INPE Ministério da Ciência e Tecnologia
Instituto Nacional de Pesquisas Espaciais

Universidade de Brasília

Thermochemistry of Molecule in the B/F/H/N system at G-2 level of Theory

Patrícia R.P. Barreto
Laboratório Associado de Plasma – LAP
Instituto Nacional de Pesquisas Espaciais – INPE
patricia@plasma.inpe.br
Alessandra F.A. Vilela and Ricardo Gargano
Instituto de Física
Universidade de Brasília - UnB

Abstract

A self-consistent set of thermochemical data, such as heats of formation, atomization energy, enthapy, entropy and heat capacity, for 39 chemical species in the B/F/H/N system are obtained at G-2 level of theory. Calculations were performed for both stable and radical species using the GAUSSIAN98 program. The geometry optimization and frequency calculation were carried out using the second order Möller-Plesset perturbation theory and the triple-zeta plus polarization 6-31G(d) basis set. Furthermore, we calculated the energies at the Gaussian-2 level of theory. Good agreement is found between the calculation and reference heats of formation and atomization energy for most molecules containing B, F, H and N, but for nine species there no experimental neither theoretical data, concerned to geometry or frequencies or energies, to compare. The maximum error, 3.9kcal mol^{-1}, in a atomization energy is found for BH_2 while for the heat of formation, error of 25.5kcal mol^{-1}, is for the BF_2. There have in general been large discrepancies between theoretical calculation and available experimental determination or estimates for BX_2 species, from the reference this value is up to 24kcal mol^{-1} for the BF_2. Polynomial fits of the predicted thermodynamic data over the 300-4000K temperature range were also determined. The species analyzed here are important in a kinetic mechanism for growth boron nitride in a CVD reactor. It is generally difficult to optimize conditions in a CVD reactor because film properties depend on complex interactions involving heat and mass transport, chemical kinetics, and thermochemistry. Developing a reliable set of thermodynamic data is a necessary first step for system optimization, since it provides important constraints on the possible reaction mechanism.

Introduction

- *There has been considerable interest in recent years, in the growth of boron nitride thin films*
- *Like carbon, boron nitride has different allotropes, the hexagonal (hBN) and cubic (cBN) phases*
- *The hexagonal phase, although electrically insulating, has properties that are very similar to graphite while the cubic phase has properties comparable to diamond*
- *There is little understanding of the chemical process which are involved in and which control the synthesis of either hBN or cBN from the vapor phase.*
- *Theoretical research found in the literature includes thermodynamic equilibrium calculations for mixtures involving B/F/N/H and B/Cl/N/H, as well as limited kinetics studies of the reactions between BCl_3 and NH_3*
- *The species analyzed here are important in a kinetic mechanism for growth boron nitride in a CVD reactor. It is generally difficult to optimize conditions in a CVD reactor because film properties depend on complex interactions involving heat and mass transport, chemical kinetics, and thermochemistry.*
- *Developing a reliable set of thermodynamic data is a necessary first step for system optimization, since it provides important constraints on the possible reaction mechanism.*

Thermodynamic Properties

- Internal energy

$$E = k_B T \left(\frac{\partial \ln Q}{\partial \ln T} \right)_v$$

- Entropy

$$S = k_B \ln Q + k_B \left(\frac{\partial \ln Q}{\partial \ln T} \right)_v$$

- Heat capacity

$$c_v = k_B \left(\frac{\partial \ln Q}{\partial \ln T} \right)_v + k_B \left(\frac{\partial^2 \ln Q}{\partial (\ln T)^2} \right)_v$$

- Enthalpy

$$H \equiv E + pV$$

- Gibbs free energy

$$G = H - ST$$

- Heat capacity

$$c_p = c_v + R$$

Partition Function

$$Q = Q_{trans} Q_{rot} Q_{vib} Q_{elet}$$

	Degrees of freedom	Partition Function	Magnetude order
Translation	3	$Q_{trans} = \left(\frac{2\pi m k_B T}{h^2} \right)^{3/2}$	$10^{33}\ m^3$
Rotation – 2D	2	$Q_{rot-2D} = \left(\frac{8\pi^2 I k_B T}{\sigma_e h^2} \right)$	$10 - 10^2$
Rotation – 3D	3	$Q_{rot-3D} = \left[\frac{\sqrt{\pi}}{\sigma_e} \left(\frac{8\pi^2 I_m k_B T}{h^2} \right)^{3/2} \right]$	$10^2 - 10^3$
Vibration	$n = 3N - 5$ $n = 3N - 6$	$Q_{vib} = \prod_{i=1}^{n} \left[1 - \exp\left(- \frac{hc\nu_i}{k_B T} \right) \right]^{-g_i}$	$1 - 10^n$
Electronic	–	$Q_{elet} = \sum_{i=0}^{n} g_i \exp\left(- \frac{\varepsilon_i}{k_B T} \right)$	1

Atomization Energies Heats of formation at 0 and 298.15K, Bound Dissociation Energies

- *Atomization Energy*

$$\Sigma D_0(A_xB_yC_z) = [x\varepsilon_0(A) + y\varepsilon_0(B) + z\varepsilon_0(C)]\ ] - \varepsilon_0(A_xB_yC_z)$$

- *Heats of formation*

$$\Delta_f H^0(A_xB_yC_z,0K) = x\ \Sigma\Delta_f H^0\,(A,0K) + y\ \Sigma\Delta_f H^0\,(B,0K) + z\ \Sigma\Delta_f H^0\,(C,0K) - \Sigma D_0(A_xB_yC_z)$$

$$\Delta_f H^0(A_xB_yC,298K) = \Delta H_f(A_xB_yC,0K) + [H^0(A_xB_yC,298K) - H^0(A_xB_yC,0K)]_{st} - x\Sigma\,[H^0(A,298K) - H^0(A,0)]_{st} - y\Sigma\,[H^0(B,298K) - H^0(B,0)]_{st} - z\Sigma\,[H^0(C,298K) - H^0(C,0)]_{st}$$

- *Bond Dissociation Energies*

$$BDE(AB–C) \equiv \Delta H_{298}{}^0 = \Delta_f H_{298}(AB,g) + \Delta_f H_{298}(C,g) - \Delta_f H_{298}(ABC)$$

Results, Discussion and Conclusion

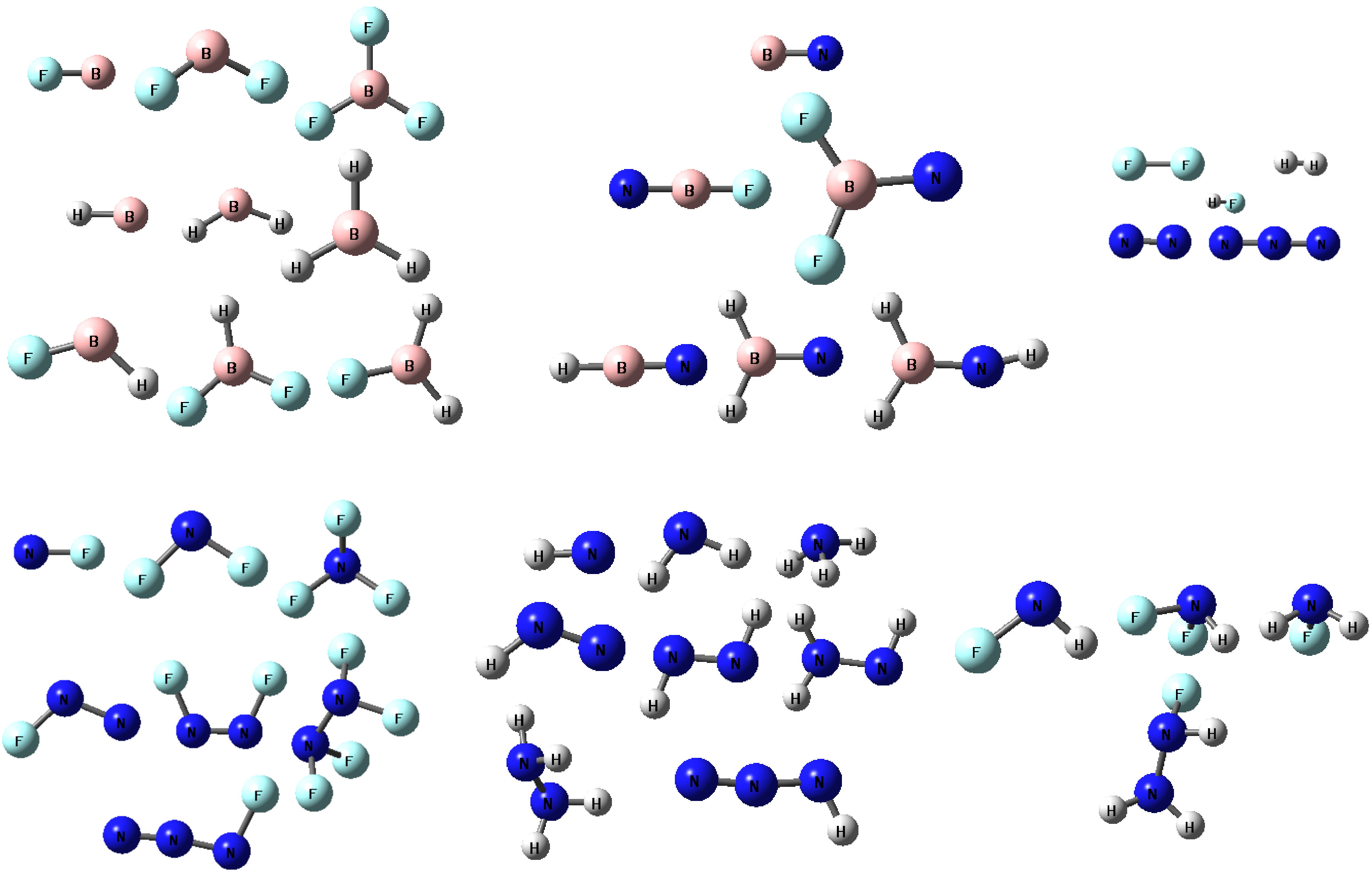
- *Geometries, frequencies and energies were obtained using GAUSSIAN98 program at G2 level (7 internal steps).*
- *Geometries, frequencies, atomization energies, heats of formation and bond dissociation energies compared with experimental and theoretical data when avaliable.*
- *Good agreement is found between the calculation and reference heats of formation and atomization energy for most molecules containing B, F, H and N, but for nine species there no experimental neither theoretical data, concerned to geometry or frequencies or energies, to compare.*
- *The maximum error, 3.9kcal mol^{-1}, in a atomization energy is found for BH_2 while for the heat of formation, error of 5.5kcal mol^{-1}, is for the BF_2.*
- *There have in general been large discrepancies between theoretical calculation and available experimental determination or estimates for BX_2 species, from the reference this value is up to 24kcal mol^{-1} for the BF_2.*

Acknowledgment

Centro Nacional de Processamento de ALTO DESEMPENHO EM SÃO PAULO

CNPq

Sub-system	*molecules*
B/F	***BF,BF_2,BF_3***
B/H	***BH, BH_2, BH_3***
B/H/F	***BHF, BHF_2, BH_2F***
B/N	***BN***
B/N/F	***BNF-a**, BNF-b, **BNF_2-a**, BNF_2-b, BNF_2-c, BNF_3-a, BNF_3-b, BNF_4*
B/N/H	***BNH-a**, BNH-b, **BNH_2-a**, BNH_2-b, BNH_2-c, **BNH_3-a**, BNH_3-b, BNH_4*
B/N/H/F	*BNHF-a, BNHF-b, BNHF-c, BNHF-d, $BNHF_2$-a, $BNHF_2$-b, $BNHF_2$-c, $BNHF_2$-d, $BNHF_2$-e, $BNHF_2$-f, $BNHF_3$-a, $BNHF_3$-b, BNH_2F-a, BNH_2F-b, BNH_2F-c, BNH_2F-d, BNH_2F-e, BNH_2F_2-a, BNH_2F_2-b, BNH_2F_2-c, BNH_2F_2-d, BNH_3F-a, BNH_3F-b*
F	***F_2***
H	***H_2***
H/F	***HF***
N	***N_3***
N/F	***NF, NF_2, NF_3, N_2F, N_2F_2-cis**, N_2F_2-trans, N_2F_3, N_2F_4, N_3F*
N/H	***NH, NH_2, NH_3, N_2H, N_2H_2-cis, N_2H_2-trans, N_2H_3, N_2H_4, N_3H,*
N/H/F	***NHF, NHF_2, NH_2F**, N_2HF-cis, N_2HF-trans, N_2HF_2-a, N_2HF_2-b, N_2HF2-c, N_2H_2F-a, N_2H_2F-b, N_2H_2F-c, $N_2H_2F_2$-a, $N_2H_2F_2$-b, $N_2H_2F_2$-c, N_2HF_3, **N_2H_3F**,*



Fully optimized geometries at the MP2/6-31G(d) level

species	geometries (Å and degrees)
BF	R_{BF}= 1.281 (1.265)
BF_2	R_{BF}= 1.321 (1.30, 1.3195$_t$), A_{FBF}= 121.1 (112, 121.10$_t$)
BF_3	R_{BF}= 1.324 (1.307), A_{FBF}= 120. (120)
BH	R_{BH}= 1.234 (1.2325)
BH_2	R_{BH}= 1.189 (1.1884 $_t$,1.186$_t$, 1.20), 1.159, A_{HBH}= 127.7 (127.57$_t$, 126.58$_t$, 180)
BH_3	R_{BH}= 1.190 (1.16), A_{HBH}= 120. (120)
BHF	R_{BF}= 1.319 (1.316$_t$), R_{BH}= 1.2001 (1.1999$_t$), A_{FBH}= 121.2 (121.24$_t$)
BHF_2	R_{BF}= 1.326 (1.30, 1.3241$_t$), R_{BH}= 1.180 (1.15, 1.1859$_t$), A_{FBF}= 118.4 (120, 118.46$_t$), A_{FBH}= 120.8 (120, 120.76$_t$)
BH_2F	R_{BF}= 1.330 (1.3298$_t$), R_{BH}= 1.190 (1.192$_t$), A_{HBH}= 124.1 (124.08$_t$), A_{FBH}= 117.9 (117.96$_t$)
BN	R_{BH}= 1.327 (1.281)
BNF-a	R_{BF}= 1.290, R_{BH}= 1.324, A_{FBN}= 180.0
BNF_2-a	R_{BF}= 1.332, R_{BH}= 1.420, A_{FBF}= 122.95, R_{FBN}= 118.5
BNH-a	R_{BH}= 1.240 (1.325 $_t$), R_{BH}= 1.170 (1.174 $_t$), A_{HBN}= 180.0
BNH_2-a	R_{BH}= 1.393 , R_{BH}= 1.190, A_{HBH}= 129.8 , A_{HBN}= 115.1
BNH_3-a	R_{BH}= 1.348 (1.398$_t$), R_{BH}= 1.000 (1.024$_t$), R_{BH}= 1.200 (1.223$_t$), A_{HBH}= 122.1 (132.2$_t$), A_{HBN}= 117.9 (113.7$_t$), A_{BNH}= 162.4 (123.5$_t$)
F_2	R_{FF}= 1.421 (1.41193)
H_2	R_{HH}= 0.738 (0.7414)
HF	R_{HF}= 0.934 (0.9168)

N_2	R_{BH}= 1.131 (1.094)
N_3	R_{BH}= 1.185 (1.1815) , A_{NNN}= 180. (180)
NF	R_{BH}= 1.330 (1.51 , 1.3173)
NF_2	R_{BH}= 1.359 (1.37), A_{FNF}= 103.3 (104.2)
NF_3	R_{BH}= 1.380 (1.371), A_{FNF}= 101.7 (102.9)
N_2F	R_{BH}= 1.345, R_{BH}= 1.370, A_{NNF}= 114.3
N_2F_2-cis	R_{BH}= 1.395 (1.384), R_{BH}= 1.230 (1.214), A_{NNF}= 113.6 (114.5)
N_2F_4	R_{BH}= 1.393 (1.37), R_{BH}= 1.460 (1.47), A_{FNF}= 102.7 (108), A_{NNF}= 105.9 (104)
N_3F	R_{N1F}= 1.432 (1.444_t), R_{N1N2}= 1.282 (1.253_t), R_{N2N3}= 1.150 (1.132_t), A_{NNF}= 103.8 (103.8_t), A_{NNN}= 171.7 (171.6_t)
NH	R_{BH}= 1.039 (1.038)
NH_2	R_{BH}= 1.020 (1.024), A_{HNH}= 103.3 (103.4)
NH_3	R_{BH}= 1.017 (1.0124), A_{HNH}= 106.4 (106.67)
N_2H	R_{BH}= 1.050, R_{BH}= 1.150, A_{NNH}= 121.2
N_2H_2-trans	R_{BH}= 1.030 (1.13), R_{BH}= 1.260(1.28), A_{NNH}= 105.4 (104)
N_2H_3	R_{BH}= 1.012, R_{BF}= 1.350, A_{HNH}= 118.6, A_{NNH}= 112.3
N_2H_4	R_{BH}= 1.020 (1.022), R_{BH}= 1.430 (1.449), A_{HNH}= 106.9 (109.47), A_{NNH}= 111.4 (112)
N_3H	R_{N1H}= 1.023 (1.019_t), R_{N1N2}= 1.250, R_{N2N3}= 1.159 (1.159_t), A_{NNH}= 110.3 (109.6_t), A_{NNN}= 171.0 (171.1_t)
NHF	R_{BH}= 1.378 (1.373), R_{BH}= 1.030 (1.035), A_{HNF}= 99.9 (102)
NHF_2	R_{BH}= 1.400 (1.400), R_{BH}= 1.020 (1.026), A_{FNF}= 103.2 (102.9), A_{FNH}= 99.6 (99.8)
NH_2F	R_{BH}= 1.434 (1.4329), R_{BH}= 1.020 (1.0225), A_{HNH}= 105.0 (106.27), A_{FNH}= 100.9 (101.08)
N_2H_3F	R_{BH}= 1.465, R_{BH}= 1.022, R_{BH}= 1.376, A_{HNH}= 113.6, A_{FNH}= 97.0, A_{HNN}= 109.4, A_{FNN}= 106.3

Scaled harmonic vibrational frequencies at the HF/6-31G(d) level for the (in cm^{-1})

species	HF/6-31G(d)
BF	1471.1
BF_2	552.8, 239.3, 1508.2
BF_3	507.9, 737.7, 942.8, 1575.0
BH	2511.2
BH_2	1125.6, 2728.9, 2868.1
BH_3	1224.0, 1305.0, 2695.3, 2816.0,
BHF	1098.7, 1388.7, 2707.5
BHF_2	569.5, 1012.7, 1200.4, 1236.9, 1538.2, 2867.6
BH_2F	1102.4, 1177.3, 1253.2, 1457.0, 2740.6, 2830.4,
BN	1890.3
BNF-a	462.5, 481.5, 1050.0, 2024.1
BNF_2-a	322.0, 476.9, 680.0, 918.0, 1521.0, 1524.7
BNH-a	947.2, 947.2, 1892.6, 3033.3
BNH_2-a	898.7, 1102.2, 1183.3, 1292.6, 2728.4, 2841.4
BNH_3-a	146.4, 464.1, 892.6, 1080.4, 1194.6, 1384.0, 2691.6, 2757.8, 3852.6
F_2	1245.0
H_2	4648.2
HF	4357.9

N_2	2757.8
N_3	530.2, 679.3, 1503.7, 1703.3
NF	1272.5
NF_2	652.8, 1189.8, 1267.6
NF_3	580.2, 756.21221.6, 1236.6
N_2F	488.1, 1064.4, 1344.4
N_2F_2-cis	416.2, 633.9, 909.0, 1153.7, 1177.8, 1965.0
N_2F_4	150.2, 336.0, 356.3, 520.6, 601.9, 693.2, 891.5, 1035.2, 1216.5, 1242.7, 1267.2, 1324.9
N_3F	282.0, 605.8, 757.8, 1045.7, 1225.7, 2384.7,
NH	3531.1
NH_2	1710.2, 3606.9, 3708.2
NH_3	1209.7, 1849.9, 3689.7, 3821.4,
N_2H	1263.8, 1662.9, 3280.4
N_2H_2-trans	1473.5, 1477.3, 1761.2, 1906.3, 3571.6, 3606.7
N_2H_3	675.8, 831.7, 1265.1, 1299.1, 1624.1, 1848.2, 3673.8, 3737.6, 3868.1
N_2H_4	474.3, 978.9, 1111.9, 1226.3, 1435.9, 1468.0, 1854.0, 1871.4, 3706.7, 3717.7, 3819.5, 3825.9
N_3H	572.1, 677.2, 1253.9, 1451.8, 2509.3, 3722.4
NHF	1185.7, 1612.0, 3632.7
NHF_2	581.0, 1163.4, 1196.0, 1468.4, 1665.5, 3747.6
NH_2F	1128.5, 1398.5, 1499.4, 1819.5, 3702.6, 3807.8
N_2H_3F	357.8, 593.9, 751.3, 1047.9, 1245.5, 1262.2, 1492.4, 1666.3, 1852.8, 3753.4, 3770.5, 3888.6

Calculated atomization energy, heats of formation at 0 and 298.15K (in kcal mol^{-1})

species	ΣD_0	$\Delta_f H^0$(0K)	$\Delta_f H^0$(298K)	species	ΣD_0	$\Delta_f H^0$(0K)	$\Delta_f H^0$(298K)
BF	181.117	-26.447	-25.707	NF	76.365	54.635	54.632
BF_2	291.213	-118.073	-117.928	NF_2	143.625	5.845	5.213
BF_3	463.770	-272.160	-272.770	NF_3	203.211	-35.271	-36.701
BH	83.087	104.743	105.517	N_2F	70.964	172.566	172.018
BH_2	160.989	78.471	78.554	N_2F_2-cis	247.394	14.606	13.208
BH_3	267.028	24.062	23.153	N_2F_4	309.592	-10.652	-13.114
BHF	226.154	-19.854	-19.800	N_3F	280.387	75.673	74.422
BHF_2	400.883	-176.113	-176.935	NH	78.240	85.920	85.944
BH_2F	331.793	-73.863	-74.787	NH_2	170.980	44.810	44.123
BN	103.703	145.027	145.772	NH_3	278.289	-10.869	-12.549
BNF-a	261.626	5.574	5.661	N_2H	215.462	61.228	60.525
BNF_2-a	353.135	-67.465	-67.918	N_2H_2-trans	280.493	47.827	46.114
BNH-a	189.355	111.005	110.823	N_2H_3	324.842	55.108	52.559
BNH_2-a	228.167	123.823	122.947	N_2H_4	407.716	23.864	20.389
BNH_3-a	360.383	43.237	41.961	N_3H	319.382	69.838	68.334
F_2	36.884	0.056	0.044	NHF	151.102	31.528	30.820
H_2	104.684	-1.424	-1.370	NHF_2	218.002	-16.902	-18.502
HF	136.587	-66.487	-66.474	NH_2F	241.665	-7.405	-9.107
N_2	224.133	0.927	0.920	N_2H_3F	385.222	13.198	9.932
N_3	230.144	107.446	106.660				

Calculated bond dissociation enthalpies (BDE) at 298K for the compounds in the B/F/H/N system at the G2 theory (in kcal mol^{-1})

species	B-F	B-H	B-N	N-F	N-H	N-N	F-F	H-H	H-F
BF	181.05								
BF_2	112.04								
BF_3	172.76								
BH		83.19							
BH_2		79.97							
BH_3		105.83							
BHF	145.10	47.24							
BHF_2	174.56	109.76							
BH_2F	170.04	104.91							
BN			105.01						
BNF-a	161.30		85.26						
BNF_2-a	90.72		63.94						
BNH-a		88.80	110.62						
BNH_2-a		40.76	-155.74						
BNH_3-a		22.91	119.83		132.54				
BNH_3-b		69.32	114.42		111.47				
F_2							38.37		
H_2								105.74	
HF									137.53

N_2						229.29			
N_3						10.20			
NF				81.19					
NF_2				66.20					
NF_3				58.49					
N_2F				-149.75			-1.65		
N_2F_2-cis				172.91			90.06		
N_2F_4				60.59			19.60		
N_3F				48.93			-22.06		
NH						84.11			
NH_2						92.36			
NH_3						107.32			
N_2H						-6.52	77.73		
N_2H_2-trans						64.65	119.21		
N_2H_3						51.14	18.01		
N_2H_4						83.82	9.48		
N_3H						89.13	15.22		
NHF				71.61		74.53			
NHF_2				-30.47		131.14			
NH_2F				69.85		90.60			
N_2H_3F				60.51		72.87	61.59		

Deviation of atomization energy, heats of formation at 0 and 298.15K calculated at G2 level of theory with experimental and theoretical data (in kcal mol^{-1})

species	ΣD_0			$\Delta_f H^0$(0K)				$\Delta_f H^0$(298K)			
	Expt.-Theory	Theory-Theory	Error bar-E	Expt. Theory	Theory Theory	Error bar-E	Error bar-T	Expt.-Theory	Theory-Theory	Error bar-E	Error bar-T
BF	1.883	-0.317	3	-2.022		3.3		-1.993	0.307	3.3	
BF_2		-0.713		-23.195		3.11		-23.172	0.628	3.11	
BF_3	-3.27	-1.37		1.155	1.36	0.41		1.35	1.37	0.41	
BH	-4.887	-0.287	2	0.401	-3.043	2.01		0.283	-3.127	2.1	1.16
BH_2	27.811	-0.889	15.2	-30.146	-2.871	15.07		-30.554	-3.004	15.07	1.16
BH_3	-4.728	-1.728	2.4	2.373	-0.662	2.39		2.147	-0.803	2.39	1.16
BHF		-0.854							0.8		
BHF_2		-70.783		1.4		0.79		1.535	1.535	0.79	
BH_2F					2.663				2.587		
BN	-10.703	2.997	5	-31.63	-5.427	29.9		-31.772	-5.472	29.9	37.35
BNH-a		14.045			-16.505				-16.503		1.03
BNH-b		1.114			-3.474				-3.539		1.59
BNH_2-a		17.533			-19.923				-20.017		1.05
BNH_2-b					-2.087				-2.157		
BNH_2-c					-0.699				-0.647		
BNH_3-a		-5.283			2.863				2.619		1.18
BNH_3-b					-3.02				-3.212		

BNH_4					-0.864				-1.055		
F_2	0.946	-0.284		-0.056	0.244			-0.044	0.256		1
H_2	-0.524			1.424	0.324			1.37	0.27		1.18
HF	-0.387	-0.287		1.296	0.287	0.19		1.333	0.274	0.19	1.2
N_2	1.807	-0.333		-0.927	0.373			-0.92	0.38		1.02
N_3		-1.794		-7.692	1.804	5		-7.65	1.74	5	
NF	-4.965	-0.265	8	4.923	-0.635	7.89	0.9	4.868	5.368	7.89	
NF_2				4.873	2.155	1.91	0.9	4.887	3.287	1.91	
NF_3				5.04	1.471	0.27	0.9	5.131	1.401	0.27	
N_2F_2-cis				3.267		1.2		3.192	4.692	1.2	8
N_2F_2-trans				4.778		1.2		4.811		1.2	
N_2F_4				11.233		2.51		11.114	8.114	2.51	2
NH	-4.22	-0.34		4.154	0.28	4		4.056	0.356	4	
NH_2	-0.98	-0.88		1.421	0.89	1.51		1.377	0.877	1.51	
NH_3	-1.569	-1.789		1.561	1.769	0.1		1.579	1.749	0.1	
N_2H								-0.268	-1.169	2.61	1
N_2H_2-cis				-0.25		5		4.586		2	
N_2H_2-trans				4.573		2		2.401	3.311		
N_2H_4	-2.316	-3.316		2.315	3.336	0.19		3.366	1.966		
NHF								-5.32		4	
NHF_2								2.902	10.702	1.5	
NH_2F								4.107	2.127		
N_2H_3F	-2.958										

Summary of average deviations and maximum deviation in kcal mol^{-1}

	Method	Experimental				Theoretical			
		Avg. dev.	Max.deviat.		n	Avg. dev.	Max.deviat.		n
ΣD_0	B3LYP	-9.85 ± 13.38	-39.13	14.11	16	-12.84 ± 12.93	-40.13	16.52	26
	G2	-0.57 ± 8.20	-10.70	27.81	16	0.41 ± 4.78	-5.28	17.53	26
	G3	-0.61 ± 8.48	-11.43	27.87	16	-0.13 ± 4.67	-7.23	15.36	26
$\Delta_f H^0(0K)$	B3LYP	8.19 ± 16.69	-45.15	39.12	25	12.13 ± 12.74	-18.95	40.15	26
	G2	-1.59 ± 10.69	-31.63	11.23	25	-1.52 ±5.39	-19.92	3.34	26
	G3	-1.57 ± 10.52	-30.91	8.00	25	-1.10 ± 5.27	-17.75	7.24	26
$\Delta_f H^0(298K)$	B3LYP	0.22 ± 12.46	-47.33	11.77	29	2.10 ± 6.99	-21.03	14.16	36
	G2	-1.22 ± 10.10	-31.77	11.11	29	-0.11 ± 5.46	-20.02	10.70	36
	G3	-1.16 ± 9.98	-31.05	7.90	29	0.006 ± 5.19	-17.85	8.10	36