800
C	-1.37525000	-2.04931800	10.94862700
C	-1.80247400	-3.24698300	11.46845800
H	-1.86338600	-5.39664400	11.20644100
H	-0.65619600	-5.38151500	9.07488200
C	0.34369000	-3.17944400	7.78760500
C	-0.17940900	-0.78692300	9.18120200
H	-1.59163600	-1.13340100	11.48343200
H	-2.34897500	-3.26769700	12.40583900
C	0.79208000	-1.97442500	7.28714300
C	-0.35771800	0.57049700	9.79054300
H	-0.81650900	0.51628100	10.77459900
H	0.61119100	1.07163100	9.87706500
H	-0.98682200	1.19347100	9.14479100
N	0.49599400	-0.83914500	8.02029200
O	1.01714700	0.34192000	7.53434900
C	1.53529800	-1.75074000	6.00465700
H	0.94941300	-1.10209400	5.34582800
H	2.48967700	-1.25153200	6.19678600
H	1.73540900	-2.69744700	5.50978700
C	0.69611600	-4.43456600	7.02359200
O	1.82206600	-4.71343800	6.67591400
O	-0.38615800	-5.18361400	6.76588500
C	-0.13871300	-6.39696600	6.01617000
H	0.54646200	-7.04794800	6.56368700
H	-1.11522700	-6.86511700	5.90095800
H	0.29396100	-6.15338600	5.04354200

Energies:

Sum of electronic and zero-point Energies = -2327.211598

Sum of electronic and thermal Enthalpies = -2327.159963

Sum of electronic and thermal Free Energies = -2327.300100

Electronic energies = -2327.8494495

Single point energies in solution = -2328.24747782

1c(R = Me)

C	0.43988000	4.29732900	1.82576800
C	0.69102200	3.60559200	0.63953700
C	-0.09257000	2.50428800	0.29458600
C	-1.13537400	2.08419800	1.13390900
C	-1.37870300	2.78745500	2.32455600
C	-0.59744300	3.88588300	2.66851700
H	1.05085000	5.15532400	2.09375600
H	1.49640100	3.92334400	-0.01701800
H	0.11341500	1.97580200	-0.63125000
H	-0.79354500	4.42362700	3.59221700
C	-2.01068700	0.90829100	0.81609200
O	-2.90733800	0.57587500	1.57653200
C	-1.76478800	0.13459300	-0.46943100
H	-1.87116500	0.78301200	-1.34737100
H	-0.75060300	-0.28186200	-0.49205700
H	-2.49008400	-0.67838700	-0.53135300
H	-2.18876300	2.44923600	2.96247400

Energies:

Sum of electronic and zero-point Energies = -384.757542

Sum of electronic and thermal Enthalpies = -384.748800

Sum of electronic and thermal Free Energies = -384.790227

Electronic energies = -384.8959884

Single point energies in solution = -384.717705773

4c

C	-5.33953300	4.75085400	2.85471400
C	-5.27222500	4.32952800	1.47525700
C	-6.01862500	3.09947400	1.34970300
C	-6.20509300	3.81571800	3.57087100
C	-6.61571200	2.80064000	2.64990200
C	-4.53602300	5.03916900	0.38547900
C	-6.24143000	2.31700200	0.09564300
C	-7.48428700	1.62967500	2.97727500
C	-6.57684700	3.88271000	5.01613800
C	-4.72456700	5.98348700	3.43445800
H	-3.86664900	6.32241600	2.84970300
H	-5.46730600	6.79297300	3.44085800
H	-4.39868000	5.82516200	4.46573300
H	-3.58790900	5.45025200	0.74159800
H	-4.32936900	4.38429100	-0.46332800
H	-5.14814700	5.87551900	0.02252500
H	-6.31006200	1.24480600	0.29661400
H	-7.18845600	2.62862800	-0.36566800
H	-5.44591800	2.48064900	-0.63470700
H	-7.20915500	1.19689800	3.94228200
H	-8.53166900	1.95521600	3.03259000
H	-7.41445000	0.84819000	2.21815300
H	-5.93862800	4.57551900	5.56767500
H	-7.61439100	4.23097500	5.10846400
H	-6.50533500	2.89899300	5.48754100
Rh	-4.44172400	2.79426900	2.78870100
C	2.52477000	3.48315800	1.80583100
C	2.23395700	2.22474000	1.27143300
C	0.91955400	1.76983000	1.23877200
C	-0.12245900	2.57455600	1.74232500
C	0.18560100	3.84046100	2.28293500
C	1.49913300	4.28969500	2.31298400
H	3.55196300	3.83518700	1.83082800
H	3.03168200	1.59944400	0.88322500
H	0.71044200	0.78864100	0.82694500
H	-0.61573100	4.45212700	2.68179400
H	1.73075200	5.26330900	2.73376700
C	-1.51843800	2.11730800	1.72378100
Sb	-3.63818700	0.46785800	5.02136000
F	-3.50519100	2.40242600	4.77134100
F	-4.26842700	0.61469500	3.16169700
F	-1.94191000	0.38363400	4.28226300
F	-3.89899000	-1.34532000	4.96464900
F	-3.05422100	0.62204600	6.74987800
F	-5.41893000	0.81900300	5.45814500
O	-2.40510500	2.90288800	2.13947500
C	-1.86771000	0.75147200	1.20068100
H	-1.46101200	0.60913000	0.19440200
H	-1.43109500	-0.01086000	1.85424500
H	-2.94693800	0.60807600	1.18574000

Energies:

Sum of electronic and zero-point Energies = -1488.538509

Sum of electronic and thermal Enthalpies = -1488.504774

Sum of electronic and thermal Free Energies = -1488.604428

Electronic energies = -1488.9177159

Single point energies in solution = -1489.63143943

c-TS1

C	-3.88453700	4.40414000	3.30920000
C	-4.09328700	4.24573300	1.87605300
C	-5.15961000	3.27147400	1.69619400
C	-4.74955600	3.47805400	3.97551700
C	-5.56720600	2.79982500	2.98052000
C	-3.50635700	5.10467100	0.79862100
C	-5.72815800	2.82137000	0.38856800

C	-6.69554100	1.86659200	3.27674700
C	-4.84391500	3.24166400	5.44782800
C	-3.01588600	5.42164800	3.98347900
H	-2.32106100	5.89029000	3.28423100
H	-3.64513600	6.21645500	4.40468700
H	-2.44193400	4.98430300	4.80567600
H	-2.48957900	5.42219000	1.03884600
H	-3.47980600	4.58631600	-0.16309100
H	-4.12107900	6.00606100	0.67212800
H	-5.97114400	1.75579300	0.40777100
H	-6.65467600	3.37383400	0.18204700
H	-5.04049600	3.00431000	-0.44010900
H	-6.45752200	1.19149600	4.09928900
H	-7.57764700	2.45791300	3.56060500
H	-6.95732600	1.25932800	2.40944400
H	-3.97104400	3.63174500	5.97608300
H	-5.73478200	3.74779000	5.84431700
H	-4.94399500	2.17416700	5.66423900
Rh	-3.36064800	2.37445500	2.64935800
C	0.66513300	4.00968400	1.36504700
C	0.94200400	3.10709600	0.33748000
C	0.17066900	1.94910500	0.20947000
C	-0.88674900	1.70881700	1.09447600
C	-1.18250000	2.60036500	2.17328600
C	-0.37412000	3.74974800	2.26607700
H	1.26485600	4.90917900	1.47443700
H	1.74981300	3.30160000	-0.36145900
H	0.37290000	1.26025300	-0.60482300
H	-1.14392100	2.21693200	3.53749500
H	-0.51842500	4.43069000	3.10060100
C	-1.84413200	0.61537400	0.85200500
Sb	-3.99973600	-1.06362800	4.19434500
F	-3.05835700	0.65841500	4.08415000
F	-5.00125100	-0.50896100	2.72760300
F	-2.64179100	-1.69134300	3.08509900
F	-4.86039000	-2.67915200	4.32633600
F	-2.91210600	-1.37958600	5.68430400
F	-5.18518000	-0.14661900	5.31540200
O	-3.00788800	0.76916400	1.27246400
C	-1.51804400	-0.66382200	0.14266000
H	-2.24372700	-0.84363800	-0.65706300
H	-0.50321300	-0.69923400	-0.25409700
H	-1.64976700	-1.46525400	0.88051100
C	1.91802500	-1.75858300	3.46256300
C	0.97592400	-2.17908100	4.40617200
C	0.14195900	-1.25220500	5.02287500
C	0.22382700	0.11000500	4.66884100
C	1.16703400	0.52405800	3.70504400
C	2.01688500	-0.40663600	3.11723300
H	2.58130700	-2.48430600	3.00065400
H	0.89317500	-3.23031900	4.66311400
H	-0.60780900	-1.58704800	5.72903600
H	2.76405100	-0.07980200	2.40026600
C	-0.60657900	1.11265400	5.33870300
O	-0.95526900	2.18464300	4.76409600
C	-1.04456100	0.93004300	6.75594600
H	-1.85009700	0.18272800	6.75772800
H	-0.23404500	0.55020100	7.38376200
H	-1.43253300	1.86979200	7.15241500
H	1.26411000	1.57727300	3.46390200

Energies:

Sum of electronic and zero-point Energies = -1873.256232

Sum of electronic and thermal Enthalpies = -1873.214084

Sum of electronic and thermal Free Energies = -1873.330403

Electronic energies = -1873.7705026

Single point energies in solution = -1874.32999439

2c(B = 1c)

C	-4.11996800	4.64329000	2.90904400
C	-4.47011200	4.41752000	1.51749200
C	-5.59851500	3.46646200	1.48755400
C	-4.86135300	3.69286500	3.67427900
C	-5.83375800	3.02427500	2.79328400
C	-4.02077900	5.24547800	0.35205100
C	-6.29050800	3.03274000	0.23352400
C	-6.87468800	2.05737800	3.26585700
C	-4.80656400	3.47404100	5.15461800
C	-3.23087700	5.73027000	3.42888500
H	-2.39857600	5.93872400	2.75202800
H	-3.81101600	6.65649800	3.53665900
H	-2.82259700	5.48756300	4.41374500
H	-2.99853700	5.60900000	0.48529200
H	-4.06245900	4.67857600	-0.58196600
H	-4.67638500	6.11984400	0.23735800
H	-6.92859200	2.16362200	0.40348900
H	-6.91582100	3.84614400	-0.15704500
H	-5.56732600	2.77009900	-0.54564700
H	-6.44898800	1.28445300	3.90917800
H	-7.64263200	2.58976700	3.84286900

H	-7.36787100	1.55769100	2.43020800
H	-3.89124500	3.87867300	5.59385000
H	-5.65934000	3.96708600	5.64051700
H	-4.86598100	2.40715600	5.39195000
Rh	-3.56625600	2.62809100	2.22163700
C	0.73521400	3.40772900	2.72875000
C	1.27665600	2.61351800	1.71228500
C	0.42423100	1.87896000	0.89416400
C	-0.96685400	1.95633100	1.08652000
C	-1.53243000	2.77340900	2.10654500
C	-0.65023700	3.48025100	2.92771800
H	1.39842900	3.98602800	3.36815300
H	2.35096100	2.57338800	1.56068600
H	0.83727400	1.25229800	0.10877300
H	-1.83497600	0.74027200	4.82413300
H	-1.02732500	4.10518600	3.73163100
C	-1.93732500	1.20683400	0.29304400
Sb	-3.93760800	-0.94790800	3.51114400
F	-2.97925700	0.79277200	3.63085300
F	-5.00421300	-0.17461800	2.20352700
F	-2.62990100	-1.33229500	2.22581300
F	-4.72111400	-2.60304200	3.44023300
F	-2.70768900	-1.40238400	4.84573800
F	-5.04955800	-0.24197300	4.82693500
O	-3.15265000	1.38515800	0.54128000
C	-1.57311600	0.20536700	-0.76298900
H	-2.42912700	0.03837600	-1.41956200
H	-0.70360100	0.51242800	-1.34995100
H	-1.33871600	-0.74551000	-0.26702200
C	1.89785100	-2.34775800	3.70494200
C	2.39873400	-1.91317000	4.93952400
C	1.70254400	-0.96306800	5.66916300
C	0.48610900	-0.42572800	5.17225600
C	0.00127800	-0.86801100	3.91725000
C	0.70273300	-1.82488600	3.19965800
H	2.44002900	-3.10035300	3.13969400
H	3.32481000	-2.32367300	5.32838200
H	2.09343600	-0.64408500	6.62859800
H	0.30466100	-2.17323400	2.25267000
C	-0.22705800	0.54015100	5.96554800
O	-1.36053400	1.05906700	5.64483600
C	0.28437300	1.05582200	7.27490000
H	0.31779500	0.24072700	8.00794000
H	1.29925200	1.45270900	7.17563400
H	-0.38136900	1.83504000	7.64685800
H	-0.92561300	-0.50191100	3.50534200

Energies:

Sum of electronic and zero-point Energies = -1873.283857

Sum of electronic and thermal Enthalpies = -1873.240855

Sum of electronic and thermal Free Energies = -1873.362280

Electronic energies = -1873.8034072

Single point energies in solution = -1874.34788137

3c(Ar = Ph)

C	-2.31816300	1.75084000	7.00314200
C	-2.00009800	1.39742600	5.70455400
C	-0.73928700	1.69885600	5.13180100
C	0.18863700	2.45451400	5.91352400
C	-0.15549400	2.75113600	7.25203800
C	-1.37992200	2.41505000	7.80513400
H	-3.29379900	1.48761500	7.40392800
H	-2.71980500	0.84250700	5.10558500
H	-1.61275400	2.67754900	8.83242500
C	1.39956500	3.10481500	5.34196200
O	1.53443900	3.30282000	4.13937500
C	2.48126800	3.61224500	6.29516200
H	2.16087900	4.53511800	6.79407400
H	2.72987900	2.88236400	7.07278000
H	3.36922800	3.83915000	5.70199100
H	0.55465000	3.30276300	7.85878900
N	-0.49939700	1.22208600	3.86178900
H	-1.28369300	0.71606900	3.47166700
C	0.79142300	0.75974700	3.34052000
H	1.44506800	0.51423600	4.18912700
H	1.28701800	1.56209300	2.78830700
C	0.60048300	-0.46085800	2.46429500
C	0.77589600	-0.37676700	1.07854500
C	0.23034800	-1.69357600	3.02276600
C	0.59059600	-1.49759700	0.26591000
H	1.06132800	0.57432700	0.63556700
C	0.04323100	-2.81447400	2.21495600
H	0.09492800	-1.77309400	4.09947100
C	0.22339300	-2.71843400	0.83237900
H	0.73264000	-1.41558400	-0.80847100
H	-0.23739500	-3.76413000	2.66309500
H	0.08001400	-3.59198800	0.20195900

Energies:

Sum of electronic and zero-point Energies = -710.334903

Sum of electronic and thermal Enthalpies = -710.318930

Sum of electronic and thermal Free Energies = -710.379464

Electronic energies = -710.6000068

Single point energies in solution = -710.261027373

c-TS2

C	-4.03885400	4.60688400	3.11392500
C	-4.41603400	4.49856100	1.71220700
C	-5.55880300	3.59547000	1.63655300
C	-4.86731200	3.70467800	3.85297500
C	-5.84119500	3.11390500	2.94755900
C	-3.90100400	5.34766600	0.59064400
C	-6.30237100	3.21754600	0.39533900
C	-6.98139200	2.24505300	3.36794300
C	-4.83704200	3.44784000	5.32515300
C	-3.06024100	5.57431200	3.70513700
H	-2.36444700	5.96159000	2.95919200
H	-3.60902300	6.43010600	4.12065800
H	-2.48421900	5.12728600	4.52022500
H	-2.85352200	5.62058700	0.73586800
H	-3.98508600	4.83720200	-0.37217100
H	-4.48709700	6.27433000	0.52669800
H	-6.60305000	2.16699300	0.42070200
H	-7.21109000	3.82827600	0.31007800
H	-5.70510800	3.38364000	-0.50404700
H	-6.66728100	1.48796100	4.08787600
H	-7.74732100	2.87390400	3.84352700
H	-7.43742200	1.73297400	2.52047300
H	-3.89498900	3.76061400	5.77968200
H	-5.64963300	4.00790900	5.80839000
H	-4.99416400	2.38645400	5.53757800
Rh	-3.71243800	2.56875800	2.32517400
C	0.16487100	4.17620600	0.83535700
C	0.25652200	3.43036500	-0.33848000
C	-0.55956600	2.30601300	-0.51257800
C	-1.47059000	1.94613200	0.48120100
C	-1.55467400	2.65575100	1.73055000
C	-0.71874500	3.78556300	1.84734200
H	0.79992500	5.04527600	0.97979500
H	0.95363600	3.71905300	-1.11951900
H	-0.50878200	1.74407100	-1.44030200
H	-1.28951100	1.96325400	2.86233000
H	-0.69841100	4.32861900	2.78335100
C	-2.51145000	0.93982600	0.20055200
Sb	-4.46308100	-0.98662700	3.56686200
F	-3.35884600	0.64430200	3.39708300
F	-5.67903400	-0.17277800	2.41792700
F	-3.51267700	-1.63729800	2.11078700
F	-5.47143400	-2.49678500	3.82898700
F	-3.06769800	-1.52844200	4.69178900
F	-5.21830800	-0.05117000	5.00381800
O	-3.61095700	1.08188500	0.77040800
C	-2.33250500	-0.19386800	-0.76145200
H	-2.33709300	0.18377800	-1.79239800
H	-1.37421400	-0.69500500	-0.59145900
H	-3.15232400	-0.90230200	-0.63572500
C	-2.07478000	1.60183300	7.37744100
C	-1.89657000	1.20312100	6.05413600
C	-0.83300300	1.68983100	5.27952400
C	0.08721800	2.60218800	5.86680800
C	-0.10919300	2.96382200	7.21416800
C	-1.17732900	2.48960300	7.96715400
H	-2.90437900	1.19253700	7.94624800
H	-2.57869200	0.47802000	5.63040800
H	-1.29587800	2.79751700	9.00121700
C	1.22166800	3.25786400	5.14095600
O	1.20696700	3.39387700	3.92291600
C	2.40177700	3.78974500	5.93791200
H	2.13879400	4.72509900	6.44753100
H	2.74043600	3.08144000	6.70046100
H	3.21360700	4.00327800	5.24036900
H	0.59107500	3.64864600	7.67860400
N	-0.73184000	1.15173200	3.93483500
H	-1.44496900	0.42520400	3.86298300
C	0.59013400	0.55764000	3.52854700
H	1.05992300	0.16260400	4.43873500
H	1.21738000	1.36328100	3.15320000
C	0.46222300	-0.53694100	2.49082000
C	1.27141500	-0.48841100	1.34690500
C	-0.37983100	-1.64233000	2.67942400
C	1.25117500	-1.52823900	0.41488900
H	1.93387500	0.36045500	1.19475600
C	-0.41709000	-2.67154600	1.73724900
H	-1.01555700	-1.71833200	3.55706000
C	0.40427200	-2.62309300	0.60854100
H	1.89998500	-1.48618900	-0.45580900
H	-1.08618400	-3.51196300	1.89279200
H	0.38847600	-3.43546700	-0.11263200

Energies:

Sum of electronic and zero-point Energies = -2198.839971

Sum of electronic and thermal Enthalpies = -2198.790723

Sum of electronic and thermal Free Energies = -2198.923199

Electronic energies = -2199.4827995

Single point energies in solution = -2199.88582829

2c(B = 3c)

C	-4.30084900	4.97627600	2.32030800
C	-5.12866800	4.49003900	1.23233500
C	-6.17535500	3.62413000	1.80994700
C	-4.68363700	4.24361200	3.48367900
C	-5.90196100	3.47038900	3.17113900
C	-5.13705000	5.01495700	-0.17071000
C	-7.26600200	2.98321600	1.00899100
C	-6.65281500	2.65753600	4.17945200
C	-4.11508300	4.38100300	4.86344600
C	-3.29976000	6.08669300	2.23380600
H	-2.75844100	6.08025500	1.28455500
H	-3.81935300	7.05086700	2.31532800
H	-2.56811700	6.04285000	3.04464300
H	-4.14432500	5.35003600	-0.48226400
H	-5.47982700	4.25501500	-0.87819700
H	-5.82104500	5.87142100	-0.24829600
H	-7.79084300	2.21722700	1.58256100
H	-7.99810400	3.73422500	0.68520400
H	-6.86310700	2.50451400	0.11019100
H	-6.00557700	1.93272100	4.68104400
H	-7.07850600	3.31595800	4.94803900
H	-7.47021400	2.10101000	3.71872900
H	-3.08827400	4.75626000	4.84355000
H	-4.71624700	5.08365500	5.45642400
H	-4.11935600	3.42101700	5.38776000
Rh	-3.98621900	2.83476300	1.92771200
C	0.31959100	3.39318000	1.29414500
C	0.55374700	2.50989100	0.23492200
C	-0.50721400	1.78606700	-0.29998700
C	-1.80171000	1.95861500	0.22000400
C	-2.05674400	2.86336400	1.28662500
C	-0.97062400	3.56413400	1.81652700
H	1.14876400	3.94869900	1.72404800
H	1.55635400	2.38373100	-0.16062900
H	-0.32900100	1.08205700	-1.10749500
H	0.09766800	1.50800900	3.80728200
H	-1.11164200	4.25774400	2.64096400
C	-2.96954500	1.22069700	-0.25276100
Sb	-4.22996800	-0.65176900	3.34149000
F	-3.20677100	1.02667000	3.22049600
F	-5.64989500	0.23537800	2.53928400
F	-3.46845400	-1.07649100	1.69851700
F	-5.11437600	-2.25005400	3.52152500
F	-2.65246700	-1.28407500	4.16396500
F	-4.74868100	-0.00435100	5.01705900
O	-4.07345900	1.46943300	0.28662000
C	-2.91188600	0.17130200	-1.32190600
H	-2.40062600	0.54255800	-2.21645900
H	-2.34813700	-0.69043600	-0.94511500
H	-3.92194000	-0.15267900	-1.57650900
C	-2.09875200	1.33352700	7.64353800
C	-1.87786100	0.91192300	6.32909400
C	-0.73360000	1.33210000	5.66353900
C	0.21572800	2.18491100	6.27316300
C	-0.03531500	2.58169900	7.59784100
C	-1.17525400	2.16106100	8.28045000
H	-2.99433500	1.00479600	8.16140900
H	-2.59744000	0.27582700	5.82992500
H	-1.34079800	2.48254200	9.30381900
C	1.41592800	2.69909600	5.54106700
O	1.56183900	2.47770700	4.33679200
C	2.45546000	3.50896400	6.28272600
H	2.03396400	4.45514800	6.64260500
H	2.83712500	2.96627700	7.15463400
H	3.27754200	3.72531700	5.59913000
H	0.66789000	3.23555600	8.10090300
N	-0.50045000	0.81937400	4.30003400
H	-1.40275100	0.72055000	3.80646900
C	0.25319300	-0.52403000	4.27004300
H	-0.42946200	-1.24793600	4.71195700
H	1.11362900	-0.38113300	4.92578200
C	0.67464500	-0.89592200	2.87354100
C	1.94727100	-0.53222000	2.40896300
C	-0.18102200	-1.63206700	2.04079700
C	2.36608900	-0.91013500	1.13351300
H	2.61393900	0.03926500	3.05026500
C	0.24276800	-2.01036000	0.76579000
H	-1.17094900	-1.90620200	2.38744400
C	1.51556700	-1.65480900	0.31244800
H	3.35949300	-0.63878100	0.78805200
H	-0.41606000	-2.60201500	0.13626400
H	1.84904500	-1.96640800	-0.67357300

Energies:

Sum of electronic and zero-point Energies = -2198.903185

Sum of electronic and thermal Enthalpies = -2198.853193

Sum of electronic and thermal Free Energies = -2198.988974

Electronic energies = -2199.5519613

Single point energies in solution = -2199.93658487

1d'

C	-1.37867700	2.16562800	1.09602100
C	-1.52887500	2.86702200	2.23449800
C	-2.42634000	1.17914300	0.70561700
O	-3.46204700	1.05707200	1.36331000
N	-2.19471300	0.41367000	-0.42044500
C	-3.26234500	-0.45002900	-0.90457500
H	-3.61906000	-0.11778200	-1.88965600
H	-2.90687600	-1.48428300	-0.99718600
H	-4.08319100	-0.40924800	-0.19051300
C	-1.00621400	0.49351600	-1.25692400
H	-0.89072000	-0.45660800	-1.78762500
H	-1.06898500	1.29369100	-2.00956300
H	-0.10412400	0.64021800	-0.65986400
H	-0.52293100	2.32914600	0.45126800
C	-0.63600600	3.88783200	2.78688800
C	0.56339000	4.28984000	2.16708200
C	-0.99064300	4.50301300	4.00147600
C	1.37051000	5.26627000	2.74105300
H	0.86637300	3.83406000	1.22889100
C	-0.18272700	5.48146500	4.57776900
H	-1.91345100	4.20413200	4.49266000
C	1.00173800	5.86709500	3.94927500
H	2.29193700	5.56220100	2.24650500
H	-0.47824600	5.94216500	5.51650900
H	1.63479600	6.62954600	4.39497200
H	-2.42541700	2.65025400	2.81296100

Energies:

Sum of electronic and zero-point Energies = -556.752330

Sum of electronic and thermal Enthalpies = -556.738434

Sum of electronic and thermal Free Energies = -556.793606

Electronic energies = -556.9703146

Single point energies in solution = -556.710742497

4d

C	-5.25804300	4.78239800	2.32796600
C	-5.72179100	4.22077300	1.07915100
C	-6.59579700	3.11663600	1.39263300
C	-5.92132200	4.07197400	3.41877000
C	-6.74194200	3.05227800	2.84719900
C	-5.35063200	4.67376900	-0.29572800
C	-7.31041400	2.25145300	0.40556100
C	-7.58320100	2.07834900	3.60568200
C	-5.75885100	4.35139800	4.87829100
C	-4.34526400	5.95478100	2.48968400
H	-3.70271600	6.09284000	1.61746700
H	-4.94214700	6.86859400	2.61468100
H	-3.70943100	5.85130100	3.37259800
H	-4.43713200	5.27155800	-0.29554400
H	-5.20392000	3.82679400	-0.97067800
H	-6.15910900	5.29479700	-0.70366500
H	-7.44123100	1.23359800	0.78151700
H	-8.30920400	2.66560200	0.21084700
H	-6.77752900	2.20073400	-0.54666000
H	-7.06177900	1.72158300	4.49664900
H	-8.51351300	2.56857900	3.92294900
H	-7.85132800	1.21345200	2.99547600
H	-4.84994900	4.92169300	5.08103700
H	-6.61351100	4.94152700	5.23520900
H	-5.71627700	3.42488800	5.45505100
Rh	-4.66053500	2.71873500	2.24061100
C	-1.16007300	2.84939800	1.38612900
C	-0.26824300	2.63104600	2.37743000
H	-0.20344700	1.62341100	2.78363200
C	-2.07005600	1.81606200	0.86997000
Sb	-3.47407300	0.49147000	4.44093700
F	-3.13285600	2.31366300	3.82269200
F	-4.59952900	0.51666600	2.85203300
F	-2.08265300	-0.01779900	3.31888300
F	-3.97644300	-1.23470900	4.80066600
F	-2.35776900	0.76205700	5.87229000
F	-4.94897800	1.22177800	5.32081400
O	-3.32111400	2.09133400	0.74456300
N	-1.64096800	0.61399700	0.48219000
C	-2.60131000	-0.45592600	0.19005500
H	-2.75801500	-0.54427700	-0.89087200
H	-2.19243600	-1.39493600	0.57134100
H	-3.54574900	-0.24658300	0.68531900
C	-0.23431000	0.24599800	0.30046200
H	0.09408100	-0.40556100	1.11723000
H	-0.13877700	-0.29860200	-0.64401000
H	0.39289200	1.13457000	0.26670100
H	-1.36737800	3.85037100	1.01690900
C	0.59087400	3.61678900	3.02846200
C	0.79022000	4.91712700	2.52247500
C	1.25886500	3.24416800	4.21047600

C	1.62188500	5.81293800	3.18490200
H	0.31266100	5.21929400	1.59442000
C	2.08699100	4.14494700	4.87675700
H	1.11610500	2.24301200	4.60954800
C	2.27018300	5.43102100	4.36561600
H	1.77602800	6.80856300	2.77903800
H	2.59134800	3.84244400	5.78951700
H	2.92121400	6.13303200	4.87838400

Energies:

Sum of electronic and zero-point Energies = -1660.542652

Sum of electronic and thermal Enthalpies = -1660.504380

Sum of electronic and thermal Free Energies = -1660.613483

Electronic energies = -1661.0024556

Single point energies in solution = -1661.63217552

d-TS1

C	-4.58723300	4.66690300	2.20629200
C	-4.24766700	4.19140100	0.87303700
C	-5.16750100	3.12276500	0.53629100
C	-5.67204700	3.86674100	2.68515400
C	-6.04016500	2.90904400	1.65460600
C	-3.28561900	4.84677700	-0.06528900
C	-5.21256200	2.36771400	-0.75318500
C	-7.19240700	1.95888600	1.71865700
C	-6.34529300	3.96113200	4.01500800
C	-3.98698000	5.85857300	2.88327500
H	-2.91428300	5.93795900	2.69286300
H	-4.46378800	6.77345900	2.50618300
H	-4.13850600	5.82798300	3.96468800
H	-2.44936200	5.30853800	0.46226100
H	-2.88006700	4.14053100	-0.79408600
H	-3.80964000	5.63524600	-0.62326600
H	-5.40927500	1.30608400	-0.58239000
H	-6.02223500	2.76328500	-1.38078000
H	-4.27963600	2.46164700	-1.31327300
H	-7.30901800	1.52977300	2.71461500
H	-8.11735100	2.49599900	1.46533700
H	-7.07367600	1.13554000	1.01235700
H	-5.75780900	4.54285300	4.72864700
H	-7.31740800	4.45882500	3.89516400
H	-6.53110000	2.96775500	4.43233100
Rh	-3.92733900	2.54876100	2.26023600
C	-1.20079600	1.47158500	1.73243100
C	-1.60051400	2.60325200	2.38586300
H	-2.03240700	2.48234400	3.69994200
C	-2.14420200	0.35392200	1.57043000
Sb	-5.23683800	-0.36340600	4.50227800
F	-4.37151500	1.35568300	4.15216100
F	-5.64768100	-0.51190700	2.69082700
F	-3.54417100	-1.09802800	4.21108700
F	-6.02613800	-1.97878800	4.88939900
F	-4.78402000	-0.05811800	6.28585100
F	-6.78956800	0.65548400	4.73628000
O	-3.38680500	0.63000500	1.60205700
N	-1.76028400	-0.90840500	1.34945400
C	-2.77253400	-1.96219500	1.20431700
H	-2.80239300	-2.30766200	0.16412400
H	-2.49952200	-2.80074900	1.85085600
H	-3.74487900	-1.57960900	1.50339600
C	-0.37263600	-1.35205900	1.23335000
H	-0.19734500	-2.17333500	1.93445000
H	-0.18060700	-1.71224000	0.21581700
H	0.32598200	-0.55452300	1.47454600
C	-1.05587600	0.52649400	5.46693500
C	0.12381000	0.70960300	4.83856900
C	-1.93890500	1.66153400	5.77019200
O	-2.07374200	2.65041100	4.95544100
N	-2.59109700	1.69305200	6.93016900
H	-1.39716100	-0.45449300	5.77698700
C	1.11149700	-0.31255700	4.49263400
C	0.93315900	-1.68278100	4.77261300
C	2.29589100	0.09079000	3.84636000
C	1.90500400	-2.61098100	4.41258700
H	0.03436500	-2.02391100	5.27764100
C	3.26827700	-0.84041300	3.48409800
H	2.45294700	1.14614800	3.63562400
C	3.07485200	-2.19415700	3.76560900
H	1.75669100	-3.66229500	4.64190400
H	4.17758200	-0.50963300	2.99084000
H	3.83282700	-2.92195200	3.49106200
H	0.40042900	1.72842400	4.57183400
H	-0.22423400	1.40760400	1.25921100
C	-0.73701800	3.80882400	2.28488300
C	-0.60972800	4.73164100	3.34432400
C	-0.01742900	4.07360600	1.09805800
C	0.21824000	5.84901900	3.22835700
H	-1.14448100	4.55801500	4.27065500
C	0.80292300	5.19350100	0.98192200
H	-0.12699900	3.40727200	0.24683700

C	0.92880900	6.08578100	2.05002400
H	0.30923600	6.53616400	4.06499100
H	1.33876600	5.37398000	0.05418000
H	1.56814700	6.95915800	1.96094300
C	-2.38287700	0.70382100	7.99283100
H	-2.49239400	1.20894200	8.95622200
H	-3.13143600	-0.08927600	7.91277400
H	-1.37710700	0.28781000	7.93806100
C	-3.63951000	2.68046500	7.18908600
H	-4.53208700	2.14946900	7.52908100
H	-3.31128300	3.38442200	7.96156500
H	-3.86148700	3.21732100	6.27063200

Energies:

Sum of electronic and zero-point Energies = -2217.265348

Sum of electronic and thermal Enthalpies = -2217.213542

Sum of electronic and thermal Free Energies = -2217.351854

Electronic energies = -2217.9405134

Single point energies in solution = -2218.33749510

2d

C	-4.31702500	4.35890400	1.85078700
C	-4.45274900	3.54909300	0.65338700
C	-5.52203700	2.56433000	0.89877300
C	-5.11435200	3.73806200	2.85786300
C	-5.91958100	2.67316100	2.23496800
C	-3.88465400	3.86946200	-0.69681900
C	-6.00043000	1.58768500	-0.12940200
C	-6.98486000	1.89317300	2.94059900
C	-5.27291100	4.17510000	4.28175500
C	-3.54783200	5.63838900	1.96805300
H	-2.66373800	5.64604200	1.32542600
H	-4.18783400	6.47769000	1.66411600
H	-3.21790600	5.82567900	2.99232900
H	-2.91055500	4.35966400	-0.61817900
H	-3.76466500	2.96768300	-1.30383100
H	-4.55727200	4.54686900	-1.24082100
H	-6.70647700	0.86951300	0.29179000
H	-6.49693400	2.11226000	-0.95571100
H	-5.15874900	1.02561400	-0.54896500
H	-6.64888700	1.55056900	3.92021900
H	-7.87008700	2.52624600	3.09054900
H	-7.29027100	1.01650500	2.36625500
H	-4.44815900	4.81755400	4.60036800
H	-6.20605500	4.74231100	4.40140700
H	-5.32219000	3.31024100	4.94917500
Rh	-3.56741300	2.29728700	2.12221700
C	-0.84536500	1.78708200	1.34875800
C	-1.55502900	2.65569400	2.11645600
H	-0.09050900	2.61685300	5.85487600
C	-1.61622600	0.72533000	0.70986900
Sb	-3.97845100	-0.23771700	4.89905700
F	-3.03950700	1.26724900	4.13308900
F	-4.86767100	-0.41539100	3.27733000
F	-2.54826800	-1.29186000	4.30593800
F	-4.82781100	-1.67600800	5.67282400
F	-2.98615500	0.11571600	6.45760000
F	-5.24863700	0.99248000	5.50276200
O	-2.85919200	0.64814500	0.98885300
N	-1.06958900	-0.17947900	-0.12435200
C	-1.86032500	-1.31376900	-0.60178500
H	-1.27674100	-2.23354500	-0.48738000
H	-2.77639800	-1.38764900	-0.01904200
H	-2.11063100	-1.18839300	-1.66235800
C	0.29844900	-0.09571800	-0.62944200
H	0.96776100	-0.76833300	-0.08061700
H	0.29919100	-0.38478600	-1.68528900
H	0.67613100	0.92405200	-0.56265000
C	-0.01994000	0.13002900	5.80605500
C	1.05101400	0.33244500	4.99937000
C	-0.31037100	1.02850100	6.90850000
O	-0.10784300	2.33701200	6.79415200
N	-0.74392200	0.61261800	8.07718700
C	-1.26035800	1.53243800	9.09993700
H	-2.28461100	1.23157000	9.33949100
H	-0.64035800	1.46431700	9.99859000
H	-1.25410500	2.55323100	8.72718900
C	-0.88364300	-0.81707500	8.39088100
H	-0.69927000	-0.94894700	9.45922500
H	-1.89595300	-1.14424300	8.14169500
H	-0.15170500	-1.40033000	7.83314700
H	-0.68954400	-0.70980900	5.67378300
C	1.48793400	-0.52973100	3.90933200
C	0.67854600	-1.55786600	3.38006800
C	2.79250500	-0.35848000	3.40429600
C	1.18578900	-2.40751800	2.40248400
H	-0.34584800	-1.67839200	3.71801900
C	3.29497300	-1.21254700	2.42582100
H	3.41970800	0.43547000	3.80265900
C	2.49515700	-2.24571600	1.93038700

H	0.56200800	-3.20602200	2.01100500
H	4.30821200	-1.08043000	2.05847500
H	2.88952900	-2.92478900	1.17950600
H	1.70870900	1.17543200	5.21449700
H	0.24061900	1.79948700	1.30688300
C	-0.87819000	3.70530500	2.89537000
C	-1.25236800	3.96578600	4.23187700
C	0.15925500	4.47410300	2.33461300
C	-0.59341700	4.94662600	4.97846400
H	-2.07025500	3.39644700	4.66442100
C	0.80639500	5.46160900	3.08010400
H	0.44255400	4.30636600	1.29934500
C	0.43859000	5.69880600	4.40525500
H	-0.89776900	5.13766500	6.00458900
H	1.59630600	6.04995000	2.62147300
H	0.93775800	6.47103100	4.98304100

Energies:

Sum of electronic and zero-point Energies = -2217.296189

Sum of electronic and thermal Enthalpies = -2217.243290

Sum of electronic and thermal Free Energies = -2217.386314

Electronic energies = -2217.976198

Single point energies in solution = -2218.36244988