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C=C/B-N substitution in five membered heterocycles. A computational analysis.

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Harmonic Oscillator Model of Aromaticity (HOMA) values were calculated using **Equation 1**.

Equation 1

$$\mathrm{HOMA} = 1 - \frac{\alpha}{n}\sum_{n=0}^{n}(\mathrm{R_{opt}} - \mathrm{R_j})^2$$

Where optimum bond distances (R_{opt}) were single or double bond distances obtained either from experiment or DFT calculations as described above and α is an empirical normalization constant. These values, if available, were taken from Krygowski et al.(*1*) For bonds shown in Table S1 experimentally derived parameters were either not available in the literature or involved use of substituted derivatives to derive parameters, thus these were calculated using model compounds shown in Table S1 and equations shown in the footnote. The force constants and optimum bond distances taken from DFT optimized (B3LYP/6-31+G(d)) geometries of model molecules.

Table S1. Optimized bond distances and empirical normalization constant for model systems used in Equation 1.

Bond	Model Molecule	α*	R_{opt} #
B-O	BH_3OH_2/ BH_2OH	17.03	1.408
B-B	H_2B-BH_2/HBBH	303.31	1.570
B-N	BH_3NH_3/BH_2NH_2	40.05	1.455
B-S	BH_3SH_2/BH_2SH	32.75	1.838
N-S	$HSNH_2$/SNH	780.42	1.704
N-N	H_2NNH_2/HNNH	58.58	1.311

* $\alpha = 2([R_{(s)} - R_{opt}]^2 + [R_{(d)} - R_{opt}]^2)^{-1}$

\# $R_{opt} = [R_{(s)} + wR_{(d)}]/(1+w)$, w = ratio of force constant

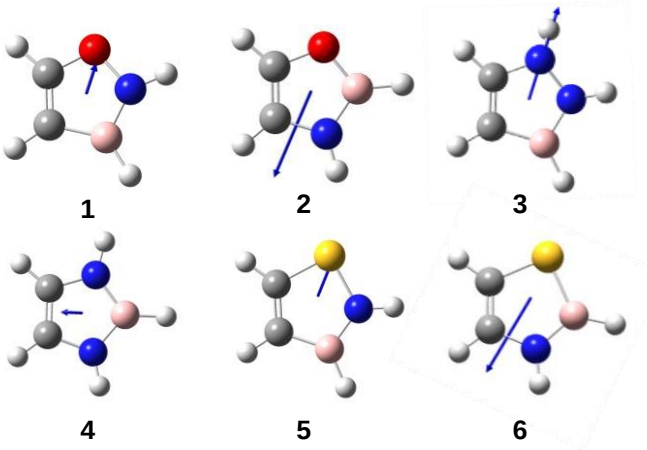


Figure S1. Direction of dipole moments in five memebered ring azaborole heterocycles (1-6).

Effect of solvent on the relative stability

Despite the larger dipole moments observed for O-B-N, S-B-N and N-N-B systems, solvent effects on the relative stability seem marginal as seen in Table S2. As the

dielectric constant of the solvent medium increased (DCM: ε=8.93, ethanol: ε=24.85 and water: ε=78.36), only a marginal increase (0.1-0.5 kcal/mol) in the stabilization of polar azaboroles (with larger dipole moments) was observed. Thus stability difference increased marginally for the oxazaborole (structures **1** and **2**) series, while it decreased for the diazaborole (structures **3** and **4**) series. For the thiazaborole series (structures **5** and **6**) the difference in dipole moment is smaller than the other two series thus solvent effect on the stability difference was minimal.

Table S2. Effect of solvent on the relative stability (kcal/mol) of azaboroles.

Entry	Molecular framework	ΔG		
		DCM	Ethanol	Water
1	**1** → **2**	-54.9	-55.0	-55.0
2	**3** → **4**	-39.1	-38.9	-38.8
3	**5** → **6**	-25.8	-25.8	-23.4
4	furan + BH_2NH_2 → CH_2=CH_2 +**1**	36.1	36.2	36.3
5	furan + BH_2NH_2 → CH_2=CH_2 +**2**	-21.9	-22.3	-22.4
6	pyrrole + BH_2NH_2 → CH_2=CH_2 + **3**	26.7	26.0	25.8
7	pyrrole + BH_2NH_2 → CH_2=CH_2 + **4**	-12.4	-12.8	-13.0
8	thiophene + BH_2NH_2 → CH_2=CH_2 + **5**	16.2	15.9	15.7
9	thiophene + BH_2NH_2 → CH_2=CH_2 + **6**	-9.6	-10.0	-10.1
10	benzene + BH_2NH_2 → CH_2=CH_2 + 1,2-azaborine	12.7	12.3	12.1

Table S3. Correlation matrix between the NICS values calculated at different points (values in bracket indicate distance in Å from the ring center).

	ASE1b	ASE2c	HOMA	NICS(0.0)	NICS(0.5)	NICS(1.0)	NICS(1.5)	NICS(2.0)	NICS(2.5)	NICS(3.0)	NICS(1.0)zz	NICS(0)zz
ASE1b	1.00	0.98	-0.34	0.79	0.87	0.92	0.92	0.90	0.87	0.85	-0.76	-0.74
ASE2c	0.98	1.00	-0.30	0.84	0.92	0.96	0.96	0.95	0.92	0.89	-0.85	-0.83
HOMA	-0.34	-0.30	1.00	-0.38	-0.29	-0.21	-0.26	-0.34	-0.40	-0.43	0.10	0.15
NICS(0.0)	0.79	0.84	-0.38	1.00	0.97	0.92	0.91	0.88	0.81	0.65	-0.74	-0.73
NICS(0.5)	0.87	0.92	-0.29	0.97	1.00	0.98	0.95	0.91	0.82	0.64	-0.77	-0.76
NICS(1.0)	0.92	0.96	-0.21	0.92	0.98	1.00	0.99	0.94	0.84	0.66	-0.82	-0.81
NICS(1.5)	0.92	0.96	-0.26	0.91	0.95	0.99	1.00	0.98	0.91	0.75	-0.89	-0.88
NICS(2.0)	0.90	0.95	-0.34	0.88	0.91	0.94	0.98	1.00	0.97	0.85	-0.92	-0.92
NICS(2.5)	0.87	0.92	-0.40	0.81	0.82	0.84	0.91	0.97	1.00	0.95	-0.93	-0.92
NICS(3.0)	0.85	0.89	-0.43	0.65	0.64	0.66	0.75	0.85	0.95	1.00	-0.92	-0.92
NICS(1.0)zz	-0.76	-0.85	0.10	-0.74	-0.77	-0.82	-0.89	-0.92	-0.93	-0.92	1.00	1.00
NICS(0)zz	-0.74	-0.83	0.15	-0.73	-0.76	-0.81	-0.88	-0.92	-0.92	-0.92	1.00	1.00

NICS values calculated at points close to each other have good correlation and the correlation is a function of the distance between the two points where NICS values are calculated.

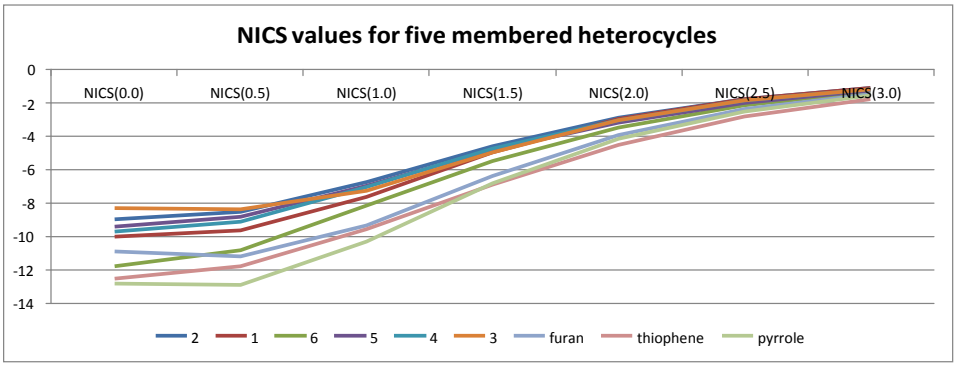


Figure S2. NICS values computed at and above the geometric ring centers of five membered rings of azaboroles (1-6), furan, thiophene and pyrrole.

Table S4. Atomic NBO charges (q) for N^{+1}, N^{-1} and N electron systems and condensed to atom local Fukui functions (f_c^+) and local electrophilicities (ω_c^+) calculated at B3LYP/6-311++G(3df,2pd)//B3LYP/6-31+G(d) level.

Molecule	NBO charge			f_x^+	ω_x^+	f_x^-	ω_x^-	N_x^+
	q_N+e	q_N-e	q_N					
1								
C5	0.248	-0.302	-0.589	-0.837	-0.946	0.287	0.324	0.254
C4	0.214	0.099	0.189	-0.024	-0.027	-0.090	-0.102	-0.080
O	0.009	-0.180	-0.356	-0.366	-0.413	0.177	0.200	0.156
N	-0.239	-0.220	-0.456	-0.217	-0.245	0.235	0.266	0.208
B	0.302	0.215	0.445	0.142	0.161	-0.230	-0.260	-0.204
BF_3 (B)	0.848	0.716	1.438	0.590	1.003	-0.722	-0.679	-0.425
BH_3 (B)	0.198	0.513	0.337	0.138	0.332	0.176	0.223	0.073
$B(CH_3)_3$ (B)	0.486	0.625	0.939	0.453	0.560	-0.314	-0.312	-0.254
2								
C5	-0.033	0.187	-0.088	-0.055	-0.049	0.275	0.246	0.307
C4	0.034	0.396	0.086	0.052	0.047	0.309	0.277	0.346
O	-0.336	-0.273	-0.653	-0.317	-0.284	0.380	0.340	0.425
N	-0.404	-0.276	-0.816	-0.412	-0.369	0.540	0.483	0.603
B	0.369	0.520	0.751	0.382	0.342	-0.231	-0.261	-0.258
3								
C5	-0.309	0.144	-0.578	-0.269	-0.267	0.722	0.716	0.399
C4	0.016	-0.059	0.028	0.013	0.012	-0.087	-0.086	0.399
N1	-0.196	-0.116	-0.460	-0.655	-0.650	0.343	0.341	0.607
N2	-0.292	-0.265	-0.610	-0.318	-0.316	0.346	0.343	-0.150
B	0.205	0.393	0.460	0.255	0.253	-0.067	-0.066	0.399
4								
C5	-0.035	0.240	-0.072	-0.038	-0.029	0.313	0.245	0.399
C4	-0.035	0.240	-0.072	-0.038	-0.029	0.313	0.245	0.399
N	-0.395	-0.314	-0.790	-0.395	-0.310	0.476	0.373	0.607
B	0.293	0.481	0.599	0.305	0.240	-0.118	-0.092	-0.150
5								
C5	-0.286	0.031	-0.580	-0.295	-0.373	0.611	0.773	0.483
C4	-0.186	-0.267	-0.404	-0.218	-0.275	0.137	0.173	0.108

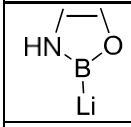
S	0.215	0.804	0.537	0.323	0.408	0.267	0.337	0.211
N	-0.246	-0.443	-0.987	-0.741	-0.937	0.544	0.689	0.430
B	0.199	0.401	0.510	0.311	0.393	-0.109	-0.138	-0.086
6								
C5	-0.001	0.235	-0.025	-0.024	-0.022	0.259	0.244	0.276
C4	-0.215	0.011	-0.417	-0.203	-0.191	0.428	0.403	0.456
S	0.036	0.273	0.126	0.090	0.085	0.147	0.138	0.156
N	-0.397	-0.333	-0.794	-0.397	-0.373	0.461	0.433	0.490
B	0.169	0.355	0.331	0.162	0.152	0.024	0.022	0.025
1,2-azaborine								
C1B	-0.248	0.087	-0.509	-0.261	-0.340	0.596	0.775	0.459
c2	-0.004	-0.139	-0.145	-0.140	-0.182	0.005	0.007	0.004
c3	-0.194	0.089	-0.293	-0.098	-0.128	0.382	0.496	0.327
C4N	0.103	0.219	0.062	-0.040	-0.053	0.157	0.204	0.092
N	-0.321	-0.326	-0.732	-0.412	-0.535	0.406	0.528	0.169
B	0.228	0.405	0.496	0.268	0.348	-0.091	-0.119	-0.074
Pyrrole								
c2	-0.024	0.364	-0.090	-0.067	-0.059	0.454	0.401	0.515
c3	-0.155	-0.064	-0.328	-0.173	-0.152	0.264	0.233	0.300
Phenol								
c2	-0.131	0.010	-0.281	-0.150	-0.159	0.291	0.309	0.274
c3	-0.090	-0.120	-0.181	-0.091	-0.096	0.061	0.065	0.058
c4	-0.124	0.208	-0.235	-0.111	-0.117	0.443	0.470	0.418
								
B	0.117	0.786	0.166	0.049	0.067	0.620	0.857	0.448

Table S5. Energy of the Highest Occupied Molecular Orbital (EHOMO, au), Lowest Unoccupied Molecular Orbital (E_{LUMO}, au), Electronegativity (χ, electronvolts), Hardness (η, electronvolts) computed in the gas phase.

Molecule	**HOMO**	**LUMO**	*X*	*η*
1	-0.262	-0.021	3.848	6.553
2	-0.229	-0.011	3.257	5.930
3	-0.205	-0.008	2.903	5.374
4	-0.235	-0.017	3.426	5.915
5	-0.237	-0.036	3.713	5.448
6	-0.231	-0.014	3.335	5.917
1,2-azaborine	-0.234	-0.039	3.712	5.301
BF_3	-0.441	-0.018	6.254	11.509
BH_3	-0.358	-0.083	5.997	7.481
$B(CH_3)_3$	-0.306	-0.018	4.402	7.842
Furan	-0.239	-0.008	3.361	6.302
Pyrrole	-0.219	-0.012	3.147	5.619
thiophene	-0.246	-0.027	3.714	5.938
	-0.181	-0.050	3.143	3.573

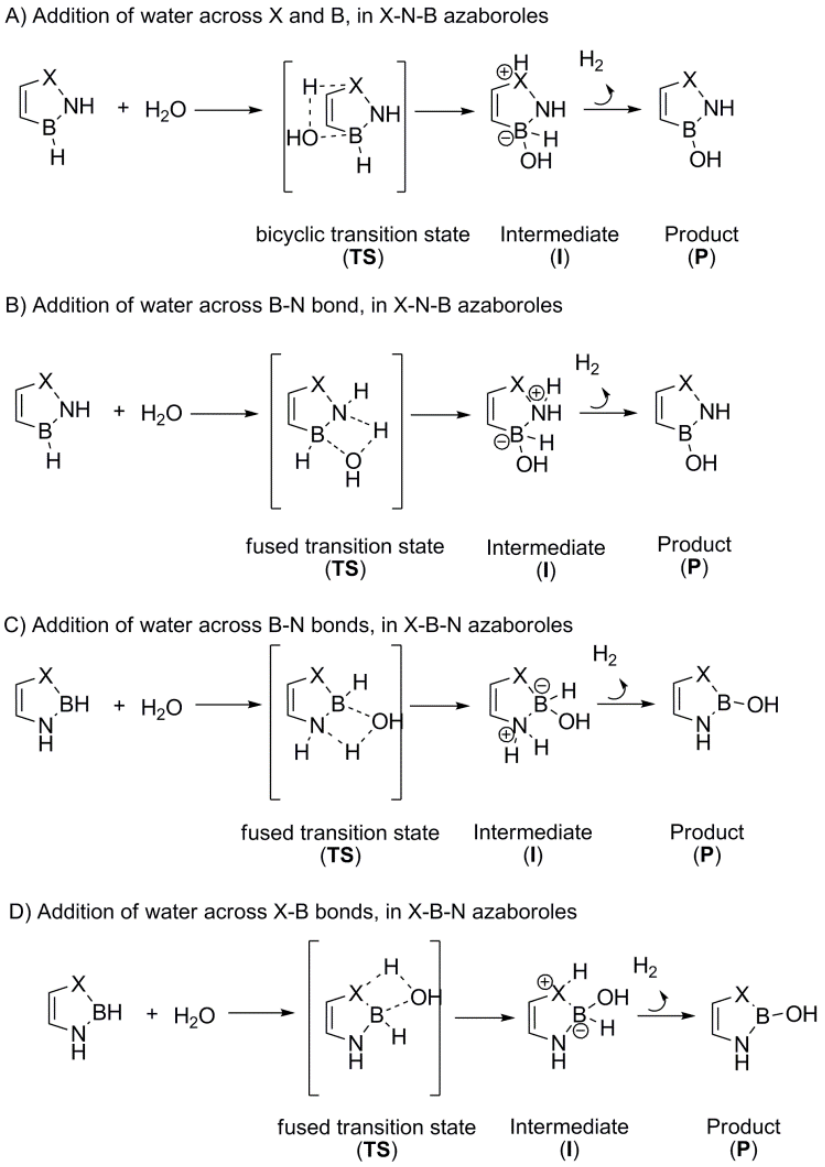


Figure S3. Hydrolysis via addition of water across X-B and B-N bonds in X-B-N and X-N-B series of azaboroles.

Table S6. Transition state, intermediate and product relative energies for hydrolysis reaction of azaboroles (Figure S3) in gas and solvent (water) phase. Values are in kcal/mol.

Sr. No.	Molecule	Mechanism	Gas phase (ΔH)			Solvent phase (ΔH)		
			TS	I	P	TS	I	P
1	**1**	A	46.7	42.5	-17.2	48.0	38.9	-15.9
2	**1**	B	26.1	3.0		27.7	1.6	
3	**2**	D	31.8	2.0	-20.8	34.3	3.1	-18.2
4	**2**	C	26.5	0.4		27.9	-1.3	
5	**3**	A	39.9	25.9	-17.7	40.9	19.9	-15.4
6	**3**	B	26.4	70.4		29.8	3.5	
7	**4**	C	31.7	7.4	-16.7	33.9	7.1	-15.1
8	**5**	A	39.4	29.5	-18.7	40.7	26.9	-17.4
9	**5**	B	26.1	3.6		28.0	2.8	
10	**6**	D	28.1	-4.4	-18.4	30.5	-2.1	-16.2
11	**6**	C	29.6	6.3		30.1	3.9	

Table S7. Enthalpies for the formation of azaborole trimers. Values are in kcal/mol.

Azaborole	ΔH
1	-40.24
2	-39.48
3	-44.99
4	-33.04
5	-46.40
6	-35.84

References:

1. Krygowski, T. M.; Szatylowicz, H.; Stasyuk, O. A.; Dominikowska, J.; Palusiak, M. *Chem. Rev.* **2014**, 6383-6422.

Coordinates

Gas Phase

benzene

Energy = -232.328722024
Free Energy = -232.185822
ZPE = 0.100573
xyz coordinates

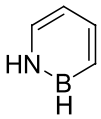
C	-0.08524	-1.39592	0.00000
C	1.16635	-0.77182	0.00000
C	1.25152	0.62410	0.00000
C	0.08524	1.39592	0.00000
C	-1.16635	0.77182	-0.00000
C	-1.25152	-0.62410	-0.00000
H	-0.15161	-2.48120	0.00000
H	2.07306	-1.37189	0.00001
H	2.22454	1.10934	0.00001
H	0.15161	2.48120	0.00000
H	-2.07306	1.37189	-0.00001
H	-2.22454	-1.10934	-0.00001

BH2NH2

Energy = -82.0806890311
Free Energy = -82.021043
ZPE = 0.047988
xyz coordinates

N	0.00002	-0.61355	0.00000
H	-0.00015	-1.17111	0.84480
H	-0.00015	-1.17111	-0.84480
B	0.00002	0.78304	0.00000
H	0.00006	1.36092	1.04824
H	0.00006	1.36092	-1.04824

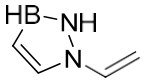
borazine



Energy = -235.764044873
Free Energy = -235.619211
ZPE = 0.097901
xyz coordinates

C	-0.04920	-1.47780	0.00000
C	-1.21234	-0.73534	0.00000
C	-1.19360	0.69052	0.00000
C	0.00000	1.36479	0.00000
H	2.02375	1.25603	0.00000
H	2.37496	-1.23978	0.00000
H	-0.13660	-2.56320	0.00000
H	-2.18651	-1.22527	0.00000
H	-2.12042	1.25553	0.00000
H	0.05171	2.44990	0.00000
B	1.28256	-0.75414	0.00000
N	1.18731	0.68349	0.00000

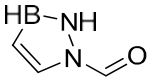
9



Energy = -291.075214788
Free Energy = -290.901702
ZPE = 0.111786
xyz coordinates

C	1.75653	0.97907	-0.00003
C	0.38811	1.07491	-0.00014
H	2.39017	1.85760	-0.00008
H	-0.25004	1.94953	-0.00045
B	2.07645	-0.51542	0.00011
H	3.07717	-1.15955	0.00002
N	0.78563	-1.12497	0.00026
N	-0.21688	-0.15876	-0.00000
H	0.46831	-2.08352	-0.00094
C	-1.56256	-0.50563	-0.00016
H	-1.71562	-1.58194	-0.00038
C	-2.61467	0.32804	0.00014
H	-2.52202	1.40892	0.00074
H	-3.61585	-0.08616	-0.00011

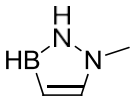
10



Energy = -327.034365728
Free Energy = -326.870695
ZPE = 0.089341
xyz coordinates

C	-2.01961	-0.46537	-0.00002
C	-0.83231	-1.13140	0.00001
H	-2.97013	-0.98482	-0.00004
H	-0.60733	-2.19189	0.00001
B	-1.66935	1.03636	-0.00001
H	-2.31560	2.03368	-0.00002
N	-0.24587	1.04829	0.00002
N	0.24261	-0.24743	0.00004
H	0.47720	1.75659	0.00004
C	1.58954	-0.51339	-0.00001
H	1.80574	-1.59374	-0.00001
O	2.44424	0.35667	-0.00002

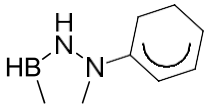
7



Energy = -252.976668897
Free Energy = -252.817623
ZPE = 0.107490
xyz coordinates

C	-1.53502	-0.73771	0.09729
C	-0.23179	-1.11282	-0.10442
H	-2.33695	-1.46104	0.18615
H	0.21094	-2.10311	-0.14762
B	-1.52393	0.78991	0.10841
H	-2.36380	1.63123	0.19089
N	-0.14040	1.11251	-0.05804
N	0.61692	-0.04116	-0.27976
H	0.32250	1.97683	-0.30449
C	1.99648	-0.04162	0.18085
H	2.45878	-0.98797	-0.11206
H	2.54776	0.77082	-0.30492
H	2.06676	0.07715	1.27232

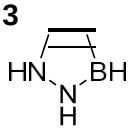
12



Energy = -444.776397802
Free Energy = -444.517875
ZPE = 0.160139
xyz coordinates

C	3.17155	0.68899	0.30829
C	1.85473	1.07693	0.32916
H	3.96810	1.35680	0.61293
H	1.40691	2.00483	0.66396
B	3.17291	-0.75222	-0.18839
H	4.01691	-1.55342	-0.44024
N	1.78064	-1.04857	-0.35914
N	1.00957	0.07906	-0.09580
C	-0.39487	0.03411	-0.03711
C	-1.06446	-1.16928	0.23944
C	-1.14056	1.20191	-0.27475
C	-2.46020	-1.19737	0.27334
H	-0.49877	-2.06862	0.46218
C	-2.53253	1.16301	-0.21488
H	-0.63152	2.12724	-0.52634
C	-3.20306	-0.03537	0.05273
H	-2.96549	-2.13465	0.49176
H	-3.09651	2.07361	-0.39976
H	-4.28848	-0.06182	0.08600
H	1.30916	-1.77391	-0.88129

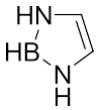
3



Energy = -213.655421392
Free Energy = -213.530084
ZPE = 0.079511
xyz coordinates

C	-1.13281	0.62917	0.01121
C	-0.90525	-0.71877	-0.01102
H	-2.13232	1.04768	0.00231
H	-1.60492	-1.54850	0.01188
B	0.25274	1.28002	0.01588
H	0.64254	2.40517	-0.02514
N	1.15007	0.16819	0.04705
H	2.12955	0.10783	-0.19523
N	0.44119	-1.03506	-0.09581
H	0.79095	-1.80660	0.46693

4



Energy = -213.722181599
Free Energy = -213.594561
ZPE = 0.080141
xyz coordinates

C	0.67939	-0.95636	-0.00012
C	-0.67939	-0.95636	-0.00006
H	1.35762	-1.79800	-0.00023
H	-1.35762	-1.79800	-0.00012
B	0.00000	1.25374	0.00012
H	0.00000	2.44243	0.00024
N	1.12773	0.36993	-0.00001
H	2.11186	0.59108	-0.00003
N	-1.12773	0.36993	0.00008
H	-2.11186	0.59108	0.00015

ethylene
Energy = -78.6218776969
Free Energy = -78.563048
ZPE = 0.051101
xyz coordinates

C	0.00000	0.00000	0.66740
H	0.00000	0.92471	1.24038
H	0.00000	-0.92471	1.24038
C	0.00000	0.00000	-0.66740
H	0.00000	-0.92471	-1.24038
H	0.00000	0.92471	-1.24038

furan

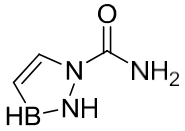
Energy = -230.106135677
Free Energy = -229.987706
ZPE = 0.070011
xyz coordinates

C	-0.71859	0.96076	0.00015
C	-1.09739	-0.34826	0.00004
H	-1.37529	1.82019	0.00029
H	-2.05235	-0.85151	0.00006
H	2.05238	-0.85143	-0.00024
O	0.00002	-1.16098	-0.00012
H	1.37522	1.82024	0.00009
C	1.09740	-0.34822	-0.00012
C	0.71855	0.96078	0.00005

hydrogen
Energy = -1.18001342918
Free Energy = -1.176824
ZPE = 0.010146
xyz coordinates

H	0.00000	0.00000	0.37138
H	0.00000	0.00000	-0.37138

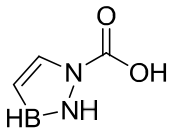
14



Energy = -382.427223177
Free Energy = -382.225637
ZPE = 0.106746
xyz coordinates

C	-0.19840	1.60090	0.06910
C	1.10310	2.00160	-0.03580
N	-0.30160	0.25360	0.37200
B	1.95210	0.75890	0.23390
N	0.98790	-0.29470	0.40450
H	3.11930	0.55300	0.33840
C	-1.47030	-0.50990	0.24220
O	-2.57760	0.00050	0.30030
N	-1.24360	-1.86920	0.12780
H	-1.12770	2.13760	-0.07420
H	1.36890	3.02690	-0.26230
H	1.06450	-1.12870	0.97380
H	-2.09040	-2.39390	-0.05570
H	-0.43580	-2.17250	-0.40440

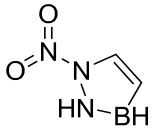
13



Energy = -402.306439749
Free Energy = -402.108914
ZPE = 0.094242
xyz coordinates

C	-0.20040	1.64100	0.04080
C	1.10510	2.02250	0.10950
N	-0.32680	0.26040	0.14100
B	1.92790	0.73330	0.27430
N	0.94480	-0.29580	0.28170
H	3.08820	0.49730	0.38080
C	-1.49700	-0.45840	0.10830
O	-2.60580	0.02250	-0.01450
O	-1.24620	-1.79080	0.23260
H	-1.11510	2.20800	-0.07340
H	1.39990	3.06300	0.04930
H	0.96230	-1.30220	0.36160
H	-2.10930	-2.24000	0.20230

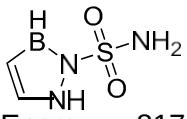
15



Energy = -418.204770759
Free Energy = -418.020313
ZPE = 0.081303
xyz coordinates

C	0.19180	1.65390	0.08630
C	1.50960	1.98890	0.07060
N	0.05440	0.28340	0.30580
B	2.30730	0.67940	0.25630
N	1.29850	-0.32240	0.35390
N	-1.08030	-0.47180	0.07700
O	-2.12390	0.14760	-0.10740
O	-0.93100	-1.69380	0.13160
H	-0.71400	2.23300	-0.02340
H	1.83460	3.01460	-0.05450
H	3.46340	0.41980	0.32650
H	1.26850	-1.31970	0.52040

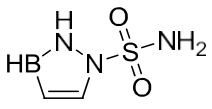
16



Energy = -817.721678312
Free Energy = -817.438268
ZPE = 0.106103
xyz coordinates

C	-1.41553	2.06087	0.29384
C	-0.32832	2.58025	-0.35576
N	-1.31414	0.70634	0.52899
B	0.58653	1.40277	-0.65707
N	-0.16488	0.26356	-0.15203
H	1.66543	1.28112	-1.13235
S	0.32530	-1.31297	0.20550
O	-0.91018	-2.07631	0.38546
O	1.34315	-1.64044	-0.78216
N	1.04387	-1.20737	1.72526
H	-2.31518	2.55170	0.65208
H	-0.22234	3.63984	-0.55401
H	-2.11822	0.09068	0.43215
H	0.62588	-1.88079	2.36327
H	2.05323	-1.31854	1.65752

11

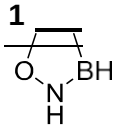


Energy = -817.722548060
Free Energy = -817.439495
ZPE = 0.105965
xyz coordinates

C	0.25288	1.55387	0.57021

C	1.61117	1.57351	0.59502
N	-0.24395	0.55285	-0.28150
B	2.07291	0.40876	-0.29847
N	0.85764	-0.20280	-0.71845
H	3.13567	0.02102	-0.66536
S	-1.62028	-0.36286	0.18989
O	-2.61776	0.62544	0.58121
O	-1.79839	-1.32605	-0.89257
N	-1.15898	-1.21323	1.56408
H	-0.48100	2.17879	1.06430
H	2.16528	2.32566	1.14425
H	0.63638	-0.83662	-1.47578
H	-1.71786	-0.94616	2.37062
H	-1.15461	-2.21687	1.40124

1



Energy = -233.507427782
Free Energy = -233.389313
ZPE = 0.066644
xyz coordinates

C	-0.97559	0.82233	0.00004
C	-1.00277	-0.53280	0.00003
H	-1.87581	1.42385	0.00008
H	-1.81102	-1.25451	0.00005
O	0.21790	-1.13224	-0.00002
B	0.51361	1.18644	-0.00001
H	1.12927	2.20387	-0.00002
N	1.14770	-0.07575	-0.00004
H	2.08257	-0.45444	-0.00008

2

Energy = -233.596485998
Free Energy = -233.475705
ZPE = 0.067646
xyz coordinates

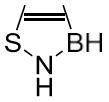
C	-0.12571	-1.14853	0.00015
C	1.04825	-0.48395	0.00004
H	-0.31004	-2.21360	0.00029
H	2.07125	-0.82810	0.00007
B	-0.54202	1.08942	-0.00013
H	-1.04298	2.16436	-0.00026
O	0.83455	0.87990	-0.00013
N	-1.15575	-0.19386	0.00005
H	-2.12954	-0.45705	0.00010

pyrrole

Energy = -210.247106547
Free Energy = -210.121669
ZPE = 0.082536
xyz coordinates

C	-0.33245	-1.12675	0.00005
C	0.98506	-0.71342	0.00008
C	0.98506	0.71343	0.00000
C	-0.33246	1.12674	-0.00008
N	-1.12343	-0.00000	-0.00005
H	-2.13237	-0.00001	-0.00009
H	-0.76857	-2.11571	0.00009
H	1.85111	-1.36215	0.00015
H	1.85111	1.36216	0.00000
H	-0.76858	2.11571	-0.00015

5



Energy = -556.525074174
Free Energy = -556.400087
ZPE = 0.063534
xyz coordinates

C	-1.37721	-0.68248	0.00018
C	-0.13252	-1.23776	0.00010
H	-2.25672	-1.32066	0.00032
H	0.13728	-2.29009	0.00015
H	0.48308	2.14747	-0.00020
H	-2.15753	1.68190	0.00009
S	1.17832	-0.09440	-0.00011
N	0.07247	1.22255	-0.00010
B	-1.30161	0.85108	0.00007

6

Energy = -556.563239743
Free Energy = -556.440780
ZPE = 0.064800
xyz coordinates

C	-1.21855	-0.74688	0.00017
C	0.04340	-1.23149	0.00010
H	-2.12915	-1.33522	0.00030
H	0.33265	-2.27343	0.00016
B	-0.04042	1.31672	-0.00011
H	0.12430	2.49157	-0.00022
N	-1.29262	0.64654	0.00006
H	-2.19971	1.09459	0.00010
S	1.26083	0.04896	-0.00012

thiophene

Energy = -553.094377258
Free Energy = -552.971874
ZPE = 0.066732
xyz coordinates

C	-0.01020	1.24351	0.00000
C	-1.27477	0.71536	0.00000
C	-1.27477	-0.71536	0.00000
C	-0.01020	-1.24351	0.00000
S	1.20034	0.00000	0.00000
H	0.28165	2.28566	0.00000
H	-2.17452	1.32185	0.00000
H	-2.17452	-1.32185	0.00000
H	0.28165	-2.28566	0.00000

Water phase

benzene

Energy = -232.331417078
Free Energy = -232.188811
ZPE = 0.100527
xyz coordinates

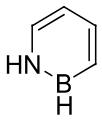
C	-0.08539	-1.39715	0.00000
C	1.16736	-0.77253	0.00000
C	1.25271	0.62465	0.00000
C	0.08539	1.39715	0.00000
C	-1.16736	0.77253	0.00000
C	-1.25271	-0.62465	0.00000
H	-0.15167	-2.48236	0.00000
H	2.07403	-1.37254	0.00001
H	2.22560	1.10996	0.00001
H	0.15167	2.48236	0.00000
H	-2.07403	1.37254	-0.00001
H	-2.22560	-1.10996	-0.00001

BH2NH2

Energy = -82.0839119957
Free Energy = -82.024882
ZPE = 0.047735
xyz coordinates

N	0.00002	-0.61221	0.00000
H	-0.00018	-1.17279	0.84396
H	-0.00018	-1.17279	-0.84396
B	0.00002	0.78053	0.00000
H	0.00006	1.36421	1.04718
H	0.00006	1.36421	-1.04718

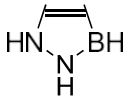
borazine



Energy = -235.768790711
Free Energy = -235.624518
ZPE = 0.097801
xyz coordinates

C	-0.04568	-1.47930	0.00000
C	-1.21281	-0.73703	0.00000
C	-1.19549	0.68751	0.00000
C	0.00000	1.36455	0.00000
H	2.02026	1.26487	0.00000
H	2.37604	-1.23742	0.00000
H	-0.13449	-2.56523	0.00000
H	-2.18599	-1.22886	0.00000
H	-2.12261	1.25182	0.00000
H	0.05192	2.44887	0.00000
B	1.28234	-0.75041	0.00000
N	1.18673	0.68623	0.00000

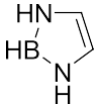
3



Energy = -213.663173912
Free Energy = -213.538607
ZPE = 0.079170
xyz coordinates

C	-1.14785	0.60267	0.00855
C	-0.88342	-0.74840	-0.00467
H	-2.16146	0.98778	-0.00024
H	-1.55725	-1.59810	0.02218
B	0.21740	1.28699	0.01263
H	0.58012	2.42398	-0.01476
N	1.14229	0.19821	0.03125
H	2.14144	0.14217	-0.11407
N	0.46032	-1.01100	-0.07899
H	0.87944	-1.82694	0.35464

4



Energy = -213.727153113
Free Energy = -213.600418
ZPE = 0.079985
xyz coordinates

C	0.68059	-0.95616	-0.00012
C	-0.68055	-0.95618	-0.00007
H	1.36171	-1.79573	-0.00023
H	-1.36161	-1.79579	-0.00011
B	-0.00003	1.25213	0.00012
H	-0.00006	2.44191	0.00025
N	1.12921	0.37053	-0.00001

H	2.11553	0.58804	-0.00005
N	-1.12922	0.37048	0.00008
H	-2.11554	0.58794	0.00013

ethylene
Energy = -78.6231648734
Free Energy = -78.564577
ZPE = 0.051017
xyz coordinates

C	0.00000	0.00000	0.66819
H	0.00000	0.92516	1.24087
H	0.00000	-0.92516	1.24087
C	0.00000	0.00000	-0.66819
H	0.00000	-0.92516	-1.24087
H	0.00000	0.92516	-1.24087

furan

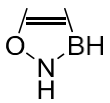
Energy = -230.109285412
Free Energy = -229.991287
ZPE = 0.069885
xyz coordinates

C	-0.71833	0.96150	0.00015
C	-1.10110	-0.34655	0.00005
H	-1.37387	1.82203	0.00029
H	-2.05731	-0.84791	0.00006
H	2.05561	-0.85215	-0.00024
O	-0.00135	-1.16201	-0.00012
H	1.37810	1.81876	0.00009
C	1.10030	-0.34890	-0.00012
C	0.72050	0.95984	0.00005

hydrogen
Energy = -1.18017598072
Free Energy = -1.176913
ZPE = 0.010143
xyz coordinates

H	0.00000	0.00000	0.37138
H	0.00000	0.00000	-0.37138

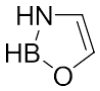
1



Energy = -233.511388093
Free Energy = -233.393812
ZPE = 0.066452
xyz coordinates

C	-0.97276	0.82674	-0.00002
C	-1.00750	-0.52947	-0.00008
H	-1.87257	1.42958	0.00008
H	-1.81976	-1.24659	0.00017
O	0.21293	-1.13149	0.00004
B	0.51894	1.18199	0.00003
H	1.13810	2.19819	0.00006
N	1.15026	-0.08023	-0.00001
H	2.08582	-0.46126	-0.00014

2



Energy = -233.601528726
Free Energy = -233.481470
ZPE = 0.067538
xyz coordinates

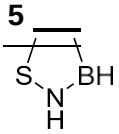
C	-0.11899	-1.14789	0.00015
C	1.05384	-0.48065	0.00004
H	-0.30087	-2.21334	0.00029
H	2.07884	-0.81891	0.00007
B	-0.55300	1.08377	-0.00013
H	-1.05534	2.15877	-0.00026
O	0.82994	0.88832	-0.00013
N	-1.15426	-0.20076	0.00005
H	-2.12635	-0.47537	0.00010

pyrrole

Energy = -210.253103535
Free Energy = -210.128247
ZPE = 0.082546
xyz coordinates

C	-0.33405	-1.12645	0.00005
C	0.98706	-0.71434	0.00008
C	0.98694	0.71448	0.00000
C	-0.33421	1.12641	-0.00008
N	-1.12273	-0.00009	-0.00005
H	-2.13320	-0.00016	-0.00009
H	-0.77368	-2.11393	0.00009
H	1.85289	-1.36437	0.00015
H	1.85269	1.36464	0.00000
H	-0.77400	2.11382	-0.00015

5



Energy = -556.529262566
Free Energy = -556.404814
ZPE = 0.063415
xyz coordinates

C	-1.38028	-0.67857	0.00019
C	-0.13565	-1.23904	0.00011
H	-2.26063	-1.31631	0.00032
H	0.13253	-2.29173	0.00015
H	0.49602	2.14709	-0.00019

H	-2.15126	1.68876	0.00009
S	1.17634	-0.09811	-0.00011
N	0.07699	1.22426	-0.00010
B	-1.29630	0.85557	0.00007

6

Energy = -556.567827636
Free Energy = -556.445994
ZPE = 0.064774
xyz coordinates

C	-1.21529	-0.74958	0.00017
C	0.04764	-1.23460	0.00010
H	-2.12538	-1.33807	0.00030
H	0.34123	-2.27546	0.00016
B	-0.04908	1.31932	-0.00011
H	0.11714	2.49402	-0.00022
N	-1.29438	0.64276	0.00006
H	-2.20638	1.08361	0.00010
S	1.26158	0.05282	-0.00012

thiophene

Energy = -553.097295454
Free Energy = -552.975189
ZPE = 0.066652
xyz coordinates

C	-0.01056	1.24581	0.00000
C	-1.27524	0.71625	0.00000
C	-1.27524	-0.71625	0.00000
C	-0.01056	-1.24581	0.00000
S	1.20089	0.00000	0.00000
H	0.28312	2.28765	0.00000
H	-2.17537	1.32236	0.00000
H	-2.17537	-1.32235	0.00000
H	0.28311	-2.28765	0.00000

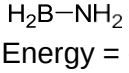
Ethanol

benzene

Energy = -232.331267813
Free Energy = -232.188660
ZPE = 0.100524
xyz coordinates

C	-0.08539	-1.39715	0.00000
C	1.16736	-0.77253	0.00000
C	1.25271	0.62465	0.00000
C	0.08539	1.39715	0.00000
C	-1.16736	0.77253	0.00000
C	-1.25271	-0.62465	0.00000
H	-0.15167	-2.48236	0.00000
H	2.07403	-1.37254	0.00001
H	2.22560	1.10996	0.00001
H	0.15167	2.48236	0.00000
H	-2.07403	1.37254	-0.00001
H	-2.22560	-1.10996	-0.00001

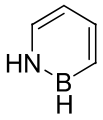
BH2NH2



Energy = -82.0837727097
Free Energy = -82.024714
ZPE = 0.047749
xyz coordinates

N	0.00002	-0.61227	0.00000
H	-0.00018	-1.17271	0.84401
H	-0.00018	-1.17271	-0.84401
B	0.00002	0.78063	0.00000
H	0.00006	1.36408	1.04721
H	0.00006	1.36408	-1.04721

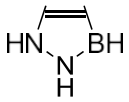
borazine



Energy = -235.768550093
Free Energy = -235.624267
ZPE = 0.097796
xyz coordinates

C	-0.04568	-1.47930	0.00000
C	-1.21281	-0.73703	0.00000
C	-1.19549	0.68751	0.00000
C	0.00000	1.36455	0.00000
H	2.02026	1.26487	0.00000
H	2.37604	-1.23742	0.00000
H	-0.13449	-2.56523	0.00000
H	-2.18599	-1.22886	0.00000
H	-2.12261	1.25182	0.00000
H	0.05192	2.44887	0.00000
B	1.28234	-0.75041	0.00000
N	1.18673	0.68623	0.00000

3

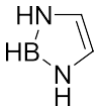


Energy = -213.662760290
Free Energy = -213.538163
ZPE = 0.079186
xyz coordinates

C	-1.14687	0.60454	0.00873
C	-0.88499	-0.74634	-0.00504
H	-2.15956	0.99198	-0.00007
H	-1.56066	-1.59466	0.02176
B	0.21988	1.28655	0.01286

H	0.58450	2.42279	-0.01526
N	1.14289	0.19614	0.03236
H	2.14107	0.13963	-0.11944
N	0.45899	-1.01269	-0.08046
H	0.87326	-1.82587	0.36331

4



Energy = -213.726911629
Free Energy = -213.600138
ZPE = 0.079995
xyz coordinates

C	0.68059	-0.95616	-0.00012
C	-0.68055	-0.95618	-0.00007
H	1.36171	-1.79573	-0.00023
H	-1.36161	-1.79579	-0.00011
B	-0.00003	1.25213	0.00012
H	-0.00006	2.44191	0.00025
N	1.12921	0.37053	-0.00001
H	2.11553	0.58804	-0.00005
N	-1.12922	0.37048	0.00008
H	-2.11554	0.58794	0.00013

ethylene
Energy = -78.6231013952
Free Energy = -78.564506
ZPE = 0.051020
xyz coordinates

C	0.00000	0.00000	0.66819
H	0.00000	0.92516	1.24087
H	0.00000	-0.92516	1.24087
C	0.00000	0.00000	-0.66819
H	0.00000	-0.92516	-1.24087
H	0.00000	0.92516	-1.24087

furan

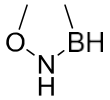
Energy = -230.109133898
Free Energy = -229.991125
ZPE = 0.069887
xyz coordinates

C	-0.71833	0.96150	0.00015
C	-1.10110	-0.34655	0.00005
H	-1.37387	1.82203	0.00029
H	-2.05731	-0.84791	0.00006
H	2.05561	-0.85215	-0.00024
O	-0.00135	-1.16201	-0.00012
H	1.37810	1.81876	0.00009
C	1.10030	-0.34890	-0.00012
C	0.72050	0.95984	0.00005

hydrogen
Energy = -1.18016870064
Free Energy = -1.176909
ZPE = 0.010143
xyz coordinates

H	0.00000	0.00000	0.37138
H	0.00000	0.00000	-0.37138

1



Energy = -233.511210919
Free Energy = -233.393613
ZPE = 0.066461
xyz coordinates

C	-0.97276	0.82674	-0.00002
C	-1.00750	-0.52947	-0.00008
H	-1.87257	1.42958	0.00008
H	-1.81976	-1.24659	0.00017
O	0.21293	-1.13149	0.00004
B	0.51894	1.18199	0.00003
H	1.13810	2.19819	0.00006
N	1.15026	-0.08023	-0.00001
H	2.08582	-0.46126	-0.00014

2

Energy = -233.601292547
Free Energy = -233.481198
ZPE = 0.067547
xyz coordinates

C	-0.11961	-1.14787	0.00015
C	1.05344	-0.48108	0.00004
H	-0.30184	-2.21326	0.00029
H	2.07826	-0.81990	0.00007
B	-0.55219	1.08417	-0.00013
H	-1.05416	2.15931	-0.00026
O	0.83040	0.88770	-0.00013
N	-1.15441	-0.20014	0.00005
H	-2.12665	-0.47397	0.00010

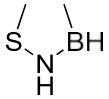
pyrrole

Energy = -210.252798592
Free Energy = -210.127925
ZPE = 0.082544
xyz coordinates

C	-0.33405	-1.12645	0.00005
C	0.98706	-0.71434	0.00008
C	0.98694	0.71448	0.00000

C	-0.33421	1.12641	-0.00008
N	-1.12273	-0.00009	-0.00005
H	-2.13320	-0.00016	-0.00009
H	-0.77368	-2.11393	0.00009
H	1.85289	-1.36437	0.00015
H	1.85269	1.36464	0.00000
H	-0.77400	2.11382	-0.00015

5



Energy = -556.529059469
Free Energy = -556.404587
ZPE = 0.063423
xyz coordinates

C	-1.38028	-0.67857	0.00019
C	-0.13565	-1.23904	0.00011
H	-2.26063	-1.31631	0.00032
H	0.13253	-2.29173	0.00015
H	0.49602	2.14709	-0.00019
H	-2.15126	1.68876	0.00009
S	1.17634	-0.09811	-0.00011
N	0.07699	1.22426	-0.00010
B	-1.29630	0.85557	0.00007

6

Energy = -556.567603890
Free Energy = -556.445748
ZPE = 0.064771
xyz coordinates

C	-1.21536	-0.74955	0.00017
C	0.04757	-1.23442	0.00010
H	-2.12535	-1.33818	0.00030
H	0.34104	-2.27530	0.00016
B	-0.04880	1.31918	-0.00011
H	0.11729	2.49391	-0.00022
N	-1.29440	0.64286	0.00006
H	-2.20621	1.08398	0.00010
S	1.26154	0.05271	-0.00012

thiophene

Energy = -553.097141663
Free Energy = -552.975030
ZPE = 0.066651
xyz coordinates

C	-0.01056	1.24581	0.00000
C	-1.27524	0.71625	0.00000
C	-1.27524	-0.71625	0.00000
C	-0.01056	-1.24581	0.00000
S	1.20089	0.00000	0.00000
H	0.28312	2.28765	0.00000
H	-2.17537	1.32236	0.00000
H	-2.17537	-1.32235	0.00000
H	0.28311	-2.28765	0.00000

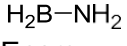
Dichloromethane

benzene

Energy = -232.330913493
Free Energy = -232.188299
ZPE = 0.100519
xyz coordinates

C	-0.08539	-1.39715	0.00000
C	1.16736	-0.77253	0.00000
C	1.25271	0.62465	0.00000
C	0.08539	1.39715	0.00000
C	-1.16736	0.77253	0.00000
C	-1.25271	-0.62465	0.00000
H	-0.15167	-2.48236	0.00000
H	2.07403	-1.37254	0.00001
H	2.22560	1.10996	0.00001
H	0.15167	2.48236	0.00000
H	-2.07403	1.37254	-0.00001
H	-2.22560	-1.10996	-0.00001

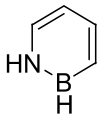
BH2NH2



Energy = -82.0834292865
Free Energy = -82.024302
ZPE = 0.047781
xyz coordinates

N	0.00002	-0.61242	0.00000
H	-0.00017	-1.17251	0.84411
H	-0.00017	-1.17251	-0.84411
B	0.00002	0.78088	0.00000
H	0.00006	1.36376	1.04730
H	0.00006	1.36376	-1.04730

borazine

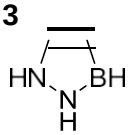


Energy = -235.767972091
Free Energy = -235.623656
ZPE = 0.097788
xyz coordinates

C	-0.04568	-1.47930	0.00000
C	-1.21281	-0.73703	0.00000
C	-1.19549	0.68751	0.00000
C	0.00000	1.36455	0.00000
H	2.02026	1.26487	0.00000

H	2.37604	-1.23742	0.00000
H	-0.13449	-2.56523	0.00000
H	-2.18599	-1.22886	0.00000
H	-2.12261	1.25182	0.00000
H	0.05192	2.44887	0.00000
B	1.28234	-0.75041	0.00000
N	1.18673	0.68623	0.00000

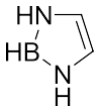
3



Energy = -213.661789751
Free Energy = -213.537108
ZPE = 0.079226
xyz coordinates

C	-1.14439	0.60906	0.00911
C	-0.88867	-0.74151	-0.00591
H	-2.15485	1.00198	0.00019
H	-1.56859	-1.58659	0.02079
B	0.22580	1.28533	0.01340
H	0.59490	2.41979	-0.01655
N	1.14418	0.19120	0.03480
H	2.13993	0.13342	-0.13159
N	0.45564	-1.01646	-0.08343
H	0.85923	-1.82366	0.38139

4



Energy = -213.726342080
Free Energy = -213.599456
ZPE = 0.080022
xyz coordinates

C	0.68031	-0.95617	-0.00012
C	-0.68031	-0.95617	-0.00006
H	1.36107	-1.79598	-0.00023
H	-1.36107	-1.79598	-0.00012
B	0.00000	1.25242	0.00012
H	-0.00000	2.44205	0.00024
N	1.12901	0.37040	-0.00001
H	2.11505	0.58813	-0.00003
N	-1.12901	0.37040	0.00008
H	-2.11505	0.58813	0.00015

ethylene
Energy = -78.6229474124
Free Energy = -78.564334
ZPE = 0.051026
xyz coordinates

C	0.00000	0.00000	0.66819
H	0.00000	0.92516	1.24087
H	0.00000	-0.92516	1.24087
C	0.00000	0.00000	-0.66819
H	0.00000	-0.92516	-1.24087
H	0.00000	0.92516	-1.24087

furan

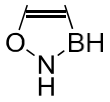
Energy = -230.108782664
Free Energy = -229.990712
ZPE = 0.069910
xyz coordinates

C	-0.71922	0.96065	0.00015
C	-1.10015	-0.34784	0.00005
H	-1.37551	1.82058	0.00029
H	-2.05570	-0.85037	0.00006
H	2.05572	-0.85033	-0.00024
O	0.00001	-1.16180	-0.00012
H	1.37548	1.82060	0.00009
C	1.10015	-0.34782	-0.00012
C	0.71920	0.96066	0.00005

hydrogen
Energy = -1.18015085475
Free Energy = -1.176900
ZPE = 0.010143
xyz coordinates

H	0.00000	0.00000	0.37138
H	0.00000	0.00000	-0.37138

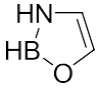
1



Energy = -233.510775882
Free Energy = -233.393125
ZPE = 0.066483
xyz coordinates

C	-0.97276	0.82674	-0.00002
C	-1.00750	-0.52947	-0.00008
H	-1.87257	1.42958	0.00008
H	-1.81976	-1.24659	0.00017
O	0.21293	-1.13149	0.00004
B	0.51894	1.18199	0.00003
H	1.13810	2.19819	0.00006
N	1.15026	-0.08023	-0.00001
H	2.08582	-0.46126	-0.00014

2



Energy = -233.600718218
Free Energy = -233.480538
ZPE = 0.067566
xyz coordinates

C	-0.12101	-1.14784	0.00015

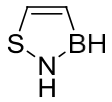
C	1.05253	-0.48204	0.00004
H	-0.30403	-2.21311	0.00029
H	2.07692	-0.82210	0.00007
B	-0.55030	1.08509	-0.00013
H	-1.05149	2.16052	-0.00026
O	0.83143	0.88628	-0.00013
N	-1.15473	-0.19872	0.00005
H	-2.12733	-0.47073	0.00010

pyrrole

Energy = -210.252081722
Free Energy = -210.127138
ZPE = 0.082547
xyz coordinates

C	-0.33380	-1.12640	0.00005
C	0.98667	-0.71424	0.00008
C	0.98667	0.71424	0.00000
C	-0.33381	1.12640	-0.00008
N	-1.12294	-0.00000	-0.00005
H	-2.13344	-0.00000	-0.00009
H	-0.77272	-2.11420	0.00009
H	1.85254	-1.36407	0.00015
H	1.85254	1.36407	-0.00000
H	-0.77273	2.11420	-0.00015

5



Energy = -556.528588301
Free Energy = -556.404035
ZPE = 0.063444
xyz coordinates

C	-1.38035	-0.67776	0.00018
C	-0.13635	-1.23875	0.00010
H	-2.26123	-1.31462	0.00032
H	0.13108	-2.29163	0.00015
H	0.49575	2.14649	-0.00020
H	-2.15102	1.68907	0.00009
S	1.17645	-0.09831	-0.00011
N	0.07758	1.22365	-0.00010
B	-1.29613	0.85543	0.00007

6

Energy = -556.567064223
Free Energy = -556.445150
ZPE = 0.064767
xyz coordinates

C	-1.21555	-0.74944	0.00017
C	0.04737	-1.23397	0.00010
H	-2.12536	-1.33839	0.00030
H	0.34054	-2.27492	0.00016
B	-0.04809	1.31886	-0.00011
H	0.11767	2.49364	-0.00022
N	-1.29441	0.64310	0.00006
H	-2.20576	1.08489	0.00010
S	1.26146	0.05245	-0.00012

thiophene

Energy = -553.096773126
Free Energy = -552.974645
ZPE = 0.066649
xyz coordinates

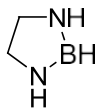
C	-0.01056	1.24581	0.00000
C	-1.27524	0.71625	0.00000
C	-1.27524	-0.71625	0.00000
C	-0.01056	-1.24581	0.00000
S	1.20089	0.00000	0.00000
H	0.28312	2.28765	0.00000
H	-2.17537	1.32236	0.00000
H	-2.17537	-1.32235	0.00000
H	0.28311	-2.28765	0.00000

cyclopentane

Energy = -196.625426215
Free Energy = -196.451091
ZPE = 0.140925
xyz coordinates

C	1.22065	-0.37217	-0.20018
C	0.05011	-1.25724	0.26293
C	-1.18612	-0.46855	-0.20335
C	-0.82215	1.01202	0.07223
C	0.73766	1.07566	0.06817
H	1.38610	-0.52230	-1.27606
H	2.16484	-0.60417	0.30640
H	0.05175	-1.34000	1.35961
H	0.09176	-2.27526	-0.14269
H	-2.11104	-0.77787	0.29747
H	-1.33326	-0.62759	-1.28072
H	-1.21211	1.32267	1.04930
H	-1.26647	1.68458	-0.67029
H	1.12119	1.77641	-0.68211
H	1.10629	1.42525	1.04026

1,3,2-diazaborolidine

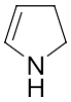


Energy = -214.928765755
Free Energy = -214.778498

ZPE = 0.103376
xyz coordinates

N	1.14269	0.46247	-0.12208
B	0.00077	1.30337	0.00005
N	-1.14218	0.46365	0.12214
C	-0.76567	-0.93564	-0.11960
C	0.76459	-0.93651	0.11958
H	2.10831	0.73198	-0.00439
H	0.00135	2.49646	-0.00018
H	-2.10739	0.73453	0.00405
H	-0.99374	-1.23443	-1.15501
H	-1.28164	-1.62928	0.55480
H	0.99228	-1.23541	1.15502
H	1.27984	-1.63066	-0.55482

2,3-dihydro-1H-pyrrole



Energy = -211.437118610
Free Energy = -211.288226
ZPE = 0.105818
xyz coordinates

C	1.22559	0.28067	-0.10393
C	0.52383	-1.08065	0.13072
N	-0.89342	-0.80185	-0.19909
C	-1.07839	0.57717	0.01867
C	0.07824	1.25652	0.08845
H	1.62760	0.34390	-1.12775
H	2.06625	0.43253	0.58280
H	0.62230	-1.37307	1.18889
H	0.91821	-1.88789	-0.49328
H	-1.56643	-1.41116	0.25474
H	-2.08874	0.97262	0.04501
H	0.17913	2.33369	0.13976

2,3-dihydro-1H-1,2-azaborole

Energy = -197.626046127
Free Energy = -197.497948
ZPE = 0.089703
xyz coordinates

N	1.18534	0.28042	-0.00002
B	0.18404	1.27808	-0.00007
C	-1.19769	0.48661	0.00002
C	-0.74111	-0.95830	-0.00006
C	0.60158	-1.01630	0.00007
H	2.19066	0.38642	-0.00010
H	0.41404	2.44914	0.00006
H	-1.82298	0.72828	-0.87456
H	-1.82243	0.72769	0.87516
H	-1.39440	-1.82389	-0.00037
H	1.24081	-1.89303	0.00010

1,2-azaborolidine

Energy = -198.852988725
Free Energy = -198.700296
ZPE = 0.114267
xyz coordinates

N	1.12721	0.52141	-0.06062
B	-0.00304	1.34580	-0.05604
C	-1.27223	0.40408	0.11919
C	-0.68487	-1.00536	-0.16949
C	0.82826	-0.90716	0.13189
H	2.09592	0.81409	-0.08355
H	0.06520	2.53714	-0.13994
H	-2.13089	0.63972	-0.52111
H	-1.63923	0.47741	1.15640
H	-0.82053	-1.24183	-1.23243
H	-1.15871	-1.80947	0.40528
H	1.05467	-1.20960	1.16587
H	1.43134	-1.53565	-0.53548

cyclopentene

Energy = -195.395941582
Free Energy = -195.244891
ZPE = 0.116940
xyz coordinates

C	-1.23669	-0.31884	0.10424
C	0.00000	-1.22750	-0.13724
C	1.23669	-0.31883	0.10424
C	0.66920	1.07663	-0.04700
C	-0.66921	1.07663	-0.04700
H	-1.65433	-0.45677	1.11408
H	-2.05364	-0.52810	-0.59849
H	0.00000	-1.56776	-1.17980
H	0.00001	-2.12058	0.49667
H	2.05365	-0.52808	-0.59848
H	1.65433	-0.45676	1.11408
H	1.29389	1.96475	-0.10575
H	-1.29390	1.96475	-0.10575

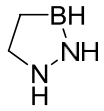
pyrrolidine

Energy = -212.661673456
Free Energy = -212.489035
ZPE = 0.129986
xyz coordinates

C	0.77914	1.03018	-0.05690
C	1.16464	-0.44736	0.17087
N	0.00027	-1.17170	-0.35072
C	-1.16443	-0.44789	0.17085

C	-0.77962	1.02982	-0.05686
H	1.16228	1.37979	-1.02101
H	1.19883	1.67901	0.71904
H	1.32678	-0.63063	1.25087
H	2.07515	-0.74281	-0.36179
H	0.00049	-2.15476	-0.08701
H	-1.32654	-0.63126	1.25083
H	-2.07478	-0.74375	-0.36187
H	-1.16296	1.37935	-1.02093
H	-1.19955	1.67841	0.71915

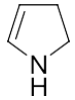
1,2,3-diazaborolidine



Energy = -214.862368319
Free Energy = -214.713605
ZPE = 0.102778
xyz coordinates

B	-0.37728	1.27470	-0.04037
N	-1.21499	0.16009	-0.04641
N	-0.53775	-1.11405	0.07662
C	0.88093	-0.77736	-0.21553
C	1.10111	0.71148	0.14850
H	-0.78701	2.38845	-0.16561
H	-2.20316	0.07208	-0.24108
H	-0.60476	-1.37504	1.06430
H	1.03673	-0.92373	-1.29170
H	1.52397	-1.48474	0.31936
H	1.43630	0.83795	1.19122
H	1.86116	1.18457	-0.48392

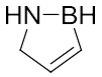
2,3-dihydro-1H-pyrrole



Energy = -211.437118610
Free Energy = -211.288226
ZPE = 0.105818
xyz coordinates

C	1.22559	0.28067	-0.10393
C	0.52383	-1.08065	0.13072
N	-0.89342	-0.80185	-0.19909
C	-1.07839	0.57717	0.01867
C	0.07824	1.25652	0.08845
H	1.62760	0.34390	-1.12775
H	2.06625	0.43253	0.58280
H	0.62230	-1.37307	1.18889
H	0.91821	-1.88789	-0.49328
H	-1.56643	-1.41116	0.25474
H	-2.08874	0.97262	0.04501
H	0.17913	2.33369	0.13976

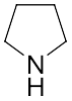
2,5-dihydro-1H-1,2-azaborole



Energy = -197.627446355
Free Energy = -197.499246
ZPE = 0.090719
xyz coordinates

B	0.12521	1.31241	0.00025
N	1.13978	0.33322	-0.00024
C	0.59550	-1.02109	0.00015
C	-0.89490	-0.80208	-0.00007
C	-1.21762	0.50973	-0.00004
H	0.34171	2.48684	0.00002
H	2.14157	0.46374	-0.00018
H	0.92003	-1.58919	0.88588
H	0.92029	-1.58967	-0.88517
H	-1.58013	-1.64758	-0.00026
H	-2.24578	0.86197	-0.00006

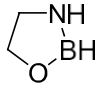
pyrrolidine



Energy = -212.661673456
Free Energy = -212.489035
ZPE = 0.129986
xyz coordinates

C	0.77914	1.03018	-0.05690
C	1.16464	-0.44736	0.17087
N	0.00027	-1.17170	-0.35072
C	-1.16443	-0.44789	0.17085
C	-0.77962	1.02982	-0.05686
H	1.16228	1.37979	-1.02101
H	1.19883	1.67901	0.71904
H	1.32678	-0.63063	1.25087
H	2.07515	-0.74281	-0.36179
H	0.00049	-2.15476	-0.08701
H	-1.32654	-0.63126	1.25083
H	-2.07478	-0.74375	-0.36187
H	-1.16296	1.37935	-1.02093
H	-1.19955	1.67841	0.71915

1,3,2-oxazaborolidine



Energy = -234.813264551
Free Energy = -234.669410
ZPE = 0.091289
xyz coordinates

N	1.16984	0.31726	0.07919
B	0.12609	1.26337	-0.00420
O	-1.09952	0.63210	-0.06991
C	-0.89167	-0.78834	0.08129
C	0.63061	-1.03613	-0.08309

H	2.16618	0.47262	0.04167
H	0.22888	2.44935	-0.01915
H	-1.49238	-1.31261	-0.66713
H	-1.24173	-1.07700	1.07946
H	1.01091	-1.73103	0.67565
H	0.87135	-1.44891	-1.07378

2,3-dihydrofuran

Energy = -231.308582848
Free Energy = -231.166902
ZPE = 0.093064
xyz coordinates

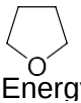
C	-0.92505	0.84820	-0.06830
C	-0.97050	-0.69281	0.08004
O	0.39808	-1.16738	-0.07708
C	1.20491	-0.06324	0.01031
C	0.56424	1.10893	0.04826
H	-1.51671	1.34455	0.71017
H	-1.32031	1.18388	-1.03821
H	-1.57989	-1.19904	-0.67197
H	-1.30449	-0.99694	1.07916
H	2.26533	-0.28496	0.02258
H	1.02985	2.08506	0.09309

2,3-dihydro-1,3,2-oxazaborole

Energy = -233.596485207
Free Energy = -233.475705
ZPE = 0.067646
xyz coordinates

N	1.15577	-0.19369	-0.00007
B	0.54183	1.08950	-0.00002
O	-0.83467	0.87979	-0.00001
C	-1.04812	-0.48410	0.00000
C	0.12585	-1.14855	0.00005
H	2.12959	-0.45686	0.00024
H	1.04284	2.16462	0.00016
H	-2.07114	-0.82819	0.00003
H	0.31026	-2.21362	-0.00009

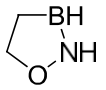
THF



Energy = -232.536113936
Free Energy = -232.370595
ZPE = 0.117299
xyz coordinates

C	0.77736	1.01783	-0.04950
C	1.13741	-0.46927	0.15607
O	0.00042	-1.20568	-0.29237
C	-1.13692	-0.47011	0.15646
C	-0.77827	1.01708	-0.05001
H	1.16553	1.38197	-1.00612
H	1.19762	1.64925	0.74048
H	1.32356	-0.68604	1.22148
H	1.99972	-0.80666	-0.42500
H	-1.32228	-0.68653	1.22207
H	-1.99928	-0.80849	-0.42397
H	-1.16614	1.37997	-1.00723
H	-1.19964	1.64880	0.73915

1,2,3-oxazaborolidine



Energy = -234.714434366
Free Energy = -234.573009
ZPE = 0.089361
xyz coordinates

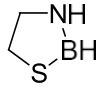
B	-0.51078	1.21963	0.05826
N	-1.21340	0.02688	0.04298
O	-0.40411	-1.13458	-0.16685
C	0.93742	-0.69981	0.16661
C	1.01877	0.80910	-0.11786
H	-1.04945	2.27611	0.16819
H	-2.18477	-0.24807	0.06723
H	1.60255	-1.32681	-0.43267
H	1.10671	-0.90216	1.23462
H	1.71558	1.31643	0.55804
H	1.35274	1.01906	-1.14525

2,3-dihydrofuran

Energy = -231.308582848
Free Energy = -231.166902
ZPE = 0.093064
xyz coordinates

C	-0.92505	0.84820	-0.06830
C	-0.97050	-0.69281	0.08004
O	0.39808	-1.16738	-0.07708
C	1.20491	-0.06324	0.01031
C	0.56424	1.10893	0.04826
H	-1.51671	1.34455	0.71017
H	-1.32031	1.18388	-1.03821
H	-1.57989	-1.19904	-0.67197
H	-1.30449	-0.99694	1.07916
H	2.26533	-0.28496	0.02258
H	1.02985	2.08506	0.09309

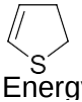
1,3,2-thiazaborolidine



Energy = -557.774823798
Free Energy = -557.629948
ZPE = 0.088431
xyz coordinates

N	1.21076	0.82286	0.09294
B	-0.08861	1.35126	0.06052
S	-1.32940	0.01929	-0.07547
C	-0.00027	-1.25632	0.19509
C	1.34182	-0.61218	-0.18307
H	2.05358	1.38283	0.08106
H	-0.35098	2.51081	0.10698
H	-0.21353	-2.14149	-0.40816
H	-0.01882	-1.53769	1.25248
H	2.15993	-1.05289	0.39971
H	1.55860	-0.77557	-1.24973

2,3-dihydrothiophene



Energy = -554.293720068
Free Energy = -554.149549
ZPE = 0.089933
xyz coordinates

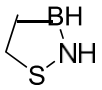
C	1.40011	-0.56193	-0.16557
C	0.07977	-1.27312	0.19673
S	-1.28377	-0.04437	-0.08338
C	-0.11666	1.28481	0.07662
C	1.17084	0.91700	0.05773
H	1.65977	-0.74067	-1.22143
H	2.22662	-0.95832	0.43699
H	0.06283	-1.55316	1.25518
H	-0.10961	-2.16268	-0.40803
H	-0.49546	2.29832	0.15733
H	1.99177	1.62587	0.12092

tetrahydrothiophene

Energy = -555.524694377
Free Energy = -555.356410
ZPE = 0.114259
xyz coordinates

C	1.28775	0.71739	0.27257
C	-0.05088	1.34599	-0.13627
S	-1.31994	0.00001	0.00003
C	-0.05091	-1.34601	0.13617
C	1.28777	-0.71738	-0.27251
H	1.36819	0.69702	1.36724
H	2.13151	1.30405	-0.11212
H	-0.02133	1.70693	-1.16970
H	-0.34001	2.17703	0.51294
H	-0.34001	-2.17695	-0.51318
H	-0.02142	-1.70711	1.16955
H	2.13149	-1.30406	0.11224
H	1.36831	-0.69700	-1.36717

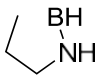
1,2,3-thiazaborolidine



Energy = -557.734787089
Free Energy = -557.588280
ZPE = 0.086376
xyz coordinates

B	1.17644	1.03396	0.04043
N	-0.19923	1.26862	0.10005
S	-1.24019	-0.14131	-0.10995
C	0.18402	-1.25887	0.25036
C	1.46227	-0.51317	-0.18890
H	1.95875	1.93238	0.13359
H	-0.68300	2.14934	0.22381
H	0.00954	-2.19845	-0.28237
H	0.20195	-1.46177	1.32693
H	2.33714	-0.90003	0.34791
H	1.65342	-0.67845	-1.26185

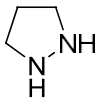
1,2-azaborolidine



Energy = -198.852987853
Free Energy = -198.700294
ZPE = 0.114267
xyz coordinates

B	-0.00321	1.34582	-0.05606
N	1.12715	0.52147	-0.06077
C	0.82830	-0.90708	0.13207
C	-0.68472	-1.00535	-0.16972
C	-1.27225	0.40393	0.11931
H	0.06502	2.53706	-0.14005
H	2.09588	0.81423	-0.08359
H	1.05435	-1.20925	1.16624
H	1.43160	-1.53575	-0.53490
H	-1.15862	-1.80973	0.40463
H	-0.82013	-1.24143	-1.23278
H	-2.13129	0.63938	-0.52057
H	-1.63878	0.47709	1.15671

pyrazolidine

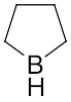


Energy = -228.673348912
Free Energy = -228.503964

ZPE = 0.118569
xyz coordinates

C	1.25008	-0.08262	-0.12489
N	0.34320	-1.20476	0.17772
N	-0.89785	-0.71106	-0.37009
C	-1.04839	0.66141	0.14564
C	0.38927	1.21529	-0.00213
H	1.61795	-0.20790	-1.14745
H	2.10356	-0.10848	0.55938
H	0.25566	-1.24566	1.20477
H	-1.65022	-1.34423	-0.10901
H	-1.36153	0.68119	1.20649
H	-1.78954	1.20968	-0.44464
H	0.48727	1.83760	-0.89728
H	0.67362	1.82406	0.86259

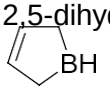
borolane



Energy = -182.754474656
Free Energy = -182.601123
ZPE = 0.122865
xyz coordinates

C	0.73861	-0.96730	0.22619
C	1.26637	0.45141	-0.11184
B	0.00000	1.38078	0.00003
C	-1.26638	0.45141	0.11180
C	-0.73860	-0.96733	-0.22616
H	0.78755	-1.12188	1.31399
H	1.32047	-1.77478	-0.23547
H	1.56065	0.49687	-1.17949
H	2.16179	0.75382	0.44598
H	0.00001	2.57895	0.00009
H	-2.16172	0.75383	-0.44614
H	-1.56081	0.49690	1.17941
H	-1.32046	-1.77479	0.23552
H	-0.78753	-1.12193	-1.31395

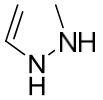
2,5-dihydro-1H-borole



Energy = -181.524822680
Free Energy = -181.396493
ZPE = 0.098775
xyz coordinates

C	-1.27680	0.38270	0.00000
B	0.00013	1.31541	-0.00002
C	1.27683	0.38249	0.00001
C	0.67133	-1.01033	-0.00000
C	-0.67150	-1.01025	0.00001
H	-1.92950	0.56857	-0.87068
H	-1.92951	0.56859	0.87068
H	0.00029	2.51198	-0.00003
H	1.92955	0.56825	0.87071
H	1.92963	0.56829	-0.87062
H	1.27670	-1.91528	-0.00007
H	-1.27703	-1.91510	-0.00001

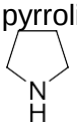
2,3-dihydro-1H-pyrazole



Energy = -227.448739456
Free Energy = -227.304116
ZPE = 0.094265
xyz coordinates

C	1.22977	0.10368	0.11707
N	0.41324	-1.13566	-0.02929
N	-0.98821	-0.73705	-0.00654
C	-1.00520	0.68140	-0.04355
C	0.21917	1.21953	-0.05455
H	2.02974	0.10382	-0.63330
H	1.71227	0.14175	1.10716
H	0.55264	-1.50456	-0.96743
H	-1.42396	-1.11571	0.83458
H	-1.96686	1.18241	-0.07877
H	0.45854	2.27358	-0.12521

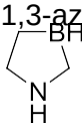
pyrrolidine



Energy = -212.661673456
Free Energy = -212.489035
ZPE = 0.129986
xyz coordinates

C	0.77914	1.03018	-0.05690
C	1.16464	-0.44736	0.17087
N	0.00027	-1.17170	-0.35072
C	-1.16443	-0.44789	0.17085
C	-0.77962	1.02982	-0.05686
H	1.16228	1.37979	-1.02101
H	1.19883	1.67901	0.71904
H	1.32678	-0.63063	1.25087
H	2.07515	-0.74281	-0.36179
H	0.00049	-2.15476	-0.08701
H	-1.32654	-0.63126	1.25083
H	-2.07478	-0.74375	-0.36187
H	-1.16296	1.37935	-1.02093
H	-1.19955	1.67841	0.71915

1,3-azaborolidine



Energy = -198.786433871
Free Energy = -198.636209
ZPE = 0.111599
xyz coordinates

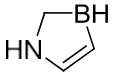
B	0.15919	1.35824	0.00019
C	1.28948	0.26282	0.10115
N	0.63104	-1.05534	-0.13461
C	-0.79481	-0.88467	0.21279
C	-1.20095	0.57886	-0.11584
H	0.31449	2.54436	0.00947
H	1.70195	0.28023	1.12881
H	2.16164	0.39390	-0.55244
H	0.70655	-1.28737	-1.12359
H	-0.90978	-1.06038	1.29188
H	-1.39346	-1.64483	-0.30135
H	-1.51531	0.66153	-1.17410
H	-2.04170	0.96672	0.47405

2,5-dihydro-1H-1,2-azaborole

Energy = -197.627446355
Free Energy = -197.499246
ZPE = 0.090719
xyz coordinates

B	0.12521	1.31241	0.00025
N	1.13978	0.33322	-0.00024
C	0.59550	-1.02109	0.00015
C	-0.89490	-0.80208	-0.00007
C	-1.21762	0.50973	-0.00004
H	0.34171	2.48684	0.00002
H	2.14157	0.46374	-0.00018
H	0.92003	-1.58919	0.88588
H	0.92029	-1.58967	-0.88517
H	-1.58013	-1.64758	-0.00026
H	-2.24578	0.86197	-0.00006

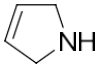
2,3-dihydro-1H-1,3-azaborole



Energy = -197.593078459
Free Energy = -197.466960
ZPE = 0.089106
xyz coordinates

B	0.12918	1.33855	-0.00000
C	-1.18587	0.42329	0.00003
N	-0.63220	-0.93290	-0.00014
C	0.72002	-0.90542	0.00000
C	1.27874	0.36364	0.00005
H	0.11727	2.53337	-0.00021
H	-1.82018	0.57962	-0.88483
H	-1.81982	0.57948	0.88519
H	-1.17647	-1.78279	0.00034
H	1.24633	-1.85910	0.00000
H	2.35502	0.49784	0.00001

2,5-dihydro-1H-pyrrole



Energy = -211.429249373
Free Energy = -211.280941
ZPE = 0.105600
xyz coordinates

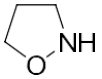
C	1.19505	-0.35091	0.09939
N	-0.00001	-1.22033	-0.02984
C	-1.19505	-0.35089	0.09939
C	-0.66797	1.06063	-0.05868
C	0.66799	1.06062	-0.05868
H	1.95470	-0.62057	-0.64599
H	1.66247	-0.48318	1.08821
H	-0.00001	-1.64029	-0.95467
H	-1.66248	-0.48316	1.08821
H	-1.95470	-0.62055	-0.64600
H	-1.30881	1.93671	-0.10473
H	1.30884	1.93669	-0.10473

1,3-oxaborolane

Energy = -218.661152218
Free Energy = -218.517587
ZPE = 0.098949
xyz coordinates

B	0.22069	1.33603	0.03000
C	1.28451	0.18113	0.06612
O	0.56275	-1.03424	-0.22251
C	-0.80295	-0.85903	0.17384
C	-1.16885	0.61533	-0.09660
H	0.43915	2.50833	0.08956
H	1.74262	0.12574	1.07617
H	2.11885	0.25843	-0.64233
H	-0.91228	-1.08594	1.24840
H	-1.39176	-1.58800	-0.39092
H	-1.49901	0.74696	-1.14290
H	-1.97925	1.00369	0.53202

isoxazolidine



Energy = -248.531856337
Free Energy = -248.369984
ZPE = 0.105423
xyz coordinates

C	1.16843	0.40321	-0.13600
N	0.77482	-0.98460	0.15756
O	-0.58473	-1.04995	-0.29661
C	-1.21441	0.17830	0.11618
C	-0.11689	1.26003	0.02636
H	1.53696	0.43996	-1.16538

H	1.98192	0.69737	0.53534
H	0.71748	-1.10294	1.17613
H	-1.59053	0.06858	1.14526
H	-2.06009	0.33761	-0.55783
H	-0.26369	1.92280	-0.83201
H	-0.09074	1.87914	0.92923

2,3-dihydro-1H-pyrrole

Energy = -211.437119037
Free Energy = -211.288226
ZPE = 0.105817
xyz coordinates

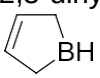
N	-0.89353	-0.80173	-0.19900
C	0.52387	-1.08070	0.13070
C	1.22553	0.28058	-0.10404
C	0.07839	1.25642	0.08877
C	-1.07832	0.57727	0.01874
H	-1.56687	-1.41112	0.25423
H	0.91808	-1.88810	-0.49318
H	0.62220	-1.37305	1.18892
H	1.62711	0.34408	-1.12799
H	2.06646	0.43222	0.58242
H	0.17951	2.33362	0.13922
H	-2.08859	0.97299	0.04441

2,3-dihydro-1,3-oxaborole

Energy = -217.459954711
Free Energy = -217.339320
ZPE = 0.077346
xyz coordinates

B	0.10963	1.32947	-0.00008
C	1.22039	0.20000	0.00013
O	0.47903	-1.06938	-0.00019
C	-0.82512	-0.77231	0.00004
C	-1.18614	0.54834	0.00005
H	0.31418	2.50446	-0.00052
H	1.86900	0.17818	0.88465
H	1.86982	0.17849	-0.88376
H	-1.45948	-1.65632	-0.00003
H	-2.22865	0.84668	0.00022

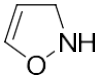
2,5-dihydro-1H-borole



Energy = -181.524822685
Free Energy = -181.396493
ZPE = 0.098775
xyz coordinates

C	-1.27680	0.38271	0.00001
B	0.00014	1.31540	0.00002
C	1.27683	0.38249	-0.00002
C	0.67133	-1.01033	0.00002
C	-0.67150	-1.01025	-0.00008
H	-1.92967	0.56864	-0.87053
H	-1.92934	0.56856	0.87082
H	0.00030	2.51198	-0.00002
H	1.92969	0.56836	0.87055
H	1.92951	0.56814	-0.87078
H	1.27669	-1.91528	0.00031
H	-1.27703	-1.91510	-0.00001

2,3-dihydroisoxazole



Energy = -247.301169836
Free Energy = -247.163467
ZPE = 0.081072
xyz coordinates

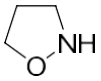
C	1.16049	0.36647	0.12632
N	0.65926	-1.02024	-0.05445
O	-0.79755	-0.92775	0.13448
C	-1.12133	0.39652	-0.02709
C	-0.07236	1.21881	-0.09419
H	1.97778	0.54512	-0.58206
H	1.56197	0.48123	1.14358
H	0.71054	-1.23907	-1.05393
H	-2.18694	0.58947	-0.04671
H	-0.09856	2.29611	-0.18580

1,3-oxaborolane

Energy = -218.661152218
Free Energy = -218.517587
ZPE = 0.098949
xyz coordinates

B	0.22069	1.33603	0.03000
C	1.28451	0.18113	0.06612
O	0.56275	-1.03424	-0.22251
C	-0.80295	-0.85903	0.17384
C	-1.16885	0.61533	-0.09660
H	0.43915	2.50833	0.08956
H	1.74262	0.12574	1.07617
H	2.11885	0.25843	-0.64233
H	-0.91228	-1.08594	1.24840
H	-1.39176	-1.58800	-0.39092
H	-1.49901	0.74696	-1.14290
H	-1.97925	1.00369	0.53202

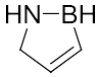
isoxazolidine



Energy = -248.531856337
Free Energy = -248.369984
ZPE = 0.105423
xyz coordinates

C	1.16843	0.40321	-0.13600
N	0.77482	-0.98460	0.15756
O	-0.58473	-1.04995	-0.29661
C	-1.21441	0.17830	0.11618
C	-0.11689	1.26003	0.02636
H	1.53696	0.43996	-1.16538
H	1.98192	0.69737	0.53534
H	0.71748	-1.10294	1.17613
H	-1.59053	0.06858	1.14526
H	-2.06009	0.33761	-0.55783
H	-0.26369	1.92280	-0.83201
H	-0.09074	1.87914	0.92923

2,5-dihydro-1H-1,2-azaborole



Energy = -197.627446355
Free Energy = -197.499246
ZPE = 0.090719
xyz coordinates

B	0.12521	1.31241	0.00025
N	1.13978	0.33322	-0.00024
C	0.59550	-1.02109	0.00015
C	-0.89490	-0.80208	-0.00007
C	-1.21762	0.50973	-0.00004
H	0.34171	2.48684	0.00002
H	2.14157	0.46374	-0.00018
H	0.92003	-1.58919	0.88588
H	0.92029	-1.58967	-0.88517
H	-1.58013	-1.64758	-0.00026
H	-2.24578	0.86197	-0.00006

2,3-dihydro-1H-borole

Energy = -181.534564252
Free Energy = -181.405864
ZPE = 0.100267
xyz coordinates

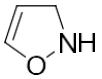
B	-0.10644	1.35088	-0.00020
C	1.20641	0.46503	0.00015
C	0.69138	-0.99843	-0.00012
C	-0.81127	-0.89200	-0.00000
C	-1.30036	0.37523	0.00006
H	-0.14308	2.54764	-0.00040
H	1.84193	0.67869	0.87272
H	1.84291	0.67873	-0.87166
H	1.03554	-1.57058	0.87469
H	1.03544	-1.57009	-0.87530
H	-1.42762	-1.79349	0.00015
H	-2.36989	0.57573	0.00025

2,3-dihydro-1,3-oxaborole

Energy = -217.459954711
Free Energy = -217.339320
ZPE = 0.077346
xyz coordinates

B	0.10963	1.32947	-0.00008
C	1.22039	0.20000	0.00013
O	0.47903	-1.06938	-0.00019
C	-0.82512	-0.77231	0.00004
C	-1.18614	0.54834	0.00005
H	0.31418	2.50446	-0.00052
H	1.86900	0.17818	0.88465
H	1.86982	0.17849	-0.88376
H	-1.45948	-1.65632	-0.00003
H	-2.22865	0.84668	0.00022

2,3-dihydroisoxazole



Energy = -247.301169836
Free Energy = -247.163467
ZPE = 0.081072
xyz coordinates

C	1.16049	0.36647	0.12632
N	0.65926	-1.02024	-0.05445
O	-0.79755	-0.92775	0.13448
C	-1.12133	0.39652	-0.02709
C	-0.07236	1.21881	-0.09419
H	1.97778	0.54512	-0.58206
H	1.56197	0.48123	1.14358
H	0.71054	-1.23907	-1.05393
H	-2.18694	0.58947	-0.04671
H	-0.09856	2.29611	-0.18580

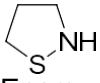
1,3-thiaborolane

Energy = -541.653613122
Free Energy = -541.508092
ZPE = 0.095904
xyz coordinates

B	-1.16770	1.08929	-0.00466
C	0.37544	1.35538	0.14422
S	1.22391	-0.26364	-0.13413
C	-0.28157	-1.26275	0.25989
C	-1.50934	-0.43250	-0.16062

H	-1.97691	1.97178	-0.02876
H	0.59456	1.74771	1.15078
H	0.75678	2.10303	-0.56218
H	-0.30903	-1.47419	1.33518
H	-0.19566	-2.21791	-0.26724
H	-1.68535	-0.55550	-1.24678
H	-2.43562	-0.76401	0.32744

isothiazolidine



Energy = -571.551727632
Free Energy = -571.384223
ZPE = 0.102740
xyz coordinates

C	-1.15875	-0.80700	-0.31034
N	0.12729	-1.29909	0.19803
S	1.28297	-0.00839	-0.07093
C	0.01454	1.36374	0.00068
C	-1.34221	0.64833	0.17191
H	-1.96086	-1.46754	0.03933
H	-1.12733	-0.84945	-1.40543
H	0.05379	-1.46134	1.20325
H	0.06962	1.92095	-0.93870
H	0.22722	2.04653	0.82776
H	-1.62804	0.64275	1.23125
H	-2.13451	1.16550	-0.38233

1,3,2-thiazaborolidine

Energy = -557.774823798
Free Energy = -557.629948
ZPE = 0.088431
xyz coordinates

N	1.21076	0.82286	0.09294
B	-0.08861	1.35126	0.06052
S	-1.32940	0.01929	-0.07547
C	-0.00027	-1.25632	0.19509
C	1.34182	-0.61218	-0.18307
H	2.05358	1.38283	0.08106
H	-0.35098	2.51081	0.10698
H	-0.21353	-2.14149	-0.40816
H	-0.01882	-1.53769	1.25248
H	2.15993	-1.05289	0.39971
H	1.55860	-0.77557	-1.24973

2,3-dihydrothiophene

Energy = -554.293720068
Free Energy = -554.149549
ZPE = 0.089933
xyz coordinates

C	1.40011	-0.56193	-0.16557
C	0.07977	-1.27312	0.19673
S	-1.28377	-0.04437	-0.08338
C	-0.11666	1.28481	0.07662
C	1.17084	0.91700	0.05773
H	1.65977	-0.74067	-1.22143
H	2.22662	-0.95832	0.43699
H	0.06283	-1.55316	1.25518
H	-0.10961	-2.16268	-0.40803
H	-0.49546	2.29832	0.15733
H	1.99177	1.62587	0.12092

2,3-dihydro-1,3-thiaborole

Energy = -540.444023551
Free Energy = -540.320963
ZPE = 0.073664
xyz coordinates

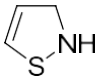
B	-1.36475	0.84319	-0.00037
C	0.14322	1.33739	0.00019
S	1.20573	-0.16678	-0.00012
C	-0.17248	-1.23198	0.00007
C	-1.42345	-0.67583	0.00007
H	-2.28210	1.61058	-0.00046
H	0.38962	1.94298	0.88218
H	0.39081	1.94441	-0.88042
H	0.04693	-2.29885	0.00032
H	-2.29683	-1.32409	0.00016

2,5-dihydro-1H-borole

Energy = -181.524822685
Free Energy = -181.396493
ZPE = 0.098775
xyz coordinates

C	-1.27680	0.38271	0.00001
B	0.00014	1.31540	0.00002
C	1.27683	0.38249	-0.00002
C	0.67133	-1.01033	0.00002
C	-0.67150	-1.01025	-0.00008
H	-1.92967	0.56864	-0.87053
H	-1.92934	0.56856	0.87082
H	0.00030	2.51198	-0.00002
H	1.92969	0.56836	0.87055
H	1.92951	0.56814	-0.87078
H	1.27669	-1.91528	0.00031
H	-1.27703	-1.91510	-0.00001

2,3-dihydroisothiazole



Energy = -570.318615157
Free Energy = -570.174970
ZPE = 0.078341
xyz coordinates

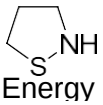
C	1.30161	-0.63226	0.20024
N	0.01312	-1.25631	-0.17592
S	-1.24100	-0.04729	0.10174
C	-0.07470	1.28699	-0.10049
C	1.19371	0.86056	-0.06588
H	2.10483	-1.12533	-0.35813
H	1.48045	-0.81161	1.27221
H	0.02174	-1.42442	-1.18380
H	-0.42639	2.30908	-0.19107
H	2.05983	1.51136	-0.13886

1,3-thiaborolane

Energy = -541.653613122
Free Energy = -541.508092
ZPE = 0.095904
xyz coordinates

B	-1.16770	1.08929	-0.00466
C	0.37544	1.35538	0.14422
S	1.22391	-0.26364	-0.13413
C	-0.28157	-1.26275	0.25989
C	-1.50934	-0.43250	-0.16062
H	-1.97691	1.97178	-0.02876
H	0.59456	1.74771	1.15078
H	0.75678	2.10303	-0.56218
H	-0.30903	-1.47419	1.33518
H	-0.19566	-2.21791	-0.26724
H	-1.68535	-0.55550	-1.24678
H	-2.43562	-0.76401	0.32744

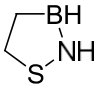
isothiazolidine



Energy = -571.551727632
Free Energy = -571.384223
ZPE = 0.102740
xyz coordinates

C	-1.15875	-0.80700	-0.31034
N	0.12729	-1.29909	0.19803
S	1.28297	-0.00839	-0.07093
C	0.01454	1.36374	0.00068
C	-1.34221	0.64833	0.17191
H	-1.96086	-1.46754	0.03933
H	-1.12733	-0.84945	-1.40543
H	0.05379	-1.46134	1.20325
H	0.06962	1.92095	-0.93870
H	0.22722	2.04653	0.82776
H	-1.62804	0.64275	1.23125
H	-2.13451	1.16550	-0.38233

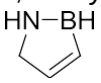
1,2,3-thiazaborolidine



Energy = -557.734787089
Free Energy = -557.588280
ZPE = 0.086376
xyz coordinates

B	1.17644	1.03396	0.04043
N	-0.19923	1.26862	0.10005
S	-1.24019	-0.14131	-0.10995
C	0.18402	-1.25887	0.25036
C	1.46227	-0.51317	-0.18890
H	1.95875	1.93238	0.13359
H	-0.68300	2.14934	0.22381
H	0.00954	-2.19845	-0.28237
H	0.20195	-1.46177	1.32693
H	2.33714	-0.90003	0.34791
H	1.65342	-0.67845	-1.26185

2,5-dihydro-1H-1,2-azaborole



Energy = -197.627446355
Free Energy = -197.499246
ZPE = 0.090719
xyz coordinates

B	0.12521	1.31241	0.00025
N	1.13978	0.33322	-0.00024
C	0.59550	-1.02109	0.00015
C	-0.89490	-0.80208	-0.00007
C	-1.21762	0.50973	-0.00004
H	0.34171	2.48684	0.00002
H	2.14157	0.46374	-0.00018
H	0.92003	-1.58919	0.88588
H	0.92029	-1.58967	-0.88517
H	-1.58013	-1.64758	-0.00026
H	-2.24578	0.86197	-0.00006

2,3-dihydro-1H-borole

Energy = -181.534564252
Free Energy = -181.405864
ZPE = 0.100267
xyz coordinates

B	-0.10644	1.35088	-0.00020
C	1.20641	0.46503	0.00015
C	0.69138	-0.99843	-0.00012
C	-0.81127	-0.89200	-0.00000

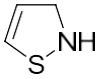
C	-1.30036	0.37523	0.00006
H	-0.14308	2.54764	-0.00040
H	1.84193	0.67869	0.87272
H	1.84291	0.67873	-0.87166
H	1.03554	-1.57058	0.87469
H	1.03544	-1.57009	-0.87530
H	-1.42762	-1.79349	0.00015
H	-2.36989	0.57573	0.00025

2,3-dihydro-1,3-thiaborole

Energy = -540.444023551
Free Energy = -540.320963
ZPE = 0.073664
xyz coordinates

B	-1.36475	0.84319	-0.00037
C	0.14322	1.33739	0.00019
S	1.20573	-0.16678	-0.00012
C	-0.17248	-1.23198	0.00007
C	-1.42345	-0.67583	0.00007
H	-2.28210	1.61058	-0.00046
H	0.38962	1.94298	0.88218
H	0.39081	1.94441	-0.88042
H	0.04693	-2.29885	0.00032
H	-2.29683	-1.32409	0.00016

2,3-dihydroisothiazole

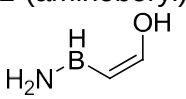


Energy = -570.318615157
Free Energy = -570.174970
ZPE = 0.078341
xyz coordinates

C	1.30161	-0.63226	0.20024
N	0.01312	-1.25631	-0.17592
S	-1.24100	-0.04729	0.10174
C	-0.07470	1.28699	-0.10049
C	1.19371	0.86056	-0.06588
H	2.10483	-1.12533	-0.35813
H	1.48045	-0.81161	1.27221
H	0.02174	-1.42442	-1.18380
H	-0.42639	2.30908	-0.19107
H	2.05983	1.51136	-0.13886

Model structures seen in Table 9.

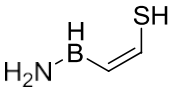
2-(aminoboryl)ethanol



Energy = -234.774258725
Free Energy = -234.624683
ZPE = 0.087879
xyz coordinates

C	0.02282	0.70250	0.00001
C	1.35906	0.54027	-0.00011
H	-0.28781	1.74959	0.00069
H	2.04964	1.38526	0.00034
H	-3.13420	-0.82116	0.00048
H	-0.73892	-1.58779	0.00059
N	-2.41015	-0.11579	-0.00015
B	-1.03617	-0.42879	0.00024
H	-2.77498	0.82918	-0.00058
O	1.96500	-0.68486	-0.00030
H	2.92678	-0.57826	0.00138

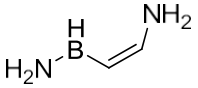
(Z)-2-(aminoboryl)ethenethiol



Energy = -557.744488790
Free Energy = -557.597951
ZPE = 0.082607
xyz coordinates

C	0.54975	0.86496	0.00001
C	-0.79928	0.90803	0.00001
H	1.02881	1.84847	-0.00022
H	-1.33279	1.85647	-0.00019
H	3.44238	-1.12394	0.00004
H	0.95408	-1.51118	0.00001
S	-1.86933	-0.51140	-0.00007
N	2.83414	-0.31631	0.00003
B	1.43190	-0.41193	0.00002
H	-3.02344	0.18624	0.00112
H	3.33893	0.56212	0.00005

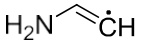
aminovinylboranamine



Energy = -214.907399902
Free Energy = -214.753765
ZPE = 0.100606
xyz coordinates

C	-0.00596	0.73430	0.01324
C	-1.35697	0.57111	0.00702
H	0.31865	1.77669	0.01576
H	-2.01925	1.43717	0.01965
B	1.03339	-0.39809	0.02504
H	0.71539	-1.56006	0.07673
N	2.42047	-0.14017	-0.01091
H	3.12142	-0.86779	0.00554
N	-2.05102	-0.61835	-0.08198
H	-2.99666	-0.63831	0.27347
H	-1.52886	-1.47184	0.07290
H	2.81380	0.79178	-0.06058

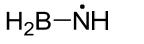
aminovinyl_Crad



Energy = -133.315189977
Free Energy = -133.234655
ZPE = 0.055088
xyz coordinates

N	0.02850	0.86493	0.03868
H	0.15412	1.77428	-0.39489
H	-1.05933	-1.68899	0.01636
H	2.36156	0.14379	1.36542
C	1.28624	-0.29983	0.02537
C	0.14730	0.37316	-0.00360
H	2.34130	-0.07461	-0.00393
H	0.17003	1.46886	-0.03009
N	-1.14879	-0.15384	-0.08926
H	-1.85725	0.38445	0.39615
H	-1.21384	-1.14181	0.13210

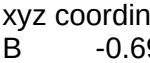
boranamine_Nrad



Energy = -81.3908398616
Free Energy = -81.353829
ZPE = 0.030488
xyz coordinates

B	-0.69749	0.01075	-0.00000
H	-1.24763	1.08898	0.00000
N	0.63821	-0.04045	0.00001
H	1.62588	0.13716	-0.00003
H	-1.35831	-0.99671	-0.00001

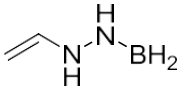
boranamine_rad



Energy = -81.4021921763
Free Energy = -81.355167
ZPE = 0.036421
xyz coordinates

B	0.83556	-0.21840	-0.00011
H	1.67935	0.62874	0.00040
N	-0.52783	0.02908	0.00000
H	-1.22821	-0.70239	0.00030
H	-0.93412	0.96210	-0.00017

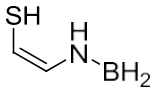
1-boryl-2-vinylhydrazine



Energy = -214.836956778
Free Energy = -214.690986
ZPE = 0.098664
xyz coordinates

C	-1.73215	-0.84007	0.07866
C	-1.29747	0.43066	0.08881
H	-2.79250	-1.04411	0.17480
H	-1.99474	1.26088	0.18210
B	2.14711	-0.38507	0.31882

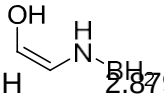
2-(borylamino)ethenethiol



Energy = -557.724244194
Free Energy = -557.581975
ZPE = 0.081716
xyz coordinates

C	-0.64332	0.84823	0.00297
C	0.69794	0.95025	0.00817
H	-1.24990	1.75002	-0.02282
H	1.15919	1.93180	-0.02230
N	-1.38275	-0.33241	0.02770
H	-0.80475	-1.16846	0.08069
B	-2.78507	-0.43977	-0.00119
H	-3.43652	0.56063	-0.06494
H	-3.27243	-1.52844	0.03887
S	1.78164	-0.46730	-0.08668
H	2.37502	-0.33389	1.12257

borylaminoethenol
(Z)-2-(borylamino)ethanol

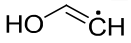


H	2.87971	-1.18632	-0.18262
N	0.99169	-0.06090	-0.39305
H	0.75200	-0.50591	-1.27943

Energy = -234.750229438
Free Energy = -234.605775 ZPE = 0.086354
xyz coordinates

C	0.07377	0.74522	-0.00003
C	-1.25311	0.56473	-0.00004
H	0.48972	1.74573	-0.00002
H	-1.94968	1.39652	0.00001
O	-1.78196	-0.71209	-0.00004
H	-2.74794	-0.67550	0.00075
N	1.00335	-0.30545	-0.00007
H	0.56843	-1.22350	-0.00024
B	2.40062	-0.19403	0.00008
H	2.89203	0.89736	0.00028
H	3.05265	-1.19533	0.00004

etheneol_Crad

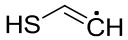


Energy = -153.186830858
Free Energy = -153.110454 ZPE = 0.042567
xyz coordinates

C	-1.23099	-0.30518	-0.00029
C	-0.11320	0.39240	0.00012

H	-2.29533	-0.13282	0.00076
H	-0.09868	1.48407	0.00049
O	1.16630	-0.10028	-0.00021
H	1.12869	-1.07231	0.00150

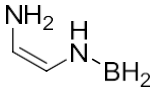
ethenethiol_Crad



Energy = -476.158741214
Free Energy = -476.085496
ZPE = 0.037249
xyz coordinates

C	-1.70625	-0.36000	-0.00010
C	-0.66631	0.44050	0.00012
H	-2.78477	-0.29419	-0.00012
H	-0.77867	1.52954	0.00040
S	1.05852	-0.02250	-0.00008
H	0.86249	-1.35837	0.00090

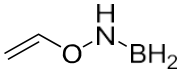
N^1-borylethene-1,2-diamine



Energy = -214.876780567
Free Energy = -214.727859
ZPE = 0.099255
xyz coordinates

C	0.09231	0.76865	-0.03043
C	-1.23997	0.59263	0.00075
H	0.52387	1.76196	0.00591
H	-1.89243	1.46041	-0.01055
N	1.01841	-0.29010	-0.10373
H	0.59978	-1.17117	-0.38997
B	2.40659	-0.22367	0.08094
H	2.90110	0.82428	0.37968
H	3.04865	-1.22133	-0.06690
N	-1.86708	-0.67399	-0.02028
H	-1.51116	-1.32837	0.67157
H	-2.87612	-0.62648	0.05178

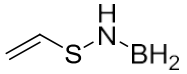
N-boryl-O-vinylhydroxylamine



Energy = -234.683413605
Free Energy = -234.544961
ZPE = 0.085400
xyz coordinates

C	-1.63872	0.85074	0.04776
C	-1.24567	-0.42194	0.13479
H	-2.68300	1.08639	0.21926
H	-1.91350	-1.24588	0.36735
O	0.01545	-0.93886	-0.04982
B	2.02743	0.39247	0.38945
H	2.82447	1.13621	-0.09899
N	0.97897	0.01313	-0.43661
H	0.84495	0.25690	-1.41308
H	-0.95994	1.66755	-0.16775
H	2.07978	-0.01733	1.50544

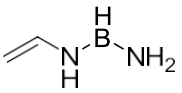
N-boryl-S-vinylthiohydroxylamine



Energy = -557.703300325
Free Energy = -557.559484
ZPE = 0.082223
xyz coordinates

C	-1.68815	1.19380	-0.02032
C	-1.49670	-0.12027	0.13624
H	-2.68421	1.61457	0.08093
H	-2.32400	-0.79241	0.36406
H	1.15200	0.36009	-1.44578
H	2.87416	1.53555	-0.10802
S	0.01380	-1.03582	0.01538
N	1.15858	0.16753	-0.44791
B	2.10482	0.77094	0.39721
H	-0.87464	1.87762	-0.24341
H	2.11078	0.50914	1.56004

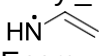
N-vinylboranediamine



Energy = -214.928988650
Free Energy = -214.777360
ZPE = 0.100158
xyz coordinates

C	2.14721	0.60757	0.00006
C	1.40329	-0.50941	-0.00004
H	3.22855	0.52462	-0.00001
H	1.90412	-1.47612	-0.00016
B	-0.97704	0.42432	-0.00009
H	-0.63753	1.56825	-0.00028
N	-2.36161	0.13074	0.00004
H	-3.05895	0.86072	-0.00005
N	0.00476	-0.61842	-0.00000
H	-0.31506	-1.57998	0.00007
H	1.72054	1.60494	0.00021
H	-2.76152	-0.79920	0.00023

nvinyl_Nrad

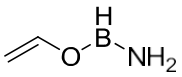


Energy = -133.354465838
Free Energy = -133.277747
ZPE = 0.055254
xyz coordinates

C	-1.20475	-0.16782	0.00002
C	0.07164	0.41044	-0.00001
H	-2.10111	0.44403	0.00005
H	0.13077	1.50656	-0.00006
N	1.15445	-0.34322	-0.00001
H	1.99368	0.24528	0.00014

H	-1.30587	-1.24899	-0.00004

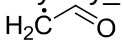
vinyloxyboranamine



Energy = -234.811553797
Free Energy = -234.666371
ZPE = 0.087551
xyz coordinates

C	-2.39765	-0.29439	-0.00000
C	-1.24949	0.38400	0.00002
H	-3.34011	0.24165	0.00005
H	-1.20674	1.47300	0.00005
O	-0.03290	-0.24008	-0.00004
H	-2.41800	-1.37992	-0.00008
B	1.15673	0.46209	0.00001
H	1.15953	1.66023	0.00012
N	2.35878	-0.26166	-0.00002
H	2.39127	-1.27364	0.00041
H	3.26498	0.18286	-0.00021

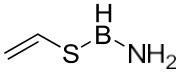
vinyloxy_Crad



Energy = -153.233250690
Free Energy = -153.164251
ZPE = 0.042678
xyz coordinates

C	1.17107	-0.17219	0.00001
C	-0.13117	0.40884	-0.00002
H	2.06282	0.44838	-0.00006
H	-0.19299	1.51366	0.00009
O	-1.17303	-0.26607	0.00000
H	1.27502	-1.25334	0.00004

vinylthioboranamine



Energy = -557.761776915
Free Energy = -557.616785
ZPE = 0.084240
xyz coordinates

C	2.70865	0.07736	0.00010
C	1.43953	0.49755	-0.00002
H	3.52253	0.79712	0.00012
H	1.19362	1.55679	-0.00012
B	-1.37087	0.55848	-0.00005
H	-1.16985	1.73541	-0.00009
N	-2.68434	0.07096	0.00009
H	-3.48403	0.68926	0.00003
S	0.04078	-0.60195	-0.00008
H	2.97647	-0.97622	0.00020
H	-2.93557	-0.90976	0.00032

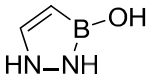
vinylthio_Srad

Energy = -476.200932863
Free Energy = -476.126850
ZPE = 0.041979
xyz coordinates

C	1.29060	1.07039	0.00000
C	0.00000	0.70849	0.00000
H	1.55785	2.12289	0.00000
H	-0.78591	1.46831	0.00000
S	-0.66366	-0.91335	0.00000
H	2.10305	0.34913	0.00000

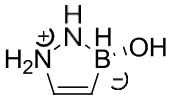
Hydrolysis (gas phase)

1H-1,2,3-diazaborol-3(2H)-ol



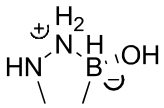
Energy = -288.962606366
Free Energy = -288.800172
ZPE = 0.085321
xyz coordinates

C	-0.20916	1.26194	0.01173
C	-1.43159	0.66835	-0.01843
H	-0.07599	2.33704	0.00625
H	-2.42053	1.11708	0.00592
B	0.79754	0.10248	0.02595
N	-0.02312	-1.09397	0.07490
H	0.18519	-1.99087	-0.34715
N	-1.38222	-0.72418	-0.10616
H	-2.00434	-1.22028	0.53046
O	2.17547	0.13923	-0.01531
H	2.60604	-0.72393	0.05631



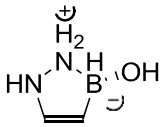
Energy = -290.083930372
Free Energy = -289.899502
ZPE = 0.106489
xyz coordinates

C	0.13671	1.26689	0.37583
C	1.26635	0.82940	-0.16684
H	-0.01136	2.32844	0.55763
H	2.16583	1.30464	-0.54693
B	-0.93779	0.03104	0.52949
H	-1.51784	-0.06859	1.59790
N	0.08908	-1.20857	0.44324
H	0.51433	-1.31721	1.36805
N	1.18714	-0.66619	-0.37399
H	0.93158	-0.87308	-1.34548
O	-1.78197	0.08241	-0.65971
H	-2.55565	-0.48707	-0.55456
H	2.06585	-1.15606	-0.18504



Energy = -290.118734270
Free Energy = -289.933813
ZPE = 0.106683
xyz coordinates

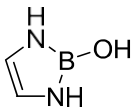
C	0.14947	1.29658	0.11743
C	1.35987	0.79310	-0.13988
H	-0.01080	2.37132	0.10702
H	2.28651	1.31005	-0.37699
B	-0.93628	0.18043	0.47288
H	-1.23009	0.03736	1.64482
N	0.16376	-1.16330	0.11264
H	0.16616	-1.91081	0.80448
N	1.50347	-0.63152	-0.00348
H	1.99364	-1.06402	-0.78564
O	-2.02815	0.02215	-0.45056
H	-2.83302	-0.27226	-0.00573
H	-0.19246	-1.52538	-0.77726



Energy = -290.118734309
Free Energy = -289.933813
ZPE = 0.106683
xyz coordinates

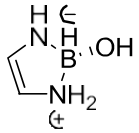
C	0.14947	1.29658	0.11743
C	1.35987	0.79310	-0.13988
H	-0.01080	2.37132	0.10702
H	2.28651	1.31005	-0.37699
B	-0.93628	0.18043	0.47288
H	-1.23009	0.03736	1.64482
N	0.16376	-1.16330	0.11264
H	0.16616	-1.91081	0.80448
N	1.50347	-0.63152	-0.00348
H	1.99364	-1.06401	-0.78564
O	-2.02815	0.02215	-0.45056
H	-2.83302	-0.27226	-0.00573
H	-0.19246	-1.52538	-0.77726

1H-1,3,2-diazaborol-2(3H)-ol



Energy = -289.027097408
Free Energy = -288.863004
ZPE = 0.085177
xyz coordinates

C	-1.44275	0.69344	0.00001
C	-1.45883	-0.66150	0.00002
H	-2.27513	1.38254	-0.00005
H	-2.31045	-1.32695	0.00002
B	0.76015	-0.01723	-0.00003
N	-0.10515	1.13625	-0.00000
H	0.11131	2.12122	-0.00001
N	-0.13829	-1.13730	-0.00002
H	0.07360	-2.12308	0.00007
O	2.13955	-0.11134	-0.00000
H	2.59709	0.73890	0.00013



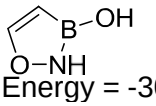
Energy = -290.179551412
Free Energy = -289.993531
ZPE = 0.106359
xyz coordinates

C	-1.46650	-0.58499	-0.23905
C	-1.32066	0.75910	-0.18560
H	-2.30931	-1.17557	-0.56593
H	-2.09248	1.46197	-0.48713
B	0.89438	0.07173	0.48207
H	1.34374	-0.07770	1.60197
N	-0.21764	-1.21723	0.21644
H	0.19922	-1.82785	-0.49194
N	-0.12801	1.20170	0.30542
H	0.13923	2.16201	0.14186
O	1.87410	0.02115	-0.56811
H	2.74277	-0.23600	-0.23400
H	-0.34532	-1.77077	1.06463

dihydrogen
Energy = -1.18001342927
Free Energy = -1.176824
ZPE = 0.010146
xyz coordinates

H	0.00000	0.00000	0.37138
H	0.00000	0.00000	-0.37138

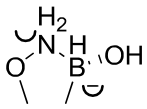
1,2,3-oxazaborol-3(2H)-ol



Energy = -308.813142230
Free Energy = -308.658692
ZPE = 0.071792
xyz coordinates

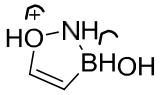
C	-0.24636	1.23921	0.00001
C	-1.44284	0.61346	0.00002
H	-0.14447	2.31696	-0.00002
H	-2.46288	0.97959	0.00000
O	-1.39237	-0.75003	0.00003
B	0.79238	0.10560	-0.00001
N	-0.01836	-1.07612	-0.00017
H	0.08082	-2.07951	0.00060

O	2.16817	0.16955	0.00003
H	2.62193	-0.68433	0.00001



Energy = -309.972354557
Free Energy = -309.795135
ZPE = 0.093516
xyz coordinates

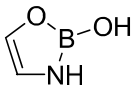
C	0.19085	1.27933	0.19047
C	1.35603	0.74813	-0.15872
H	0.07144	2.35765	0.22958
H	2.30908	1.17853	-0.44554
O	1.45487	-0.66180	-0.19002
B	-0.93120	0.17671	0.48720
H	-1.28490	0.02230	1.64031
N	0.15799	-1.15681	0.17142
H	-0.18563	-1.68208	-0.63739
O	-1.97415	0.06067	-0.49296
H	-2.80925	-0.21970	-0.09770
H	0.32226	-1.79831	0.94813



Energy = -309.906712420
Free Energy = -309.729175
ZPE = 0.090785
xyz coordinates

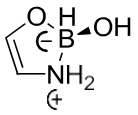
C	0.18136	1.22960	0.39499
C	1.29751	0.80122	-0.15344
H	0.04546	2.28516	0.61203
H	2.24442	1.19590	-0.49816
O	1.28724	-0.69339	-0.33414
B	-0.92883	0.02561	0.50406
H	-1.48018	-0.10910	1.58692
N	0.01577	-1.24771	0.38692
O	-1.79947	0.16209	-0.64890
H	-2.61735	-0.33965	-0.53568
H	0.46344	-1.43882	1.28863
H	1.10256	-0.92205	-1.26752

1,3,2-oxazaborol-2(3H)-ol



Energy = -308.908395282
Free Energy = -308.750930
ZPE = 0.073152
xyz coordinates

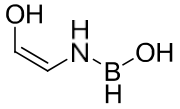
C	1.47556	0.58631	-0.00015
C	1.35862	-0.75577	-0.00022
H	2.37258	1.18963	-0.00034
H	2.09492	-1.54431	-0.00036
B	-0.73144	0.04669	0.00058
O	0.02094	-1.13088	0.00019
N	0.18442	1.14314	0.00025
O	-2.09855	0.10251	-0.00050
H	-2.50681	-0.77485	0.00078
H	0.02140	2.13776	-0.00001



Energy = -310.065515914
Free Energy = -309.885788
ZPE = 0.094411
xyz coordinates

C	-1.43715	0.57774	-0.22105
C	-1.28759	-0.76007	-0.18106
H	-2.28310	1.16775	-0.54246
H	-2.04675	-1.48760	-0.45492
B	0.85062	-0.11100	0.48209
O	-0.11870	-1.23495	0.23574
N	-0.18173	1.19952	0.21390
H	-0.29298	1.78379	1.04373
H	1.23519	-0.10661	1.62960
O	1.84233	0.03797	-0.53471
H	2.70535	-0.29963	-0.26667
H	0.26079	1.77056	-0.51265

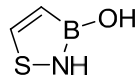
(Z)-2-(hydroxyborylamino)ethanol



Energy = -310.061287340
Free Energy = -309.879302
ZPE = 0.092678
xyz coordinates

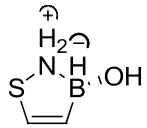
C	-0.83453	1.06916	0.03582
C	-1.86326	0.20893	0.02613
H	-1.08731	2.12165	0.11888
H	-2.87889	0.58325	0.11770
B	1.28463	-0.39818	0.11670
O	-1.71013	-1.15878	-0.05453
N	0.54013	0.79968	-0.04623
H	1.09669	1.62589	-0.24185
H	0.77971	-1.43779	0.40218
O	2.65091	-0.27715	-0.05717
H	3.11813	-1.11136	0.07656
H	-2.57193	-1.56964	-0.21156

1,2,3-thiazaborol-3(2H)-ol



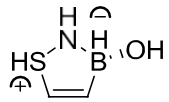
Energy = -631.833476437
Free Energy = -631.671596
ZPE = 0.068966
xyz coordinates

C	0.32449	1.36750	0.00000
C	-1.01490	1.15701	0.00000
H	0.72756	2.37627	0.00000
H	-1.81294	1.89387	-0.00000
H	0.27779	-2.04320	0.00000
S	-1.50560	-0.52123	0.00000
N	0.14045	-1.04066	0.00000
B	1.09943	0.03330	0.00000
O	2.47126	-0.11142	0.00000
H	2.78924	-1.02470	-0.00000



Energy = -632.988780435
Free Energy = -632.807022
ZPE = 0.090151
xyz coordinates

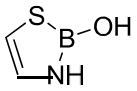
C	-0.37712	1.38356	0.16685
C	0.92424	1.23919	-0.09430
H	-0.79035	2.39236	0.16977
H	1.65946	2.00940	-0.31550
H	-0.32429	-1.65264	-0.65482
S	1.59265	-0.42524	-0.10439
N	-0.01421	-1.14781	0.17930
B	-1.26753	0.09126	0.46425
H	-1.58389	-0.09336	1.62488
O	-2.28509	-0.19765	-0.50241
H	-3.05418	-0.62260	-0.10193
H	0.04606	-1.80636	0.95548



Energy = -632.943773613
Free Energy = -632.755603
ZPE = 0.086245
xyz coordinates

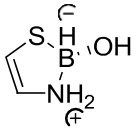
C	-0.43596	1.33978	0.32642
C	0.83800	1.30341	-0.06285
H	-0.91532	2.31287	0.43740
H	1.56006	2.07593	-0.30928
S	1.41452	-0.42412	-0.15073
N	0.02657	-1.14778	0.40686
B	-1.22667	-0.08067	0.47718
H	-1.74417	-0.28781	1.56315
O	-2.09935	-0.20274	-0.66817
H	-2.77016	-0.88393	-0.52939
H	0.25273	-1.62327	1.27862
H	1.31446	-0.60740	-1.49863

1,3,2-thiazaborol-2(3H)-ol



Energy = -631.871213196
Free Energy = -631.711747
ZPE = 0.070263
xyz coordinates

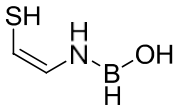
C	-1.28187	1.12800	-0.00015
C	-1.64665	-0.17122	-0.00003
H	-1.96032	1.97365	0.00006
H	-2.65517	-0.56029	0.00008
B	0.88865	0.16373	0.00018
N	0.09514	1.35067	0.00004
H	0.45690	2.29523	0.00052
S	-0.25849	-1.27932	0.00002
O	2.25991	0.17976	-0.00018
H	2.67710	-0.69155	0.00041



Energy = -633.022726228
Free Energy = -632.842188
ZPE = 0.091490
xyz coordinates

C	0.90687	1.37007	-0.21307
C	1.49630	0.17639	-0.37651
H	1.29705	2.34190	-0.48984
H	2.48028	0.08731	-0.82783
B	-1.01591	-0.22354	0.45039
H	-1.48263	-0.47445	1.53593
N	-0.41185	1.31076	0.43489
H	-1.11090	1.85896	-0.07630
S	0.66284	-1.26063	0.16431
O	-1.91441	-0.21652	-0.66111
H	-2.56089	-0.93270	-0.62754
H	-0.36954	1.68492	1.38688

(Z)-2-(hydroxyborylamino)ethenethiol



Energy = -633.036443430
Free Energy = -632.855633
ZPE = 0.088124
xyz coordinates

C	0.24451	1.44729	0.04693
C	1.43785	0.82933	0.10206
H	0.24353	2.53110	0.15075
H	2.31457	1.43791	0.29920
B	-1.53447	-0.38516	0.24611
H	-0.88872	-1.15892	0.88428
N	-1.02466	0.88662	-0.12931
S	1.72878	-0.92060	-0.04017
O	-2.83557	-0.65294	-0.11723
H	-3.14474	-1.51439	0.19084
H	-1.69674	1.52271	-0.54906
H	2.94701	-0.80557	-0.61470

3_TS_A (Transition state for **3** formed via mechanism A)
Energy = -290.057525537
Free Energy = -289.874153
ZPE = 0.102183
xyz coordinates

C	-0.72221	-1.19373	0.30519
C	-1.39061	-0.21521	-0.30964
H	-1.11486	-2.19950	0.40874
H	-2.35299	-0.16875	-0.80876
B	0.70783	-0.53020	0.68017
H	1.52426	-0.97506	1.43670
N	0.21836	0.92288	0.91314
H	0.97076	1.61318	0.81484
N	-0.54664	0.98891	-0.36220
H	0.46313	0.51450	-1.03994
O	1.34452	-0.36826	-0.84380
H	2.23552	0.01412	-0.81426
H	-1.04629	1.86970	-0.47762

3_TS_B
Energy = -290.078189368
Free Energy = -289.895854
ZPE = 0.101583
xyz coordinates

C	0.43115	1.30916	0.17925
C	1.44675	0.53544	-0.24455
H	0.50476	2.39163	0.18879
H	2.41029	0.83324	-0.65194
B	-0.75051	0.37016	0.62306
H	-1.37447	0.47680	1.64654
N	-0.10780	-1.05653	0.32229
H	-0.13503	-1.76376	1.05274
N	1.26600	-0.86318	-0.08754
H	1.46405	-1.39992	-0.93146
O	-1.82508	0.11012	-0.60620
H	-2.73645	-0.01714	-0.29170
H	-1.15474	-0.88230	-0.53008

4_TS_C
Energy = -290.135210003
Free Energy = -289.951927
ZPE = 0.100759
xyz coordinates

C	-1.21934	-0.88690	-0.17263
C	-1.46894	0.43421	-0.29436
H	-1.82502	-1.72037	-0.50006
H	-2.35662	0.88055	-0.72867
B	0.70092	0.36950	0.61025
H	1.34849	0.61994	1.59134
N	0.10472	-1.08458	0.37229
H	1.16275	-0.93755	-0.47664
N	-0.42429	1.22119	0.17919
H	-0.55411	2.20790	0.33672
O	1.77662	0.07863	-0.63661
H	2.70066	0.02627	-0.33831
H	0.17289	-1.79340	1.09886

1_TS_B
Energy = -309.930606579
Free Energy = -309.755141
ZPE = 0.088495
xyz coordinates

C	0.47171	1.28102	0.19371
C	1.44676	0.47690	-0.24723
H	0.58757	2.35880	0.20487
H	2.42828	0.68819	-0.65899
O	1.21892	-0.88783	-0.20340
B	-0.74139	0.37742	0.62764
H	-1.35227	0.49158	1.65757
N	-0.12080	-1.05028	0.30856
H	-1.15437	-0.87789	-0.54818
O	-1.80557	0.13956	-0.59096
H	-2.72161	0.02968	-0.28447
H	-0.05267	-1.78688	1.00709

1_TS_ A
Energy = -309.898067928
Free Energy = -309.720903
ZPE = 0.088771
xyz coordinates

C	0.74921	1.13544	0.35593
C	1.41012	0.17600	-0.27655
H	1.19422	2.10255	0.56762
H	2.39128	0.01547	-0.70307
O	0.55251	-1.01457	-0.43871
B	-0.73739	0.49858	0.65149
H	-1.47770	0.94582	1.48391

N	-0.27778	-0.96543	0.88574
O	-1.39261	0.31575	-0.76499
H	-1.42093	1.12437	-1.29690
H	-0.28660	-0.54723	-1.00830
H	-1.00402	-1.65397	0.65245

2_TS_ C
Energy = -310.018672354
Free Energy = -309.840843
ZPE = 0.089289
xyz coordinates

C	-1.23607	0.80474	-0.21023
C	-1.38278	-0.52808	-0.28234
H	-1.90805	1.57424	-0.56533
H	-2.20438	-1.09642	-0.70015
B	0.68829	-0.32003	0.61401
O	-0.34841	-1.24537	0.25068
N	0.05559	1.11355	0.35035
H	0.06203	1.83380	1.06845
H	1.32045	-0.53778	1.60942
O	1.70322	-0.07111	-0.63673
H	2.64156	-0.05758	-0.38494
H	1.13240	0.96087	-0.50606

2_TS_D
Energy = -310.009518308
Free Energy = -309.830868
ZPE = 0.088415
xyz coordinates

C	-1.47459	0.35920	-0.29591
C	-1.15129	-0.92990	-0.10110
H	-2.41301	0.72597	-0.69521
H	-1.69216	-1.84500	-0.28513
B	0.71539	0.44609	0.54437
O	0.14055	-1.04610	0.46608
N	-0.44415	1.22540	0.06836
H	-0.66872	2.16672	0.35309
H	1.31438	0.75354	1.53701
O	1.73752	0.02394	-0.60277
H	2.65705	-0.01620	-0.29194
H	1.06525	-0.99175	-0.34256

5_TS_B
Energy = -632.948303155
Free Energy = -632.768129
ZPE = 0.085373
xyz coordinates

C	-0.19142	1.49294	0.20498
C	1.04836	1.13503	-0.17100
H	-0.46432	2.54645	0.21050
H	1.85281	1.78083	-0.51643
H	-1.22269	-1.09295	-0.49389
S	1.42586	-0.59818	-0.14333
N	-0.20157	-1.01688	0.40861
B	-1.11886	0.28043	0.59554
H	-1.80591	0.27757	1.58499
O	-2.02945	-0.22933	-0.66510
H	-2.92807	-0.49053	-0.40228
H	-0.14636	-1.66775	1.18932

5_TS_A
Energy = -632.926541132
Free Energy = -632.742563
ZPE = 0.084832
xyz coordinates

C	-0.42879	1.45561	0.32013
C	0.80518	1.29539	-0.16361
H	-0.83877	2.45820	0.44656
H	1.56053	1.99006	-0.51751
S	1.16281	-0.52195	-0.25228
N	-0.00475	-0.96858	0.93079
B	-1.18198	-0.00539	0.56127
H	-2.11360	-0.06923	1.32165
O	-1.49698	-0.54214	-0.84860
H	-1.90732	0.12938	-1.41324
H	0.39247	-0.83539	1.86097
H	-0.03763	-0.68371	-1.13425

6_TS_thiazaborole132_C
Energy = -632.980624483
Free Energy = -632.801976
ZPE = 0.086384
xyz coordinates

C	0.65389	1.48812	-0.10859
C	1.46315	0.44829	-0.36404
H	0.87383	2.52859	-0.32255
H	2.43665	0.53828	-0.83269
B	-0.81398	-0.41084	0.57206
H	-1.36702	-0.83076	1.54785
N	-0.63269	1.15076	0.42705
H	-1.59600	0.74825	-0.46976
S	0.86643	-1.15274	0.10720
O	-1.84112	-0.40334	-0.67486
H	-2.74282	-0.68432	-0.44212
H	-0.94207	1.75099	1.18911

6_TS_D
Energy = -632.981013708
Free Energy = -632.802064
ZPE = 0.084335
xyz coordinates

C	1.36806	0.91257	-0.24204
C	1.44484	-0.43163	-0.37529
H	2.16976	1.58140	-0.54513
H	2.27906	-0.97504	-0.79746
B	-0.90183	0.54200	0.56703
H	-1.58838	0.69198	1.53590
N	0.23100	1.45120	0.32334

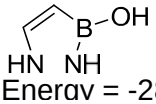
S	0.04771	-1.31208	0.29096
O	-1.75835	0.27779	-0.71493
H	-2.70598	0.17959	-0.51521
H	0.29081	2.37560	0.72728
H	-1.12702	-0.83658	-0.73596

water
Energy = -76.4640659845
Free Energy = -76.419138
ZPE = 0.021095
xyz coordinates

O	0.00000	0.00000	0.11731
H	0.00000	0.77122	-0.46923
H	0.00000	-0.77122	-0.46923

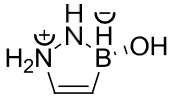
Hydrolysis (water phase)

1H-1,2,3-diazaborol-3(2H)-ol



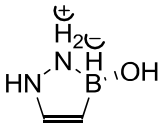
Energy = -288.973401121
Free Energy = -288.812659
ZPE = 0.085047
xyz coordinates

C	-0.21084	1.26172	0.01293
C	-1.43850	0.66340	-0.01554
H	-0.08875	2.33912	0.00769
H	-2.42861	1.10753	0.01396
B	0.79655	0.10280	0.02463
N	-0.02232	-1.08566	0.06856
H	0.18551	-2.02178	-0.25706
N	-1.37601	-0.71877	-0.10492
H	-2.02465	-1.25376	0.46883
O	2.18184	0.14085	-0.01205
H	2.60345	-0.73164	0.01004



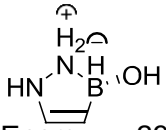
Energy = -290.108577010
Free Energy = -289.925686
ZPE = 0.106556
xyz coordinates

C	0.08714	1.25635	0.32485
C	1.27110	0.87011	-0.13546
H	-0.11303	2.31578	0.47230
H	2.16609	1.39829	-0.44691
B	-0.92249	-0.00743	0.48849
H	-1.41856	-0.16493	1.60215
N	0.11060	-1.21085	0.26948
H	0.41182	-1.56702	1.17597
N	1.32996	-0.61816	-0.30046
H	1.38236	-0.86850	-1.29363
O	-1.94563	0.06970	-0.57489
H	-2.65249	-0.56874	-0.40373
H	2.16791	-1.02103	0.13104



Energy = -290.134969413
Free Energy = -289.951425
ZPE = 0.106871
xyz coordinates

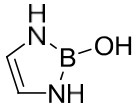
C	0.15328	1.29555	0.11292
C	1.36778	0.78717	-0.13638
H	-0.00330	2.37179	0.10658
H	2.29611	1.30042	-0.37439
B	-0.91032	0.15249	0.46203
H	-1.19407	0.00305	1.64073
N	0.15058	-1.15721	0.08602
H	0.13976	-1.92156	0.76056
N	1.49832	-0.62835	0.00966
H	2.01997	-1.07911	-0.74068
O	-2.05401	0.06190	-0.42629
H	-2.79196	-0.39818	-0.00232
H	-0.15149	-1.53138	-0.81940



Energy = -290.134969413
Free Energy = -289.951425
ZPE = 0.106871
xyz coordinates

C	0.15328	1.29555	0.11292
C	1.36778	0.78717	-0.13638
H	-0.00330	2.37179	0.10658
H	2.29611	1.30042	-0.37439
B	-0.91032	0.15249	0.46203
H	-1.19407	0.00305	1.64073
N	0.15058	-1.15721	0.08602
H	0.13976	-1.92156	0.76056
N	1.49832	-0.62835	0.00966
H	2.01997	-1.07911	-0.74068
O	-2.05401	0.06190	-0.42629
H	-2.79196	-0.39818	-0.00232
H	-0.15149	-1.53138	-0.81940

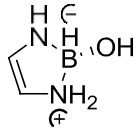
1H-1,3,2-diazaborol-2(3H)-ol



Energy = -289.036131731
Free Energy = -288.873673
ZPE = 0.085099
xyz coordinates

C	-1.43774	0.70109	-0.00003

C	-1.46377	-0.65617	-0.00001
H	-2.26387	1.39824	-0.00005
H	-2.31708	-1.31984	-0.00002
B	0.75834	-0.02200	0.00001
N	-0.09839	1.13461	-0.00001
H	0.13042	2.11815	-0.00002
N	-0.14424	-1.14074	0.00001
H	0.05252	-2.13094	0.00003
O	2.14094	-0.11575	0.00003
H	2.58626	0.74375	0.00003



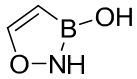
Energy = -290.191845799
Free Energy = -290.007339
ZPE = 0.106245
xyz coordinates

C	-1.43580	-0.58527	-0.28119
C	-1.30841	0.75711	-0.20254
H	-2.26606	-1.18542	-0.62270
H	-2.06937	1.46313	-0.52221
B	0.88397	0.05640	0.48640
H	1.38328	-0.09916	1.58633
N	-0.21236	-1.21396	0.24680
H	0.18947	-1.89417	-0.40389
N	-0.13281	1.19833	0.35423
H	0.13753	2.15891	0.18740
O	1.85026	0.05554	-0.59427
H	2.67587	-0.37092	-0.32438
H	-0.39119	-1.72037	1.11685

dihydrogen
Energy = -1.18017610744
Free Energy = -1.176923
ZPE = 0.010134
xyz coordinates

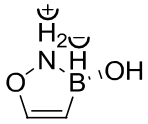
H	0.00000	0.00000	0.37151
H	0.00000	0.00000	-0.37151

1,2,3-oxazaborol-3(2H)-ol



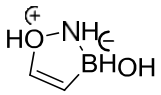
Energy = -308.821790051
Free Energy = -308.668815
ZPE = 0.071644
xyz coordinates

C	-0.25220	1.23968	-0.00006
C	-1.44814	0.60900	-0.00000
H	-0.16246	2.31920	-0.00012
H	-2.46917	0.97225	-0.00001
O	-1.38739	-0.75448	0.00006
B	0.78988	0.10717	-0.00002
N	-0.01167	-1.07619	-0.00003
H	0.10383	-2.07932	0.00035
O	2.16827	0.17659	-0.00001
H	2.61505	-0.68361	0.00004



Energy = -309.985668961
Free Energy = -309.809460
ZPE = 0.093616
xyz coordinates

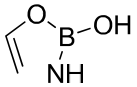
C	0.19166	1.27431	0.23495
C	1.34506	0.74722	-0.16588
H	0.08314	2.35198	0.31690
H	2.29157	1.18602	-0.46298
O	1.42900	-0.65401	-0.24608
B	-0.91971	0.14840	0.48844
H	-1.31559	-0.02254	1.62658
N	0.15871	-1.15988	0.20660
H	-0.17034	-1.78474	-0.53402
O	-1.95981	0.10289	-0.51588
H	-2.74836	-0.34983	-0.18503
H	0.37331	-1.72391	1.03136



Energy = -309.923578976
Free Energy = -309.747002
ZPE = 0.090982
xyz coordinates

C	0.14764	1.23151	0.34226
C	1.30512	0.82646	-0.13758
H	-0.01965	2.29060	0.51946
H	2.24712	1.25573	-0.45287
O	1.36567	-0.65512	-0.25342
B	-0.91872	0.00869	0.47729
H	-1.41705	-0.14937	1.58610
N	0.04330	-1.24483	0.27361
O	-1.91507	0.13634	-0.59274
H	-2.68867	-0.41317	-0.40342
H	0.40346	-1.56378	1.17613
H	1.44395	-0.94720	-1.18596

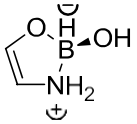
1,3,2-oxazaborol-2(3H)-ol



Energy = -308.915569761
Free Energy = -308.759593
ZPE = 0.072782
xyz coordinates

C	1.47441	0.58867	-0.00020
C	1.36442	-0.75443	-0.00017

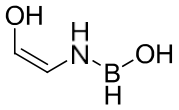
H	2.36739	1.19800	-0.00033
H	2.10200	-1.54209	-0.00025
B	-0.73150	0.04614	0.00010
O	0.02204	-1.13356	0.00002
N	0.18288	1.14152	-0.00004
O	-2.10120	0.10245	0.00027
H	-2.51878	-0.77243	0.00040
H	0.02701	2.13870	-0.00003



Energy = -310.080115393
Free Energy = -309.901789
ZPE = 0.094356
xyz coordinates

C	-1.45845	0.55001	-0.22656
C	-1.28829	-0.77898	-0.16018
H	-2.32367	1.11726	-0.53758
H	-2.03261	-1.53176	-0.39969
B	0.84880	-0.07211	0.47054
O	-0.08504	-1.22127	0.24397
N	-0.21485	1.21007	0.18232
H	-0.34691	1.80097	1.00574
H	1.22893	0.00358	1.61927
O	1.87625	-0.05266	-0.52863
H	2.72014	0.25032	-0.16708
H	0.16493	1.81492	-0.55191

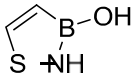
(Z)-2-(hydroxyborylamino)ethanol



Energy = -310.071255396
Free Energy = -309.891681
ZPE = 0.092532
xyz coordinates

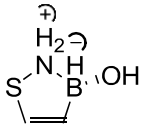
C	-0.83177	1.06764	0.02540
C	-1.86888	0.21562	0.01958
H	-1.07777	2.12312	0.07670
H	-2.88205	0.60054	0.07542
B	1.29435	-0.40459	0.07488
O	-1.73579	-1.15585	-0.04257
N	0.54793	0.79679	-0.03224
H	1.10042	1.64040	-0.15487
H	0.78646	-1.46574	0.25927
O	2.66817	-0.27792	-0.03603
H	3.12684	-1.12504	0.05375
H	-2.61629	-1.55732	-0.10010

1,2,3-thiazaborol-3(2H)-ol



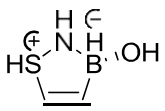
Energy = -631.842304611
Free Energy = -631.681714
ZPE = 0.068914
xyz coordinates

C	0.31917	1.37107	-0.00000
C	-1.02175	1.15516	0.00000
H	0.71200	2.38469	-0.00001
H	-1.82369	1.88760	0.00000
H	0.29176	-2.04093	0.00002
S	-1.50080	-0.52590	0.00000
N	0.14471	-1.03848	-0.00000
B	1.09610	0.03650	-0.00000
O	2.47206	-0.10753	0.00000
H	2.77832	-1.02722	-0.00002



Energy = -633.001344556
Free Energy = -632.820918
ZPE = 0.090279
xyz coordinates

C	-0.37863	1.38458	0.21313
C	0.91739	1.23935	-0.08441
H	-0.78249	2.39668	0.26261
H	1.65405	2.01153	-0.29490
H	-0.30616	-1.77066	-0.49279
S	1.56937	-0.42468	-0.15009
N	-0.01639	-1.14328	0.26185
B	-1.25499	0.07023	0.46171
H	-1.64872	-0.11468	1.60030
O	-2.25064	-0.17051	-0.55739
H	-2.95804	-0.74507	-0.23206
H	0.09368	-1.71063	1.10358

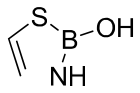


Energy = -632.959185089
Free Energy = -632.773108
ZPE = 0.086409
xyz coordinates

C	-0.41976	1.34146	0.28222
C	0.86740	1.28886	-0.06110
H	-0.88372	2.32510	0.37070
H	1.60162	2.05618	-0.28441
S	1.44892	-0.43095	-0.11510
N	-0.00243	-1.14638	0.30937
B	-1.20944	-0.06637	0.45895
H	-1.68272	-0.25616	1.57390

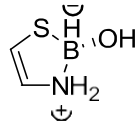
O	-2.20770	-0.18444	-0.60961
H	-2.84969	-0.87680	-0.39827
H	0.17669	-1.71267	1.13638
H	1.49508	-0.59020	-1.46683

1,3,2-thiazaborol-2(3H)-ol



Energy = -631.878759012
Free Energy = -631.720759
ZPE = 0.070086
xyz coordinates

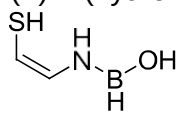
C	-1.28473	1.12547	-0.00001
C	-1.64989	-0.17462	-0.00008
H	-1.96206	1.97174	0.00000
H	-2.65772	-0.56632	-0.00014
B	0.89101	0.16916	0.00005
N	0.09170	1.35097	0.00006
H	0.44220	2.30103	0.00012
S	-0.25559	-1.27983	-0.00007
O	2.26236	0.18191	0.00010
H	2.67881	-0.69212	0.00010



Energy = -633.037920369
Free Energy = -632.859240
ZPE = 0.091434
xyz coordinates

C	1.01504	1.30255	-0.22067
C	1.52599	0.07543	-0.37185
H	1.47531	2.24316	-0.49639
H	2.50484	-0.09386	-0.80941
B	-1.03504	-0.13336	0.43805
H	-1.53119	-0.32272	1.52056
N	-0.30489	1.34390	0.42088
H	-0.93404	1.98688	-0.07014
S	0.56451	-1.29466	0.17241
O	-1.93095	-0.16961	-0.68021
H	-2.81505	-0.45948	-0.41760
H	-0.22118	1.70905	1.37484

(Z)-2-(hydroxyborylamino)ethenethiol



Energy = -633.044201858
Free Energy = -632.865037
ZPE = 0.088018
xyz coordinates

C	0.23801	1.44622	0.04762
C	1.43396	0.83229	0.10616
H	0.23490	2.52979	0.14455
H	2.31132	1.44169	0.29486
B	-1.54005	-0.38924	0.23151
H	-0.88020	-1.17761	0.83675
N	-1.03210	0.88588	-0.13451
S	1.74157	-0.91744	-0.04600
O	-2.84864	-0.65808	-0.10642
H	-3.14518	-1.52616	0.20215
H	-1.70594	1.54411	-0.51695
H	3.00224	-0.79428	-0.51265

3_TS_B
Energy = -290.070765430
Free Energy = -289.888960
ZPE = 0.102268
xyz coordinates

C	-0.73528	-1.19145	0.30098
C	-1.39266	-0.19822	-0.31032
H	-1.14051	-2.19478	0.38721
H	-2.35127	-0.14399	-0.81547
B	0.70084	-0.53963	0.67649
H	1.51249	-1.00054	1.43385
N	0.22976	0.91528	0.91444
H	0.98513	1.59985	0.81121
N	-0.54450	0.99182	-0.35293
H	0.48005	0.49454	-1.03641
O	1.34804	-0.37576	-0.84295
H	2.21911	0.05506	-0.81137
H	-1.02273	1.88238	-0.48243

3_TS_A
Energy = -290.087498575
Free Energy = -289.906814
ZPE = 0.101172
xyz coordinates

C	0.43222	1.30844	0.18178
C	1.44935	0.53236	-0.24681
H	0.50966	2.39174	0.18840
H	2.40755	0.82964	-0.66665
B	-0.74780	0.36256	0.62723
H	-1.37394	0.47670	1.64975
N	-0.10808	-1.05272	0.31672
H	-0.15663	-1.78861	1.01727
N	1.26787	-0.85905	-0.08147
H	1.48820	-1.41153	-0.90938
O	-1.83200	0.11893	-0.60447
H	-2.73421	-0.06082	-0.28292
H	-1.15361	-0.86381	-0.55347

4_TS_C
Energy = -290.143251990
Free Energy = -289.961703
ZPE = 0.100359
xyz coordinates

C	-1.21573	-0.89426	-0.16791
C	-1.48108	0.42429	-0.29375
H	-1.81897	-1.73618	-0.47962
H	-2.37835	0.86341	-0.71575
B	0.69048	0.37198	0.61140
H	1.32634	0.63746	1.59551
N	0.10998	-1.07954	0.36921
H	1.16989	-0.91908	-0.48032
N	-0.42708	1.22599	0.15246
H	-0.60725	2.18362	0.41701
O	1.79344	0.09029	-0.63032
H	2.70644	-0.00674	-0.30436
H	0.20254	-1.80998	1.07140

1_TS_B
Energy = -309.938700539
Free Energy = -309.764623
ZPE = 0.088211
xyz coordinates

C	0.47452	1.27913	0.19245
C	1.45304	0.47480	-0.24476
H	0.59703	2.35696	0.20717
H	2.43746	0.68744	-0.64942
O	1.22089	-0.88858	-0.20055
B	-0.74200	0.37268	0.62535
H	-1.34544	0.49469	1.65853
N	-0.12551	-1.05161	0.30223
H	-1.15944	-0.86695	-0.55828
O	-1.81015	0.15102	-0.58750
H	-2.71964	0.00357	-0.27132
H	-0.07262	-1.80096	0.98914

1_TS_A
Energy = -309.906591949
Free Energy = -309.731030
ZPE = 0.088437
xyz coordinates

C	0.75532	1.12626	0.37268
C	1.41038	0.16984	-0.27066
H	1.20179	2.09402	0.57780
H	2.37983	0.01581	-0.72494
O	0.54257	-1.01745	-0.43911
B	-0.73354	0.49778	0.65238
H	-1.47733	0.93663	1.49127
N	-0.28902	-0.97651	0.87207
O	-1.38533	0.33936	-0.76501
H	-1.34478	1.14218	-1.30822
H	-0.30106	-0.53650	-1.01333
H	-1.01975	-1.65732	0.63183

2_TS_C
Energy = -310.028321856
Free Energy = -309.852114
ZPE = 0.088978
xyz coordinates

C	-1.23887	0.80365	-0.20530
C	-1.39261	-0.52768	-0.27968
H	-1.91682	1.57565	-0.54353
H	-2.21765	-1.09615	-0.68995
B	0.69410	-0.30721	0.61299
O	-0.34459	-1.24713	0.24941
N	0.05385	1.11016	0.34237
H	0.08178	1.85980	1.02927
H	1.31626	-0.53342	1.61312
O	1.70844	-0.08200	-0.63268
H	2.64301	-0.01196	-0.36780
H	1.12412	0.94825	-0.52664

2_TS_D
Energy = -310.017106737
Free Energy = -309.840293
ZPE = 0.088023
xyz coordinates

C	-1.47254	0.36080	-0.29489
C	-1.15153	-0.92951	-0.10152
H	-2.41269	0.72897	-0.68909
H	-1.69172	-1.84302	-0.29797
B	0.72129	0.44679	0.54013
O	0.14057	-1.05302	0.46920
N	-0.43788	1.23164	0.06092
H	-0.68491	2.14753	0.41008
H	1.31059	0.74884	1.53985
O	1.73049	0.02897	-0.60346
H	2.65108	-0.03749	-0.29472
H	1.06230	-0.99555	-0.34269

5_TS_B
Energy = -632.956157530
Free Energy = -632.777279
ZPE = 0.085093
xyz coordinates

C	-0.18733	1.49135	0.20447
C	1.05428	1.13467	-0.17227
H	-0.45685	2.54653	0.21278
H	1.86183	1.77873	-0.51344
H	-1.22668	-1.07634	-0.51294
S	1.42683	-0.59993	-0.13925
N	-0.20347	-1.01677	0.39582
B	-1.11622	0.27497	0.59660
H	-1.79468	0.27942	1.59180
O	-2.04029	-0.21576	-0.65842
H	-2.92367	-0.51819	-0.38092
H	-0.16318	-1.69884	1.15127

5_TS_A
Energy = -632.935487082
Free Energy = -632.753739
ZPE = 0.084673
xyz coordinates

C	-0.43887	1.45660	0.31200
C	0.79580	1.29137	-0.16889
H	-0.85194	2.45920	0.42337
H	1.54726	1.98287	-0.53562
S	1.16500	-0.51924	-0.25150
N	-0.00429	-0.95871	0.94919
B	-1.17696	0.00316	0.56313
H	-2.12464	-0.06861	1.31002
O	-1.48801	-0.56175	-0.85005
H	-1.85451	0.11247	-1.44440
H	0.39889	-0.78451	1.87114
H	-0.07769	-0.69226	-1.11884

6_TS_C
Energy = -632.991171650
Free Energy = -632.814045
ZPE = 0.086247
xyz coordinates

C	0.67406	1.47883	-0.10328
C	1.48084	0.43676	-0.35853
H	0.90909	2.51880	-0.30272
H	2.45945	0.51559	-0.81787
B	-0.83464	-0.39267	0.57218
H	-1.37517	-0.80991	1.55458
N	-0.61633	1.15579	0.41586
H	-1.57131	0.75793	-0.49712
S	0.85105	-1.16275	0.10681
O	-1.84502	-0.39692	-0.67008
H	-2.76364	-0.61170	-0.42434
H	-0.95688	1.78788	1.13803

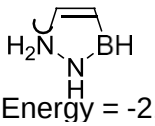
6_TS_D
Energy = -632.988243217
Free Energy = -632.811252
ZPE = 0.084001
xyz coordinates

C	1.33127	0.95773	-0.24477
C	1.45195	-0.38505	-0.37232
H	2.11436	1.64909	-0.54539
H	2.30861	-0.89209	-0.79708
B	-0.94163	0.55147	0.55731
H	-1.62989	0.68092	1.52562
N	0.17789	1.47093	0.31759
S	0.09699	-1.33028	0.29401
O	-1.75395	0.22379	-0.71702
H	-2.69712	0.06708	-0.52533
H	0.24541	2.36958	0.77907
H	-1.09790	-0.87042	-0.71204

water
Energy = -76.4708080511
Free Energy = -76.427898
ZPE = 0.021018
xyz coordinates

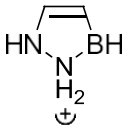
O	0.00000	0.00000	0.11861
H	0.00000	0.76836	-0.47443
H	0.00000	-0.76836	-0.47443

Protonation



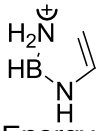
Energy = -213.981912900
Free Energy = -213.841199
ZPE = 0.093173
xyz coordinates

C	1.26510	0.42241	-0.00003
C	0.85561	-0.84537	0.00003
H	2.31735	0.68428	0.00006
H	1.35883	-1.80561	0.00002
B	-0.00042	1.34777	0.00002
H	-0.14597	2.51940	0.00034
N	-1.09401	0.44541	-0.00024
H	-2.10149	0.56088	0.00065
N	-0.64508	-0.91931	0.00004
H	-0.98856	-1.42155	-0.83332
H	-0.98867	-1.42124	0.83355



Energy = -213.976809574
Free Energy = -213.837103
ZPE = 0.092616
xyz coordinates

C	-1.28491	0.39532	0.01326
C	-0.77752	-0.88171	0.00518
H	-2.34974	0.58826	0.01970
H	-1.31610	-1.82539	0.02659
B	-0.13586	1.33556	-0.00424
H	0.09838	2.49226	-0.03703
N	1.13077	0.35464	0.01547
H	1.77993	0.53093	-0.76401
N	0.58895	-0.96745	-0.08962
H	1.14158	-1.72908	0.29364
H	1.66176	0.47323	0.89068



Energy = -214.047200675
Free Energy = -213.905517
ZPE = 0.093401
xyz coordinates

C	-0.65236	-1.01323	0.00012
C	0.68364	-0.98124	0.00007
H	-1.35050	-1.83676	0.00023
H	1.35718	-1.82885	0.00012
B	0.15060	1.27372	-0.00013
H	0.12765	2.45167	-0.00024
N	-1.14736	0.38802	0.00001
H	-1.73944	0.59031	0.81910
N	1.17965	0.34226	-0.00008
H	2.17793	0.51973	-0.00014
H	-1.73951	0.59015	-0.81908

H_2S
Energy = -399.429465021
Free Energy = -399.391688
ZPE = 0.015152
xyz coordinates

S	0.00000	0.00000	0.10335
H	0.00000	0.97798	-0.82683
H	0.00000	-0.97798	-0.82683

H_3O^+
Energy = -76.7362627589
Free Energy = -76.676395
ZPE = 0.034288
xyz coordinates

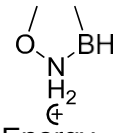
O	0.00000	0.07792	0.00000
H	-0.94624	-0.20778	0.00000
H	0.47312	-0.20778	0.81946
H	0.47312	-0.20778	-0.81946

NH_3
Energy = -56.5874909560
Free Energy = -56.541539
ZPE = 0.034523
xyz coordinates

N	0.00000	0.11043	0.00000
H	-0.94908	-0.25766	0.00000
H	0.47454	-0.25766	0.82193
H	0.47454	-0.25766	-0.82193

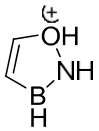
NH_4^+
Energy = -56.9239710104
Free Energy = -56.862004
ZPE = 0.049905
xyz coordinates

N	0.00000	0.00000	0.00000
H	0.59427	0.59427	0.59427
H	-0.59427	-0.59427	0.59427
H	-0.59427	0.59427	-0.59427
H	0.59427	-0.59427	-0.59427



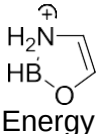
Energy = -233.815428409
Free Energy = -233.682588
ZPE = 0.079727
xyz coordinates

C	1.18164	0.59743	-0.00009
C	0.89872	-0.73130	-0.00007
H	2.19756	0.97180	-0.00018
H	1.53878	-1.60929	-0.00013
O	-0.41865	-1.09431	0.00003
B	-0.12313	1.32150	0.00000
H	-0.54872	2.42252	0.00004
N	-1.16536	0.13923	0.00009
H	-1.77378	0.09526	-0.83145
H	-1.77363	0.09527	0.83174



Energy = -233.781238879
Free Energy = -233.646952
ZPE = 0.077495
xyz coordinates

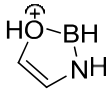
C	1.08671	0.74276	0.01427
C	1.05731	-0.58022	-0.02381
H	2.02053	1.29437	0.01781
H	1.74600	-1.41601	-0.04524
O	-0.34491	-1.07365	-0.08632
B	-0.37961	1.27044	0.01222
H	-0.85437	2.35182	-0.01944
N	-1.20969	0.12094	0.06517
H	-2.09895	-0.11314	-0.37138
H	-0.55216	-1.70189	0.64878



Energy = -233.903393642
Free Energy = -233.768138
ZPE = 0.080370
xyz coordinates

C	-0.42982	-1.10353	0.00015
C	0.86729	-0.80422	0.00004
H	-0.94345	-2.05407	0.00029
H	1.73786	-1.44588	0.00007
B	-0.03922	1.24926	-0.00014

H	-0.22092	2.41276	-0.00026
O	1.11566	0.56921	-0.00013
N	-1.18776	0.17163	0.00005
H	-1.80655	0.26620	0.82025
H	-1.80664	0.26601	-0.82011



Energy = -233.893706488
Free Energy = -233.756145
ZPE = 0.078990
xyz coordinates

C	0.64638	-0.99229	0.00000
C	-0.68920	-0.98953	0.00000
H	1.28795	-1.86318	0.00003
H	-1.49065	-1.70974	0.00002
B	0.13634	1.26320	0.00000
H	0.05395	2.43561	0.00006
O	-1.06590	0.41722	-0.00001
N	1.15663	0.31346	-0.00001
H	2.15634	0.48031	0.00001
H	-2.00159	0.69990	0.00002

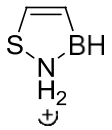
Energy = -210.558565457
Free Energy = -210.418891
ZPE = 0.095730
xyz coordinates

C	-0.24835	1.18278	-0.00006
C	1.01334	0.73506	-0.00008
C	1.01337	-0.73503	-0.00000
C	-0.24832	-1.18278	0.00008
N	-1.15033	-0.00002	0.00005
H	-1.76914	-0.00007	-0.82644
H	-0.69336	2.16798	-0.00010
H	1.89844	1.35928	-0.00015
H	1.89850	-1.35920	-0.00000
H	-0.69328	-2.16800	0.00015
H	-1.76907	0.00002	0.82659

SH_3^+

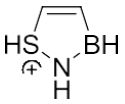
Energy = -399.708564770
Free Energy = -399.656579
ZPE = 0.026492
xyz coordinates

S	0.00000	0.11227	0.00000
H	-1.15670	-0.59878	0.00000
H	0.57835	-0.59878	1.00173
H	0.57835	-0.59878	-1.00173



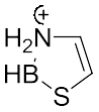
Energy = -556.835716478
Free Energy = -556.698563
ZPE = 0.076223
xyz coordinates

C	1.39019	-0.75124	-0.00019
C	0.11893	-1.25044	-0.00011
H	2.23881	-1.42805	-0.00032
H	-0.16307	-2.30295	-0.00015
H	-0.25171	1.86106	-0.82223
H	2.25728	1.58205	-0.00010
S	-1.22035	-0.13530	0.00011
N	-0.06673	1.26809	0.00010
B	1.42166	0.74505	-0.00008
H	-0.25155	1.86093	0.82256



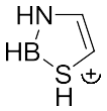
Energy = -556.824070554
Free Energy = -556.681726
ZPE = 0.073113
xyz coordinates

C	1.45332	-0.59042	0.01650
C	0.30224	-1.27214	-0.00914
H	2.39743	-1.12993	0.03256
H	0.07426	-2.33364	-0.02649
H	2.03382	1.84688	-0.02909
S	-1.12547	-0.15322	-0.09035
N	-0.15624	1.23151	0.04340
B	1.25113	0.96168	0.01087
H	-0.62481	2.11871	-0.12637
H	-1.56849	-0.30414	1.19274



Energy = -556.865962578
Free Energy = -556.729155
ZPE = 0.077214
xyz coordinates

C	-1.19561	-0.83865	0.00017
C	0.07387	-1.23965	0.00010
H	-2.09849	-1.43633	0.00030
H	0.39528	-2.27532	0.00016
B	0.07323	1.30219	-0.00012
H	0.17560	2.47675	-0.00023
N	-1.33841	0.63578	0.00006
H	-1.87948	0.96156	0.81715
S	1.31374	0.05127	-0.00012
H	-1.87963	0.96142	-0.81698



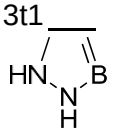
Energy = -556.862772511
Free Energy = -556.725120
ZPE = 0.073964
xyz coordinates

C	1.19796	-0.80361	0.00921
C	-0.06214	-1.26512	0.03499
H	2.07965	-1.43553	-0.00658
H	-0.41124	-2.28784	-0.00060
B	0.21006	1.37462	0.00594
H	0.03559	2.53853	0.04384
N	1.36041	0.59298	0.00175
H	2.30364	0.97218	0.01084
S	-1.23240	0.08623	-0.09610
H	-1.67730	0.22132	1.18292

water
Energy = -76.4640659845
Free Energy = -76.419138
ZPE = 0.021095
xyz coordinates

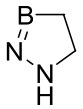
O	0.00000	0.00000	0.11731
H	0.00000	0.77122	-0.46923
H	0.00000	-0.77122	-0.46923

Tautomer (gas phase)

3t1


Energy = -213.511215440
Free Energy = -213.386873
ZPE = 0.077975
xyz coordinates

C	-1.29198	-0.61812	-0.05768
C	-0.74599	0.82906	0.16933
H	-0.82339	1.16700	1.22050
B	-0.01524	-1.15005	-0.01572
N	1.27193	-0.55880	-0.00235
N	0.69375	0.80050	-0.31998
H	-2.33626	-0.83426	-0.20030
H	-1.27928	1.54423	-0.46736
H	1.26591	1.47500	0.19142
H	1.71732	-0.55922	0.92074

3t2


Energy = -213.543430496
Free Energy = -213.423920
ZPE = 0.079018
xyz coordinates

C	1.30982	-0.47404	-0.11003
C	0.58405	0.90671	0.12551
B	-0.05303	-1.12174	0.19118
N	-1.28361	-0.69976	0.01862
N	-0.87592	0.71061	-0.24237
H	2.14830	-0.61864	0.57121
H	0.68737	1.14650	1.19359
H	-1.45174	1.28792	0.37240
H	1.63763	-0.60399	-1.14757
H	0.99709	1.72497	-0.47221

3t3


Energy = -213.598639417
Free Energy = -213.484732
ZPE = 0.076164
xyz coordinates

C	-1.16979	0.47783	0.00013
C	-0.64592	-0.96077	-0.00002
B	0.17590	1.27840	0.00007
N	1.30269	0.28331	-0.00008
N	0.85003	-0.89292	-0.00012
H	-1.79022	0.71549	0.87569
H	-0.92472	-1.55502	0.87930
H	-1.79038	0.71562	-0.87530
H	-0.92484	-1.55488	-0.87940
H	0.37590	2.45172	0.00013

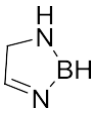
3t4


Energy = -213.657020709
Free Energy = -213.537162
ZPE = 0.078133
xyz coordinates

C	-1.07699	0.67993	0.00002
C	-0.82586	-0.80661	-0.00011
N	0.41294	-1.15660	-0.00010
H	-1.58389	-1.58491	-0.00022
H	-1.66400	0.99480	0.87612
B	0.42069	1.21100	0.00014
H	0.87800	2.30977	0.00027
N	1.18262	0.03204	0.00005
H	2.17851	-0.13764	0.00008

H	-1.66392	0.99498	-0.87607

4t1



Energy = -213.689840372
Free Energy = -213.568731
ZPE = 0.079065
xyz coordinates

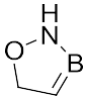
C	-0.97734	-0.62577	-0.00010
C	0.47053	-1.07308	0.00017
N	1.14952	0.21287	0.00014
H	-1.79456	-1.35287	-0.00016
H	0.70229	-1.68058	0.88824
H	0.70256	-1.68076	-0.88772
N	-1.16917	0.64236	-0.00023
B	0.19371	1.24919	-0.00007
H	2.15824	0.26065	0.00035
H	0.44122	2.41401	-0.00012

1t2

Energy = -233.399080714
Free Energy = -233.288011
ZPE = 0.065200
xyz coordinates

C	1.07092	-0.83674	-0.07354
C	0.89708	0.66917	0.30898
B	-0.46697	-0.63795	-0.27137
N	-1.65620	-0.34543	0.28515
H	1.68211	-0.95392	-0.97149
H	0.78493	0.84482	1.38145
H	1.58296	1.38856	-0.14723
O	-0.41655	0.85596	-0.37867
H	1.40270	-1.51397	0.71485

1t1



Energy = -233.365502724
Free Energy = -233.249488
ZPE = 0.064863
xyz coordinates

C	-1.25097	-0.67828	-0.04505
C	-0.79081	0.78556	0.13849
B	0.05659	-1.12343	-0.01341
N	1.31517	-0.46317	-0.02910
H	-2.28070	-0.96587	-0.16701
H	-1.26154	1.44922	-0.59317
H	-0.92037	1.19854	1.15092
O	0.67570	0.86791	-0.19234
H	1.81851	-0.40952	0.85809

2t1

Energy = -233.483268751
Free Energy = -233.369136
ZPE = 0.067404
xyz coordinates

C	0.79907	0.80705	0.00007
C	-0.80761	0.79193	-0.00006
O	-1.20698	-0.66042	-0.00013
H	1.16176	1.32433	0.89329
H	-1.23850	1.23238	-0.89990
B	0.08860	-0.99385	0.00001
N	1.34537	-0.63637	0.00014
H	-1.23865	1.23234	0.89972
H	1.16191	1.32429	-0.89312

2t2

Energy = -233.569199539
Free Energy = -233.454269
ZPE = 0.066906
xyz coordinates

C	-0.78335	-0.83753	0.00015
C	0.72554	-0.89058	0.00004
H	-1.39913	-1.74134	0.00029
H	1.13643	-1.38493	-0.88969
B	-0.06976	1.21905	-0.00012
H	-0.04627	2.40683	-0.00025
O	1.09535	0.49092	-0.00013
N	-1.27068	0.35004	0.00006
H	1.13657	-1.38474	0.88981

5t2

Energy = -556.441075625
Free Energy = -556.321659
ZPE = 0.063716
xyz coordinates

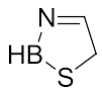
C	1.65040	0.27963	-0.10255
C	0.78046	-1.00212	0.13187
H	2.09322	0.30368	-1.10359
H	0.99586	-1.79533	-0.58639
S	-1.06435	-0.50934	-0.06807
N	-0.87280	1.27991	0.09176
B	0.42210	1.20072	0.03342
H	2.43998	0.38688	0.64413
H	0.91442	-1.37381	1.14962

6t2

Energy = -556.455011979
Free Energy = -556.339083
ZPE = 0.064707
xyz coordinates

C	-1.39608	0.49993	0.14536
C	0.01707	1.15999	-0.13540
H	-2.12095	0.96973	-0.52855
H	0.09030	1.51912	-1.16350
S	1.39106	-0.17062	0.05397
B	-0.12160	-1.08770	-0.07675
N	-1.41362	-0.99293	-0.08402
H	-1.69888	0.70214	1.17964
H	0.25001	1.96845	0.56091

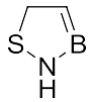
6t1



Energy = -556.529489542
Free Energy = -556.414256
ZPE = 0.063392
xyz coordinates

C	-1.37339	-0.45427	-0.00013
C	-0.08775	-1.24341	0.00011
H	-2.32028	-1.00518	-0.00019
H	-0.01949	-1.88897	0.88478
S	1.25970	0.00312	0.00015
H	-0.01927	-1.88916	-0.88440
B	0.02375	1.33003	-0.00013
N	-1.35384	0.82723	-0.00025
H	0.32888	2.47873	-0.00020

5t1

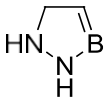


Energy = -556.411160622
Free Energy = -556.287647
ZPE = 0.063169
xyz coordinates

C	1.61433	0.46527	-0.08669
C	0.97009	-0.90406	0.17053
H	2.68295	0.59190	-0.16453
H	1.22043	-1.64029	-0.60011
S	-0.91971	-0.65578	-0.09158
H	1.16289	-1.32704	1.16549
N	-0.96372	1.14693	0.02728
B	0.44075	1.21041	-0.11514
H	-1.31522	1.42015	0.94611

Tautomer (water phase)

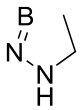
3t1



Energy = -213.520926423
Free Energy = -213.397726
ZPE = 0.078208
xyz coordinates

C	-1.29131	-0.62719	-0.06023
C	-0.75691	0.82632	0.16070
H	-0.83771	1.16651	1.20732
B	-0.00894	-1.14720	-0.00787
N	1.28024	-0.55723	-0.01060
N	0.69378	0.81109	-0.31387
H	-2.33799	-0.85355	-0.17016
H	-1.28869	1.53848	-0.47967
H	1.24321	1.46695	0.24443
H	1.73708	-0.55424	0.90588

3t2



Energy = -213.555205612
Free Energy = -213.436619
ZPE = 0.079068
xyz coordinates

C	1.31438	-0.49210	-0.08059
C	0.60688	0.90547	0.09659
B	-0.06550	-1.11057	0.14533
N	-1.30760	-0.70339	0.02161
N	-0.88477	0.73321	-0.22673
H	2.09993	-0.65404	0.65682
H	0.72866	1.21315	1.14070
H	-1.40322	1.27431	0.46714
H	1.70574	-0.64608	-1.09085
H	1.01540	1.67657	-0.56065

3t3

Energy = -213.606849099
Free Energy = -213.493764
ZPE = 0.076170
xyz coordinates

C	-1.16700	0.47493	0.00005
C	-0.64162	-0.96153	-0.00006
B	0.16687	1.28146	-0.00009
N	1.30251	0.28511	0.00002
N	0.84835	-0.89176	0.00005
H	-1.78656	0.70789	0.87711
H	-0.91999	-1.55527	0.87962

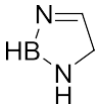
H	-1.78705	0.70800	-0.87655
H	-0.91989	-1.55486	-0.88007
H	0.37488	2.45310	-0.00011

3t4

Energy = -213.662022826
Free Energy = -213.542760
ZPE = 0.077926
xyz coordinates

C	-1.07158	0.68683	0.00003
C	-0.83391	-0.79918	-0.00003
N	0.40437	-1.15863	0.00006
H	-1.60057	-1.56895	-0.00021
H	-1.65885	1.00174	0.87562
B	0.42762	1.20609	0.00001
H	0.89468	2.30109	0.00019
N	1.18645	0.02370	-0.00017
H	2.18279	-0.14828	0.00047
H	-1.65898	1.00256	-0.87538

4t1



Energy = -213.698472378
Free Energy = -213.577957
ZPE = 0.079035
xyz coordinates

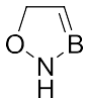
C	-1.01133	-0.57223	-0.00008
C	0.40359	-1.09541	0.00005
N	1.15969	0.14744	-0.00033
H	-1.86702	-1.25144	0.00014
H	0.59980	-1.71602	0.88640
H	0.60028	-1.71665	-0.88573
N	-1.12954	0.71070	-0.00002
B	0.27093	1.23381	0.00019
H	2.17021	0.12741	0.00090
H	0.57746	2.38653	-0.00002

1t2

Energy = -233.403580863
Free Energy = -233.293552
ZPE = 0.065146
xyz coordinates

C	1.23526	-0.61763	-0.09108
C	0.69875	0.82269	0.17655
B	-0.23116	-1.04242	-0.00868
N	-1.44021	-0.52575	0.13236
H	1.68847	-0.73352	-1.07903
H	0.76023	1.06978	1.24066
H	1.17084	1.59553	-0.43205
O	-0.73653	0.83922	-0.22654
H	1.90587	-0.98361	0.68684

1t1



Energy = -233.372881184
Free Energy = -233.257662
ZPE = 0.064930
xyz coordinates

C	-1.24627	-0.68091	-0.05182
C	-0.79356	0.78467	0.14619
B	0.06117	-1.12937	-0.01802
N	1.31877	-0.45731	-0.02226
H	-2.27833	-0.96645	-0.16403
H	-1.27576	1.46046	-0.56558
H	-0.90707	1.17707	1.16697
O	0.67066	0.86979	-0.20463
H	1.79768	-0.40395	0.87932

2t1

Energy = -233.493969684
Free Energy = -233.380546
ZPE = 0.067447
xyz coordinates

C	0.80163	0.81015	0.00010
C	-0.79982	0.80250	-0.00001
O	-1.20940	-0.66065	-0.00013
H	1.16460	1.32218	0.89424
H	-1.22625	1.23891	-0.90169
B	0.07880	-0.99559	0.00039
N	1.34202	-0.64784	-0.00021
H	-1.22682	1.23883	0.90144
H	1.16463	1.32224	-0.89398

2t2

Energy = -233.577256749
Free Energy = -233.463002
ZPE = 0.066919
xyz coordinates

C	-0.80966	-0.81163	0.00015
C	0.69012	-0.91946	0.00004
H	-1.45291	-1.69381	0.00029
H	1.07954	-1.42764	-0.89004
B	-0.02637	1.22067	-0.00012
H	0.03651	2.40873	-0.00025

O	1.11228	0.45531	-0.00013
N	-1.25599	0.39726	0.00006
H	1.07968	-1.42745	0.89017

5t2

Energy = -556.451328714
Free Energy = -556.332925
ZPE = 0.063794
xyz coordinates

C	1.65318	0.27719	-0.08269
C	0.78097	-1.00979	0.10708
H	2.13416	0.31090	-1.06420
H	0.97793	-1.76625	-0.65264
S	-1.06969	-0.50868	-0.05513
N	-0.86873	1.29171	0.07562
B	0.43120	1.19929	0.02410
H	2.40851	0.38040	0.69832
H	0.91473	-1.42889	1.10446

6t2

Energy = -556.463738466
Free Energy = -556.348309
ZPE = 0.064760
xyz coordinates

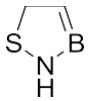
C	-1.39673	0.50489	0.14256
C	0.01572	1.16087	-0.13322
H	-2.11514	0.97067	-0.53853
H	0.09363	1.52527	-1.15777
S	1.39239	-0.17215	0.05253
B	-0.11862	-1.07682	-0.07365
N	-1.41746	-1.00276	-0.08266
H	-1.70197	0.70769	1.17425
H	0.24659	1.95963	0.57239

6t1

Energy = -556.536267970
Free Energy = -556.421561
ZPE = 0.063440
xyz coordinates

C	-1.37295	-0.45150	-0.00015
C	-0.09557	-1.24257	0.00006
H	-2.31880	-1.00069	-0.00057
H	-0.03155	-1.88779	0.88439
S	1.25808	-0.00208	-0.00002
H	-0.03144	-1.88837	-0.88378
B	0.03169	1.32967	-0.00006
N	-1.34760	0.83525	0.00020
H	0.33841	2.47934	-0.00026

5t1

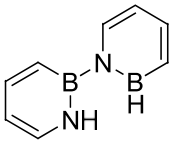


Energy = -556.416897733
Free Energy = -556.294336
ZPE = 0.063061
xyz coordinates

C	1.61234	0.46490	-0.09269
C	0.96942	-0.90577	0.17132
H	2.68229	0.58765	-0.16696
H	1.22344	-1.65033	-0.58898
S	-0.91842	-0.65820	-0.09182
H	1.15568	-1.31879	1.17032
N	-0.96350	1.14813	0.02368
B	0.44235	1.21922	-0.10423
H	-1.32446	1.42490	0.93841

Dimer trimer

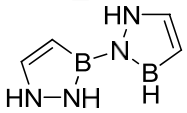
dimer_borazine



Free Energy = -470.070773
ZPE = 0.177218
xyz coordinates

C	1.54649	1.30117	-0.22046
C	2.91951	1.18604	-0.19770
C	3.57425	-0.06284	0.01464
C	2.82990	-1.19822	0.19557
H	0.98566	-2.04045	0.31282
H	1.13432	2.29034	-0.41044
H	3.54654	2.06401	-0.35279
H	4.65722	-0.12689	0.02808
H	3.28613	-2.17096	0.35431
B	0.70469	0.05236	-0.01490
N	1.46383	-1.15526	0.18521
C	-1.48862	1.14258	0.20273
C	-2.85752	1.19566	0.21169
H	-0.90284	2.03895	0.37663
C	-3.02572	-1.19835	-0.21256
H	-0.89138	-2.26751	-0.40577
C	-3.63328	0.02009	-0.00094
H	-3.34119	2.15162	0.38858
H	-3.65659	-2.07174	-0.37066
H	-4.71947	0.11588	0.01135
B	-1.51496	-1.26031	-0.22062
N	-0.78341	-0.02478	-0.00126

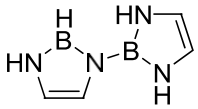
dimer_ 3



Free Energy = -425.901194
ZPE = 0.140803
xyz coordinates

C	1.57815	1.23722	0.09006
C	2.84035	0.72701	0.00090
H	1.39400	2.30319	0.16052
H	3.79738	1.23866	0.03402
C	-3.07901	-0.66861	0.01145
C	-2.89374	0.69012	-0.05468
H	-4.06407	-1.11886	0.03747
H	-3.62026	1.49405	-0.12405
N	2.86959	-0.64993	-0.15873
H	3.55902	-1.15968	0.39009
N	-1.57030	1.04249	0.02322
H	-1.19402	1.84799	-0.46335
N	1.54972	-1.11347	0.02479
N	-0.78655	-0.12097	0.01030
B	0.65461	0.01154	0.06152
B	-1.67674	-1.25631	0.05895
H	-1.25369	-2.36962	0.13999
H	1.38062	-2.03322	-0.36044

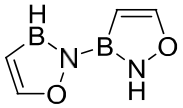
dimer_ 4



Free Energy = -426.024241
ZPE = 0.141639
xyz coordinates

C	1.57316	1.10118	-0.00026
C	2.87963	0.73736	-0.00015
H	1.16343	2.10194	-0.00054
H	3.75948	1.36579	-0.00028
C	-2.91637	-0.67523	-0.00013
C	-2.90723	0.68043	0.00015
H	-3.76285	-1.34716	-0.00025
H	-3.74282	1.36570	0.00031
N	0.75218	-0.04310	-0.00003
N	-1.59340	-1.14054	-0.00023
B	1.62738	-1.19024	0.00025
B	-0.70063	-0.01522	-0.00001
N	2.95376	-0.66115	0.00017
H	3.83980	-1.14339	0.00031
N	-1.57461	1.12677	0.00022
H	-1.36083	2.11204	0.00055
H	-1.38139	-2.12642	-0.00046
H	1.31076	-2.33749	0.00051

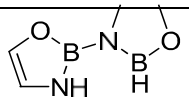
dimer_ 1



Free Energy = -465.618257
ZPE = 0.114899
xyz coordinates

C	-3.08963	0.59065	-0.00000
C	-2.81084	-0.73704	-0.00004
H	-4.10066	0.97753	-0.00002
H	-3.44367	-1.61770	-0.00009
O	-1.49523	-1.05653	-0.00002
B	-1.71907	1.25824	0.00006
N	-0.78538	0.18029	0.00005
C	1.56382	-1.21965	0.00004
C	2.81739	-0.71087	0.00001
H	1.35355	-2.28082	0.00009
H	3.79648	-1.17501	0.00003
B	0.65322	0.01072	0.00002
N	1.56288	1.10292	-0.00010
O	2.89541	0.64754	-0.00002
H	-1.35016	2.39123	0.00010
H	1.54535	2.11080	0.00016

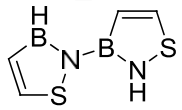
dimer_ 2



Free Energy = -465.791253
ZPE = 0.116970
xyz coordinates

C	-2.91663	0.58195	-0.00000
C	-2.78918	-0.75907	0.00000
H	-3.81598	1.18163	-0.00000
H	-3.51829	-1.55437	-0.00001
O	-1.45077	-1.12177	0.00000
C	1.54609	-1.08619	0.00000
C	2.83767	-0.70923	-0.00000
H	1.12006	-2.07918	0.00000
H	3.75481	-1.27864	-0.00000
O	2.94661	0.67073	-0.00000
N	-1.62910	1.14553	0.00000
N	0.73567	0.07448	0.00000
B	-0.70654	0.05660	0.00000
B	1.65578	1.17427	0.00000
H	-1.48059	2.14295	-0.00000
H	1.41349	2.33679	0.00000

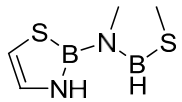
dimer_ 5



Free Energy = -1111.638726
ZPE = 0.108836
xyz coordinates

C	-3.11563	1.19888	-0.00022
C	-3.36151	-0.14244	0.00009
H	-3.93785	1.90906	-0.00035
H	-4.32267	-0.64998	0.00023
C	1.33579	-1.34337	-0.00039
C	2.67695	-1.11973	-0.00025
H	0.95563	-2.36132	-0.00069
H	3.47804	-1.85305	-0.00038
S	3.14675	0.55627	0.00018
S	-1.94585	-1.14387	0.00027
N	1.50435	1.05690	0.00020
N	-0.88337	0.22657	-0.00008
B	-1.61044	1.46498	-0.00031
B	0.55783	-0.01437	-0.00010
H	-1.02079	2.50489	-0.00054
H	1.33587	2.05458	0.00041

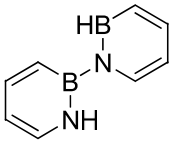
dimer_ 6



Free Energy = -1111.714661
ZPE = 0.111063
xyz coordinates

C	-2.93088	1.20796	-0.00024
C	-3.34785	-0.07520	0.00003
H	-3.57011	2.08343	-0.00040
H	-4.37064	-0.42490	0.00014
C	1.31287	-1.20014	-0.00038
C	2.65965	-1.13323	-0.00032
H	0.73207	-2.11553	-0.00068
H	3.34209	-1.97242	-0.00056
N	-1.54515	1.36902	-0.00027
N	0.64599	0.03857	-0.00003
B	-0.80478	0.15144	-0.00002
B	1.56184	1.14223	0.00030
S	3.26308	0.52729	0.00017
S	-2.00631	-1.23229	0.00030
H	-1.15246	2.30121	-0.00046
H	1.25693	2.29041	0.00064

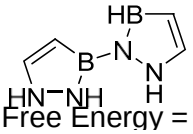
dimertrans_borazine



Free Energy = -470.067351
ZPE = 0.176937
xyz coordinates

C	-1.58871	1.29347	0.38561
C	-2.95485	1.13373	0.34168
C	-3.56139	-0.10161	-0.04254
C	-2.78042	-1.17162	-0.38301
H	-0.91398	-1.91117	-0.66322
H	-1.19058	2.25894	0.68900
H	-3.61627	1.95876	0.60582
H	-4.64145	-0.20225	-0.07202
H	-3.20206	-2.12341	-0.69228
B	-0.70297	0.11484	0.02695
N	-1.41134	-1.08357	-0.35286
C	1.44862	-1.05307	0.41070
C	2.81409	-1.16249	0.38862
H	0.83829	-1.88148	0.76348
C	3.05209	1.13087	-0.40573
H	0.93184	2.24262	-0.68533
C	3.62224	-0.06511	-0.03034
H	3.27070	-2.09434	0.70878
H	3.71064	1.94157	-0.71432
H	4.70399	-0.20289	-0.03644
N	0.78356	0.09732	0.04526
B	1.54163	1.26364	-0.37498

dimertrans_3

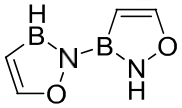


Free Energy = -425.900314
ZPE = 0.141044
xyz coordinates

C	-1.72057	1.26855	-0.16905
C	-2.90901	0.61799	-0.03172
H	-1.64874	2.34035	-0.30608
H	-3.92094	1.00798	-0.09077
C	3.09973	0.60872	0.14236
C	2.84768	-0.72048	-0.05446
H	4.10227	0.99642	0.27938
H	3.53375	-1.55733	-0.14770
N	-2.77747	-0.74242	0.22987
H	-3.39622	-1.36180	-0.29008
N	1.49571	-1.00837	-0.10162
H	1.15680	-1.67997	-0.78589
N	-1.40726	-1.06294	0.06263
N	0.78579	0.21238	-0.08093
B	-0.65953	0.17060	-0.06338
B	1.72865	1.28196	0.13099

H	1.36877	2.40708	0.28161
H	-1.12570	-1.85484	0.62902

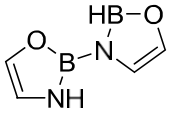
dimertrans_1



Free Energy = -465.619897
ZPE = 0.114956
xyz coordinates

C	3.10837	0.55095	-0.00004
C	2.76361	-0.75922	0.00004
H	4.13785	0.88582	-0.00006
H	3.34971	-1.67171	0.00009
O	1.42980	-1.00939	0.00005
B	1.77348	1.29427	-0.00008
N	0.78492	0.26652	-0.00002
C	-1.74699	1.25653	-0.00006
C	-2.90654	0.55958	-0.00001
H	-1.70864	2.33800	-0.00012
H	-3.94513	0.86819	-0.00002
B	-0.65857	0.17782	-0.00001
N	-1.38810	-1.03853	0.00004
O	-2.77466	-0.79530	0.00006
H	1.46965	2.44390	-0.00015
H	-1.20757	-2.03008	0.00016

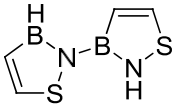
dimertrans_2



Free Energy = -465.789007
ZPE = 0.116807
xyz coordinates

C	2.89800	0.62028	-0.00008
C	2.81955	-0.72401	0.00007
H	3.77297	1.25481	-0.00017
H	3.57864	-1.49092	0.00016
O	1.49935	-1.13827	0.00014
C	-1.58546	1.09313	0.00015
C	-2.86475	0.67501	0.00006
H	-1.21009	2.10724	0.00033
H	-3.79864	1.21692	0.00012
O	-2.92704	-0.70388	-0.00011
N	1.58714	1.13364	-0.00013
N	-0.73499	-0.03669	0.00003
B	0.70700	0.00716	0.00001
B	-1.61854	-1.17111	-0.00013
H	1.41129	2.12630	-0.00034
H	-1.34400	-2.32251	-0.00027

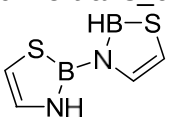
dimertrans_5



Free Energy = -1111.638648
ZPE = 0.108727
xyz coordinates

C	3.23839	1.00374	0.00056
C	3.32194	-0.35495	0.00049
H	4.14072	1.60904	0.00075
H	4.21233	-0.97812	0.00059
C	-1.52445	1.48825	-0.00029
C	-2.81680	1.07171	-0.00046
H	-1.28669	2.54744	-0.00032
H	-3.71720	1.67907	-0.00063
S	-3.03872	-0.65758	-0.00040
S	1.78984	-1.17557	0.00017
N	-1.33580	-0.91268	-0.00015
N	0.90129	0.31437	0.00012
B	1.77473	1.45684	0.00034
B	-0.55797	0.28958	-0.00009
H	1.31792	2.55763	0.00034
H	-1.04168	-1.88106	0.00003

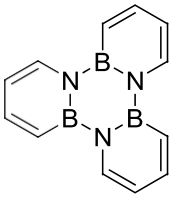
dimertrans_6



Free Energy = -1111.713735
ZPE = 0.110820
xyz coordinates

C	3.01183	1.06769	0.00007
C	3.33309	-0.24177	0.00001
H	3.70996	1.89691	0.00013
H	4.32974	-0.66083	-0.00001
C	-1.42990	1.29845	-0.00010
C	-2.76403	1.10062	-0.00008
H	-0.95330	2.27207	-0.00019
H	-3.52384	1.87072	-0.00014
N	1.63740	1.32638	0.00007
N	-0.64240	0.13228	-0.00001
B	0.81279	0.16120	0.00000
B	-1.44605	-1.05725	0.00008
S	-3.20143	-0.60989	0.00005
S	1.91592	-1.30148	-0.00008
H	1.32810	2.28891	0.00015
H	-1.02702	-2.16609	0.00017

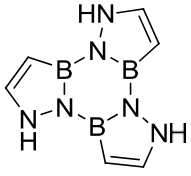
trimer_borazine



Free Energy = -703.382356
ZPE = 0.236566
xyz coordinates

C	1.17039	2.77032	0.00000
C	2.53975	2.86503	-0.00000
C	3.35944	1.69817	-0.00001
C	2.79384	0.45553	0.00001
H	0.61317	3.70444	0.00001
H	3.03113	3.83791	-0.00001
H	4.44177	1.78182	-0.00002
H	3.42028	-0.42735	0.00001
B	0.53694	1.38629	0.00001
N	1.42909	0.23922	0.00002
C	-1.79162	2.19168	-0.00001
C	-3.15056	2.05993	-0.00001
H	-1.34097	3.17600	-0.00002
C	-2.98439	-0.37177	0.00001
C	-3.75125	0.76663	0.00000
H	-3.76418	2.95543	-0.00002
H	-3.51433	-1.32165	0.00001
H	-4.83947	0.70566	0.00001
B	-1.46894	-0.22794	0.00000
N	-0.92167	1.11801	-0.00000
N	-0.50739	-1.35702	0.00001
B	0.93206	-1.15802	0.00001
C	-1.00233	-2.64708	0.00001
H	-2.08014	-2.74847	0.00002
C	-0.20894	-3.75821	-0.00001
H	-0.67776	-4.73731	0.00000
C	1.21147	-3.63193	-0.00002
H	1.80821	-4.54399	-0.00003
C	1.81420	-2.39874	-0.00001
H	2.90179	-2.38306	-0.00002

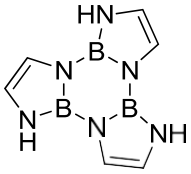
trimer_3



Free Energy = -637.128473
ZPE = 0.182605
xyz coordinates

C	-2.15646	2.04951	-0.02819
C	-3.19565	1.15772	-0.00727
H	-2.31758	3.11957	-0.08225
H	-4.26474	1.34614	0.00208
C	-0.69687	-2.89224	-0.02376
C	0.59533	-3.34577	-0.02566
H	-1.54383	-3.56784	-0.02999
H	0.96745	-4.36498	-0.06078
C	2.85363	0.84253	0.02667
C	2.60048	2.18819	0.00075
H	3.86237	0.44721	0.03130
H	3.29752	3.02038	0.01110
N	-2.79114	-0.16292	-0.05520
H	-3.28494	-0.87054	0.47869
N	1.53486	-2.33721	0.07813
H	2.40766	-2.39434	-0.43612
N	1.25663	2.49558	-0.09765
H	0.87524	3.29322	0.39998
N	-1.39494	-0.19703	0.04049
N	0.86785	-1.10908	0.00262
N	0.52664	1.30658	0.01388
B	-0.90804	1.16883	0.00340
B	-0.55850	-1.37065	-0.00473
B	1.46627	0.20182	0.03231

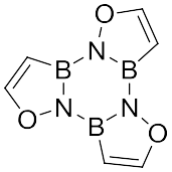
trimer_4



Free Energy = -637.304644
ZPE = 0.183637
xyz coordinates

C	2.72156	0.78905	0.00030
C	3.38558	-0.39324	0.00024
H	3.13863	1.78695	0.00026
H	4.45287	-0.56659	0.00044
C	-0.67768	-2.75155	0.00001
C	-2.03363	-2.73504	-0.00002
H	-0.02261	-3.61218	0.00000
H	-2.71778	-3.57236	-0.00003
C	-2.04417	1.96240	0.00037
C	-1.35204	3.12853	0.00006
H	-3.11700	1.82516	0.00075
H	-1.73534	4.13960	0.00013
N	1.33458	0.55495	-0.00017
N	-0.18650	-1.43342	-0.00009
N	-1.14803	0.87816	0.00023
B	1.14455	-0.88811	-0.00019
B	-1.34110	-0.54717	-0.00006
B	0.19666	1.43499	-0.00022
N	2.46221	-1.45450	-0.00006
H	2.77197	-2.41387	-0.00011
N	-2.49066	-1.40456	-0.00006
H	-3.47626	-1.19256	0.00000
N	0.02871	2.85931	-0.00041
H	0.70510	3.60688	-0.00082

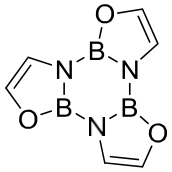
trimer_1



Free Energy = -696.698306
ZPE = 0.144508
xyz coordinates

C	-1.34056	2.65448	0.00005
C	-2.59114	2.13187	0.00009
H	-1.14915	3.71925	0.00012
H	-3.56941	2.59877	0.00019
O	-2.67967	0.77091	0.00001
B	-0.44193	1.42181	-0.00012
N	-1.35116	0.29992	-0.00016
C	-1.62866	-2.48774	0.00010
C	-0.55102	-3.30981	0.00014
H	-2.64666	-2.85380	0.00031
H	-0.46654	-4.39050	0.00027
B	-1.01002	-1.09351	-0.00015
N	0.41602	-1.32027	-0.00023
C	2.96888	-0.16656	0.00006
C	3.14201	1.17774	0.00011
H	3.79484	-0.86520	-0.00001
H	4.03569	1.79123	0.00012
N	0.93539	1.02050	-0.00000
B	1.45207	-0.32795	-0.00007
O	0.67202	-2.70646	-0.00002
O	2.00789	1.93525	0.00002

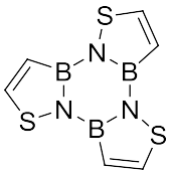
trimer_2



Free Energy = -696.958200
ZPE = 0.146984
xyz coordinates

C	-1.61502	2.31484	-0.00066
C	-2.84562	1.76597	-0.00061
H	-1.33886	3.35996	-0.00066
H	-3.82829	2.21262	-0.00104
O	-2.78834	0.37567	0.00017
C	-1.19732	-2.55590	0.00005
C	-0.10670	-3.34724	-0.00025
H	-2.24052	-2.83923	-0.00016
H	-0.00219	-4.42157	-0.00057
C	2.81215	0.24093	-0.00036
C	2.95233	1.58110	-0.00012
H	3.57911	-0.52087	-0.00064
H	3.83062	2.20857	-0.00018
O	1.06870	-2.60253	-0.00023
O	1.71976	2.22688	0.00036
N	-0.65968	1.27843	0.00065
N	-0.77717	-1.21042	0.00045
N	1.43683	-0.06782	-0.00012
B	-1.43861	0.05620	0.00068
B	0.67063	-1.27393	0.00017
B	0.76808	1.21791	0.00029

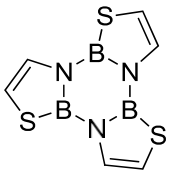
trimer_5



Free Energy = -1665.740287
ZPE = 0.135105
xyz coordinates

C	-1.34341	-2.67579	-0.00003
C	-0.31379	-3.56335	-0.00042
H	-2.37180	-3.02592	0.00012
H	-0.37016	-4.64849	-0.00076
C	2.98866	0.17406	-0.00040
C	3.24347	1.50926	-0.00078
H	3.80532	-0.54232	-0.00058
H	4.21166	2.00252	-0.00142
C	-1.64614	2.50133	0.00035
C	-2.92967	2.05354	-0.00052
H	-1.43477	3.56690	0.00083
H	-3.84128	2.64485	-0.00099
S	1.83928	2.54492	-0.00022
S	-3.12340	0.31949	-0.00067
S	1.28481	-2.86457	-0.00009
N	-1.41754	0.06022	0.00100
N	0.76068	1.19807	0.00098
N	0.65660	-1.25736	0.00058
B	-0.68041	1.30967	0.00108
B	-0.79381	-1.24358	0.00059
B	1.47363	-0.06525	0.00059

trimer_6



Free Energy = -1665.846248
ZPE = 0.137783
xyz coordinates

C	1.61966	-2.32993	-0.00014
C	2.92940	-2.01400	0.00014
H	1.21635	-3.33636	0.00001
H	3.75591	-2.71159	0.00041
C	1.20793	2.56757	0.00002
C	0.27930	3.54376	0.00013
H	2.28111	2.72228	-0.00001
H	0.47024	4.60832	0.00022

C	-2.82759	-0.23759	0.00006
C	-3.20880	-1.52987	0.00024
H	-3.49767	0.61483	0.00029
H	-4.22619	-1.89681	0.00036
N	0.73959	-1.23651	-0.00026
N	0.70115	1.25863	-0.00016
N	-1.44068	-0.02224	-0.00006
B	1.44376	0.02738	-0.00013
B	-0.74551	1.23650	-0.00012
B	-0.69811	-1.26388	-0.00021
S	-1.39134	2.94327	-0.00002
S	-1.85347	-2.67657	0.00001
S	3.24479	-0.26668	0.00012

TS_dimer_borazine
Free Energy = -470.064109
ZPE = 0.176494
xyz coordinates

C	-1.57769	1.15642	-0.67725
C	-2.94727	1.00857	-0.61184
C	-3.55647	-0.09855	0.04988
C	-2.78041	-1.05749	0.64597
H	-0.90263	-1.70834	1.08637
H	-1.17275	2.02541	-1.19269
H	-3.60632	1.74649	-1.06931
H	-4.63690	-0.19111	0.09064
H	-3.20701	-1.91185	1.16292
B	-0.70507	0.10697	-0.02458
N	-1.41389	-0.97120	0.61145
C	1.45891	-0.63937	-0.95626
C	2.82894	-0.71943	-0.99309
H	0.84964	-1.14343	-1.70370
C	3.02889	0.69669	0.98713
H	0.87696	1.40381	1.83984
C	3.61593	-0.04929	-0.01417
H	3.30045	-1.29873	-1.78127
H	3.67882	1.18963	1.70902
H	4.70036	-0.14309	-0.08340
B	1.51781	0.79512	1.03157
N	0.78969	0.07626	0.00632

TS_dimertrans_3
Free Energy = -425.888745
ZPE = 0.140323
xyz coordinates

C	-3.09748	-0.35212	-0.53759
C	-2.89203	0.31908	0.63776
H	-4.08607	-0.63647	-0.87904
H	-3.60230	0.69744	1.36674
B	-1.70236	-0.56974	-1.12434
N	-0.80368	0.02860	-0.18234
C	1.70285	1.11463	-0.57110
C	2.91962	0.56858	-0.26536
H	1.60052	2.06778	-1.07614
H	3.92033	0.96766	-0.39750
B	0.66861	0.09084	-0.10158
N	1.45664	-0.94628	0.49666
H	-1.30175	-1.11652	-2.10657
H	1.21785	-1.91076	0.68784
N	2.81457	-0.70124	0.27315
H	3.43415	-0.96588	1.03398
N	-1.55243	0.48397	0.92053
H	-1.21746	1.33472	1.36201

TS_dimertrans_4
Free Energy = -426.017253
ZPE = 0.141662
xyz coordinates

C	2.91757	0.67904	-0.01598
C	2.91738	-0.67951	-0.00290
H	3.75915	1.35692	-0.03664
H	3.75880	-1.35787	-0.01061
C	-1.56251	-0.01119	-1.09924
C	-2.87573	-0.00783	-0.75487
H	-1.12783	-0.02130	-2.08978
H	-3.74604	-0.01451	-1.39652
N	1.59179	1.12879	0.00371
N	-0.76058	0.00085	0.06040
B	0.70609	0.00047	0.03546
B	-1.64905	0.01233	1.19348
H	1.36450	2.11204	0.00818
H	-1.34843	0.02410	2.34453
N	1.59153	-1.12847	0.02550
H	1.36401	-2.11139	0.04868
N	-2.96945	0.00650	0.64114
H	-3.86260	0.01121	1.11017

TS_dimertrans_1
Free Energy = -465.606271
ZPE = 0.114709
xyz coordinates

C	3.12045	0.20702	0.48505
C	2.78310	-0.30470	-0.72277
H	4.14793	0.32908	0.80429
H	3.37132	-0.67009	-1.55734
B	1.77834	0.51609	1.15471
N	0.80276	0.11746	0.20724
C	-1.68392	1.16945	-0.41211
C	-2.88532	0.55871	-0.27404
H	-1.57437	2.17818	-0.78917
H	-3.90245	0.87337	-0.47485
B	-0.66558	0.13281	0.06629
N	-1.47324	-0.97354	0.42752
H	1.46894	0.97684	2.20831
H	-1.35161	-1.90725	0.79216
O	-2.82991	-0.71133	0.21585
O	1.45040	-0.39055	-0.96442

TS_dimertrans_2
Free Energy = -465.780840

ZPE = 0.116781
xyz coordinates

C	2.91176	0.51059	0.33478
C	2.82039	-0.59732	-0.42915
H	3.79194	1.03447	0.68002
H	3.57249	-1.22713	-0.87909
O	1.49833	-0.93802	-0.63589
C	-1.57322	0.66502	-0.86570
C	-2.86134	0.41419	-0.56085
H	-1.16973	1.26985	-1.66637
H	-3.78523	0.74143	-1.01355
O	-2.94705	-0.42009	0.53478
N	1.60634	0.92177	0.64672
N	-0.74523	-0.02069	0.05503
B	0.71265	-0.00155	0.03376
B	-1.64535	-0.70615	0.93012
H	1.41745	1.72555	1.22691
H	-1.38697	-1.40315	1.85485

TS_dimertrans_5
Free Energy = -1111.628794
ZPE = 0.108497
xyz coordinates

C	-3.19842	0.98678	-0.40334
C	-3.34083	-0.30327	0.01001
H	-4.07285	1.58261	-0.65162
H	-4.25569	-0.87511	0.14137
C	1.46760	0.57410	1.30158
C	2.77882	0.36365	1.00320
H	1.17627	0.95759	2.27527
H	3.64955	0.52943	1.63089
S	3.07571	-0.25325	-0.59855
S	-1.84743	-1.11668	0.36573
N	1.39715	-0.25711	-0.94740
N	-0.90489	0.27992	-0.03697
B	-1.71707	1.38554	-0.44027
B	0.56583	0.20958	0.11375
H	-1.20644	2.42233	-0.74182
H	1.12393	-0.56070	-1.87440

TS_dimertrans_6
Free Energy = -1111.706487
ZPE = 0.110771
xyz coordinates

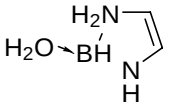
C	-2.97317	1.11078	-0.22105
C	-3.34449	-0.17457	-0.02894
H	-3.63935	1.95311	-0.36767
H	-4.35705	-0.55261	0.00544
C	1.37195	0.29803	1.20571
C	2.71551	0.22181	1.09028
H	0.82869	0.49897	2.12283
H	3.43444	0.35168	1.88802
N	-1.59269	1.31129	-0.22273
N	0.65409	0.08541	0.01537
B	-0.81326	0.13861	-0.03099
B	1.50525	-0.18318	-1.10069
S	3.23718	-0.13662	-0.55676
S	-1.96815	-1.26246	0.16719
H	-1.21948	2.24060	-0.37241
H	1.13974	-0.39695	-2.20932

Structure of intermediate involved in hydrolysis via stepwise proton transfer

hydroxide-ion
[OH]
-
hydroxide-ion.out Energy: -47646.4050758

O	0.00000	0.00000	0.10800
H	0.00000	0.00000	-0.86399

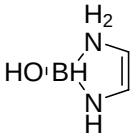
4c



Free energy= -290.415643
ZPE= 0.119298

C	1.45410	-0.59607	-0.33070
C	1.36096	0.74139	-0.24886
B	-0.70698	0.05255	0.63795
N	0.24242	-1.19499	0.28082
H	2.11333	1.44607	-0.58306
H	-1.30683	-0.03788	1.66446
H	-0.22105	-1.85999	-0.34672
O	-1.87518	-0.04775	-0.53480
H	-1.85052	0.71749	-1.14483
H	-2.78943	-0.13529	-0.20156
H	2.22161	-1.23152	-0.74322
H	0.47941	-1.72989	1.12259
N	0.17152	1.18730	0.31032
H	0.10187	2.13215	0.66037

4d

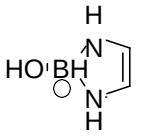


Free energy= -290.007322
ZPE= 0.106254

C	1.43555	-0.58475	-0.28180
C	1.30768	0.75752	-0.20271
B	-0.88405	0.05592	0.48657
N	0.21288	-1.21409	0.24704
H	2.06810	1.46389	-0.52290
H	-1.38386	-0.10071	1.58609
H	-0.18885	-1.89480	-0.40317
O	-1.84955	0.05565	-0.59470
H	-2.67461	-0.37277	-0.32620

H	2.26611	-1.18443	-0.62341
H	0.39242	-1.71997	1.11725
N	0.13246	1.19829	0.35556
H	-0.13939	2.15801	0.18598

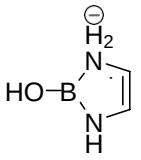
4e



Free energy= -289.532278
ZPE= 0.090514

C	-1.35183	0.67795	-0.25234
C	-1.35183	-0.67794	-0.25235
B	0.81976	-0.00001	0.50219
N	-0.19203	1.18099	0.38397
H	-2.15467	-1.33250	-0.57977
H	1.47171	-0.00003	1.56155
H	0.14744	2.06699	0.01849
O	1.82888	0.00003	-0.62947
H	2.72342	-0.00019	-0.26138
H	-2.15465	1.33252	-0.57975
N	-0.19204	-1.18100	0.38395
H	0.14742	-2.06700	0.01847

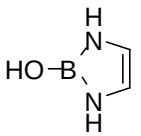
4f



Free energy= -289.279798
ZPE= 0.099337

C	-1.51651	-0.59346	-0.00002
C	-1.41277	0.74057	-0.00009
B	0.79522	0.07755	-0.00001
N	-0.15091	-1.17062	-0.00000
H	-2.22705	1.45279	-0.00000
H	0.01050	-1.77355	0.81702
O	2.12255	-0.10930	0.00020
H	2.66805	0.69423	0.00017
H	-2.37430	-1.24628	0.00010
H	0.01044	-1.77371	-0.81691
N	-0.07869	1.18213	-0.00018
H	0.13875	2.16983	0.00002

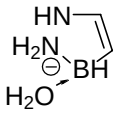
4g



Free energy= -288.873675
ZPE= 0.085098

C	-1.46368	-0.65629	-0.00001
C	-1.43782	0.70100	-0.00002
B	0.75833	-0.02187	-0.00000
N	-0.14412	-1.14073	0.00013
H	-2.26402	1.39806	0.00003
O	2.14098	-0.11567	-0.00001
H	2.58672	0.74364	0.00007
H	-2.31694	-1.32003	0.00000
H	0.05257	-2.13094	-0.00054
N	-0.09856	1.13466	-0.00005
H	0.12998	2.11827	0.00011

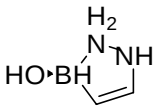
3c



Free energy= -290.358027
ZPE= 0.120369

C	1.31785	0.80038	-0.21072
B	-0.77010	0.07826	0.65017
N	0.23410	-1.15023	0.31187
H	2.19068	1.33902	-0.56682
H	-1.37893	-0.11944	1.65905
H	-0.19529	-1.91118	-0.22169
O	-1.88522	-0.02996	-0.52393
H	-2.81058	-0.08951	-0.21808
H	-1.83244	0.66253	-1.21238
H	0.57663	-1.55158	1.19132
C	0.20395	1.27675	0.37463
H	0.06215	2.33601	0.55659
N	1.33493	-0.59341	-0.45348
H	2.20599	-1.07477	-0.23956

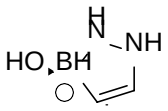
3d



Free energy= -289.950502
ZPE= 0.106954

C	1.31063	0.79566	-0.17275
B	-0.93684	0.13536	0.49497
N	0.18455	-1.15887	0.28292
H	2.21859	1.31807	-0.46372
H	-1.40588	-0.04429	1.60682
H	-0.20265	-1.91592	-0.28256
O	-1.92438	0.06886	-0.56848
H	-2.70762	-0.42458	-0.28675
H	0.44532	-1.54716	1.19251
C	0.15445	1.29075	0.28952
H	0.02600	2.36334	0.41342
N	1.34692	-0.61614	-0.39021
H	2.19470	-1.07052	-0.05630

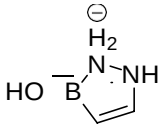
4e



Free energy= -289.476898
ZPE= 0.091179

C	1.36285	0.69797	-0.19971
B	-0.85317	0.08434	0.51058
N	0.12066	-1.15992	0.38167
H	2.29336	1.17616	-0.50728
H	-1.43530	0.07658	1.61382
H	-0.29986	-1.86028	-0.23137
O	-1.93624	0.08114	-0.55814
H	-2.74449	-0.30743	-0.19480
C	0.22388	1.25927	0.25350
H	0.12178	2.34355	0.30984
N	1.32970	-0.71147	-0.31286
H	2.14731	-1.14313	0.11770

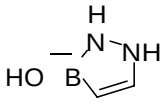
4f



Free energy= -289.217293
ZPE= 0.099344

C	1.39890	0.73432	-0.00242
B	-0.84067	0.18571	0.01254
N	0.07515	-1.13021	0.03648
H	2.37074	1.21669	0.01751
H	-0.13355	-1.80992	-0.70423
O	-2.17722	0.12940	-0.02327
H	-2.62106	-0.73379	-0.01752
C	0.16642	1.30708	0.02939
H	0.02431	2.37917	0.05176
H	-0.01581	-1.62806	0.93245
N	1.42324	-0.64771	-0.13537
H	2.11588	-1.19085	0.37384

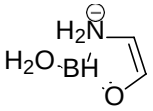
4g



Free energy= -288.812659
ZPE= 0.085047

C	1.43848	0.66342	-0.01551
B	-0.79655	0.10278	0.02458
N	0.02234	-1.08567	0.06852
H	2.42859	1.10756	0.01404
O	-2.18184	0.14084	-0.01205
H	-2.60349	-0.73162	0.01033
C	0.21083	1.26172	0.01290
H	0.08870	2.33912	0.00768
H	-0.18542	-2.02180	-0.25710
N	1.37604	-0.71876	-0.10492
H	2.02461	-1.25368	0.46897

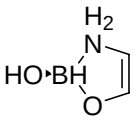
2c



Free energy= -310.299564
ZPE= 0.107665

C	-1.46089	0.49085	-0.35215
C	-1.26340	-0.82106	-0.20460
O	-0.08987	-1.17305	0.40265
B	0.69679	0.00888	0.62087
N	-0.30338	1.20527	0.22156
H	-1.91874	-1.63107	-0.49727
H	1.25702	0.15089	1.66149
H	0.11060	1.87218	-0.43889
O	1.82103	0.03563	-0.52479
H	1.81054	-0.74547	-1.11610
H	2.73658	0.16103	-0.20595
H	-2.28705	1.03445	-0.78359
H	-0.57292	1.75734	1.04261

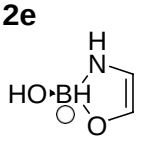
2d



Free energy= -309.901798
ZPE= 0.094353

C	-1.45837	0.55035	-0.22620
C	-1.28859	-0.77870	-0.16012
O	-0.08537	-1.22142	0.24347
B	0.84858	-0.07235	0.47051
N	-0.21434	1.20998	0.18219
H	-2.03326	-1.53118	-0.39948
H	1.22849	0.00268	1.61935
H	0.16569	1.81411	-0.55252
O	1.87625	-0.05238	-0.52847
H	2.72077	0.24744	-0.16579
H	-2.32353	1.11794	-0.53675
H	-0.34596	1.80147	1.00524

2e

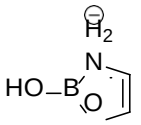


Free energy= -309.433122
ZPE= 0.078848

C	-1.35113	0.65910	-0.22413
C	-1.32685	-0.68995	-0.23659
O	-0.15630	-1.20508	0.27311
B	0.79820	-0.02929	0.48812
N	-0.17665	1.16896	0.37494
H	-2.09915	-1.38840	-0.54090
H	1.35650	-0.17617	1.58556

H	0.17627	2.02747	-0.03894
O	1.83526	0.06118	-0.57631
H	2.60972	-0.46438	-0.32699
H	-2.16163	1.30147	-0.55406

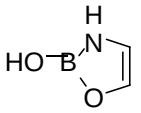
2f



Free energy= -309.154427
ZPE= 0.086837

C	-1.51902	0.52808	-0.00009
C	-1.34309	-0.79124	0.00001
O	-0.00869	-1.18483	0.00005
B	0.76827	-0.05953	0.00002
N	-0.18781	1.17178	-0.00001
H	-2.07436	-1.58634	0.00018
H	-0.04816	1.78016	-0.81842
O	2.08555	0.09627	-0.00001
H	2.61806	-0.71792	-0.00007
H	-2.41624	1.12670	-0.00005
H	-0.04820	1.78000	0.81853

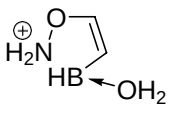
2g



Free energy= -308.759593
ZPE= 0.072781

C	-1.47440	0.58868	0.00002
C	-1.36450	-0.75442	0.00002
O	-0.02204	-1.13358	-0.00002
B	0.73150	0.04614	-0.00001
N	-0.18286	1.14152	-0.00004
H	-2.10207	-1.54208	0.00001
H	-0.02704	2.13871	0.00008
O	2.10123	0.10243	0.00002
H	2.51885	-0.77244	-0.00002
H	-2.36735	1.19805	0.00001

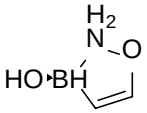
1c



Free energy= -310.211651
ZPE= 0.106969

C	1.34403	0.76011	-0.20560
B	-0.76047	0.07394	0.62956
N	0.22161	-1.15471	0.25214
H	2.24833	1.22667	-0.57905
H	-1.30940	-0.12977	1.66929
H	-0.14904	-1.83695	-0.41739
O	-1.91270	0.00841	-0.48014
H	-2.82920	-0.05346	-0.14744
H	-1.87850	0.68822	-1.18260
H	0.54174	-1.66904	1.07861
C	0.23357	1.25603	0.34361
H	0.10649	2.31910	0.51053
O	1.41958	-0.62445	-0.35395

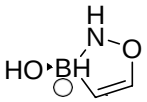
1d



Free energy= -309.809461
ZPE= 0.093616

C	1.34513	0.74720	-0.16584
B	-0.91965	0.14841	0.48840
N	0.15864	-1.15987	0.20645
H	2.29169	1.18595	-0.46287
H	-1.31542	-0.02251	1.62659
H	-0.17042	-1.78446	-0.53439
O	-1.95989	0.10287	-0.51578
H	-2.74853	-0.34950	-0.18468
H	0.37302	-1.72416	1.03108
C	0.19169	1.27433	0.23482
H	0.08317	2.35201	0.31665
O	1.42905	-0.65405	-0.24590

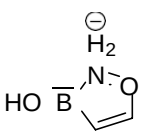
1e



Free energy= -309.344010
ZPE= 0.078155

C	1.37506	0.63832	-0.19768
B	-0.84913	0.09418	0.50412
N	0.09399	-1.17758	0.38599
H	2.32195	1.05055	-0.54234
H	-1.40686	0.07706	1.61203
H	-0.26223	-1.80933	-0.33595
O	-1.92038	0.12427	-0.55961
H	-2.74259	-0.24205	-0.20444
C	0.26345	1.23539	0.25627
H	0.19912	2.32056	0.31274
O	1.37629	-0.73263	-0.24240

1f

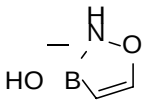


Free energy= -309.064176
ZPE= 0.086171

C	1.41179	0.68333	0.00029
B	-0.83209	0.19429	-0.00066
N	0.06400	-1.12776	-0.00039

H	2.42163	1.07700	0.00058
H	-0.03830	-1.72765	-0.82962
O	-2.16256	0.16881	0.00049
H	-2.63309	-0.68127	0.00026
C	0.21139	1.28890	-0.00041
H	0.10500	2.36524	-0.00042
O	1.43229	-0.69591	0.00038
H	-0.03968	-1.72706	0.82906

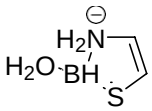
1g



Free energy= -308.668816
ZPE= 0.071642

C	1.44814	0.60904	-0.00002
B	-0.78988	0.10712	0.00001
N	0.01174	-1.07624	0.00008
H	2.46916	0.97234	-0.00002
H	-0.10375	-2.07939	-0.00026
O	-2.16831	0.17657	-0.00002
H	-2.61541	-0.68348	-0.00003
C	0.25217	1.23968	0.00001
H	0.16239	2.31920	0.00001
O	1.38743	-0.75444	-0.00002

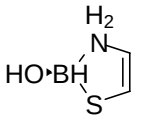
6c



Free energy= -633.255514
ZPE= 0.104783

C	-1.15774	1.20375	-0.27909
C	-1.52967	-0.06707	-0.43306
B	0.87795	-0.01944	0.58090
N	0.11902	1.37817	0.44109
H	-2.45465	-0.36461	-0.91371
H	1.50505	-0.11368	1.58630
H	0.71433	2.07306	-0.02495
O	1.93841	0.00017	-0.60969
H	1.74503	-0.59747	-1.36194
H	2.86777	-0.13717	-0.33786
H	-1.68417	2.09649	-0.58917
H	-0.05824	1.76429	1.37657
S	-0.45255	-1.31827	0.21394

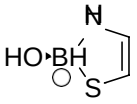
6d



Free energy= -632.858741
ZPE= 0.091906

C	-1.03826	1.27739	-0.23732
C	-1.50789	0.03295	-0.37910
B	1.04837	-0.10036	0.45693
N	0.26783	1.36743	0.42526
H	-2.47372	-0.17589	-0.82799
H	1.55022	-0.22950	1.54367
H	0.87998	2.04070	-0.04614
O	2.01562	-0.16967	-0.59254
H	1.61877	-0.29190	-1.46898
H	-1.52501	2.19754	-0.53604
H	0.15378	1.72063	1.38089
S	-0.51055	-1.30227	0.19575

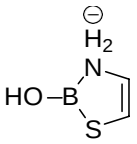
6e



Free energy= -632.405082
ZPE= 0.076677

C	-0.95696	1.32111	-0.14072
C	-1.56246	0.13242	-0.37256
B	1.03774	-0.03570	0.45842
N	0.28963	1.30013	0.46876
H	-2.54631	0.00672	-0.80945
H	1.55490	-0.37029	1.51777
H	0.82408	2.15997	0.40502
O	2.00939	-0.08269	-0.64066
H	2.67846	-0.76147	-0.46588
H	-1.40758	2.28344	-0.37763
S	-0.57989	-1.26878	0.14761

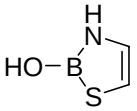
6f



Free energy= -632.109830
ZPE= 0.083402

C	-1.34862	1.09291	-0.00005
C	-1.62672	-0.20886	0.00005
B	0.90135	0.06344	-0.00007
N	0.09387	1.39772	-0.00002
H	-2.62850	-0.62039	0.00020
H	0.35130	1.97326	-0.81515
O	2.22714	0.17177	0.00004
H	2.74625	-0.64961	0.00012
H	-2.03507	1.92814	0.00006
H	0.35125	1.97298	0.81534
S	-0.24463	-1.33651	-0.00002

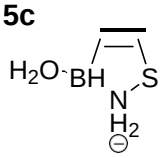
6g



Free energy= -631.720758
ZPE= 0.070087

C	-1.28477	1.12543	0.00001
C	-1.64991	-0.17467	0.00002
B	0.89104	0.16922	-0.00003
N	0.09167	1.35099	-0.00001
H	-2.65772	-0.56639	0.00016
H	0.44211	2.30108	-0.00036
O	2.26239	0.18192	0.00009
H	2.67878	-0.69215	-0.00018
H	-1.96213	1.97168	0.00009
S	-0.25556	-1.27983	-0.00003

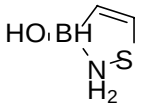
5c



Free energy= -633.223368
ZPE= 0.103781

C	0.92383	1.23007	-0.08826
B	-1.10747	0.03458	0.61259
N	0.02638	-1.11267	0.43934
H	1.63254	2.00886	-0.35908
H	-1.75048	-0.17730	1.59775
H	-0.29083	-1.88436	-0.15644
O	-2.11342	-0.25713	-0.60946
H	-3.04364	-0.42051	-0.36059
H	-2.09850	0.39368	-1.33937
H	0.25362	-1.52373	1.34913
C	-0.33337	1.37930	0.35731
H	-0.73824	2.38001	0.49002
S	1.54706	-0.42250	-0.25615

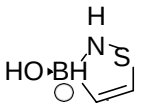
5d



Free energy= -632.820915
ZPE= 0.090280

C	0.91731	1.23937	-0.08437
B	-1.25506	0.07021	0.46172
N	-0.01629	-1.14329	0.26225
H	1.65394	2.01158	-0.29485
H	-1.64914	-0.11471	1.60018
H	-0.30606	-1.77113	-0.49200
O	-2.25040	-0.17057	-0.55768
H	-2.95786	-0.74519	-0.23258
H	0.09401	-1.71016	1.10429
C	-0.37868	1.38458	0.21333
H	-0.78253	2.39668	0.26298
S	1.56928	-0.42464	-0.15029

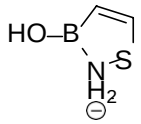
5e



Free energy= -632.355893
ZPE= 0.075708

C	0.90293	1.22469	-0.07049
B	-1.17038	-0.05103	0.47403
N	-0.02485	-1.15674	0.43515
H	1.61765	2.00212	-0.33921
H	-1.77538	-0.23072	1.54402
H	0.21861	-1.41074	1.39291
O	-2.11359	-0.16372	-0.68299
H	-2.63601	-0.97414	-0.58792
C	-0.37181	1.35638	0.33497
H	-0.78246	2.36240	0.45469
S	1.44409	-0.47333	-0.25023

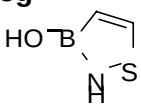
5f



Free energy= -632.078787
ZPE= 0.082987

C	0.97624	1.19239	-0.00015
B	-1.15126	0.10556	-0.00017
N	-0.12751	-1.10898	-0.00035
H	1.75957	1.94645	-0.00019
H	-0.24544	-1.71511	-0.82281
O	-2.47067	-0.10112	0.00043
H	-2.81604	-1.00879	0.00071
C	-0.35829	1.40198	-0.00036
H	-0.75933	2.40996	-0.00051
H	-0.24594	-1.71566	0.82162
S	1.56336	-0.46494	0.00026

5g



Free energy= -631.681715
ZPE= 0.068912

C	1.02184	1.15517	0.00004
B	-1.09610	0.03662	-0.00006
N	-0.14480	-1.03850	-0.00034
H	1.82382	1.88756	-0.00008
H	-0.29196	-2.04096	0.00065
O	-2.47213	-0.10751	0.00009
H	-2.77825	-1.02727	0.00021
C	-0.31909	1.37117	-0.00003
H	-0.71182	2.38482	-0.00006
S	1.50080	-0.52598	0.00007