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Supporting Information

Mechanism of B-H Redistribution during Reduction of Polyborazylene by Hydrazine

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Contents

1. Methodology adapted for determination of Free Energy barrier in Solution Phase:

We have optimized each intermediates and transition states using M052x functional using 6-31++G(d,p) basis set for all the atoms. Frequency analysis of each intermediate and transition states has been done at the same level of theory. The thermodynamic parameter obtained after optimization and frequency is listed below-

H_{corr} = Enthalpic correction obtained from gas phase harmonic frequency computation.

G_{corr} = Free energy correction obtained from gas phase harmonic frequency computation.

We have included the effect of the solvent in energy by carrying out single point calculation using M052X in CPCM solvent model along with 6-31++G(d,p) on each atom. E_{sol} is denoted as the single point energy obtained in CPCM solvent model. We have determined solution phase free energy of each solute by the approximation mentioned below-

$G^{0.5}_{sol} = E_{sol} + H_{corr} + 0.5\,(G_{corr} - H_{corr})$, where $G^{0.5}_{sol}$ is corrected solution phase free energy.

Using those solution phase corrected free energies we have determined free energy activation barriers and free energy change of each step.

$\Delta G^{\#}_{0.5} = G^{0.5}_{sol}(Ts) - G^{0.5}_{sol}(r)$

$\Delta G_{0.5} = G^{0.5}_{sol}(p) - G^{0.5}_{sol}(r)$

where,

$\Delta G^{\#}_{0.5}$ = free energy activation barrier,

$\Delta G_{0.5}$ = Free energy change of a reaction step,

Ts = transition state of a reaction step,

p=product of a reaction step,

and r = reactant of a reaction step.

The justification of this approximation: Admittedly getting accurate free energy estimates for solution phase reactions is always challenging and at times questionable with quantum chemistry. Several recipes are used and its common to find questions being raised on their accuracy. Our general philosophy is that we always use the empirical correction to the entropy estimates derived from

quantum chemistry based on Wertz's approximation [1]. It must be noted that generally the entropy computation in quantum chemical computations follows from frequency computations which computes entropy through Sakur-Tetrode Equation which essentially uses an ideal gas model, where each particle is considered to behave in a non-interacting ideal way.[2] It has been shown experimentally that the entropic reduction of noble gases is about 50% when they are dissolved in solution phase. This forms the basis for Wertz's approximation that there is reduction of entropy when a species is moved from gas phase to liquid phase.[1] One can easily see that this arises from substantial loss of translational freedom within a liquid. Hence, it has evolved as a general practice that a 50% scaling factor to gas phase entropy of a species is applied to estimate the solvent phase entropy. This reduction shows a marked effect for reaction free energy changes which involve association and also in free energy activation barriers where the transition states are formed through associative pathways.[3]

Reference:

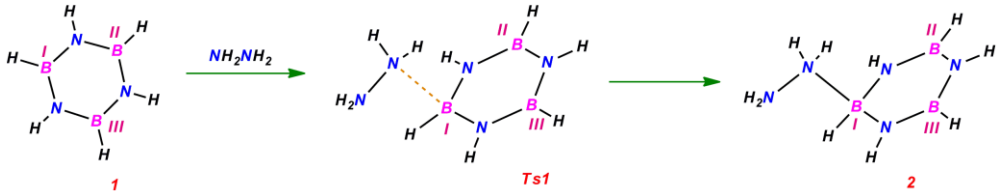
[1] (a)Wertz, D. H. *J. Am. Chem. Soc.* **1980**, *102*, 5316−5322; (b) Spickermann, C. *Entropies of Condensed Phases and Complex Systems*; Springer Theses; Springer: Berlin, **2010**, pp 76−80, and references therein.

[2] http://www.gaussian.com/g_whitepap/thermo.htm.

[3] Plata, R. E.; Singleton, D. A. *J. Am. Chem. Soc.* **2015**, *137*, 3811−3826.

2. Standardization of theoretical methods:

For calibration of our used theoretical approach, we have checked the thermodynamics and kinetics involved with the adduct formation between **Bz** and **Hz**. We have used two different gas phase optimized geometry at the M052X/6-31++G(d,p) and MP2/cc-pVTZ levels of theory for the comparisons.



	$\Delta G^{\#}$(TS1) (kcal/mol)	**ΔG(1 ⟶ 2) (kcal/mol)**
CCSD(t)(CPCM)/aug-cc-pVTZ//MP2/cc-pVTZ	5.5	1.8
MP2(CPCM)/cc-pVQZ//MP2/cc-pVTZ	5.2	0.6
MP2(CPCM)/aug-cc-pVTZ//MP2/cc-pVTZ	5.0	0.4
RI-MP2(CPCM)/aug-cc-pVQZ//MP2/cc-pVTZ	6.2	0.7
DLPNO-CCSD(t)(CPCM)/aug-cc-pVTZ//MP2/cc-pVTZ	6.4	1.8
DLPNO-CCSD(t)(CPCM)/ cc-pVQZ//MP2/cc-pVTZ	6.6	2.1
M052x(CPCM)/6-31++g**//M052x/6-31++g**	2.8	0.3
M052x(CPCM)/aug-cc-pVTZ//M052x/6-31++g**	6.9	5.0
DLPNO-CCSD(t)(CPCM)/aug-cc-pVTZ//M052x/6-31++g**	4.6	0.6

Our theoretical calculation shows that the predicted thermodynamics and kinetics at the DLPNO-CCSD(t)(CPCM)/aug-cc-pVTZ//M052x/6-31++g** level of theory agrees well with the more accurate CCSD(t)(CPCM)/aug-cc-pVTZ//MP2/cc-pVTZ and MP2(CPCM)/cc-pVQZ//MP2/cc-pVTZ level of values.

So we have calculated all the rate determining free energy activation barriers in CCSD(t)(CPCM)/aug-cc-pVTZ//M052x/6-31++g** level of theory.

3. Digestion of polyborazylene framework*:*

We have investigated the formation of a single B-containing unit by opening of a borazine type ring of a anthracene types of polyborazylene framework. We have found that the rate determining free energy activation barrier of the whole process is 22.8 kcal/mol at M052X(SMD)/6-31++G(d,p)//M052x/6-31++G(d,p) level of theory, which is comparable with the overall rate determinination barrier for the borazine digestion process (ΔG= 18.8 kcal/mol). So our results shows that the estimated activation barrier for borazine (**Bz**) digestion agrees well with the polyborazylene (**PBz**) digestion.

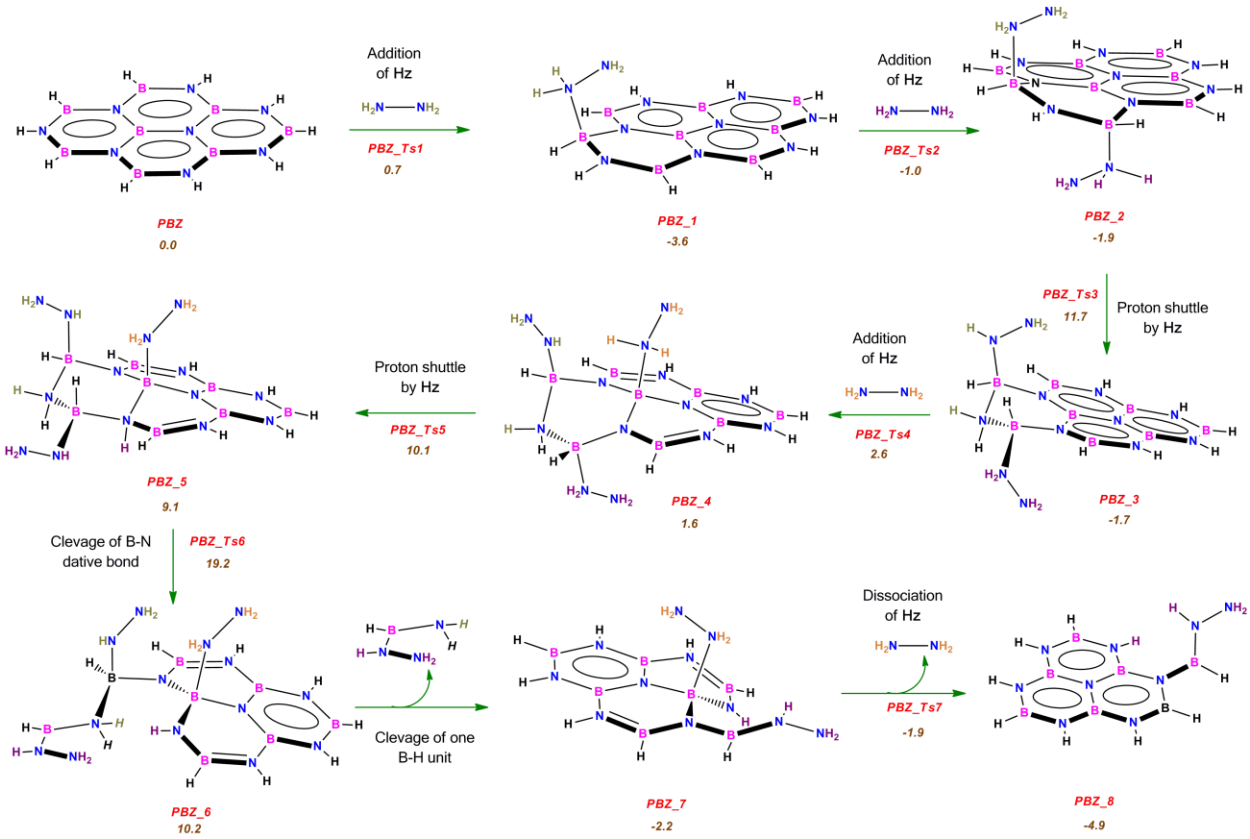


Fig 1. Overall scheme of single B-containing unit formation from Polyborazylene (**PBz**) in presence of hydrazine (**Hz**).

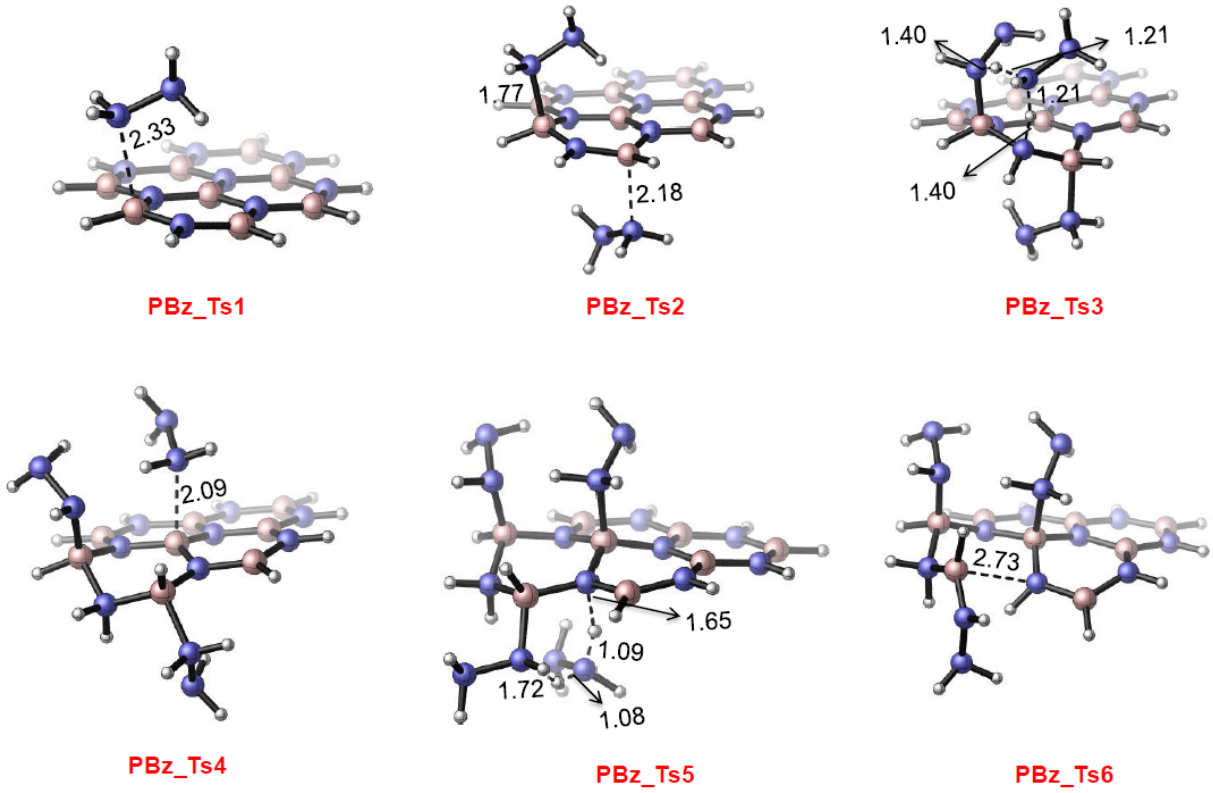
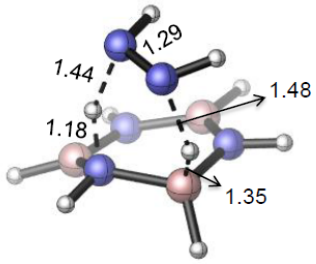


Fig 2. Optimized geometries of the important transition states for formation of a single B-containing unit from Polyborazylene (**PBz**) in presence of hydrazine (**Hz**). Bond distances are shown in Å. H, B and N atoms are shown in white, light pink and blue colors respectively.

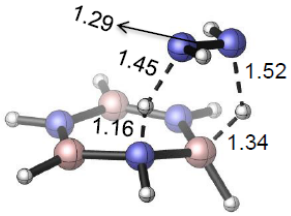
4. Various routes for diimide and diimide type moiety formation from digested B-containing units:

(**I**) Concerted dihydrogen transfer from hydrazine (**Hz**):

(a) hydrogenation of borazine (**Bz**):



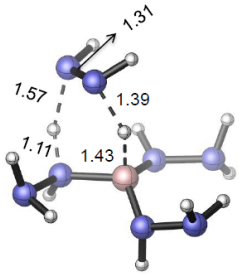
TS_BZ_Hz_cis



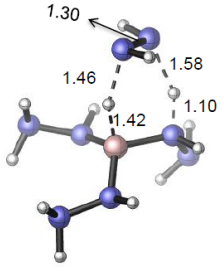
TS_BZ_Hz_trans

	Free energy activation barrier of the transition state ($\Delta G^{\#}$) **(kcal/mol)**
TS_BZ_Hz_cis	75.1
TS_BZ_Hz_trans	71.7

(b) hydrogenation of $B(NHNH_2)_3$ (**12**):



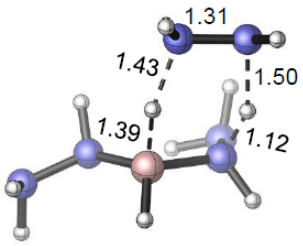
TS_12_Hz_cis



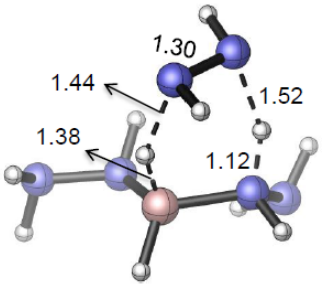
TS_12_Hz_trans

	Free energy activation barrier of the transition state ($\Delta G^{\#}$) (kcal/mol)
TS_12_Hz_cis	70.7
TS_12_Hz_trans	70.0

(c) hydrogenation of $BH(NHNH_2)_2$ (**9**):



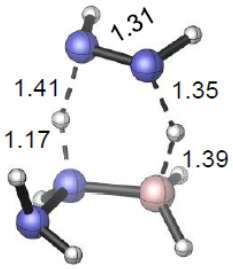
TS_9_Hz_cis



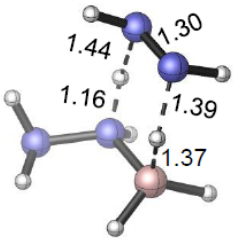
TS_9_Hz_trans

	Free energy activation barrier of the transition state ($\Delta G^{\#}$) **(kcal/mol)**
TS_9_Hz_cis	70.2
TS_9_Hz_trans	63.7

(d) hydrogenation of $BH_2(NHNH_2)_2$ (**13**):



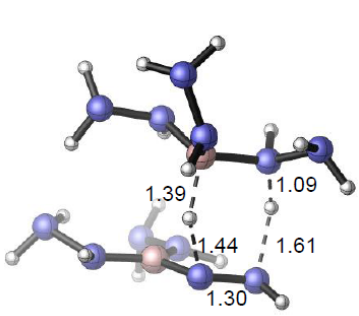
TS_13_Hz_cis



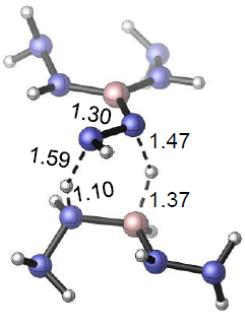
TS_13_Hz_trans

	Free energy activation barrier of the transition state ($\Delta G^{\#}$) **(kcal/mol)**
TS_13_Hz_cis	55.7
TS_13_Hz_trans	51.8

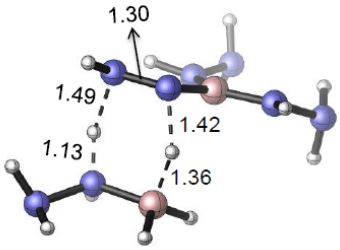
(**II**) Concerted dihydrogen transfer from $B(NHNH_2)_3$ (**12**):



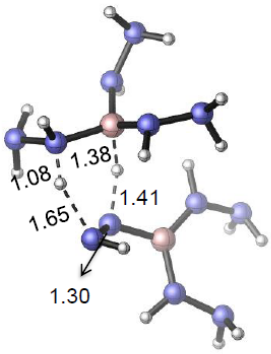
TS_12_12_trans



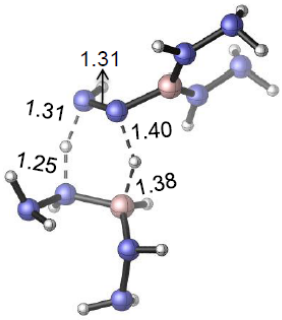
TS_9_12_trans



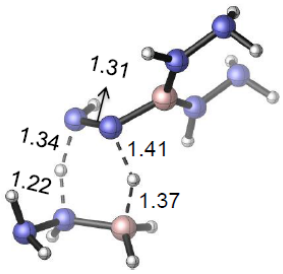
TS_13_12_trans



TS_12_12_cis



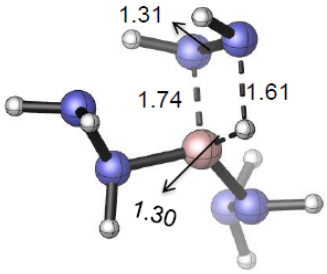
TS_9_12_cis



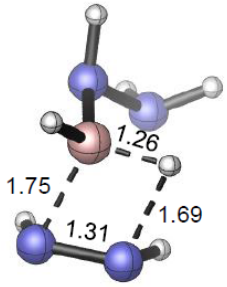
TS_13_12_cis

	Free energy activation barrier of the transition state ($\Delta G^{\#}$) **(kcal/mol)**
TS_12_12_cis	76.8
TS_12_12_trans	75.2
TS_9_12_cis	78.3
TS_9_12_trans	72.6
TS_13_12_cis	64.8
TS_13_12_trans	60.2

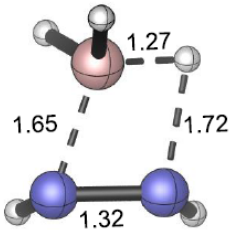
(**III**) Hydride transfer routes:



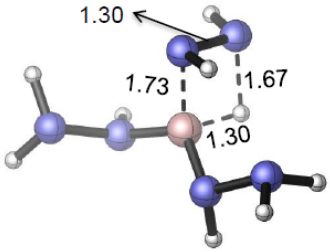
TS_12_Hydride_cis



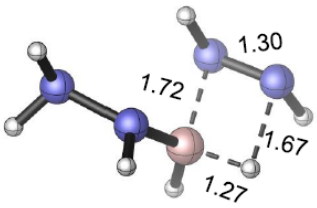
TS_9_Hydride_cis



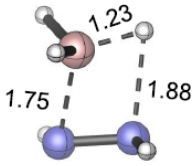
TS_13_Hydride_cis



TS_12_Hydride_trans



TS_9_Hydride_trans



TS_13_Hydride_trans

	Free energy activation barrier of the transition state (ΔG‡) (kcal/mol)
TS_12_hydride_cis	93.4
TS_12_hydride_trans	90.7
TS_9_hydride_cis	88.8
TS_9_hydride_trans	83.1
TS_13_hydride_cis	69.5
TS_13_hydride_trans	67.4

(**IV**) Oligomerization routes:

We know that free N_2 can be formed from the azide, so we have investigated the formation of tri-nitrogen containing species similar to **Hz**, which can be considered as a precursor of azide. We have found two different ways for such type of species formation- (i) intermolecular pathway and (ii) intramolecular pathway. We have found the rate determining barriers for both the routes are very high which cannot be surmountable at room temperature. In case of intermolecular route a intermediate (**Int_oligomer_inter**) is formed before the N-N bond formation from two units of **12**. Formation of **Int_oligomer_inter** is endoergic by 7.6 kcal/mol in terms of free energy activation barrier.

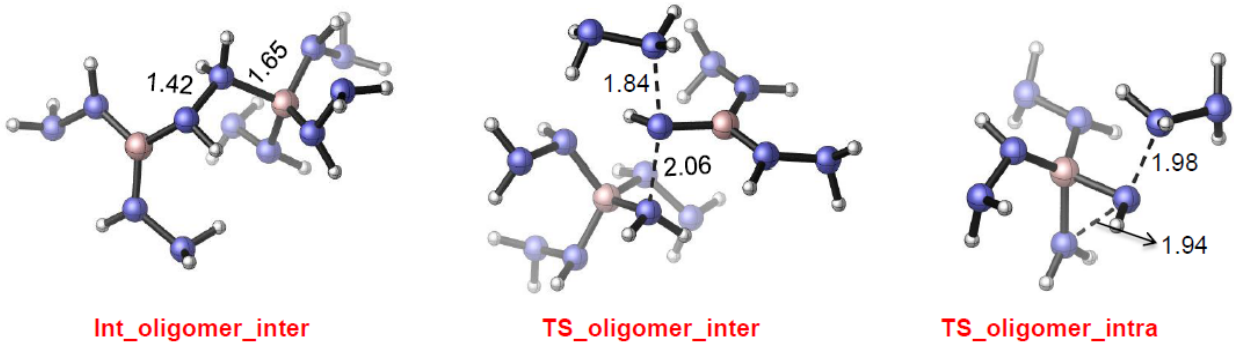


Fig 3. Important intermediate and transition states associated with the N-N bond formation transition state.

	Free energy activation barrier of the transition state ($\Delta G^{\ddagger}$) **(kcal/mol)**
TS_oligomer_inter	58.8
TS_oligomer_intra	50.1

(**V**) Formation of dimer of **12** and the associated pathways of hydride transfer:

(a) Formation of **12_dimer**, dimer of **12**:

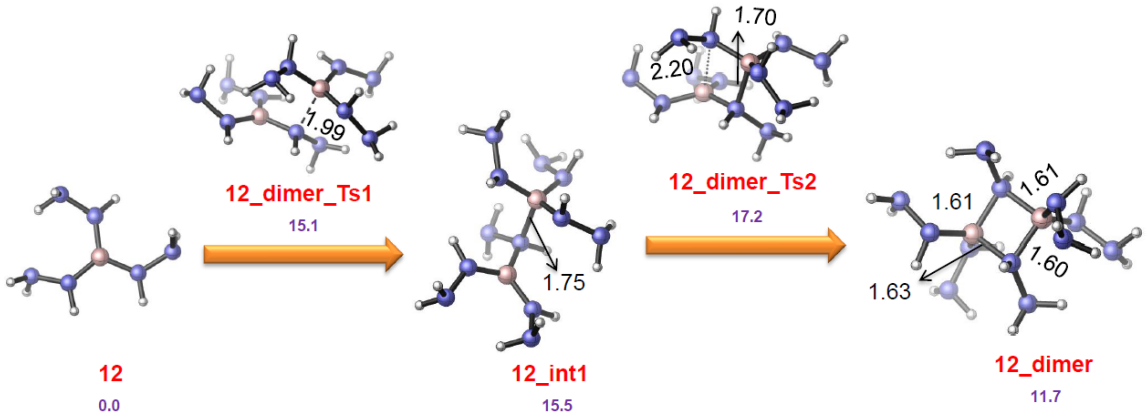


Fig 4. Overall scheme of the pathway corresponding to the dimerization of **12** .

Formation of **12_dimer**, dimer of **12,** occurs via rate determining free energy activation barrier of 17.2 kcal/mol, which is associated to **12_dimer_Ts2**. We have found that formation of **12_dimer** from two unit of **12** is an endoergic process by 11.7 kcal/mol.

(b) Hydride transfer routes from **12_dimer**:

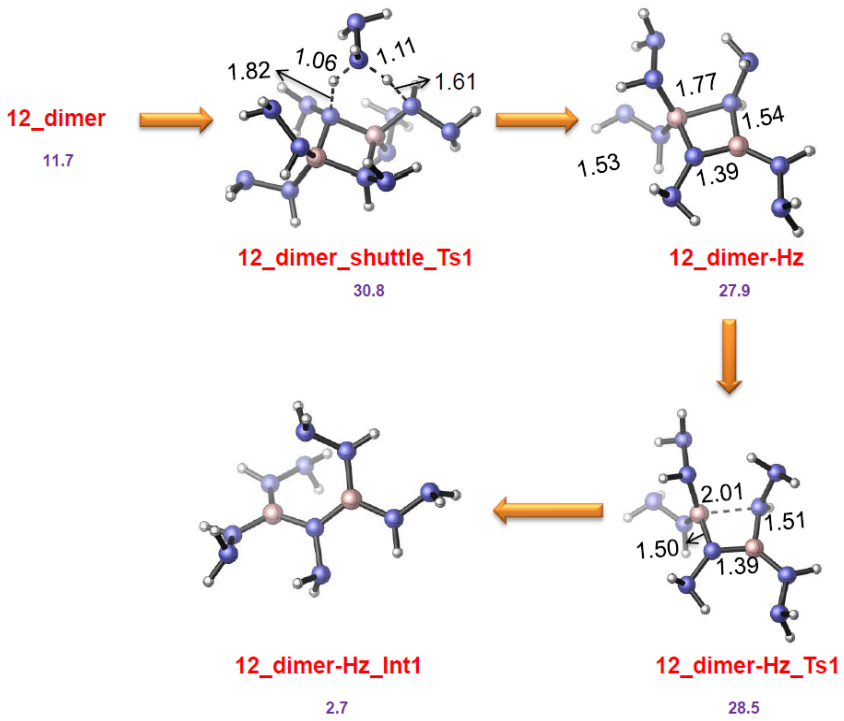


Fig 5. Overall scheme of one B-N bond dissociation of **12_dimer** to form **12_dimer-Hz_Int1**.

Our theoretical calculations shows that **12_dimer** yielded **12_dimer-Hz** via a intra-molecular proton transfer followed by B-N bond cleavage and it is an highly endoergic process. We have found that free energy activation barrier associated with **12_dimer_shuttle_Ts1**, the **Hz** assisted intra-molecular proton transfer transition state, is 30.8 kcal/mol. Later **12_dimer-Hz** converted to **12_dimer-Hz_Int1** via a B-N bond dissociation transition state (**12_dimer-Hz_Ts1**) which has activation barrier of 28.5 kcal/mol. Also, formation of **12_dimer-Hz_Int1** from **12_dimer** is exoergic by 9.0 kcal/mol.

After that, we have investigated the two possible hydride transfer modes (cis and trans) which will convert a N-H proton to B-H hydride and simultaneously a N-N double bond is formed. We have seen that the free energy barrier associated with the hydride transfer process are 95.7 kcal/mol and 102.4 kcal/mol respectively associated with the *trans* and *cis* pathways respectively.

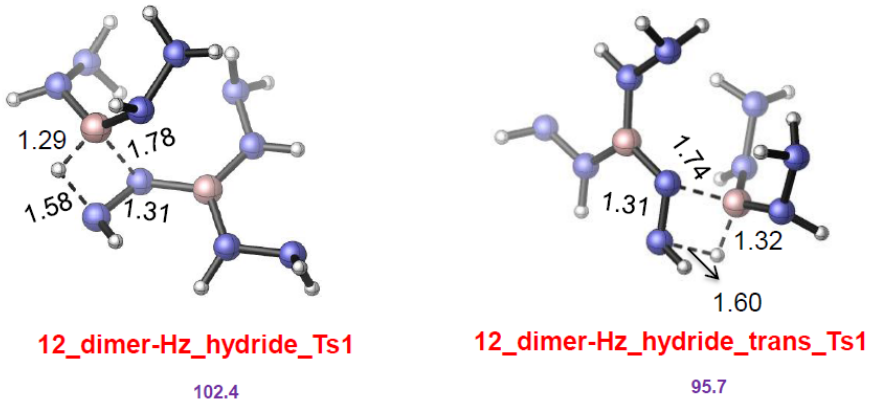


Fig 6. Transition state geometries associated with the hydride transfer process by (i) *cis* pathway (**12_dimer-Hz_hydride_Ts1**) and (ii) *trans* pathway (**12_dimer-Hz_hydride_trans_Ts1**).

After that we have checked the possibility of concerted dihydrogen transfer from **Hz** to 12_dimer-Hz. The dihydrogen transfer process has been checked for both *cis* and *trans* pathway. Also we have considered dihydrogen transfer from two different faces of the B-N bond which are distinct compared to each other. We have found that all the possible concerted dihydrogen transfer process is high barrier process and are not viable in experimental temperature.

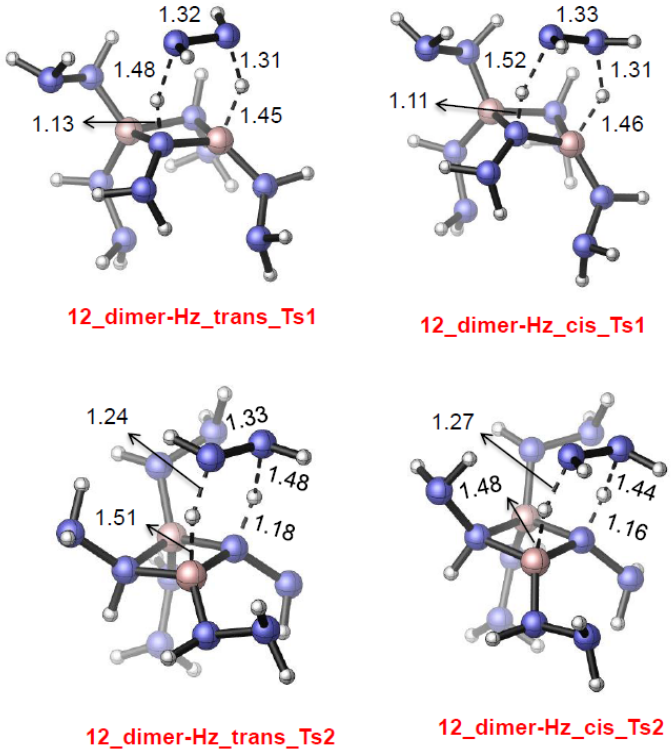


Fig 7. Transition state geometries associated with the concerted dihydrogen transfer process by (i) *cis* pathway (**12_dimer-Hz_cis_Ts1** & **12_dimer-Hz_cis_Ts2**; for two possible faces of B-N bond) and (ii) *trans* pathway (**12_dimer-Hz_ trans_Ts1** & **12_dimer-Hz_ trans_Ts1**; for two possible faces of B-N bond).

	Free energy activation barrier of the transition state ($\Delta G^{\#}$) (kcal/mol)
12_dimer-Hz_cis_Ts1	83.1
12_dimer-Hz_cis_Ts2	82.7
12_dimer-Hz_trans_Ts1	79.9
12_dimer-Hz_trans_Ts2	77.3

5. Cartesian coordinates of optimized geometries of some important transition states and intermediates:

Bz

H	-2.53531200	0.74924400	0.00002100
H	-1.75331400	-1.66500200	0.00003300
H	0.61795800	-2.57018900	0.00017100
H	2.31869400	-0.68603100	0.00004300
H	1.91681700	1.82045200	-0.00010500
H	-0.56534700	2.35092500	0.00004600
B	-1.39010800	0.41134400	0.00000700
B	1.05116400	0.99819700	-0.00002900
B	0.33886000	-1.40937800	0.00004600
N	-0.33011000	1.37289800	0.00004900
N	1.35413400	-0.40058200	-0.00001900
N	-1.02389100	-0.97234700	-0.00007700

Zero-point correction= 0.094896 (Hartree/Particle)
Thermal correction to Energy= 0.100091
Thermal correction to Enthalpy= 0.101035
Thermal correction to Gibbs Free Energy= 0.066769
Sum of electronic and zero-point Energies= -242.558767
Sum of electronic and thermal Energies= -242.553572
Sum of electronic and thermal Enthalpies= -242.552628
Sum of electronic and thermal Free Energies= -242.586894

Hz

N	0.00000000	0.73109500	-0.00016600
H	0.57019100	0.99124100	-0.79814800
H	0.56803700	0.99138200	0.79930700
N	0.00000000	-0.73109500	-0.00016600
H	-0.56803700	-0.99138200	0.79930700
H	-0.57019100	-0.99124100	-0.79814800

Zero-point correction= 0.053982 (Hartree/Particle)
Thermal correction to Energy= 0.056926
Thermal correction to Enthalpy= 0.057870
Thermal correction to Gibbs Free Energy= 0.032145
Sum of electronic and zero-point Energies= -111.791886
Sum of electronic and thermal Energies= -111.788942
Sum of electronic and thermal Enthalpies= -111.787998
Sum of electronic and thermal Free Energies= -111.813723

Ts1

H	2.62069000	-1.94195500	-0.54025800
H	3.04022600	0.50627500	-1.06582900
H	1.71137800	2.53817100	-0.32727500
H	-0.36555200	1.87067400	0.94779800
H	0.48971800	-2.24961800	0.77811500
B	1.88581100	-1.05069500	-0.22477900
B	-0.24482600	-0.25272200	0.88484800
B	1.38852400	1.40774600	-0.10191600
N	0.68732000	-1.30398600	0.49832600
N	0.20564600	1.10766100	0.62561600
N	2.19240600	0.30962400	-0.56237400
H	-1.08114200	-0.46469100	1.72374700
N	-1.80087300	-0.40562900	-0.66348500
H	-2.01288700	-1.36531900	-0.91326100
H	-1.38077000	0.07233600	-1.44943900
N	-2.91325800	0.33150200	-0.19736800
H	-3.77650600	0.06052000	-0.64977500
H	-2.99138700	0.17776100	0.80041000

Zero-point correction= 0.150831 (Hartree/Particle)
Thermal correction to Energy= 0.159531
Thermal correction to Enthalpy= 0.160475
Thermal correction to Gibbs Free Energy= 0.117272
Sum of electronic and zero-point Energies= -354.356240
Sum of electronic and thermal Energies= -354.347541
Sum of electronic and thermal Enthalpies= -354.346597
Sum of electronic and thermal Free Energies= -354.389800

1

H	2.60878500	-1.94699000	-0.39494400
H	3.05163000	0.48715200	-0.95487200

H	1.74660100	2.53273800	-0.22049200
H	-0.40241100	1.90913700	0.91788400
H	0.42218800	-2.23934500	0.79654600
B	1.83761300	-1.05620300	-0.17132800
B	-0.41239800	-0.24319700	0.75531200
B	1.36608300	1.40678100	-0.06318700
N	0.58853200	-1.30906900	0.45107600
N	0.13402000	1.13040000	0.57474600
N	2.16441700	0.29845400	-0.52171100
H	-1.14933100	-0.42990700	1.70681900
N	-1.62605400	-0.41729800	-0.55020000
H	-1.79989800	-1.41068500	-0.68170900
H	-1.16111400	-0.04630600	-1.37306500
N	-2.79202900	0.34557400	-0.28527400
H	-3.59057600	-0.01218700	-0.79223300
H	-2.96456100	0.28306300	0.71162300

Zero-point correction= 0.152227 (Hartree/Particle)
Thermal correction to Energy= 0.160920
Thermal correction to Enthalpy= 0.161865
Thermal correction to Gibbs Free Energy= 0.119156
Sum of electronic and zero-point Energies= -354.356700
Sum of electronic and thermal Energies= -354.348007
Sum of electronic and thermal Enthalpies= -354.347063
Sum of electronic and thermal Free Energies= -354.389771

Ts2

H	-1.79605700	1.63959600	2.14137900
H	-3.45563600	1.24164400	0.27024000
H	-3.25125000	-0.27876600	-1.74639400
H	-1.24111200	-1.74168800	-1.61325600
H	0.22918300	0.24109000	1.87944600
B	-1.61299200	0.90940000	1.20962500
B	-0.27569200	-1.15864800	0.25709200
B	-2.41850100	-0.22290200	-0.88549300
N	-0.32198500	0.24859300	1.02944300
N	-1.28010900	-1.03794600	-0.89261600
N	-2.59370600	0.72700100	0.20974500
H	-0.49995600	-2.06172000	1.06115500
N	1.15368000	-1.32875300	-0.34398000
H	1.31454100	0.19397200	-0.94635800
H	1.18209900	-2.08274100	-1.01951500
N	2.17679500	-1.60196500	0.61991000
H	2.57784400	-0.72040700	0.91676100
H	1.75879500	-2.05177900	1.43141100
N	1.15743100	1.25779200	-0.80082300
H	0.78740300	1.73441400	-1.61878200
H	0.34677800	0.96824600	0.13085200
N	2.33454400	1.82615200	-0.24420500
H	3.06522700	1.89000000	-0.94165900

H	2.13151800	2.75276700	0.10627300

Zero-point correction= 0.202804 (Hartree/Particle)
Thermal correction to Energy= 0.214412
Thermal correction to Enthalpy= 0.215356
Thermal correction to Gibbs Free Energy= 0.164867
Sum of electronic and zero-point Energies= -466.137772
Sum of electronic and thermal Energies= -466.126165
Sum of electronic and thermal Enthalpies= -466.125220
Sum of electronic and thermal Free Energies= -466.175709

Ts2'

H	-1.92197900	2.48616800	-0.00816000
H	-3.16226000	0.41006800	-0.73776700
H	-2.56373600	-2.00620400	-0.39227100
H	-0.30075200	-2.30959500	0.59957600
H	0.30693400	1.89202700	0.99337700
B	-1.47094700	1.37925600	0.00177100
B	0.53621000	-0.33219900	0.66231400
B	-1.80070100	-1.11373200	-0.16069100
N	-0.08270500	1.15660300	0.41832700
N	-0.52382100	-1.35497200	0.36806200
N	-2.22581300	0.25996300	-0.40170500
H	1.13365300	-0.42919500	1.71146800
N	1.56434300	-0.19044000	-0.55873000
H	0.71187700	0.89576400	-0.50005400
H	1.48889500	-0.91441300	-1.26234800
N	2.94128100	0.05637500	-0.28623100
H	3.12899400	1.04733400	-0.36347300
H	3.14255900	-0.23128000	0.66462300

Zero-point correction= 0.146807 (Hartree/Particle)
Thermal correction to Energy= 0.155030
Thermal correction to Enthalpy= 0.155974
Thermal correction to Gibbs Free Energy= 0.114299
Sum of electronic and zero-point Energies= -354.314664
Sum of electronic and thermal Energies= -354.306441
Sum of electronic and thermal Enthalpies= -354.305497
Sum of electronic and thermal Free Energies= -354.347172

2

H	0.96770400	-2.65773500	-0.48151500
H	2.85210100	-1.49407700	0.50615900
H	3.64849600	0.78747500	0.58341000
H	2.18871400	2.45948800	-0.58162800
H	-1.08743300	-1.32262900	-0.75807400
B	0.90924000	-1.50041700	-0.16931000
B	-0.87619100	0.19878000	0.59793500
B	2.56581400	0.51232500	0.15082000
N	-0.36153500	-0.84112800	-0.24235000
N	1.83276700	1.52554700	-0.49565600

N	2.11196000	-0.85406000	0.26308500
H	-0.20262300	0.75335300	1.40932700
N	-2.23435300	0.58276600	0.49622800
H	-2.62998800	1.29118700	1.09294500
H	0.93540800	1.37377600	-0.92332500
N	-3.10807000	-0.04092500	-0.41322600
H	-3.87796400	-0.47980300	0.07502000
H	-3.47410600	0.63013100	-1.07611800

Zero-point correction= 0.150260 (Hartree/Particle)
Thermal correction to Energy= 0.160077
Thermal correction to Enthalpy= 0.161021
Thermal correction to Gibbs Free Energy= 0.115461
Sum of electronic and zero-point Energies= -354.354006
Sum of electronic and thermal Energies= -354.344190
Sum of electronic and thermal Enthalpies= -354.343246
Sum of electronic and thermal Free Energies= -354.388805

Ts3

H	-1.38046300	-2.71050600	-1.21628100
H	-3.27904600	-1.57953000	-0.66296300
H	-4.20286500	0.41444900	0.08730600
H	-2.72180600	2.07734600	1.14767600
H	0.74984700	-1.92946200	-0.64995600
B	-1.27191900	-1.70339000	-0.56791800
B	0.69356400	-0.36435600	0.65252400
B	-3.02410800	0.22371400	0.20549200
N	0.05390100	-1.33836700	-0.21210700
N	-2.26507000	1.25921300	0.78681400
N	-2.51807100	-1.03066300	-0.29265900
N	2.12854200	-0.41205600	0.79682900
H	2.56258900	-0.09520300	1.64923000
H	-1.30275100	1.16405500	1.06208600
N	2.89872100	-1.27976500	-0.00350000
H	3.68422200	-0.79109700	-0.41153200
H	3.24381000	-2.06567100	0.53374000
H	0.12818000	0.19272800	1.54525600
N	0.52557200	1.41105900	-0.77751200
H	0.72106300	0.93294700	-1.65032900
H	-0.40054900	1.81807500	-0.81076600
N	1.48015800	2.39217200	-0.42466300
H	2.23359800	1.90348900	0.04635500
H	1.85021700	2.87738200	-1.23273700

Zero-point correction= 0.207118 (Hartree/Particle)
Thermal correction to Energy= 0.220243
Thermal correction to Enthalpy= 0.221187
Thermal correction to Gibbs Free Energy= 0.167307
Sum of electronic and zero-point Energies= -466.151195
Sum of electronic and thermal Energies= -466.138070
Sum of electronic and thermal Enthalpies= -466.137126
Sum of electronic and thermal Free Energies= -466.191006

3

H	-1.33402400	-2.91270300	-0.35945800
H	-2.79123700	-1.32331900	-1.40584100
H	-3.76570500	0.79714100	-0.79191600
H	-2.70622400	1.90850100	1.19910500
H	0.47094100	-2.11009400	0.89077200
B	-1.18295200	-1.73340000	-0.17392100
B	0.77257800	-0.02450900	0.75281300
B	-2.80422600	0.35228100	-0.23252900
N	-0.03212100	-1.31597900	0.51984500
N	-2.26787100	1.07124500	0.85993700
N	-2.21449700	-0.85995500	-0.72070200
N	2.27649800	-0.20325800	0.66466700
H	2.70438800	-0.61781900	1.48375100
H	-1.53810900	0.71739300	1.46031900
N	2.67552500	-0.83101100	-0.55322100
H	3.65646400	-0.65505900	-0.72106200
H	2.52042700	-1.83442900	-0.54543800
H	0.49302400	0.60145800	1.75615200
N	0.46918000	0.92542400	-0.53403000
H	0.76164600	0.35161600	-1.32791700
H	-0.52638000	1.12998800	-0.57959900
N	1.18919000	2.15402200	-0.44211100
H	2.05954400	1.90585400	0.02386500
H	1.39691100	2.48619500	-1.37523900

Zero-point correction= 0.209651 (Hartree/Particle)
Thermal correction to Energy= 0.221974
Thermal correction to Enthalpy= 0.222918
Thermal correction to Gibbs Free Energy= 0.171943
Sum of electronic and zero-point Energies= -466.159293
Sum of electronic and thermal Energies= -466.146970
Sum of electronic and thermal Enthalpies= -466.146026
Sum of electronic and thermal Free Energies= -466.197000

Ts4

H	-0.69900300	-2.41650400	-2.03125400
H	-2.50073800	-1.01678800	-1.76116000
H	-1.52209600	2.73632800	-0.44491700
H	1.35911500	-1.94582000	-1.00017700
B	-0.57590000	-1.44237000	-1.33166200
B	1.17557200	-0.29400800	0.34422500
B	-2.10748000	0.77077700	-0.87454600
N	0.67782300	-1.26508500	-0.69892600
N	-1.15411900	1.79932300	-0.47156900
N	-1.74210500	-0.60111300	-1.24067300
N	2.44581500	-0.65772800	1.08876200
H	2.30566000	-1.28262700	1.87248100

H	-0.53102900	1.64732800	0.30714400
N	3.49049500	-1.09504400	0.22003600
H	4.38642100	-0.92483900	0.65709500
H	3.43275300	-2.08794700	0.01408200
H	0.32577300	0.07687400	1.13022500
N	1.66786600	1.03262800	-0.51713700
H	2.42042100	0.66673600	-1.10303500
H	0.87490700	1.34540900	-1.08174000
N	2.07774700	2.08675000	0.34757400
H	2.55549300	1.61906800	1.11489600
H	2.72686200	2.69681400	-0.13282500
H	-3.11662300	1.18151500	-1.38325500
N	-3.04187500	0.32122900	1.09516200
H	-2.33028600	0.65055600	1.73868200
H	-3.88864300	0.85865600	1.22148300
N	-3.33289800	-1.05745500	1.23315100
H	-2.69167100	-1.54397500	0.61494300
H	-3.18951700	-1.37731800	2.18259500

Zero-point correction= 0.266788 (Hartree/Particle)
Thermal correction to Energy= 0.282202
Thermal correction to Enthalpy= 0.283146
Thermal correction to Gibbs Free Energy= 0.224448
Sum of electronic and zero-point Energies= -577.955670
Sum of electronic and thermal Energies= -577.940256
Sum of electronic and thermal Enthalpies= -577.939312
Sum of electronic and thermal Free Energies= -577.998010

4

H	-0.61662200	-2.60489200	-1.79151200
H	-2.39297100	-1.16381800	-1.90636400
H	-1.77437900	2.57177400	-0.38588700
H	1.24728300	-2.12654400	-0.50596400
B	-0.58947900	-1.58983700	-1.13814200
B	1.16149500	-0.23100500	0.44645500
B	-2.32048400	0.52786400	-0.68419300
N	0.58512400	-1.37947400	-0.36037900
N	-1.38633100	1.64536500	-0.30563000
N	-1.75437600	-0.76561500	-1.23437000
N	2.56406800	-0.42492400	0.99170600
H	2.61533700	-0.96614400	1.84558700
H	-0.81452000	1.59150400	0.52652000
N	3.49875400	-0.85927800	0.00501900
H	4.43167800	-0.58379200	0.28112700
H	3.49878700	-1.86721900	-0.11897900
H	0.44870300	0.20373200	1.33535400
N	1.36497100	0.99152900	-0.63030000
H	1.99732000	0.60054800	-1.32997100
H	0.43932300	1.21222800	-1.02260900
N	1.87430600	2.15885000	0.00757900

H	2.53834900	1.81243200	0.69622900
H	2.35524100	2.73707400	-0.66923900
H	-3.23918500	0.94122300	-1.36785200
N	-3.13818900	0.02923400	0.72864000
H	-3.58201800	0.81963800	1.18910800
H	-3.88463200	-0.61315300	0.47722300
N	-2.33472800	-0.65060100	1.71618300
H	-1.80501300	-1.33795600	1.18086000
H	-1.63553300	0.02264400	2.01663100

Zero-point correction= 0.267995 (Hartree/Particle)
Thermal correction to Energy= 0.283301
Thermal correction to Enthalpy= 0.284245
Thermal correction to Gibbs Free Energy= 0.226577
Sum of electronic and zero-point Energies= -577.958162
Sum of electronic and thermal Energies= -577.942857
Sum of electronic and thermal Enthalpies= -577.941913
Sum of electronic and thermal Free Energies= -577.999580

Ts5

H	-0.01590300	0.76707900	3.35371100
H	-2.04644800	0.40261500	2.32967600
H	-0.44465900	-2.35752500	1.82946700
H	1.97140400	0.71845700	2.02750100
B	-0.04964700	0.52980800	2.17059200
B	1.40605900	0.44587200	-0.04598400
B	-1.88502300	-1.12491700	0.88801600
N	1.15246600	0.57491200	1.45462100
N	-0.73773200	-2.16054500	0.87789600
N	-1.37621300	0.25529300	1.58396400
N	2.69115000	1.05845400	-0.57530900
H	2.63284700	2.04757900	-0.78090100
H	-1.07859500	-3.04315900	0.50991600
N	3.83123500	0.73618200	0.22047600
H	4.66294700	0.75682700	-0.35466000
H	3.96755200	1.39451700	0.98190700
H	0.46446700	0.80039800	-0.71314900
N	1.62423600	-1.14508500	-0.28891300
H	2.47014700	-1.36617900	0.23887700
H	0.78367100	-1.62609300	0.12653500
N	1.73865800	-1.46032100	-1.67465000
H	2.26156100	-0.68909300	-2.08280300
H	2.26880500	-2.31477600	-1.78938700
H	-2.86957900	-1.47037100	1.53773300
N	-2.43908900	-0.88242000	-0.55462600
H	-3.23114900	-1.48340000	-0.73620900
H	-2.76418100	0.62856400	-0.52017500
N	-1.57218800	-0.97124900	-1.69874800
H	-1.16985300	-0.05500400	-1.86238500
H	-0.78471900	-1.57835400	-1.49620200

N	-2.48659000	1.68040100	-0.24348100
H	-3.24761600	2.22318100	0.15863100
H	-1.78887100	1.20685900	0.62723700
N	-1.81010400	2.31854000	-1.31603200
H	-2.47595200	2.68511000	-1.98335900
H	-1.23362500	3.06982300	-0.96145600

Zero-point correction= 0.318354 (Hartree/Particle)
Thermal correction to Energy= 0.336277
Thermal correction to Enthalpy= 0.337221
Thermal correction to Gibbs Free Energy= 0.274365
Sum of electronic and zero-point Energies= -689.745735
Sum of electronic and thermal Energies= -689.727812
Sum of electronic and thermal Enthalpies= -689.726868
Sum of electronic and thermal Free Energies= -689.789724

5

H	-3.06117300	-1.17359800	-1.14511300
H	-3.98130800	0.59876300	0.38644100
H	-0.62923300	-1.48437600	-0.99866300
B	-2.36330400	-0.53513300	-0.40429500
B	0.07155400	-0.05668300	0.46176200
N	-0.96393600	-0.77476600	-0.36498900
N	-2.98660100	0.47010000	0.38556000
N	1.34577600	-0.79452300	0.81516700
H	1.26930000	-1.36323800	1.64914000
N	1.86809800	-1.52496600	-0.29552300
H	2.86187800	-1.66449700	-0.16989200
H	1.43703300	-2.44057400	-0.38493500
H	-0.36732500	0.53551200	1.42181200
N	0.67319100	1.11685400	-0.57704900
H	1.05148300	0.55462600	-1.34152300
H	-0.10588300	1.67246900	-0.91379300
N	1.64293700	1.95533700	0.04179200
H	2.10198300	1.34905200	0.71866800
H	2.32446700	2.25552200	-0.64387900
H	-2.49872700	0.98317000	1.09970100

Zero-point correction= 0.177069 (Hartree/Particle)
Thermal correction to Energy= 0.187432
Thermal correction to Enthalpy= 0.188376
Thermal correction to Gibbs Free Energy= 0.141473
Sum of electronic and zero-point Energies= -385.311569
Sum of electronic and thermal Energies= -385.301206
Sum of electronic and thermal Enthalpies= -385.300262
Sum of electronic and thermal Free Energies= -385.347165

6

H	2.50871400	-0.45699700	0.00016000
B	0.72037400	0.68754000	-0.00001000
N	1.50615600	-0.49165600	-0.00009900

H	1.12882200	-1.42294800	0.00068000
H	1.25105400	1.75839300	0.00008200
N	-0.69309600	0.64136500	0.00017200
H	-1.25544000	1.47296000	-0.00060200
N	-1.47837500	-0.52589800	-0.00017900
H	-1.28809300	-1.07823000	-0.82700300
H	-1.28973000	-1.07755600	0.82747800

Zero-point correction= 0.086197 (Hartree/Particle)
Thermal correction to Energy= 0.091492
Thermal correction to Enthalpy= 0.092436
Thermal correction to Gibbs Free Energy= 0.059053
Sum of electronic and zero-point Energies= -192.656256
Sum of electronic and thermal Energies= -192.650961
Sum of electronic and thermal Enthalpies= -192.650017
Sum of electronic and thermal Free Energies= -192.683400

Ts6

H	-1.99032700	0.02673100	-1.73105600
H	-2.15119600	2.15025600	-0.37600500
H	0.00911700	-1.34276800	-1.12256600
B	-1.34651800	0.20861300	-0.71899300
B	0.92135800	-0.19610600	0.47183800
N	-0.19128900	-0.62356600	-0.44593400
N	-1.32625600	1.59443500	-0.21498600
N	2.10204000	-1.12531200	0.67555800
H	1.94924100	-1.83497400	1.38150000
N	2.58684100	-1.67403700	-0.54996200
H	3.55260700	-1.95123400	-0.43613000
H	2.06107500	-2.49360400	-0.83974800
H	0.55310700	0.25679600	1.54188200
N	1.64541300	1.08199300	-0.32957300
H	2.00816700	0.63083700	-1.17057600
H	0.89654300	1.73067900	-0.57318600
N	2.64785400	1.72461700	0.44985800
H	3.06042900	0.97426200	0.99960400
H	3.35822900	2.11333600	-0.15756100
H	-0.99458500	1.73374900	0.72990700
N	-2.80566900	-0.68930100	0.46694500
H	-2.70245400	-1.68104900	0.28501500
N	-4.08881400	-0.16586700	0.19040100
H	-4.10572100	0.08353200	-0.79174700
H	-4.82638500	-0.83296400	0.37771300
H	-2.54287700	-0.48684800	1.42257300

Zero-point correction= 0.233137 (Hartree/Particle)
Thermal correction to Energy= 0.246676
Thermal correction to Enthalpy= 0.247620
Thermal correction to Gibbs Free Energy= 0.193453
Sum of electronic and zero-point Energies= -497.103723
Sum of electronic and thermal Energies= -497.090185
Sum of electronic and thermal Enthalpies= -497.089240

Sum of electronic and thermal Free Energies= -497.143407

7

H	2.02282100	-0.09395200	1.78086500
H	2.17861400	2.10446100	0.61739600
H	-0.12357900	-1.22211300	1.30822800
B	1.43287000	0.09196500	0.72813900
B	-0.85497700	-0.21646500	-0.44229900
N	0.20055100	-0.70842700	0.50236000
N	1.38235000	1.54828900	0.34442500
N	-2.08442700	-1.07532800	-0.68850700
H	-1.93136300	-1.79586200	-1.38420600
N	-2.60017500	-1.61506300	0.53006300
H	-3.56833700	-1.87610800	0.40017900
H	-2.08901600	-2.44292200	0.82327800
H	-0.41024000	0.20031100	-1.50179300
N	-1.53471000	1.11338200	0.31383300
H	-1.95643700	0.70177700	1.14721300
H	-0.74861500	1.71312000	0.57373800
N	-2.46792100	1.80165200	-0.51171200
H	-2.91828700	1.06536100	-1.05095600
H	-3.16434600	2.25835100	0.06375000
H	1.16580900	1.74895700	-0.62462700
N	2.56326000	-0.70210300	-0.39870400
H	2.49199800	-1.68253200	-0.14233400
N	3.88243000	-0.17936800	-0.38464700
H	4.06089000	0.13230600	0.56322800
H	4.55938000	-0.88879000	-0.63368900
H	2.15173400	-0.58111300	-1.31924200

Zero-point correction= 0.234428 (Hartree/Particle)
Thermal correction to Energy= 0.248040
Thermal correction to Enthalpy= 0.248984
Thermal correction to Gibbs Free Energy= 0.194942
Sum of electronic and zero-point Energies= -497.103247
Sum of electronic and thermal Energies= -497.089634
Sum of electronic and thermal Enthalpies= -497.088690
Sum of electronic and thermal Free Energies= -497.142732

Ts7

H	-0.10562200	0.30366500	-2.09988100
H	-0.01620200	-2.68639300	-1.89134600
B	-0.96088600	0.44131400	-0.19557400
B	1.13816400	-1.07899200	-1.07941400
N	0.29777900	-2.39298600	-0.97312400
N	0.21235500	0.19343200	-1.14153400
H	0.83868000	-3.16801200	-0.60606100
H	1.88969900	-1.05850000	-2.05415400
N	2.08676300	-0.94370300	0.16506800

H	2.86212900	-1.59368700	0.12367600
H	2.45655900	0.37109500	-0.04553800
N	1.50619800	-1.04160000	1.47830700
H	1.24279200	-0.10271800	1.75800000
H	0.63763500	-1.56659300	1.42981800
N	2.26210200	1.53596700	-0.33096900
H	2.87955100	1.94543800	-1.02770000
H	1.23302400	1.16115300	-0.78736300
N	2.11805900	2.30738100	0.85452700
H	3.02546600	2.48626000	1.26475100
H	1.66952200	3.19066600	0.64921500
H	-0.62222300	0.89919200	0.89307300
N	-2.05086000	1.24755400	-0.89294800
H	-1.68577100	2.11055700	-1.28498600
N	-3.11882100	1.50890200	0.02015200
H	-2.87019600	2.23133700	0.69163800
H	-3.93736500	1.81128900	-0.49057900
N	-1.72809200	-0.96842400	0.18258900
H	-2.63041500	-0.90774600	-0.28721800
N	-1.85750300	-1.20147700	1.58480500
H	-2.16901200	-0.32832900	1.99539900
H	-2.57108500	-1.90329300	1.74159100
H	-1.10939800	-1.72231400	-0.22550600

Zero-point correction= 0.284695 (Hartree/Particle)
Thermal correction to Energy= 0.300484
Thermal correction to Enthalpy= 0.301428
Thermal correction to Gibbs Free Energy= 0.242589
Sum of electronic and zero-point Energies= -608.896555
Sum of electronic and thermal Energies= -608.880767
Sum of electronic and thermal Enthalpies= -608.879822
Sum of electronic and thermal Free Energies= -608.938662

8

H	2.46431300	0.36810700	-0.83217100
B	0.71530000	0.08687700	0.39597400
N	2.14607000	-0.10532500	0.00044400
H	0.50907800	0.04290500	1.59720400
N	0.04322200	1.21525100	-0.36993000
H	0.61987000	2.04947200	-0.33161900
N	-1.28304200	1.49272000	0.09134300
H	-1.27363300	1.96454300	0.99182600
H	-1.75434700	2.08550800	-0.57894300
N	-0.04422500	-1.29836900	-0.19038500
H	0.11792600	-1.23927200	-1.19503800
N	-1.41882900	-1.45675000	0.15891000
H	-1.80538800	-0.51328800	0.18426600
H	-1.89154100	-2.00108700	-0.55131400
H	0.49474700	-2.07572900	0.17697100
H	2.84010500	-0.04822800	0.72628000

Zero-point correction= 0.144755 (Hartree/Particle)
Thermal correction to Energy= 0.152758
Thermal correction to Enthalpy= 0.153702
Thermal correction to Gibbs Free Energy= 0.113510
Sum of electronic and zero-point Energies= -304.451089
Sum of electronic and thermal Energies= -304.443087
Sum of electronic and thermal Enthalpies= -304.442143
Sum of electronic and thermal Free Energies= -304.482335

Ts8

B	0.30241400	0.86769100	0.58963900
N	1.04349500	-0.39669700	0.76228700
H	1.65815200	-0.42877400	1.56359900
N	1.60965000	-0.95770000	-0.41351100
H	2.49247800	-0.51635400	-0.65213000
H	1.76984100	-1.94629100	-0.27566800
N	0.43382600	1.57367500	-0.66189300
H	0.58029000	1.04797100	-1.50837000
H	0.10601100	1.49470300	1.59784200
N	-1.60353200	0.00667100	0.51172900
H	-1.59828300	-0.54504000	1.36260400
H	-2.38470800	0.64935200	0.51697500
N	-1.65199900	-0.77795500	-0.66998400
H	-0.69342900	-1.01219700	-0.91233400
H	-2.17136200	-1.63400500	-0.52314500
H	-0.09114300	2.41622200	-0.81796300

Zero-point correction= 0.142800 (Hartree/Particle)
Thermal correction to Energy= 0.151067
Thermal correction to Enthalpy= 0.152011
Thermal correction to Gibbs Free Energy= 0.111063
Sum of electronic and zero-point Energies= -304.447540
Sum of electronic and thermal Energies= -304.439273
Sum of electronic and thermal Enthalpies= -304.438328
Sum of electronic and thermal Free Energies= -304.479277

Ts9

H	0.08970900	-2.27192500	-0.86781900
B	0.57227400	-0.48164900	0.24478800
N	-0.27506600	-1.79252800	-0.04875000
H	0.36108000	-0.16391200	1.41691100
N	2.03606200	-0.75326100	-0.09657500
H	2.39936300	-1.57230100	0.38242200
N	2.82693000	0.39846100	0.20631900
H	3.02245300	0.46712300	1.20174300
H	3.70581400	0.34841300	-0.29089900
N	0.08497700	0.68625700	-0.68957400
H	0.82703400	0.81305100	-1.37332500
N	-0.11477600	1.91893100	0.03244500
H	0.75553500	2.16437200	0.49904900

H	-0.31486700	2.65214800	-0.63807300
H	-1.51072100	0.25941600	-0.94150000
H	-0.23247600	-2.44588300	0.72384500
N	-2.30775200	-0.31314100	-0.49328800
H	-3.13402000	-0.43169200	-1.06656900
H	-1.58368600	-1.21864200	-0.32015000
N	-2.65007500	0.30510000	0.75631900
H	-2.49032100	-0.38321300	1.48373700
H	-1.95837300	1.04255200	0.89840200

Zero-point correction= 0.197945 (Hartree/Particle)
Thermal correction to Energy= 0.208402
Thermal correction to Enthalpy= 0.209346
Thermal correction to Gibbs Free Energy= 0.162765
Sum of electronic and zero-point Energies= -416.241833
Sum of electronic and thermal Energies= -416.231376
Sum of electronic and thermal Enthalpies= -416.230432
Sum of electronic and thermal Free Energies= -416.277013

9

B	0.06206300	0.78283200	-0.00022800
H	0.50342000	1.89621100	-0.00037600
N	-1.34528500	0.60499600	0.00068500
H	-1.98644500	1.38092400	-0.00185700
N	-1.90095400	-0.68675400	0.00018300
H	-2.46794100	-0.83521200	0.82468800
H	-2.46492500	-0.83633700	-0.82620100
N	0.93285900	-0.32335400	-0.00076000
H	0.57868000	-1.26528100	0.00025500
N	2.34120600	-0.26722900	0.00028600
H	2.66646300	0.22677300	-0.81998400
H	2.66564500	0.22515100	0.82186400

Zero-point correction= 0.104333 (Hartree/Particle)
Thermal correction to Energy= 0.110772
Thermal correction to Enthalpy= 0.111717
Thermal correction to Gibbs Free Energy= 0.075101
Sum of electronic and zero-point Energies= -247.944254
Sum of electronic and thermal Energies= -247.937815
Sum of electronic and thermal Enthalpies= -247.936870
Sum of electronic and thermal Free Energies= -247.973486

Ts_9_dimer

B	-1.07885500	0.73643300	0.25366400
N	-0.18594200	-0.61857200	0.77240900
H	0.20264700	-0.33111500	1.66848700
N	-1.00370700	-1.78385900	0.87792100
H	-0.56422500	-2.45908200	1.49028700
H	-1.89505800	-1.49400800	1.26888900
H	-1.63466100	1.13650900	1.25947300
B	0.85995100	-0.66531900	-0.32810700

H	0.52049600	-1.00759800	-1.41049600
N	0.12857500	1.51910200	-0.26227400
H	-0.12725100	2.23375300	-0.93521300
N	0.91228500	2.03582300	0.81197200
H	1.79450800	2.37555800	0.45002600
H	0.43324900	2.80571200	1.27062400
N	2.21596700	-0.66678900	0.05225500
H	2.49215300	-0.32787700	0.96397500
N	3.23204600	-0.72719600	-0.91841500
H	3.67074400	0.17657000	-1.04124300
H	3.93004600	-1.40702800	-0.64992100
N	-2.00551500	0.42658400	-0.85684900
H	-1.58425900	0.13285300	-1.72874500
N	-3.16982400	-0.31984900	-0.53488200
H	-3.95887200	0.04999700	-1.04828300
H	-3.05218400	-1.29652700	-0.78060300

Zero-point correction= 0.210254 (Hartree/Particle)
Thermal correction to Energy= 0.222960
Thermal correction to Enthalpy= 0.223905
Thermal correction to Gibbs Free Energy= 0.171622
Sum of electronic and zero-point Energies= -495.871579
Sum of electronic and thermal Energies= -495.858873
Sum of electronic and thermal Enthalpies= -495.857929
Sum of electronic and thermal Free Energies= -495.910211

9_dimer

B	-0.93444400	-0.62617400	-0.38606300
N	-0.41610700	0.90038100	-0.55378800
H	-0.10365700	1.00766500	-1.51515400
N	-1.27845400	1.96902300	-0.14440300
H	-1.08495100	2.78042300	-0.71592700
H	-2.23422700	1.65925900	-0.29632400
H	-1.16506600	-1.13432700	-1.46480800
B	0.78767400	0.49270100	0.39123200
H	0.52249600	0.77956800	1.53498600
N	0.47915000	-1.08377200	0.19784000
H	0.45291800	-1.55946100	1.09441800
N	1.30719900	-1.73878400	-0.76163300
H	2.26528800	-1.65661000	-0.43732300
H	1.03010900	-2.70982800	-0.82716000
N	2.12856600	0.88447300	-0.16681300
H	2.26015100	1.89100200	-0.12199200
N	3.16363700	0.20604100	0.54979300
H	4.03240500	0.29754900	0.04026700
H	3.29466700	0.59053200	1.48189500
N	-1.99476800	-0.72459300	0.67227200
H	-2.10010000	-1.67184600	1.02231600
N	-3.23208800	-0.22679200	0.16310300
H	-3.68795700	-0.89517200	-0.45154900

H	-3.84817100	-0.01322800	0.93591600

Zero-point correction= 0.212985 (Hartree/Particle)
Thermal correction to Energy= 0.225104
Thermal correction to Enthalpy= 0.226048
Thermal correction to Gibbs Free Energy= 0.175506
Sum of electronic and zero-point Energies= -495.881167
Sum of electronic and thermal Energies= -495.869048
Sum of electronic and thermal Enthalpies= -495.868104
Sum of electronic and thermal Free Energies= -495.918647

Ts10

B	-0.07133800	-0.44355600	0.81643600
N	-1.53071700	-0.26214900	0.64007500
H	-2.11326900	-0.66266700	1.36159800
N	-2.03925300	-0.45531800	-0.67272000
H	-2.28516200	-1.42555500	-0.84207000
H	-2.86692800	0.11018800	-0.80335200
N	0.63612500	-1.16391700	-0.22548900
H	0.22976400	-1.26386600	-1.14036300
N	2.04487000	-1.20059200	-0.29512700
H	2.42819900	-0.26050800	-0.25984100
H	2.40098200	-1.72662100	0.49201200
H	0.29637700	-0.57902100	1.96018800
N	0.51173100	1.42291400	0.61724000
H	-0.23955600	1.86242600	1.13903500
H	1.40506700	1.65885100	1.03088400
N	0.52249600	1.75929900	-0.76131100
H	-0.09713000	1.10272400	-1.22780500
H	0.18158700	2.70017200	-0.91114500

Zero-point correction= 0.161115 (Hartree/Particle)
Thermal correction to Energy= 0.170459
Thermal correction to Enthalpy= 0.171403
Thermal correction to Gibbs Free Energy= 0.127475
Sum of electronic and zero-point Energies= -359.737012
Sum of electronic and thermal Energies= -359.727668
Sum of electronic and thermal Enthalpies= -359.726723
Sum of electronic and thermal Free Energies= -359.770651

10

B	0.01945500	-0.47414600	0.65169600
N	0.11134200	1.03563100	0.79781200
H	-0.51303900	1.40369400	1.50676500
N	-0.06322200	1.70395400	-0.45795000
H	-1.03562000	1.67630000	-0.75034600
H	0.25874900	2.65851400	-0.37997700
N	-1.26286300	-1.09207800	0.11714500
H	-1.64148300	-1.83144800	0.69217700
N	-2.27730800	-0.20783000	-0.34872400

H	-2.78825500	-0.64712000	-1.10330100
H	-2.93973900	0.01847300	0.38583400
H	0.42097700	-1.06884600	1.63943100
N	1.14552800	-0.73268800	-0.50987200
H	1.11885200	-1.68622100	-0.85492500
N	2.49823000	-0.38984800	-0.16094800
H	2.43125500	0.59462600	0.08904500
H	2.66110300	-0.85823100	0.72691500
H	0.86797000	-0.10899600	-1.27233600

Zero-point correction= 0.163172 (Hartree/Particle)
Thermal correction to Energy= 0.172325
Thermal correction to Enthalpy= 0.173269
Thermal correction to Gibbs Free Energy= 0.129676
Sum of electronic and zero-point Energies= -359.742257
Sum of electronic and thermal Energies= -359.733105
Sum of electronic and thermal Enthalpies= -359.732161
Sum of electronic and thermal Free Energies= -359.775754

Ts11

B	-0.88478100	-0.32455900	-0.09557600
N	-1.87375600	-0.32002500	0.98634700
H	-1.81099000	-1.18241800	1.51636900
N	-3.18613100	-0.13147300	0.44607500
H	-3.52907000	-0.98535700	0.01608300
H	-3.81387400	0.12091000	1.19809800
N	-0.54570800	-1.51918200	-0.82739400
H	0.33595800	-1.46349600	-1.33152300
N	-0.65329800	-2.71741400	-0.06564500
H	-0.87723300	-3.47962700	-0.69120900
H	0.24963700	-2.89357700	0.36984700
H	0.44809800	-0.01322700	0.81873100
N	-0.81043400	0.95850700	-0.96243700
H	0.26167200	1.26405700	-0.95334800
N	-1.51587100	2.13256600	-0.51172000
H	-2.40923400	1.79290000	-0.16435800
H	-0.97579900	2.46735700	0.28288000
H	-1.09549600	0.76772900	-1.91828100
B	1.65699100	0.31645300	0.55408600
H	2.16895900	0.46198700	1.66214400
N	1.60690300	1.62777700	-0.26309500
H	2.47731600	1.77856000	-0.76651300
N	1.28069000	2.74611500	0.56920000
H	1.93597500	2.81072500	1.34265600
H	1.32509800	3.59759600	0.02396800
N	2.28857400	-0.75597000	-0.32685900
H	3.23315300	-0.46929100	-0.57503400
N	2.34234100	-2.00883400	0.36745400
H	2.79139700	-2.69316500	-0.22810900
H	2.89022100	-1.92560400	1.22156800

Zero-point correction= 0.267203 (Hartree/Particle)
Thermal correction to Energy= 0.282078
Thermal correction to Enthalpy= 0.283023
Thermal correction to Gibbs Free Energy= 0.226083
Sum of electronic and zero-point Energies= -607.662086
Sum of electronic and thermal Energies= -607.647211
Sum of electronic and thermal Enthalpies= -607.646267
Sum of electronic and thermal Free Energies= -607.703206

11

H	0.48220900	1.78855700	0.87137200
H	-1.71735400	0.60725100	1.21608300
B	0.04440100	1.12623900	-0.06178100
H	-0.52823300	1.78397700	-0.90641100
N	-1.04495600	0.13742500	0.61923100
H	-0.48823400	-0.48596100	1.20871000
N	-1.76759600	-0.70317400	-0.30520000
H	-2.25242100	-0.05416400	-0.91928700
H	-1.02080400	-1.08770700	-0.88372400
N	1.00972400	0.11767200	-0.66608200
H	1.66334300	0.53447900	-1.31822100
N	1.67877900	-0.59222300	0.38068800
H	2.12401900	-1.41899100	0.00595700
H	2.38381300	-0.01654100	0.83397400

Zero-point correction= 0.126632 (Hartree/Particle)
Thermal correction to Energy= 0.133226
Thermal correction to Enthalpy= 0.134170
Thermal correction to Gibbs Free Energy= 0.097120
Sum of electronic and zero-point Energies= -249.081381
Sum of electronic and thermal Energies= -249.074787
Sum of electronic and thermal Enthalpies= -249.073843
Sum of electronic and thermal Free Energies= -249.110893

12

B	0.20391200	-0.23238100	0.01787700
N	0.02367300	1.16959400	-0.14193300
H	0.73710700	1.74616100	-0.55102900
N	-1.16681800	1.89476900	0.08404700
H	-1.93188300	1.37801200	-0.33236300
H	-1.33924900	1.93009100	1.08186700
N	-0.89020200	-1.13186800	0.28972700
H	-0.68755900	-2.09346300	0.51923200
N	-2.18013000	-0.89385600	-0.22542700
H	-2.35741200	-1.46097200	-1.04554100
H	-2.87953900	-1.10016300	0.47534800
N	1.52384200	-0.78507000	-0.04875100
N	2.71798600	-0.04531700	0.01598500
H	2.85095500	0.48713200	-0.83455200
H	2.69218500	0.59149600	0.80271100

H	1.69737800	-1.77415500	-0.02058200

Zero-point correction= 0.140690 (Hartree/Particle)
Thermal correction to Energy= 0.149779
Thermal correction to Enthalpy= 0.150724
Thermal correction to Gibbs Free Energy= 0.107645
Sum of electronic and zero-point Energies= -358.607974
Sum of electronic and thermal Energies= -358.598885
Sum of electronic and thermal Enthalpies= -358.597940
Sum of electronic and thermal Free Energies= -358.641019

Ts12

H	-0.65144000	1.72794600	-1.07206800
H	2.30151800	0.98453300	-0.29287800
B	-0.58463300	1.36782000	0.06346600
H	-0.21668100	2.09567900	0.94468000
N	1.49720100	0.38282000	-0.42183300
H	1.38176200	0.16347500	-1.40095600
N	1.55532200	-0.81756000	0.32508200
H	2.50310700	-1.14991800	0.45102600
H	1.14154100	-0.63874000	1.23118500
N	-1.27767700	0.19927500	0.45836300
H	-1.33187300	-0.08203700	1.42615200
N	-1.59381900	-0.79853500	-0.48389600
H	-0.93562300	-1.56592400	-0.40556300
H	-2.53633300	-1.13610700	-0.34292600

Zero-point correction= 0.123632 (Hartree/Particle)
Thermal correction to Energy= 0.130969
Thermal correction to Enthalpy= 0.131914
Thermal correction to Gibbs Free Energy= 0.092607
Sum of electronic and zero-point Energies= -249.067147
Sum of electronic and thermal Energies= -249.059810
Sum of electronic and thermal Enthalpies= -249.058865
Sum of electronic and thermal Free Energies= -249.098172

13

H	1.35936600	1.44255300	-0.00060500
B	1.33708800	0.25209800	-0.00007200
H	2.31873600	-0.43017700	-0.00010400
N	0.10914800	-0.40582900	0.00028200
H	0.05524900	-1.41450900	0.00011600
N	-1.12420200	0.27462400	-0.00025900
H	-1.65706100	0.02861100	-0.82438100
H	-1.65634500	0.03147000	0.82516800

Zero-point correction= 0.066899 (Hartree/Particle)
Thermal correction to Energy= 0.070996
Thermal correction to Enthalpy= 0.071940
Thermal correction to Gibbs Free Energy= 0.041994
Sum of electronic and zero-point Energies= -137.265313
Sum of electronic and thermal Energies= -137.261216
Sum of electronic and thermal Enthalpies= -137.260272

Sum of electronic and thermal Free Energies= -137.290218

Ts13

B	-0.83778100	0.00281600	-0.28815400
N	-1.89080700	0.86394300	0.19527500
H	-2.67172900	0.34106300	0.57236600
N	-1.52895300	2.01868900	0.92952000
H	-2.25972700	2.71206000	0.84599300
H	-1.38912100	1.79903900	1.91122800
N	-1.20957500	-1.31386000	-0.77721900
H	-0.42712900	-1.92949300	-0.96768100
N	-2.22656800	-1.94163600	-0.01497400
H	-2.75243000	-2.56960600	-0.60640300
H	-1.82011500	-2.46418900	0.75520800
H	0.09550800	-0.13174100	0.99756300
N	0.31845100	0.58655900	-1.15406400
H	1.08267800	-0.14943100	-1.00446800
N	0.85982700	1.88161200	-0.82258000
H	0.18242100	2.31721200	-0.19853900
H	1.70113100	1.68258400	-0.28448700
H	0.03408200	0.59605900	-2.13033100
B	1.02599900	-0.98672400	1.28255700
H	1.51190300	-0.55411500	2.31075200
N	2.02633400	-1.02874600	0.10377700
H	2.45997700	-1.94498900	0.06294300
N	3.02650100	-0.00045800	0.21834800
H	3.48912400	-0.06608100	1.12124900
H	3.71979800	-0.11904700	-0.51059200
H	0.47607000	-2.06250200	1.40660500

Zero-point correction= 0.231042 (Hartree/Particle)
Thermal correction to Energy= 0.243652
Thermal correction to Enthalpy= 0.244596
Thermal correction to Gibbs Free Energy= 0.193600
Sum of electronic and zero-point Energies= -497.009719
Sum of electronic and thermal Energies= -496.997108
Sum of electronic and thermal Enthalpies= -496.996164
Sum of electronic and thermal Free Energies= -497.047161

HzB

H	-1.27950700	-0.98076900	1.00426400
B	-1.36131700	-0.29007100	0.00756100
H	-2.22166400	0.56000700	0.07483600
N	0.05394400	0.54940000	0.00128000
H	0.07244300	1.10247300	0.85368000
N	1.18869500	-0.30850700	-0.11878400
H	1.95286200	0.03331300	0.44922600
H	0.89282500	-1.21680100	0.21987400
H	0.05516300	1.18278300	-0.79162400

H	-1.36401000	-0.91690100	-1.02552700

Zero-point correction= 0.089215 (Hartree/Particle)
Thermal correction to Energy= 0.093914
Thermal correction to Enthalpy= 0.094858
Thermal correction to Gibbs Free Energy= 0.063423
Sum of electronic and zero-point Energies= -138.414725
Sum of electronic and thermal Energies= -138.410027
Sum of electronic and thermal Enthalpies= -138.409083
Sum of electronic and thermal Free Energies= -138.440518

Ts14

B	-1.44540400	-0.68641300	0.69910600
N	-2.29302900	-0.25286500	-0.32839700
H	-1.95080800	-0.12784800	-1.26730300
N	-3.47270000	0.49560000	-0.11465500
H	-4.20841600	-0.12230300	0.20070400
H	-3.30366600	1.18826400	0.60397800
N	-0.13074400	-1.25514000	0.40042000
N	0.26220200	-1.55731000	-0.94066700
H	-0.49190700	-2.05764500	-1.40187000
H	0.37813000	-0.65465000	-1.39723900
H	0.18961200	-1.98607500	1.01876000
H	0.91212600	-0.00136000	2.28868500
H	2.89318000	-0.87699700	1.12962000
H	0.57037400	2.23038600	1.02826300
B	1.07060800	0.20731200	1.11120200
N	2.40707800	-0.12778800	0.65746300
N	0.29981400	1.36487500	0.57274200
H	-1.80204500	-0.65632700	1.83671100
N	2.84306300	0.10944200	-0.66677400
H	3.80702900	0.41586800	-0.65328000
H	2.77235900	-0.73643200	-1.22269400
N	0.27796400	1.48776400	-0.85076800
H	-0.43113000	2.16174700	-1.10812800
H	1.18360000	1.76682800	-1.21329600

Zero-point correction= 0.211230 (Hartree/Particle)
Thermal correction to Energy= 0.223533
Thermal correction to Enthalpy= 0.224477
Thermal correction to Gibbs Free Energy= 0.174077
Sum of electronic and zero-point Energies= -495.869894
Sum of electronic and thermal Energies= -495.857591
Sum of electronic and thermal Enthalpies= -495.856647
Sum of electronic and thermal Free Energies= -495.907047

14

B	1.71492700	-1.02174500	-0.07272600
N	2.24464200	0.23684100	-0.22871600
H	1.61318200	1.02164000	-0.38697400
N	3.61433800	0.57965900	-0.18084300

H	4.00856200	0.25841000	0.69336900
H	4.10153500	0.12103200	-0.93970500
N	0.19726700	-1.17043600	-0.10310400
N	-0.19524700	-1.41694400	1.28273100
H	-0.16927000	-0.48388600	1.69638100
H	-1.18890900	-1.63290000	1.20975700
H	0.00529100	-2.05178300	-0.57364300
H	-0.39811200	-0.19042600	-2.07007800
H	-2.60589600	-0.89832400	-1.56708600
H	-0.87739100	2.02326900	-0.91809400
B	-0.74297900	-0.07857000	-0.90414400
N	-2.17650300	-0.58601600	-0.70637700
N	-0.39609100	1.30817000	-0.38116300
H	2.38540700	-1.99320400	0.09604400
N	-3.06315200	0.25291800	0.03363600
H	-3.52871600	0.92377500	-0.56986900
H	-3.77962900	-0.31550600	0.46669400
N	-0.60699400	1.48859300	1.02604600
H	-0.15176000	2.34151800	1.32240500
H	-1.60184900	1.52846600	1.22967100

Zero-point correction= 0.212153 (Hartree/Particle)
Thermal correction to Energy= 0.224754
Thermal correction to Enthalpy= 0.225698
Thermal correction to Gibbs Free Energy= 0.174004
Sum of electronic and zero-point Energies= -495.868268
Sum of electronic and thermal Energies= -495.855667
Sum of electronic and thermal Enthalpies= -495.854723
Sum of electronic and thermal Free Energies= -495.906417

Ts15

B	1.35345900	-0.77902300	0.39638500
N	2.34946500	0.11990600	-0.11641900
H	2.02351700	0.94138400	-0.60648800
N	3.54323000	-0.36113500	-0.70894500
H	4.20513100	-0.58099200	0.02243800
H	3.36578700	-1.20281200	-1.24420400
N	0.15709900	-0.12223100	1.10069700
N	0.29854400	1.20644800	1.60639700
H	1.26567000	1.47919300	1.47647100
H	-0.31049600	1.79562800	1.04077800
H	-0.22268100	-0.70626300	1.83455300
H	0.42267800	-1.18669700	-0.80240700
H	-1.53495400	-2.34933800	0.10143800
H	-0.91606400	0.54922600	-2.09685000
B	-0.54646400	-0.47651200	-0.33842100
N	-1.69503100	-1.42102700	-0.27026200
N	-0.64412400	0.77744200	-1.14604400
H	1.66332900	-1.88075200	0.74272700
N	-2.93010600	-0.84323400	0.12357100

H	-3.69142300	-1.32341500	-0.33694800
H	-3.08032300	-0.88685200	1.12632300
N	-1.54331700	1.73578500	-0.57120400
H	-1.47880600	2.59852600	-1.09420600
H	-2.49666000	1.38715000	-0.57798500

Zero-point correction= 0.211490 (Hartree/Particle)
Thermal correction to Energy= 0.223245
Thermal correction to Enthalpy= 0.224189
Thermal correction to Gibbs Free Energy= 0.174819
Sum of electronic and zero-point Energies= -495.858020
Sum of electronic and thermal Energies= -495.846266
Sum of electronic and thermal Enthalpies= -495.845322
Sum of electronic and thermal Free Energies= -495.894691

15

B	-1.28301800	-0.25074400	0.87192500
N	-2.70950000	0.09265800	0.57017200
H	-3.22458500	0.49938400	1.33421700
N	-3.52221300	-0.90157000	-0.04326200
H	-3.50086800	-0.78498000	-1.04826100
H	-3.16942300	-1.82724000	0.18256300
N	-0.41797700	0.05095100	-0.54562400
N	-0.78971400	1.29829800	-1.17459500
H	-1.74280800	1.44855700	-0.83747500
H	-0.20818300	2.00716300	-0.73366800
H	-0.68744200	-0.67478600	-1.20468800
H	-0.79603100	0.48962400	1.70211300
H	0.89534900	-2.24965700	-0.39318500
H	2.82638800	0.62848800	0.47337400
B	1.03814800	-0.13754300	-0.22833600
N	1.52860600	-1.46702100	-0.32515200
N	1.90085500	0.89868300	0.17252900
H	-1.06852900	-1.44364700	1.07261200
N	2.82662600	-1.74783800	0.13816200
H	2.79517000	-2.27838500	1.00004800
H	3.34059600	-2.27023900	-0.55827700
N	1.49567000	2.22287800	0.40690000
H	1.41782500	2.40177000	1.40065700
H	2.16042100	2.86610600	-0.00188600

Zero-point correction= 0.211956 (Hartree/Particle)
Thermal correction to Energy= 0.224674
Thermal correction to Enthalpy= 0.225619
Thermal correction to Gibbs Free Energy= 0.173533
Sum of electronic and zero-point Energies= -495.886343
Sum of electronic and thermal Energies= -495.873625
Sum of electronic and thermal Enthalpies= -495.872680
Sum of electronic and thermal Free Energies= -495.924766

Ts16

B	-1.50824500	-1.16078200	0.55865400
N	-2.66022900	-0.37079600	0.80343800
H	-2.82064100	0.11160500	1.67042000
N	-3.71965600	-0.16542700	-0.10906100
H	-3.35852800	0.30086800	-0.93450500
H	-4.09489100	-1.06317600	-0.38866200
N	-0.27216000	0.17423400	-0.76546000
N	-0.91964100	1.43784500	-0.74311800
H	-1.53762300	1.43261300	0.06494000
H	-0.21838300	2.15400900	-0.59143500
H	-0.47244900	-0.29282500	-1.63742300
H	-0.72634900	-1.26787200	1.46202000
H	0.93663600	-2.15985100	-0.59031100
H	2.78112500	0.53998600	0.75276500
B	1.07275300	-0.06880700	-0.25685500
N	1.58059700	-1.39653300	-0.44404800
N	1.88915300	0.87456100	0.41782900
H	-1.55851200	-1.98833200	-0.31411300
N	2.82709400	-1.73971400	0.11434000
H	2.70950100	-2.32529600	0.93229900
H	3.39077200	-2.23144100	-0.56578900
N	1.70330900	2.26862800	0.36686400
H	1.69622800	2.65260000	1.30293200
H	2.45130000	2.70546700	-0.15762200

Zero-point correction= 0.210525 (Hartree/Particle)
Thermal correction to Energy= 0.223531
Thermal correction to Enthalpy= 0.224476
Thermal correction to Gibbs Free Energy= 0.171364
Sum of electronic and zero-point Energies= -495.882999
Sum of electronic and thermal Energies= -495.869992
Sum of electronic and thermal Enthalpies= -495.869048
Sum of electronic and thermal Free Energies= -495.922159

Ts17

B	-1.71771500	-1.51795200	0.33926700
N	-1.40490300	-0.41103700	-0.51983600
N	-2.18124300	0.77033100	-0.54418200
H	-3.02766100	0.59169500	-0.01898300
H	-1.64078000	1.47239100	-0.04195200
H	-0.91171200	-0.55074400	-1.39132700
H	-0.31952100	-0.95356600	1.61403600
H	1.18128800	-2.13034900	0.01062200
H	0.70976800	1.33473900	1.74721500
B	0.15524000	-0.36686400	0.64555000
N	1.14886700	-1.13265200	-0.14337100
N	0.28482800	1.07899900	0.86482600
H	-1.24336800	-2.58372500	0.09833400
N	2.42520200	-0.55426600	-0.35034100
H	3.09785100	-0.89105200	0.32865600

H	2.75828400	-0.78601100	-1.27676700
N	0.78335900	1.80415300	-0.25510200
H	0.62541500	2.79187400	-0.11219100
H	1.76857500	1.61026900	-0.39660000
H	-2.57853800	-1.37013700	1.15091600

Zero-point correction= 0.172983 (Hartree/Particle)
Thermal correction to Energy= 0.183111
Thermal correction to Enthalpy= 0.184055
Thermal correction to Gibbs Free Energy= 0.138413
Sum of electronic and zero-point Energies= -385.183813
Sum of electronic and thermal Energies= -385.173685
Sum of electronic and thermal Enthalpies= -385.172741
Sum of electronic and thermal Free Energies= -385.218383

16

B	-1.30875800	-1.40192300	1.21473600
N	-0.90516500	-0.90293500	-0.29822600
N	-1.99163300	-0.26755700	-1.01430700
H	-2.82468800	-0.74207900	-0.67668100
H	-2.03339200	0.67792200	-0.63709900
H	-0.67953200	-1.73359700	-0.83753700
H	-1.51512900	-0.38917100	1.85223600
H	1.60620100	-1.78385900	-0.25260900
H	1.23110800	1.74348300	0.25815500
B	0.34817500	-0.07562400	-0.18027800
N	1.57676100	-0.77623500	-0.30017700
N	0.34164400	1.31018800	0.05542100
H	-0.35742400	-2.04186600	1.62088600
N	2.77211000	-0.10026100	0.00382300
H	3.15667100	-0.42538900	0.88244300
H	3.45034800	-0.24214100	-0.73237900
N	-0.82334000	2.05784700	0.29499700
H	-0.94832100	2.21753100	1.28744400
H	-0.77130200	2.94331300	-0.19019300
H	-2.30425900	-2.08374100	1.06231700

Zero-point correction= 0.175158 (Hartree/Particle)
Thermal correction to Energy= 0.185458
Thermal correction to Enthalpy= 0.186403
Thermal correction to Gibbs Free Energy= 0.140819
Sum of electronic and zero-point Energies= -385.225945
Sum of electronic and thermal Energies= -385.215645
Sum of electronic and thermal Enthalpies= -385.214700
Sum of electronic and thermal Free Energies= -385.260284

Ts18

B	1.54266800	-0.24868100	0.03886900
N	-0.37857200	-0.74140400	-0.89988500
N	-0.49088100	-2.15214400	-0.74886100
H	0.21672600	-2.43419600	-0.07869100

H	-1.39949400	-2.35893700	-0.34999200
H	-0.14310000	-0.52300600	-1.85744400
H	1.03843200	-0.28845200	1.12997500
H	-0.18291800	1.89107000	-0.87869600
H	-2.88926000	0.64863100	0.97822100
B	-1.30324600	0.19985600	-0.27817900
N	-1.09813200	1.58601800	-0.58461900
N	-2.36332200	-0.12980800	0.60788100
H	1.66275700	0.79795100	-0.54310100
N	-1.90047800	2.55822300	0.04472200
H	-1.37924500	3.04857400	0.76160600
H	-2.23193400	3.22863100	-0.63584800
N	-2.92956800	-1.40980100	0.75028000
H	-2.97238500	-1.66403300	1.72875200
H	-3.86666800	-1.42754400	0.36738600
H	2.00681300	-1.24674900	-0.45165800
N	3.59441000	0.07969100	0.90906800
H	3.78157600	-0.78745700	1.39719100
N	4.44753700	0.30949200	-0.19571400
H	5.34920400	-0.13603800	-0.08494700
H	3.98738300	-0.06316900	-1.01712600
H	3.65805200	0.85698000	1.55083200

Zero-point correction= 0.230210 (Hartree/Particle)
Thermal correction to Energy= 0.244899
Thermal correction to Enthalpy= 0.245844
Thermal correction to Gibbs Free Energy= 0.188378
Sum of electronic and zero-point Energies= -497.005089
Sum of electronic and thermal Energies= -496.990400
Sum of electronic and thermal Enthalpies= -496.989456
Sum of electronic and thermal Free Energies= -497.046921

Dz

H	1.01326400	0.83592300	0.00005000
N	0.61620500	-0.11941400	-0.00001200
N	-0.61620000	-0.11941800	0.00001200
H	-1.01330200	0.83590500	-0.00005000

Zero-point correction= 0.028356 (Hartree/Particle)
Thermal correction to Energy= 0.031214
Thermal correction to Enthalpy= 0.032158
Thermal correction to Gibbs Free Energy= 0.006737
Sum of electronic and zero-point Energies= -110.585274
Sum of electronic and thermal Energies= -110.582416
Sum of electronic and thermal Enthalpies= -110.581472
Sum of electronic and thermal Free Energies= -110.606893

Ts19

B	-0.41987800	0.01239700	0.09592200
N	-0.86181800	-1.36741300	0.17049000
H	-0.17223700	-2.10252600	0.12836600

N	-2.04387200	-1.78590500	-0.47921300
H	-2.84451300	-1.49368100	0.06407000
H	-2.10967200	-1.40361800	-1.41684300
N	-1.39268400	1.09013100	-0.04254300
H	-2.16033800	0.95460800	-0.68507000
N	-0.83476100	2.38903500	-0.06874200
H	-0.62169600	2.69026800	-1.01375300
H	-1.47328700	3.04649800	0.35688300
N	0.82729700	0.35507100	0.87805100
N	1.13535000	-0.42211200	2.04087500
H	0.34027400	-1.02213100	2.23235100
H	1.93548200	-1.00874300	1.82966100
H	0.79499900	1.34447900	1.11790600
H	0.48294700	0.08303000	-1.30245400
N	1.60325800	-0.22284800	-1.79586600
N	2.44745300	-0.22419700	-0.97875400
H	1.76587900	0.16750100	0.13918500

Zero-point correction= 0.165322 (Hartree/Particle)
Thermal correction to Energy= 0.176475
Thermal correction to Enthalpy= 0.177420
Thermal correction to Gibbs Free Energy= 0.128715
Sum of electronic and zero-point Energies= -469.165473
Sum of electronic and thermal Energies= -469.154320
Sum of electronic and thermal Enthalpies= -469.153376
Sum of electronic and thermal Free Energies= -469.202081

Ts20

B	0.45793000	0.06399200	0.75654600
N	1.42727700	0.12936300	-0.31689500
H	1.12496400	0.16154000	-1.27909500
N	2.64939300	-0.57965700	-0.23360800
H	3.28839800	-0.05835100	0.35125800
H	2.50309400	-1.49095100	0.18543700
N	-0.78127900	0.90104900	0.57518300
N	-0.75421600	1.99131300	-0.35053800
H	0.21716300	2.18706500	-0.56852800
H	-1.22565100	1.71095500	-1.20296200
H	-1.15991200	1.23609800	1.45282600
H	-0.33395400	-1.26459300	0.59085900
N	-1.29064400	-1.81284200	-0.04886700
N	-2.09153700	-1.02522400	-0.37877100
H	-1.64838400	0.09500700	0.08314300
H	0.83167700	-0.12474500	1.87880100

Zero-point correction= 0.128923 (Hartree/Particle)
Thermal correction to Energy= 0.137424
Thermal correction to Enthalpy= 0.138368
Thermal correction to Gibbs Free Energy= 0.095933
Sum of electronic and zero-point Energies= -358.500436
Sum of electronic and thermal Energies= -358.491936
Sum of electronic and thermal Enthalpies= -358.490992

Sum of electronic and thermal Free Energies= -358.533426

Ts21

H	-0.72840300	1.68892900	-1.15476100
B	-0.38091600	1.40725100	-0.04607300
H	-0.16691400	2.22604600	0.80208400
N	-0.82704900	0.09545000	0.46851900
H	-1.15195800	0.10261400	1.43043600
N	-1.60626700	-0.71671400	-0.40357400
H	-1.74410900	-1.63135200	0.00707700
H	-2.50268000	-0.27769700	-0.56909300
H	1.01209400	1.01603900	-0.38313600
N	1.90491600	0.11582700	-0.31829300
N	1.50327100	-0.85382900	0.19652100
H	0.36245300	-0.64597400	0.49555700

Zero-point correction= 0.091890 (Hartree/Particle)
Thermal correction to Energy= 0.097816
Thermal correction to Enthalpy= 0.098760
Thermal correction to Gibbs Free Energy= 0.062928
Sum of electronic and zero-point Energies= -247.836408
Sum of electronic and thermal Energies= -247.830481
Sum of electronic and thermal Enthalpies= -247.829537
Sum of electronic and thermal Free Energies= -247.865370

Ts22

H	-2.50969100	1.36669800	-1.31140700
H	-2.53785300	-1.14779700	-1.02588600
H	-1.07250100	-2.60409100	0.45198000
H	0.60532700	-1.22195800	1.68232800
H	1.51441600	0.99540600	0.36145200
H	-0.77635200	2.44668700	0.16213100
B	-1.73016500	0.77957300	-0.62351100
B	0.23594000	0.76932000	1.01274700
B	-0.93574500	-1.43338700	0.26982600
N	-0.76929400	1.44006800	0.16072100
N	0.22138700	-0.73736000	0.88006200
N	-1.79175800	-0.67574200	-0.54190500
H	0.53170700	1.21736100	2.08741000
N	2.36308600	0.49943600	-0.55497400
N	2.15129600	-0.62321700	-0.75518600
H	1.17177700	-0.95212200	-0.02433100

Zero-point correction= 0.117971 (Hartree/Particle)
Thermal correction to Energy= 0.125527
Thermal correction to Enthalpy= 0.126471
Thermal correction to Gibbs Free Energy= 0.085935
Sum of electronic and zero-point Energies= -353.107304
Sum of electronic and thermal Energies= -353.099748
Sum of electronic and thermal Enthalpies= -353.098804
Sum of electronic and thermal Free Energies= -353.139340

PBz

H	-3.52599700	2.28129800	-0.00016700
H	1.16240100	-3.36113400	0.00023300
H	-1.33543800	-3.54904000	0.00021900
H	1.16244600	3.36115500	0.00004500
H	4.79685600	-0.00005400	-0.00014200
H	3.37772600	2.08858100	-0.00016100
H	3.37767700	-2.08864200	-0.00007400
H	-1.33534700	3.54905300	0.00022700
H	-4.60634900	0.00003400	-0.00047300
H	-3.52609100	-2.28123000	-0.00032800
B	-2.91704800	1.25483400	-0.00009800
B	-0.74665000	-0.00000400	0.00007100
B	-2.91711800	-1.25479800	-0.00006800
N	-3.59997700	0.00004700	-0.00006700
N	-1.47494400	1.25856100	0.00013000
N	-1.47498400	-1.25859200	0.00001100
N	0.67320400	-2.48116600	0.00004500
B	-0.74928600	2.50913900	0.00017800
B	1.42665100	1.25417100	-0.00003200
B	1.42661800	-1.25417000	0.00003400
B	-0.74934000	-2.50913300	0.00008200
B	3.60251900	-0.00003500	-0.00007200
N	2.86413500	-1.22295700	-0.00003700
N	2.86416500	1.22290900	-0.00009500
N	0.69948100	0.00001200	0.00003100
N	0.67326100	2.48118100	0.00000200

Zero-point correction= 0.194330 (Hartree/Particle)
Thermal correction to Energy= 0.206457
Thermal correction to Enthalpy= 0.207401
Thermal correction to Gibbs Free Energy= 0.157001
Sum of electronic and zero-point Energies= -643.432178
Sum of electronic and thermal Energies= -643.420052
Sum of electronic and thermal Enthalpies= -643.419107
Sum of electronic and thermal Free Energies= -643.469507

PBz_Ts1

H	2.47136600	3.00562200	-0.77404000
H	-1.13478500	-3.38089000	-0.52674100
H	1.30639400	-3.10732800	-1.01809500
H	-2.18887000	3.19020300	0.40963200
H	-5.15678000	-0.75873700	0.68438800
H	-4.11389700	1.54178200	0.69156700
H	-3.46423200	-2.54253100	0.10269900
H	0.18071300	3.83387800	-0.08924400
H	3.88776100	0.98704700	-1.23688400
H	3.19400800	-1.44572400	-1.44829100
B	2.06568400	1.88167400	-0.72493400
B	0.19036100	0.24681100	-0.41287400

B	2.50670900	-0.60003800	-0.95832100
N	2.93892800	0.78681400	-0.96704300
N	0.68289900	1.61922800	-0.40135600
N	1.08323300	-0.84706100	-0.73220600
N	-0.80067900	-2.43201200	-0.49162800
B	-0.21405800	2.70633300	-0.09674400
B	-2.10476700	1.07960700	0.18545800
B	-1.71437600	-1.36988100	-0.16414300
B	0.57686000	-2.19095400	-0.77106700
B	-4.00609500	-0.54186500	0.44566500
N	-3.10562800	-1.60247600	0.12553800
N	-3.48551700	0.78762500	0.46951500
N	-1.20814300	-0.01336700	-0.12920200
N	-1.57760200	2.41919400	0.19681800
N	3.27715600	-1.20460500	1.15238300
H	2.75934900	-2.03988800	1.39045500
H	4.26973000	-1.41149500	1.15197400
N	2.91043900	-0.15979600	2.03110700
H	3.50165500	-0.11655800	2.85128500
H	2.98040400	0.71138900	1.51862700

Zero-point correction= 0.250313 (Hartree/Particle)
Thermal correction to Energy= 0.266078
Thermal correction to Enthalpy= 0.267022
Thermal correction to Gibbs Free Energy= 0.207745
Sum of electronic and zero-point Energies= -755.233131
Sum of electronic and thermal Energies= -755.217366
Sum of electronic and thermal Enthalpies= -755.216422
Sum of electronic and thermal Free Energies= -755.275699

PBz_1

H	2.38862200	3.08535100	-0.76357100
H	-1.05909900	-3.38629000	-0.49282300
H	1.40054100	-3.06921300	-0.82650600
H	-2.27405600	3.16396600	0.38096000
H	-5.18337700	-0.83179900	0.51216200
H	-4.17641000	1.48506900	0.57479300
H	-3.43439200	-2.58697400	0.01324200
H	0.09661000	3.85382000	-0.03973700
H	3.87605200	1.13495600	-1.14626500
H	3.20424800	-1.29739300	-1.48324500
B	2.03966600	1.94652200	-0.63898000
B	0.20248000	0.26070100	-0.32493800
B	2.60675600	-0.56374200	-0.72496500
N	2.96019100	0.88972600	-0.80692500
N	0.66073800	1.64839900	-0.29900800
N	1.12814300	-0.81461100	-0.58057300
N	-0.74663100	-2.43096300	-0.44307300
B	-0.26982800	2.71605300	-0.04582100
B	-2.13804500	1.05504800	0.16452700
B	-1.69195700	-1.38483100	-0.16560300

B	0.64153400	-2.15605300	-0.63852300
B	-4.02519500	-0.59644200	0.33129300
N	-3.09346000	-1.64104900	0.05471100
N	-3.52696400	0.74040100	0.38350700
N	-1.20863500	-0.02126300	-0.10698000
N	-1.63858400	2.40413700	0.20215900
N	3.30528000	-1.11440000	0.78778500
H	3.02316200	-2.08443300	0.89447700
H	4.31525100	-1.07945800	0.66950400
N	2.84117700	-0.37322300	1.90877500
H	3.53973500	-0.35893800	2.64024300
H	2.68727800	0.57498100	1.57916900

Zero-point correction= 0.251783 (Hartree/Particle)
Thermal correction to Energy= 0.267452
Thermal correction to Enthalpy= 0.268397
Thermal correction to Gibbs Free Energy= 0.209786
Sum of electronic and zero-point Energies= -755.235835
Sum of electronic and thermal Energies= -755.220166
Sum of electronic and thermal Enthalpies= -755.219222
Sum of electronic and thermal Free Energies= -755.277832

PBz_Ts2

H	-2.73286200	2.18100500	-1.09606800
H	1.76787400	-2.94835700	1.67303000
H	-0.73135500	-3.09026800	1.61433300
H	2.00098100	2.84598400	-1.71940500
H	5.51778500	-0.16120800	0.03587100
H	4.16549100	1.67690200	-1.05331300
H	4.02351400	-1.91372300	1.07796200
H	-0.48442600	3.14238400	-1.74835100
H	-3.90943300	0.22301100	-0.00973900
H	-2.90484600	-1.79144800	1.18252600
B	-2.17260600	1.30249400	-0.49576200
B	-0.04028700	0.00200600	-0.05880200
B	-2.29801400	-1.15359700	0.34333700
N	-2.90895000	0.13269700	-0.08216400
N	-0.71279100	1.13616500	-0.67318500
N	-0.80223100	-1.08418900	0.52425400
N	1.31180300	-2.17640500	1.21618300
B	0.05599000	2.18459300	-1.27068100
B	2.18578300	1.01549900	-0.65608900
B	2.10061300	-1.13798900	0.61161200
B	-0.11646200	-2.16628200	1.15315300
B	4.32239000	-0.12586900	0.01532200
N	3.54341300	-1.15363500	0.62572100
N	3.62651200	0.94527600	-0.62093500
N	1.41623600	-0.04101600	-0.03656100

N	1.48257000	2.10011600	-1.28607500
N	-2.52182200	-2.25158600	-1.03084000
H	-2.09847500	-3.13996000	-0.78042500
H	-3.52634000	-2.38071000	-1.12247100
N	-1.90699400	-1.76361100	-2.21708500
H	-2.44024900	-2.03820700	-3.03166200
H	-1.91441700	-0.74924800	-2.14590000
N	-2.15756400	2.47129100	1.33897700
H	-1.59290800	3.29920100	1.19979000
H	-3.11655000	2.74273000	1.52667900
N	-1.58059000	1.67249700	2.35507600
H	-1.96535900	1.88211100	3.26703500
H	-1.77260500	0.70234200	2.12609500

Zero-point correction= 0.307200 (Hartree/Particle)
Thermal correction to Energy= 0.326606
Thermal correction to Enthalpy= 0.327550
Thermal correction to Gibbs Free Energy= 0.259571
Sum of electronic and zero-point Energies= -867.035275
Sum of electronic and thermal Energies= -867.015869
Sum of electronic and thermal Enthalpies= -867.014924
Sum of electronic and thermal Free Energies= -867.082904

PBz_2

H	-2.82501800	-2.05527100	1.03202000
H	1.88681400	2.95159300	-1.60325000
H	-0.60369300	3.18855100	-1.54273400
H	1.88702400	-2.95145400	1.60339000
H	5.52428700	0.00020400	0.00014300
H	4.09985200	-1.82861300	1.00990600
H	4.09974800	1.82883800	-1.00979800
H	-0.60354800	-3.18851900	1.54300200
H	-3.92704700	0.00004600	0.00061800
H	-2.82499100	2.05504300	-1.03226700
B	-2.24136800	-1.27581000	0.30335100
B	-0.03940100	-0.00006200	-0.00006800
B	-2.24142400	1.27554000	-0.30363900
N	-2.91975600	-0.00007000	0.00004500
N	-0.75636000	-1.14189300	0.53845600
N	-0.75641800	1.14176800	-0.53843100
N	1.40044500	2.17904300	-1.17993000
B	-0.02854300	-2.22232800	1.11970100
B	2.14699200	-1.09713500	0.59882100
B	2.14692700	1.09712900	-0.59895800
B	-0.02867400	2.22230200	-1.11960100
B	4.32794300	0.00010500	0.00002100
N	3.59024200	1.06881400	-0.59096200
N	3.59030500	-1.06871900	0.59088400

N	1.41982300	-0.00007600	-0.00015700
N	1.40057600	-2.17903600	1.17991800
N	-2.34064300	2.24433700	1.21589500
H	-1.84729100	3.11681600	1.05545100
H	-3.32789100	2.44409700	1.35175900
N	-1.74578600	1.56773900	2.31532100
H	-2.22821500	1.79019500	3.17594900
H	-1.84507200	0.57313500	2.12648500
N	-2.34038700	-2.24422500	-1.21565200
H	-1.84660800	-3.11648400	-1.05526700
H	-3.32758200	-2.44446200	-1.35124000
N	-1.74610100	-1.56755500	-2.31536700
H	-2.22876300	-1.79034700	-3.17578100
H	-1.84584800	-0.57297300	-2.12667100

Zero-point correction= 0.308388 (Hartree/Particle)
Thermal correction to Energy= 0.327941
Thermal correction to Enthalpy= 0.328885
Thermal correction to Gibbs Free Energy= 0.261400
Sum of electronic and zero-point Energies= -867.035486
Sum of electronic and thermal Energies= -867.015933
Sum of electronic and thermal Enthalpies= -867.014988
Sum of electronic and thermal Free Energies= -867.082474

PBz_Ts3

H	-2.37187200	2.37196800	-0.02117100
H	2.56049300	-2.83704400	1.55523100
H	0.11058900	-2.99812700	2.03212300
H	1.96840100	2.83894500	-1.99038500
H	5.80754400	-0.16126000	-1.06865600
H	4.24060400	1.66140000	-1.84817800
H	4.61493900	-1.85338300	0.38014700
H	-0.40718200	3.22006600	-1.31397700
H	-3.09415200	0.29263500	1.58255800
H	-2.18942500	-1.84414500	1.78619900
B	-1.72650300	1.47153600	0.48740000
B	0.40829800	0.08667000	0.23789400
B	-1.74179500	-1.19239500	0.85938500
N	-2.48780800	0.19621400	0.77549200
N	-0.36629500	1.25999500	-0.13337400
N	-0.20952200	-1.00403800	0.95484600
N	2.01465200	-2.06870200	1.20185500
B	0.21910300	2.25511000	-0.97412300
B	2.42055800	1.05101200	-0.93494300
B	2.64118800	-1.06510700	0.38938200
B	0.59744500	-2.07732000	1.43883600
B	4.64708100	-0.10571200	-0.78512700
N	4.04262300	-1.09683900	0.04421900
N	3.82172900	0.95656700	-1.26464700

N	1.82763700	0.02756300	-0.10271400
N	1.58311100	2.12571500	-1.39396200
N	-2.09614900	-2.02906200	-0.46135900
H	-2.15542000	-3.01912400	-0.26052700
H	-3.28502700	-1.45666600	-0.91990800
N	-1.25036100	-1.89248100	-1.61889700
H	-1.47294100	-0.99810500	-2.04546300
H	-0.28409800	-1.83763800	-1.30745400
N	-3.99350800	-0.51157600	-1.17745300
H	-5.00029700	-0.61611900	-1.08357400
H	-3.41075200	0.00604200	-0.25330800
N	-3.57099000	0.08148300	-2.39858100
H	-3.90882500	-0.45188700	-3.18907300
H	-3.90631400	1.03383400	-2.46513100
N	-1.38448000	2.20633700	2.02542600
H	-0.65818400	2.88027600	1.79377200
H	-2.19942100	2.71717800	2.35011800
N	-0.98631500	1.29357100	3.05120300
H	-0.67664900	0.43702200	2.59515300
H	-0.21915200	1.68195200	3.58360800

Zero-point correction= 0.359638 (Hartree/Particle)
Thermal correction to Energy= 0.381180
Thermal correction to Enthalpy= 0.382124
Thermal correction to Gibbs Free Energy= 0.310397
Sum of electronic and zero-point Energies= -978.822427
Sum of electronic and thermal Energies= -978.800885
Sum of electronic and thermal Enthalpies= -978.799941
Sum of electronic and thermal Free Energies= -978.871669

PBz_3

H	-2.95799300	-0.76681900	1.32511500
H	2.45092600	2.92652600	-1.31348400
H	0.02807700	3.53238800	-1.29880200
H	1.45255600	-3.13645400	1.39333500
H	5.54229500	-0.69624200	0.04859900
H	3.82203300	-2.35654300	0.87006500
H	4.44679600	1.41612100	-0.81021200
H	-1.02999200	-2.96456900	1.32362900
H	-2.66577500	0.22704700	-1.61363000
H	-2.34103500	2.61886400	-1.16735600
B	-2.35498100	-0.74918000	0.27644600
B	0.04062200	0.18051200	-0.07524700
B	-1.95512300	1.84034200	-0.31932300
N	-2.78886800	0.42725300	-0.62392800
N	-0.85744400	-0.91238500	0.32189700
N	-0.47167400	1.45339400	-0.48558300
N	1.84047300	2.19712900	-0.98457300
B	-0.30502200	-2.09033100	0.91012100

B	2.02323200	-1.29524700	0.48277700
B	2.39302900	0.96487400	-0.51299300
B	0.42904800	2.46170400	-0.94519700
B	4.36188600	-0.50806100	0.02300800
N	3.81417800	0.70546700	-0.48185100
N	3.44767800	-1.49781200	0.50250800
N	1.48338800	-0.06567600	-0.04446200
N	1.10077100	-2.28870000	0.98080500
N	-2.38259400	2.31108300	1.04482700
H	-2.55115700	3.30165800	1.11109000
N	-1.66243700	1.90442500	2.20190500
H	-2.01965500	1.01133500	2.51507300
H	-0.67914300	1.77821300	1.97562700
H	-3.75543000	0.69045700	-0.46552700
N	-2.93452000	-2.13350700	-0.48708000
H	-2.72670100	-2.90789500	0.14296300
H	-3.94283300	-2.05273500	-0.58185900
N	-2.36307900	-2.29250400	-1.78416200
H	-1.38088000	-2.04575600	-1.68868700
H	-2.43665700	-3.25583000	-2.08604200

Zero-point correction= 0.310333 (Hartree/Particle)
Thermal correction to Energy= 0.328875
Thermal correction to Enthalpy= 0.329820
Thermal correction to Gibbs Free Energy= 0.265106
Sum of electronic and zero-point Energies= -867.030556
Sum of electronic and thermal Energies= -867.012013
Sum of electronic and thermal Enthalpies= -867.011069
Sum of electronic and thermal Free Energies= -867.075783

PBz_Ts4

H	2.95995600	1.14430600	1.35372600
H	-2.07468000	-2.39301400	-2.28865500
H	0.39157900	-2.78645600	-2.29650600
H	-1.72545300	2.85663400	1.87961300
H	-5.52098600	0.62273000	-0.38364200
H	-3.99810900	2.09014100	1.00050500
H	-4.21515100	-1.13959400	-1.64159800
H	0.75802100	3.01840500	1.77105800
H	2.64126500	0.56424200	-1.68851200
H	2.63228300	-1.88293600	-1.64893000
B	2.30549400	1.19788200	0.33608800
B	0.01127200	0.01579200	-0.07746900
B	2.16451500	-1.25687900	-0.70342800
N	2.85265300	0.22699200	-0.75167000
N	0.81293300	1.16751500	0.42510000
N	0.66283300	-1.03403000	-0.85598200
N	-1.55102600	-1.75733700	-1.71039200
B	0.13685200	2.14148400	1.21240700

B	-2.10024700	1.24540200	0.53215100
B	-2.22841100	-0.69388000	-1.02183100
B	-0.11723100	-1.90699100	-1.65860000
B	-4.33168300	0.50114200	-0.33695700
N	-3.66187100	-0.51039300	-1.08412500
N	-3.53472900	1.37304200	0.46813900
N	-1.44322100	0.22201500	-0.23122500
N	-1.28393200	2.14123300	1.32632400
N	2.53393300	-1.86996100	0.65028300
H	3.50280400	-1.76993300	0.92549200
N	2.25208000	-3.27548300	0.68001100
H	1.26268300	-3.38032500	0.87053300
H	2.39408000	-3.66291100	-0.25260900
H	3.85981400	0.11532100	-0.69612700
N	2.67236200	2.74078100	-0.25055900
H	2.36094100	3.38182500	0.47931700
H	3.67669300	2.84117200	-0.36469700
N	2.03983900	2.96766200	-1.50933000
H	1.10830600	2.56436000	-1.42068200
H	1.95471200	3.96091400	-1.68583300
N	-0.03266900	-1.02657900	1.90266300
H	-0.23361500	-0.43240900	2.69565300
N	-0.92451500	-2.12891800	1.91104600
H	-1.13420400	-2.36808100	0.94815600
H	-0.52207000	-2.93572700	2.37258800
H	0.95563500	-1.28421300	1.86734600

Zero-point correction= 0.366770 (Hartree/Particle)
Thermal correction to Energy= 0.388310
Thermal correction to Enthalpy= 0.389254
Thermal correction to Gibbs Free Energy= 0.318555
Sum of electronic and zero-point Energies= -978.831030
Sum of electronic and thermal Energies= -978.809491
Sum of electronic and thermal Enthalpies= -978.808547
Sum of electronic and thermal Free Energies= -978.879246

PBz_4

H	-2.68618100	2.19711900	-1.17217900
H	1.54923200	-2.34353000	2.58236500
H	-0.94842900	-2.25779200	2.60612000
H	2.14941400	2.19698600	-2.32138600
H	5.48701000	-0.23678000	0.41520000
H	4.25869600	1.21657900	-1.24994200
H	3.88533000	-1.57051500	1.84421200
H	-0.20079200	3.00358300	-2.05193500
H	-2.48244500	1.07796300	1.66455200
H	-3.01823100	-1.25919100	1.58950300
B	-1.96377300	1.75344800	-0.30593200

B	-0.07723500	-0.13766100	-0.22347700
B	-2.40884700	-0.75444100	0.65359200
N	-2.74764900	0.85148200	0.70757100
N	-0.63488700	1.21480800	-0.69506600
N	-0.90312400	-0.85988800	0.80456500
N	1.14999000	-1.76144600	1.86526500
B	0.20714300	1.99138900	-1.52991400
B	2.23557600	0.71841100	-0.78544100
B	2.00923600	-0.95287600	1.04066200
B	-0.29305400	-1.65029000	1.80320300
B	4.29505700	-0.19286300	0.31354700
N	3.45367700	-0.96976300	1.16189500
N	3.67258700	0.65192000	-0.65814800
N	1.41145200	-0.08965400	0.05981100
N	1.58167600	1.61832000	-1.72406100
N	-2.91153600	-1.27934700	-0.70788100
H	-3.77078100	-0.86687600	-1.04770000
N	-3.13044500	-2.69822300	-0.68690000
H	-2.22616400	-3.14581100	-0.77507100
H	-3.46917300	-2.96163900	0.23783400
H	-3.74963800	0.99527900	0.63793900
N	-1.59586800	3.14643000	0.61208200
H	-1.09810600	3.75562300	-0.03721400
H	-2.43879200	3.62134100	0.92202300
N	-0.82497100	2.78082700	1.75579700
H	-0.17878800	2.05718200	1.43697900
H	-0.29166900	3.57361600	2.09028500
N	-0.25932600	-1.06028900	-1.65733200
H	0.14535000	-0.54914400	-2.43555000
N	0.34009100	-2.35338900	-1.60282700
H	0.40282000	-2.60740800	-0.62122600
H	-0.25580100	-3.02253900	-2.07377400
H	-1.29504900	-1.09214200	-1.71563400

Zero-point correction= 0.367933 (Hartree/Particle)
Thermal correction to Energy= 0.389503
Thermal correction to Enthalpy= 0.390447
Thermal correction to Gibbs Free Energy= 0.319378
Sum of electronic and zero-point Energies= -978.834408
Sum of electronic and thermal Energies= -978.812838
Sum of electronic and thermal Enthalpies= -978.811894
Sum of electronic and thermal Free Energies= -978.882963

PBz_Ts5

H	2.73720000	-0.40063200	-1.79503900
H	-2.55706800	1.93873700	2.36726000
H	-0.16068300	2.64205400	2.42113500
H	-1.62095400	-2.74653300	-2.34634800

H	-5.56731500	-1.44340400	0.35216300
H	-3.92159100	-2.48668900	-1.26262300
H	-4.48989600	0.39940000	1.70681800
H	0.85913400	-2.62632400	-2.24510000
H	2.71959100	-0.08528100	1.27830400
H	2.15214000	2.26437200	1.52640300
B	2.24376400	-0.72816700	-0.72140000
B	-0.25478500	0.25742900	-0.33575900
B	1.74838000	1.64967600	0.54383300
N	2.67076800	0.35398900	0.35910000
N	0.70259800	-0.87761500	-0.75920700
N	0.29601000	1.17690100	0.73217000
N	-1.97515800	1.47197000	1.69172100
B	0.15413800	-1.87251000	-1.62433400
B	-2.17554100	-1.33689600	-0.84346300
B	-2.51390900	0.39022900	0.90826100
B	-0.56732100	1.81781500	1.64588400
B	-4.42580500	-1.10225400	0.23969600
N	-3.88440900	-0.05841300	1.04595900
N	-3.55571300	-1.73783300	-0.69873600
N	-1.65835000	-0.26567000	-0.04307400
N	-1.26862800	-2.01656100	-1.74917700
N	1.87236900	2.50272400	-0.74391300
H	2.79485200	2.53857100	-1.15874200
N	1.46593900	3.86453500	-0.53490100
H	0.45562000	3.85948400	-0.45341800
H	1.79612700	4.15913100	0.38409800
H	3.63040300	0.61981700	0.16236600
N	2.85847700	-2.08955500	-0.21848700
H	1.85749500	-2.35633000	1.15500200
H	2.62874600	-2.80748800	-0.90277300
N	4.28178100	-1.96129600	-0.10571600
H	4.66202600	-2.78270800	0.34474000
H	4.69864200	-1.88111100	-1.02923800
N	-0.33851200	1.19433000	-1.73645000
H	-0.44992200	0.59737400	-2.55001400
N	-1.37514000	2.17858300	-1.75735100
H	-1.71575700	2.28291500	-0.80694800
H	-0.98025500	3.06138700	-2.05744400
H	0.60819900	1.65226200	-1.70985800
N	0.95164100	-2.02154600	1.64570400
H	0.29637800	-2.75467000	1.90546600
H	0.57356800	-1.49978000	0.76178500
N	1.26406500	-1.09877900	2.68844300
H	0.65168800	-0.29239500	2.58630400
H	1.14286800	-1.53913100	3.58951000

Zero-point correction=	0.420995 (Hartree/Particle)
Thermal correction to Energy=	0.445310
Thermal correction to Enthalpy=	0.446254

Thermal correction to Gibbs Free Energy= 0.370472
Sum of electronic and zero-point Energies= -1090.632142
Sum of electronic and thermal Energies= -1090.607827
Sum of electronic and thermal Enthalpies= -1090.606882
Sum of electronic and thermal Free Energies= -1090.682664

PBz_5

H	-2.54836400	-0.90189300	1.16263000
H	2.53925700	2.47783600	-1.93675900
H	0.11330700	3.05588400	-2.03454000
H	1.52550500	-3.27554700	1.36880400
H	5.62086900	-1.07737000	-0.34801800
H	3.90012600	-2.61244600	0.69254000
H	4.54043800	0.97373600	-1.35510900
H	-0.92348800	-3.31120300	0.93469800
H	-2.64781500	-0.00008400	-1.81104600
H	-2.22817400	2.41110900	-1.41457900
B	-2.30252100	-1.06465100	-0.02680700
B	0.14547400	0.07095500	0.02365800
B	-1.85449900	1.57646400	-0.60511700
N	-2.70445900	0.23578000	-0.82099200
N	-0.73244900	-1.26355400	-0.19976700
N	-0.36998300	1.22636200	-0.76593700
N	1.94351100	1.83824000	-1.43834700
B	-0.19259200	-2.43784400	0.57696100
B	2.12997000	-1.47941500	0.35384800
B	2.49750300	0.65843100	-0.84948000
B	0.51558600	2.08934900	-1.44832900
B	4.45044800	-0.83978100	-0.30813400
N	3.91019800	0.33934700	-0.89268000
N	3.53716900	-1.75054900	0.32082200
N	1.61169600	-0.25585700	-0.16357300
N	1.17318100	-2.46780900	0.87874400
N	-2.10460900	2.05174500	0.85699800
H	-3.06217400	2.01059700	1.18326100
N	-1.65885600	3.40389400	1.06188700
H	-0.64739400	3.38319700	0.98203300
H	-1.96081800	3.95848900	0.26062000
H	-3.69937100	0.37432600	-0.65871400
N	-3.00983400	-2.22439100	-0.70578200
H	-2.76639900	-3.13003300	-0.32060000
N	-4.42429600	-2.02517500	-0.67340700
H	-4.85483900	-2.54683400	-1.42445500
H	-4.82769800	-2.33235600	0.20649000
N	-0.15721200	0.40292200	1.62126900
H	-0.29129800	-0.41719400	2.20526300
N	0.84282300	1.21451000	2.24460600
H	1.54124000	1.44064700	1.54480600
H	0.40529700	2.07019800	2.56375700

H	-1.07520100	0.97793200	1.54273800
H	-0.59800800	-1.47478500	-1.19369800

Zero-point correction= 0.366243 (Hartree/Particle)
Thermal correction to Energy= 0.387549
Thermal correction to Enthalpy= 0.388493
Thermal correction to Gibbs Free Energy= 0.318762
Sum of electronic and zero-point Energies= -978.831537
Sum of electronic and thermal Energies= -978.810231
Sum of electronic and thermal Enthalpies= -978.809287
Sum of electronic and thermal Free Energies= -978.879019

PBz_Ts6

H	-3.22761300	-0.35714200	1.52765200
H	2.42431600	2.42796600	-2.07592300
H	-0.00394200	2.92155300	-2.15320400
H	1.65539900	-3.33477700	1.22359300
H	5.67429500	-0.85841000	-0.21020700
H	4.01381200	-2.44866800	0.83409700
H	4.52111600	1.08335800	-1.34387400
H	-0.61730800	-3.61616900	0.17589600
H	-2.90179000	-0.11409800	-1.59734500
H	-2.23628000	2.38158100	-1.43039400
B	-3.21801100	-0.68795700	0.38658500
B	0.13989500	-0.04005700	-0.05153800
B	-1.84981700	1.59731800	-0.57780000
N	-3.00111100	0.34472600	-0.69183300
N	-0.63287700	-1.35242400	-0.20267200
N	-0.43580700	1.12673600	-0.81295700
N	1.86213700	1.78331100	-1.54623500
B	-0.04976400	-2.55644800	0.26851400
B	2.17991600	-1.45041400	0.38911200
B	2.47950600	0.66927900	-0.88049900
B	0.43153000	1.98339700	-1.54195700
B	4.48930000	-0.68951100	-0.21701400
N	3.90996800	0.43657700	-0.87381000
N	3.61310600	-1.62425400	0.41925500
N	1.63540700	-0.25106300	-0.17558900
N	1.26098400	-2.48381600	0.85629500
N	-2.04770800	2.13815100	0.85500700
H	-3.00331700	2.23521400	1.17528000
N	-1.45241100	3.43938500	0.99518600
H	-0.44827200	3.30138400	0.96991700
H	-1.65680600	3.98149800	0.15515200
H	-3.86019000	0.88892500	-0.76433900
N	-3.64263800	-1.97186600	0.03443000
H	-3.79234400	-2.67295900	0.74442100
N	-3.50920000	-2.43810700	-1.28802400
H	-2.80515200	-3.16749900	-1.32626500

H	-4.38846600	-2.81488900	-1.61814900
N	-0.11062000	0.28627900	1.61321200
H	-0.15745500	-0.58610700	2.13104000
N	0.85402800	1.13032300	2.24519800
H	1.57046200	1.33134900	1.55437900
H	0.39778600	1.99066900	2.52088600
H	-1.02398800	0.78084400	1.61684400
H	-1.26984400	-1.42936500	-0.97870300

Zero-point correction= 0.365675 (Hartree/Particle)
Thermal correction to Energy= 0.387292
Thermal correction to Enthalpy= 0.388236
Thermal correction to Gibbs Free Energy= 0.317833
Sum of electronic and zero-point Energies= -978.811906
Sum of electronic and thermal Energies= -978.790289
Sum of electronic and thermal Enthalpies= -978.789345
Sum of electronic and thermal Free Energies= -978.859748

PBz_6

H	-4.51665200	0.25980800	-2.30970900
H	2.40006700	2.77495600	-1.58080300
H	-0.07161100	3.01650300	-1.78291200
H	2.11687800	-3.48736900	0.77891800
H	5.84313400	-0.65111400	-0.73371100
H	4.32978400	-2.47970300	0.14137900
H	4.52620400	1.44078500	-1.28569100
H	-0.40120500	-3.52677000	0.95465400
H	-1.82602300	-0.98598200	-1.21538400
H	-2.27164000	2.12126700	-1.25501200
B	-3.82926000	-0.37415900	-1.57477200
B	0.34156300	-0.01967300	0.18732800
B	-1.83970500	1.17476900	-0.61874200
N	-2.36646800	-0.19696800	-1.57434100
N	-0.41244300	-1.31914900	0.38192700
N	-0.34280200	1.08931300	-0.58558400
N	1.87791600	2.04263500	-1.12879300
B	0.23189300	-2.54883600	0.65970600
B	2.44790800	-1.48384600	0.14082400
B	2.56451800	0.84196400	-0.71509200
B	0.43910000	2.09485900	-1.20720800
B	4.66281800	-0.53158800	-0.57331500
N	3.99062700	0.68223200	-0.89821200
N	3.87473700	-1.60618300	-0.06418100
N	1.79939200	-0.23050200	-0.13711500
N	1.66245300	-2.60694400	0.60402700
N	-2.49139300	1.03567200	0.76401400
H	-3.43452900	0.67107300	0.77030000
N	-2.57328900	2.31737100	1.41150600
H	-1.65352000	2.54272300	1.77112700

H	-2.76561200	3.03240800	0.71028300
H	-1.98870700	0.07653100	-2.47379400
N	-4.41792300	-1.26187200	-0.67164600
H	-5.41921400	-1.37595800	-0.62465700
N	-3.64458900	-2.02872700	0.22056700
H	-3.88594100	-1.80838800	1.17920200
H	-3.78731600	-3.01730600	0.05729500
N	0.29239800	0.56591200	1.86551600
H	0.68933700	-0.17263100	2.43746600
N	0.98184500	1.77982100	2.13435400
H	1.03567200	2.29846600	1.26369300
H	0.48937400	2.32751400	2.82768000
H	-0.72174200	0.60997200	2.00388900
H	-1.39414700	-1.27251300	0.61787900

Zero-point correction= 0.365214 (Hartree/Particle)
Thermal correction to Energy= 0.388154
Thermal correction to Enthalpy= 0.389098
Thermal correction to Gibbs Free Energy= 0.315121
Sum of electronic and zero-point Energies= -978.825025
Sum of electronic and thermal Energies= -978.802085
Sum of electronic and thermal Enthalpies= -978.801141
Sum of electronic and thermal Free Energies= -978.875118

PBz_7

H	-1.12329100	-3.35919800	-0.61038900
H	1.33934400	-3.21509500	-0.92149200
H	-1.99180400	3.26031000	-0.09341400
H	-5.13978100	-0.53627000	0.05932300
H	-3.99707800	1.71712800	0.12354000
H	-3.47387800	-2.40995000	-0.27186600
H	0.22209100	3.73476600	-1.18957800
H	3.34676800	-1.90193100	-0.69922700
B	0.39482600	0.23586000	-0.19078600
B	2.70129500	-0.91757200	-0.47742300
N	0.79578900	1.55459300	-0.79513500
N	1.26463200	-0.96698000	-0.49517200
N	-0.74583000	-2.43343200	-0.49260100
B	-0.08347500	2.66380800	-0.74892800
B	-1.95914400	1.13830500	-0.09390100
B	-1.64730600	-1.31670400	-0.30279100
B	0.66091100	-2.26311600	-0.66811100
B	-3.95751400	-0.37831400	-0.02765100
N	-3.07653100	-1.48746800	-0.21057800
N	-3.38126000	0.92621900	0.03444300
N	-1.08825700	-0.00142900	-0.20679300
N	-1.37596600	2.46492100	-0.14160200

N	3.45287100	0.24333200	-0.14596000
H	3.06497400	1.16569900	-0.03618100
N	4.86668000	0.28818700	-0.11073800
H	5.20451000	-0.37017800	0.57838300
H	5.23659300	0.01356400	-1.01176100
N	0.72980400	0.53726600	1.53730800
H	0.25665400	1.40464100	1.77734000
N	0.27836300	-0.49413600	2.41119100
H	0.13755200	-1.32445800	1.84468300
H	0.98745400	-0.69655600	3.10339400
H	1.73479100	0.68143000	1.59581300
H	1.60506700	1.60726300	-1.39115700

Zero-point correction= 0.275772 (Hartree/Particle)
Thermal correction to Energy= 0.293557
Thermal correction to Enthalpy= 0.294501
Thermal correction to Gibbs Free Energy= 0.231867
Sum of electronic and zero-point Energies= -786.179164
Sum of electronic and thermal Energies= -786.161379
Sum of electronic and thermal Enthalpies= -786.160435
Sum of electronic and thermal Free Energies= -786.223069

PBz_Ts7

H	-1.11162700	-3.33555600	-0.68301400
H	1.35401000	-3.18177000	-1.00579800
H	-1.99562500	3.28579900	-0.09568800
H	-5.11189400	-0.53663600	0.14688200
H	-3.98295800	1.72354300	0.15638500
H	-3.44584500	-2.40171900	-0.23017800
H	0.31263800	3.81376400	-0.96162800
H	3.35012000	-1.84049000	-0.84353800
B	0.38053700	0.24578500	-0.34917200
B	2.70367600	-0.87729500	-0.54674700
N	0.81275200	1.59193800	-0.76093400
N	1.26271400	-0.93066100	-0.59049900
N	-0.73515400	-2.40784500	-0.57813500
B	-0.05145700	2.71408800	-0.66014700
B	-1.95263900	1.16274500	-0.13856100
B	-1.63346100	-1.29746500	-0.35277200
B	0.66860700	-2.23423800	-0.75761700
B	-3.93567900	-0.37132200	0.00938300
N	-3.05445300	-1.47522200	-0.20018000
N	-3.36648800	0.93719600	0.03675100
N	-1.07717800	0.02720300	-0.30018700
N	-1.38346500	2.49063800	-0.17599900
N	3.44515000	0.25170200	-0.12094100
H	3.03973600	1.12580100	0.16785000

N	4.85680500	0.30245300	-0.05701900
H	5.19379600	-0.45054800	0.52805700
H	5.24101300	0.17404100	-0.98399900
N	0.70484400	0.43762000	1.74204600
H	0.19408000	1.26381100	2.02989900
N	0.20136800	-0.69146900	2.43557300
H	0.25431100	-1.48626900	1.80841300
H	0.74362900	-0.89231000	3.26581900
H	1.69841700	0.58394100	1.88609500
H	1.70002000	1.70824300	-1.22073100

Zero-point correction= 0.274335 (Hartree/Particle)
Thermal correction to Energy= 0.292053
Thermal correction to Enthalpy= 0.292997
Thermal correction to Gibbs Free Energy= 0.229971
Sum of electronic and zero-point Energies= -786.179355
Sum of electronic and thermal Energies= -786.161636
Sum of electronic and thermal Enthalpies= -786.160692
Sum of electronic and thermal Free Energies= -786.223718

PBz_8

H	0.98457200	-3.37912300	0.19012300
H	-1.49178400	-3.21486100	0.44417900
H	1.94990800	3.26671100	0.00070400
H	5.00859900	-0.58034700	-0.50030100
H	3.91232600	1.68913800	-0.33925800
H	3.31974200	-2.44389300	-0.24268600
H	-0.47161600	3.80600800	0.48255500
H	-3.46579100	-1.76421600	0.59043200
B	-0.44129200	0.21156300	0.22646500
B	-2.79599700	-0.85883400	0.18532700
N	-0.90977800	1.56370700	0.39264000
N	-1.34639500	-0.93362700	0.26599600
N	0.62357900	-2.43963800	0.17352900
B	-0.04683800	2.70056300	0.32449000
B	1.88152800	1.14520600	-0.05429500
B	1.52769000	-1.33480700	-0.00107800
B	-0.78189900	-2.26348400	0.31207700
B	3.83777400	-0.40927600	-0.33468900
N	2.94090600	-1.51245000	-0.20009100
N	3.28656900	0.90498200	-0.25790700
N	0.98405700	0.00768600	0.04547600
N	1.33596000	2.47142800	0.06094300
N	-3.48402000	0.22808100	-0.38962300
H	-3.02737300	0.95165100	-0.92113600
N	-4.88854900	0.30231200	-0.53021500
H	-5.23296800	-0.55602900	-0.94055500
H	-5.31188500	0.40999700	0.38163800
H	-1.87486800	1.71293900	0.63757300

Zero-point correction=	0.218535 (Hartree/Particle)
Thermal correction to Energy=	0.232746
Thermal correction to Enthalpy=	0.233690
Thermal correction to Gibbs Free Energy=	0.178308
Sum of electronic and zero-point Energies=	-674.380947
Sum of electronic and thermal Energies=	-674.366736
Sum of electronic and thermal Enthalpies=	-674.365792
Sum of electronic and thermal Free Energies=	-674.421173