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Supplementary Text

Correlation of BDE's with changes in spin populations: invariance with respect to definition of atomic populations. Various schemes exist for calculating atomic electron populations, and from them atomic charges, using molecular wave functions.[1] The most common is the Mulliken definition,[2] although its shortcomings are well documented.[3,4] The great variety of procedures available for defining atomic populations, and the wide disparity in the numerical results obtained from them, leads to some level of difficulty in drawing useful conclusions from such analyses. It is not unusual for the population of an atom to vary by an entire electron, or even more, depending on the particular definition of charge used to perform the calculation. However, the paragraphs below demonstrate that the correlation between B-H BDE and spin density delocalization described in the main body of the paper and illustrated graphically in Figure 6 is not an artifact of using a partcular definition of atomic population.

Despite the large and well-documented inconsistencies between definitions, atomic populations derived for an entire series of molecules using a given procedure usually correlate very closely with those calculated for the same series of molecules using some other procedure.[1] These correlations are not equally good for all pairs of definitions of charge, nor do the best fit lines generally have a slope of one or an intercept of zero. Nonetheless, *differences* in atomic populations, when assessed consistently using a single reasonable definition, are still likely to be meaningful. Using two quite different procedures and comparing the results provides an even greater degree of confidence if both approaches lead to the same conclusions.

Many of the procedures that yield atomic populations can equally well provide atomic spin density populations, and it is possible to quantify the earlier discussion of spin density distribution using such an approach. Two quite dissimilar definitions have been chosen for the present application: the Atoms in Molecules (AIM) approach of Bader[5,6,7] and the Natural Population Analysis (NPA) of Weinhold.[8,9] The former is based on a division of physical space according to

topological principles into regions belonging to the various atoms comprising a molecule, while the latter represents a modification of the Mulliken procedure that largely removes the problem of basis set dependence.

Table 4 lists both the AIM and NPA atomic spin density populations of the borane radicals, and shows that the B-H BDE is correlated with the delocalization of spin density, as described previously. The data are presented graphically in Figure 6, which plots the BDE against the fraction of alpha spin density found on atoms *other* than the BH_2 fragment in each radical (R^2 = 0.96). Importantly, the correlation is demonstrated equally well using the NPA populations, as shown in Figure A (R^2 = 0.97). The similarity results from the aforementioned fact that the NPA and AIM populations, while numerically very dissimilar, nonetheless often show an excellent correlation, as illustrated in Figure B (slope = 1.022, correlation coefficient = 0.98). This close correspondence suggests that the foregoing discussion is not invalidated by the unavoidably arbitrary nature of all definitions of atomic charge.

Correlation of BDE's with changes in atomic population. Interestingly, the correlation between electron population and BDE extends to the total populations as well as the spin densities, if one considers the change in the electronic population of the BH_n fragment that takes place upon hydrogen atom abstraction. This change is defined simply as the population of the BH_2 fragment in the radical minus that of the BH_3 fragment in the parent complex. Figure C shows the relationship between this population difference and the BDE for the hydrogen abstraction process. The excellent correlation (R^2 = 0.97) mirrors that in Figure 6 (BDE versus spin density). Once again, the AIM and NPA procedures for defining electronic population yield the same qualitative result; a plot of the population difference computed via NPA versus that computed via AIM yields a best fit line with a correlation coefficient of 0.998 and a slope of 0.79. The changes are consistently ~25% larger with AIM than with NPA, but are related in a rigorously linear fashion.

Demonstration that geometric constraints do not significantly complicate the interpretation of difference densities for complexation. Figures 9 and 10 illustrate the reorganization of charge density that occurs as the result of complexation of various Lewis bases with borane. A complication arises in their interpretation because of the changes in geometry that occur during complexation. To avoid artifacts associated with the movement of atoms, the geometries of the "isolated" molecules in the subtraction procedure must be identical to the geometries used in the complexes. For instance, in the calculation for $BH_3{\cdot}NH_3$, the BH_3 and NH_3 wave functions were those for BH_3 and NH_3 *at the exact geometries they hold in the* $BH_3{\cdot}NH_3$ *complex.*

As the changes in molecular geometry that accompany complexation can be quite substantial, there is some ambiguity in the interpretation of the difference density distributions.[10] How much of the charge redistribution derives from complexation, and how much from geometric change within the fragments? In order to answer this question, NPA atomic populations were computed for the isolated component molecules both at their equilibrium geometries and also at their geometries in the complexes. The resulting differences, which are listed in Table C, were taken to indicate the amount of charge redistribution directly related to the changes in geometry. The calculated differences were generally much smaller than the charge redistribution resulting from complexation, with a mean absolute value of 0.010 electrons, and a maximal value of 0.070 electrons for the case of $BH_2{\cdot}OCH_2$. Consequently, the charge density perturbations depicted in Figures 9 and 10 mostly reflect the complexation process itself, and are only modestly "contaminated" by the associated geometry changes.

Correlation of strength of association with orbital energies. In so far as the complexation of borane to Lewis bases can be described in terms of frontier molecular orbital interactions (HOMO on the Lewis base, LUMO on the borane), one might expect the strength of coordination to correlate with the HOMO-LUMO energy gap. Since the LUMO is the same in all cases -- the empty p orbital on boron -- one might predict a correlation between the HOMO

energy of the Lewis base and the complexation enthalpy. The LUMO energies are listed in Table D. However, plotting the HF/6-311++G**(6d)//MP2/6-31G* HOMO energy against the dissociation enthalpy yields a correlation coefficient of only 0.49.

It is likely that not only the energy but also the spatial orientation and diffuseness of the HOMO influences its interaction with the LUMO on boron. A diffuse lone pair orbital cannot overlap with the LUMO as effectively as a compact one. It might be possible to compensate for this effect in at least an approximate fashion by using localized MO's instead of the canonical MO's, since the localized MO's ought in general to have shapes and orientations optimal for intermolecular interaction. The optimization process might minimize differences in lone pair "availability" from one species to the next.

The NBO procedure of Weinhold and Reed[8,9,11] that is included in the Gaussian 94 ab initio package[12] yields localized MO's that can be used for this purpose. The use of localized orbitals substantially improved the correlation of HOMO-LUMO gap with complexation enthalpy, raising the correlation coefficient to 0.84, but still did not provide a truly convincing quantitative relationship. Use of QCISD orbital energies instead of HF energies made essentially no difference at all. The absence of a strong correlation probably results from the dependence of interaction strength on not only orbital energy but also the extent of orbital overlap, for which the localization procedure does not adequately compensate. The orbital energies relevant to the above discussion are provided in Table D.

Notes and References.

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Table A. G-2 and CBS-4 total enthalpies (Hartrees).

Structure	Symmetry	State	0 K[a]		0 K to 298 K Increment[b]	
			G-2	CBS-4	G-2	CBS-4
H	K_h	2	-0.50000	-0.50335	0.00236	0.00236
BH_2	C_{2v}	2	-25.85726[c]	-25.86744	0.00381	0.00381
BH_3	D_{3h}	1	-26.52486[c]	-26.53660	0.00384	0.00384
B_2H_5	C_{2v}	2	-52.44782	-52.47117	0.00482	0.00476
B_2H_6	D_{2h}	1	-53.10751	-53.13182	0.00456	0.00451
NH_3	C_{3v}	1	-56.45865	-56.47365	0.00381	0.00386
H_2O	C_{2v}	1	-76.33205	-76.34858	0.00379	0.00379
PH_3	C_{3v}	1	-342.67903	-342.68642	0.00385	0.00384
H_2S	C_{2v}	1	-398.93070	-398.93532	0.00379	0.00379
CO	$C_{\infty v}$	1	-113.17750	-113.18898	0.00330	0.00331
H_2CO	C_{2v}	1	-114.33892	-114.35829	0.00381	0.00381
HCN	$C_{\infty v}$	1	-93.28489	-93.29258	0.00346	0.00341
HNC	$C_{\infty v}$	1	-93.26210	-93.27309	0.00378	0.00357
CH_3OCH_3	C_{2v}	1		-154.78280		0.00535
CH_3CN	C_{3v}	1		-132.54562		0.00442
CH_3SCH_3	C_{2v}	1		-477.40125		0.00583
$(CH_3)_2CO$	C_{2v}	1		-192.85938		0.00627
$N(CH_3)_3$	C_{3v}	1		-174.15521		0.00654
$P(CH_3)_3$	C_{3v}	1		-460.41718		0.00757
$(CH_3)_2SO$	C_s	1		-552.52964		0.00650
THF	C_2	1		-232.07369		0.00590
pyridine	C_{2v}	1		-247.88073		0.00510
BH_2NH_3	C_s	1	-82.36231	-82.38843	0.00492	0.00486
BH_3NH_3	C_{3v}	1	-83.02505	-83.05293	0.00495	0.00486
BH_2OH_2	C_1	2	-102.20693	-102.23145	0.00538	0.00527
BH_3OH_2	C_s	1	-102.87330	-102.89892	0.00547	0.00525
BH_2PH_3	C_s	2	-368.58897	-368.61216	0.00542	0.00541
BH_3PH_3	C_{3v}	1	-369.23661	-369.25969	0.00565	0.00557
BH_2SH_2	C_s	2	-424.82515	-424.83979	0.00698	0.00686
BH_3SH_2	C_s	1	-425.47471	-425.48169	0.00657	0.00630
BH_2CO	C_{2v}	2	-139.11144	-139.13684	0.00473	0.00462
BH_3CO	C_{3v}	1	-139.73669	-139.76045	0.00508	0.00493
BH_2COH	C_s	1	-139.64708	-139.67048	0.00528	0.00500
BH_2CHO	C_s	1	-139.69483	-139.72013	0.00523	0.00538
BH_2OC	C_{2v}	2	-139.03573	-139.05168	0.00545	0.00514
BH_3OC	C_{3v}	1	-139.70374	-139.72506	0.00754	0.00668
BH_2OCH	C_s	1	-139.64784	-139.66299	0.00502	0.00546
BH_2OCH_2	C_1	2	-140.29401	-140.32278	0.00537	0.00547
BH_3OCH_2	C_s	1	-140.88347	-140.91223	0.00589	0.00565
BH_2OCH_3	C_s	1	-140.95150	-140.98178	0.00538	0.00536
BH_2NCH	C_s	2	-119.21832	-119.24398	0.00502	0.00491
BH_3NCH	C_{3v}	1	-119.83433	-119.85332	0.00543	0.00536
BH_2NCH_2	C_{2v}	1	-119.86778	-119.89399	0.00517	0.00500
BH_2CNH	C_s	2	-119.21424	-119.23856	0.00504	0.00497
BH_3CNH	C_{3v}	1	-119.83411	-119.85834	0.00549	0.00515

BH_2CNH_2	C_{2v}	1	-119.80878	-119.83586	0.00528	0.00501
BH_2CHNH	C_s	1	-119.82235	-119.84674	0.00509	0.00494
$BH_2O(CH_3)_2$	C_1	2		-180.67987		0.00755
$BH_3O(CH_3)_2$	C_s	1		-181.34638		0.00743
BH_2NCCH_3	C_s	2		-158.49385		0.00643
BH_3NCCH_3	C_{3v}	1		-159.11238		0.00703
$BH_2S(CH_3)_2$	C_1	2		-503.32159		0.00808
$BH_3S(CH_3)_2$	C_s	1		-503.97478		0.00817
$BH_2OC(CH_3)_2$	C_1	2		-218.81399		0.00822
$BH_3OC(CH_3)_2$	C_s	1		-219.41957		0.00841
$BH_2N(CH_3)_3$	C_s	2		-200.08546		0.00790
$BH_3N(CH_3)_3$	C_{3v}	1		-200.75000		0.00790
$BH_2P(CH_3)_3$	C_s	2		-486.36736		0.01001
$BH_3P(CH_3)_3$	C_{3v}	1		-487.01613		0.00995
$BH_2OS(CH_3)_2$	C_1	2		-578.43472		0.00877
$BH_3OS(CH_3)_2$	C_1	1		-579.09587		0.00881
BH_2-THF	C_1	2		-257.97436		0.00826
BH_3-THF	C_1	1		-258.64017		0.00822
BH_2-pyridine	C_{2v}	2		-273.85723		0.00698
BH_3-pyridine	C_s	1		-274.46831		0.00736

Notes: (a) Enthalpies at absolute zero, in Hartrees. (b) Increments in enthalpies on going from absolute zero to 298 K, in Hartrees. (c) These values are taken from Curtiss, L. A.; Raghavachari, K.; Trucks, G. W.; Pople, J. A. *J. Chem. Phys.* **1991**, *94*, 7221-7230 and are reproduced here only for the reader's convenience.

Table B. Atomic charges, QCISD/6-311+G**(6D).

	AIM		NPA	
Species	BH_n	X	BH_n	X
H_3N-BH_3	-0.103	+0.099	-0.356	+0.356
H_3N-BH_2	-0.058	+0.057	-0.320	+0.320
Change	+0.045	-0.042	+0.036	-0.036
H_2O-BH_3	-0.076	+0.082	-0.245	+0.245
H_2O-BH_2	-0.062	+0.057	-0.227	+0.227
Change	+0.014	-0.025	+0.018	-0.018
H_3P-BH_3	-0.139	+0.141	-0.616	+0.616
H_3P-BH_2	+0.089	-0.089	-0.499	+0.499
Change	+0.228	-0.230	+0.117	-0.117
OC-BH_3	+0.141	-0.142	-0.455	+0.455
OC-BH_2	+0.564	-0.565	-0.127	+0.127
Change	+0.423	-0.423	+0.328	-0.328
H_2CO-BH_3	-0.051	+0.056	-0.246	+0.246
H_2CO-BH_2	+0.753	-0.750	+0.370	-0.370
Change	+0.804	-0.806	+0.616	-0.616
HCN-BH_3	+0.020	-0.019	-0.309	+0.309
HCN-BH_2	+0.695	-0.695	+0.220	-0.220
Change	+0.675	-0.676	+0.529	-0.529
HNC-BH_3	+0.077	-0.077	-0.474	+0.474
HNC-BH_2	+0.593	-0.593	-0.048	+0.048
Change	+0.516	-0.516	+0.426	-0.426

Table C. Differences in atomic charges resulting from difference density geometry modifications (based on QCISD/6-311+G**(6D)//MP2/6-31G* NPA charges).

Complex	Species	Atoms		
H_3B-BH_3	BH_3	B: +0.036	H: -0.012	
	BH_3	B: +0.036	H: -0.012	
H_3B-BH_2	BH_2	B: -0.003	H: +0.001	
	BH_3	B: +0.022	H: -0.007	
H_3N-BH_3	BH_3	B: +0.032	H: -0.011	
	NH_3	N: +0.010	H: -0.003	
H_3N-BH_2	BH_2	B: -0.008	H: +0.004	
	NH_3	N: +0.008	H: -0.003[a]	
H_2O-BH_3	BH_3	B: +0.020	H: -0.007[a]	
	H_2O	O: +0.006	H: -0.003	
H_2O-BH_2	BH_2	B: -0.006	H: +0.003[a]	
	H_2O	O: +0.006	H: -0.003[a]	
H_3P-BH_3	BH_3	B: +0.028	H: -0.009	
	PH_3	P: +0.011	H: -0.004	
H_3P-BH_2	BH_2	B: -0.002	H: +0.001	
	PH_3	P: +0.012	H: -0.004[a]	
OC-BH_3	BH_3	B: +0.029	H: -0.010	
	CO	C: +0.001	O: -0.001	
OC-BH_2	BH_2	B: -0.003	H: +0.002	
	CO	C: -0.005	O: +0.005	
H_2CO-BH_3	BH_3	B: +0.021	H: -0.007[a]	
	H_2CO	O: +0.004	C: +0.012	H: -0.008[a]
H_2CO-BH_2	BH_2	B: -0.007	H: +0.003[a]	
	H_2CO	O: +0.003	C: +0.070	H: -0.037[a]
HCN-BH_3	BH_3	B: +0.028	H: -0.009	
	HCN	N: +0.001	C: -0.001	H: 0.000
HCN-BH_2	BH_2	B: -0.008	H: +0.004	
	HCN	N: -0.040	C: +0.047	H: -0.007
HNC-BH_3	BH_3	B: +0.034	H: -0.011	
	HNC	C: +0.005	N: -0.005	H: 0.000
HNC-BH_2	BH_2	B: -0.007	H: +0.004	
	HNC	C: -0.034	N: +0.021	H: +0.013

Notes: a. Average value for slightly different hydrogen atoms.

Table D. HOMO energies of Lewis bases (Hartrees).[a]

Lewis Base	HF[b]	HF/NBO[b,c]	QCISD/NBO[c,d]
H_3N	0.09852	-0.52359	-0.52187
H_2O[e]	0.14267	-0.71688	-0.71662
H_3P	0.06317	-0.55901	-0.56928
OC[f]	0.07838	-0.66950	-0.67398
CO[g]	0.07838	-1.04540	-1.05222
H_2CO[e]	0.06553	-0.72953	-0.73361
HCN	0.06008	-0.75520	-0.76160
HNC	0.06230	-0.60309	-0.60654

Notes:

a. All calculations were performed at the MP2/6-31G* optimized geometries.
b. Hartree-Fock calculations performed using the 6-311+G(3df,2p) basis set.
c. NBO implies orbitals were localized according to the NBO procedure of Weinhold.
d. QCISD calculations performed using the 6-311+G**(6D) basis set.
e. The average energy of the two lone pairs on oxygen was used for the localized (NBO) orbital energies.
f. Lone pair on the carbon end.
g. Lone pair on the oxygen end.

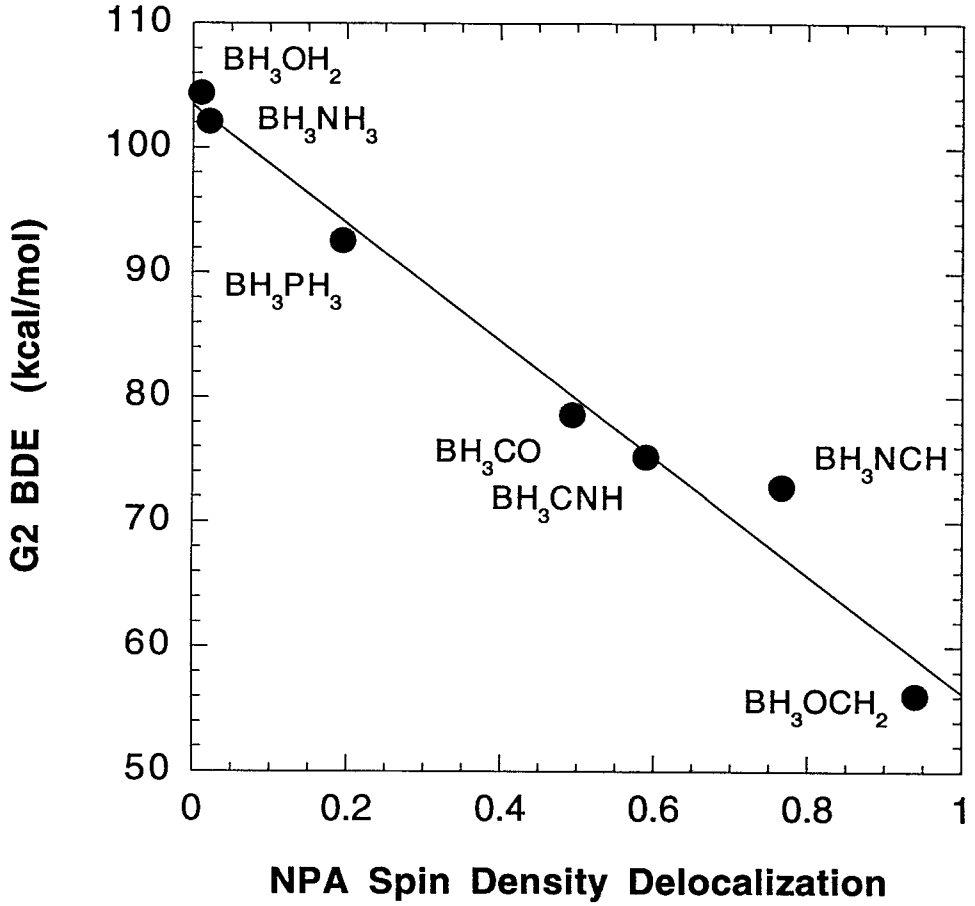

Figure A

Figure A. Plot of calculated B-H bond dissociation enthalpy versus spin density delocalization calculated via the NPA procedure. The enthalpies were calculated via the G2 procedure and correspond to absolute zero. The spin density populations were computed using QCISD/6-311+G**(6D) wave functions at the MP2/6-31G* optimized geometries. The spin density delocalization is defined here as the total quantity of α spin density on atoms other than the BH_2 fragment. Correlation coefficient = 0.97.

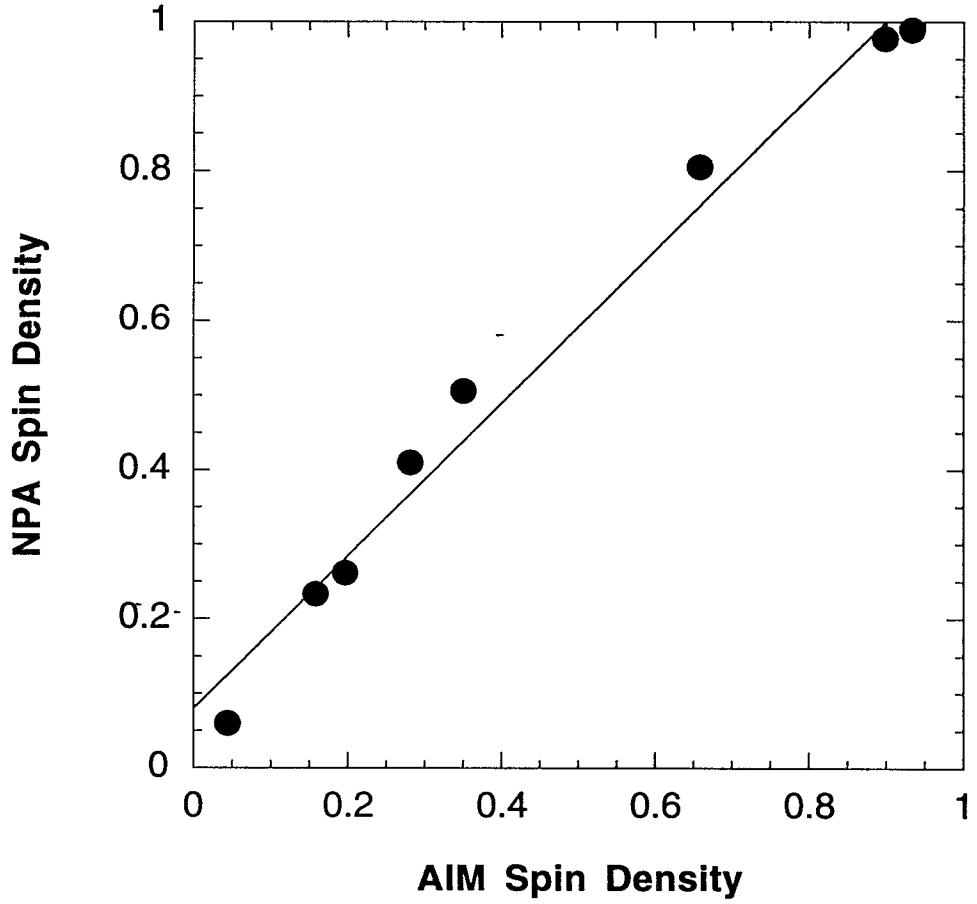

Figure B

Figure B. Plot of NPA spin density versus AIM spin density. The spin density populations are for the BH_2 fragments and were computed using QCISD/6-311+G**(6D) wave functions at the MP2/6-31G* optimized geometries. Best fit equation: NPA = 1.022 * AIM + 0.080; correlation coefficient = 0.98.

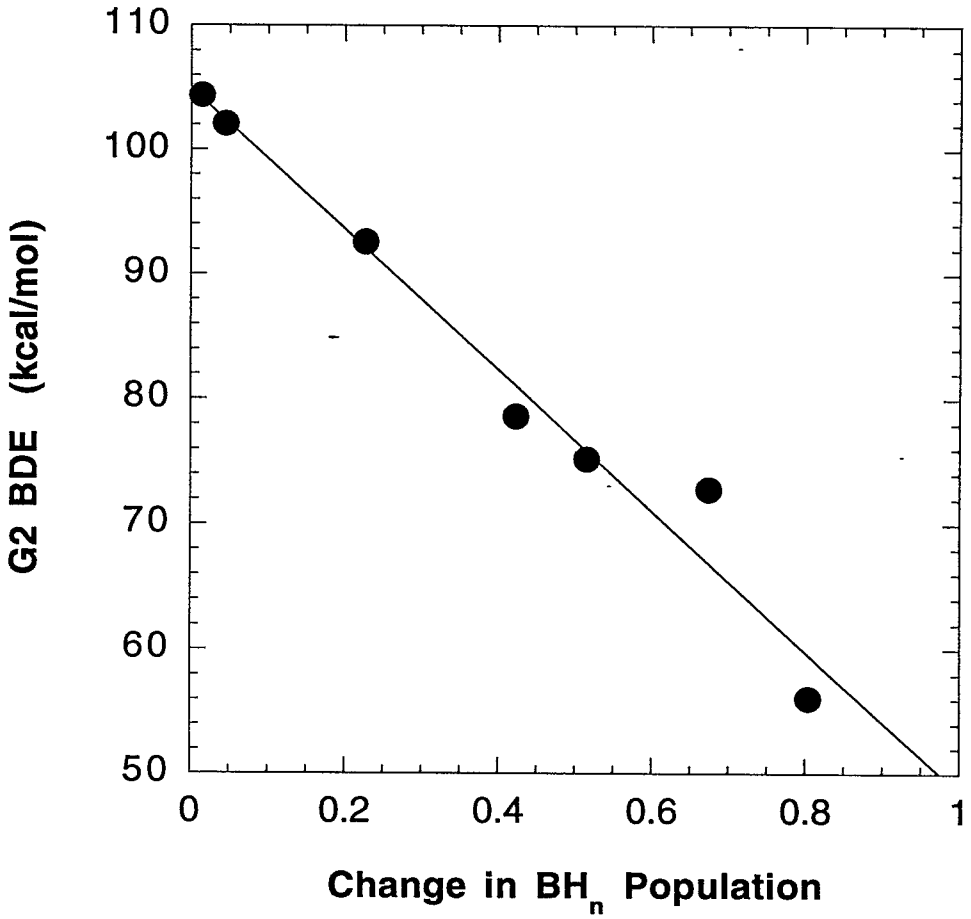

Figure C

Figure C. Plot of calculated B-H bond dissociation enthalpy versus change in BH_n population upon hydrogen abstraction. The enthalpies were calculated via the G2 procedure and correspond to absolute zero. The atomic populations were computed using the AIM procedure and QCISD/6-311+G**(6D) wave functions at the MP2/6-31G* optimized geometries. The population difference is defined here as the BH_3 population in the closed-shell complex minus the BH_2 population in the corresponding radical obtained by abstraction of a single hydrogen atom from boron. Correlation coefficient = 0.97.

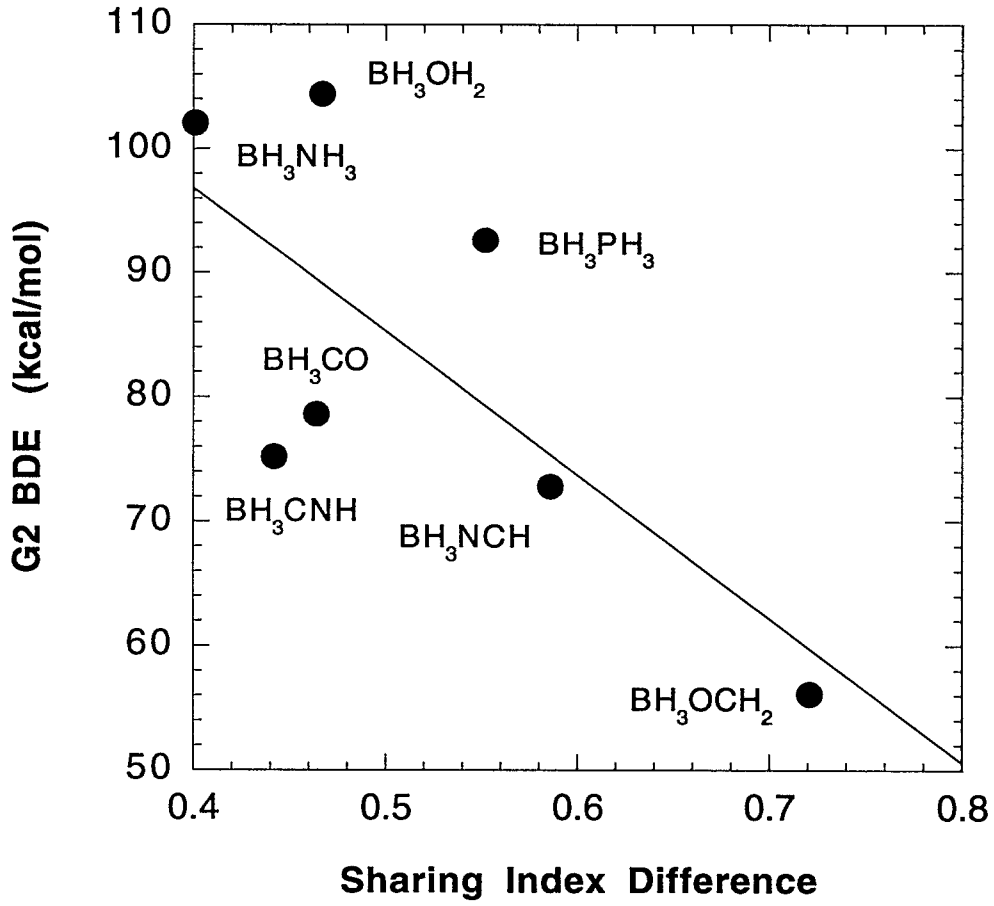

Figure D

Figure D. Plot of B-H bond dissociation enthalpy versus sharing index difference. The BDE's were calculated via the G2 procedure and correspond to absolute zero. The sharing indices were computed using QCISD/6-311+G**(6D) wave functions at the MP2/6-31G* optimized geometries. The sharing index difference is defined as the B-X sharing index in the closed-shell complex minus the B-X sharing index in the corresponding radical obtained by abstraction of a single hydrogen atom from boron. Correlation coefficient = 0.53.

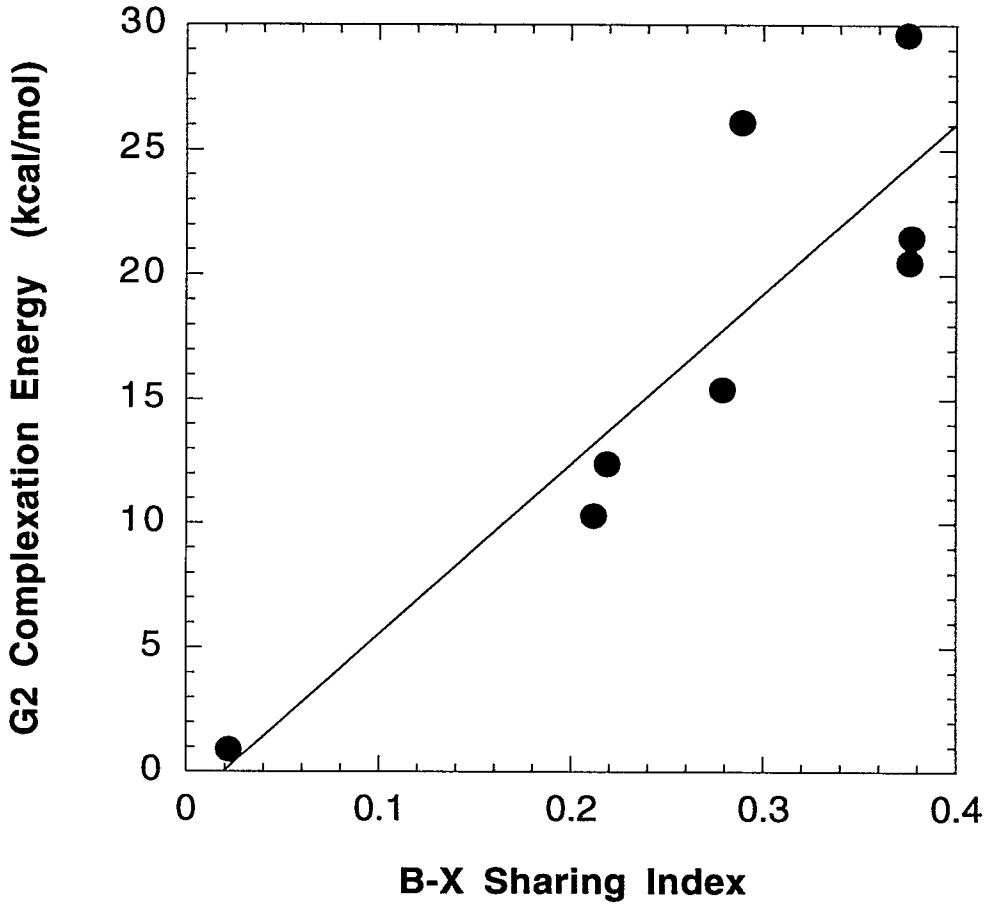

Figure E

Figure E. Plot of calculated complexation enthalpy of borane radical with various Lewis bases versus the calculated sharing index for the B-X bond. The enthalpies were calculated via the G2 procedure and correspond to absolute zero. The sharing indices were computed using QCISD/6-311+G**(6D) wave functions at the MP2/6-31G* optimized geometries. Correlation coefficient = 0.27.

MP2/6-31G* Optimized Geometries (G-2 calculations):

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 BH2 C2V G2 calculation
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Molecule:
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Stoichiometry    = BH2(2)
Charge           = 0
Multiplicity     = 2
Alpha Electrons  = 4
Alpha Valence    = 3
Beta Electrons   = 3
Beta Valence     = 2

Z-matrix: MP2
----------------------------------------------------------------

0  2
B
H        1        rbh
H        1        rbh      2        a

rbh = 1.188294
a = 127.651137
----------------------------------------------------------------
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 BH3 D3H G2 calculation
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Molecule:
---------
Stoichiometry    = BH3
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 4
Alpha Valence    = 3
Beta Electrons   = 4
Beta Valence     = 3

Z-matrix: MP2
----------------------------------------------------------------

0  1
B
H        1        rbh
H        1        rbh      2        a
H        1        rbh      2        a        3        t        0

rbh = 1.191189
a = 120.000000
t = 180.000000
----------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

```
-----------------------------------------------------
 Diborane radical (B2H5) C2V symmetry G2 calculation
-----------------------------------------------------

Molecule:
---------
Stoichiometry    = B2H5(2)
Charge           = 0
Multiplicity     = 2
Alpha Electrons  = 8
Alpha Valence    = 6
Beta Electrons   = 7
Beta Valence     = 5

Z-matrix: MP2
-----------------------------------------------------------------

0  2
X
H        1        1.
B        2        rbh1     1        a1
B        2        rbh1     1        a1       3        180.     0
X        3        1.       2        90.      1        0.       0
H        3        rbh2     2        a2       5        t1       0
H        3        rbh2     2        a2       5        -t1      0
X        4        1.       2        90.      1        0.       0
H        4        rbh2     2        a2       8        t1       0
H        4        rbh2     2        a2       8        -t1      0

rbh1 = 1.322885
rbh2 = 1.186729
t1 = 73.504535
a1 = 138.270464
a2 = 111.356457
-----------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------------------------------------
 Diborane (B2H6) D2H symmetry G-2 calculation
-----------------------------------------------

Molecule:
---------
Stoichiometry    = B2H6
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 8
Alpha Valence    = 6
Beta Electrons   = 8
Beta Valence     = 6

Z-matrix: MP2
-----------------------------------------------------------------

0  1
X
X        1        1.
B        1        rbx      2        90.
B        1        rbx      2        90.      3        180.     0
```

```
H         1         rhx       2         90.       3         90.       0
H         1         rhx       2         90.       3         -90.      0
H         3         rbh       1         a1        2         0.        0
H         3         rbh       1         a1        2         180.      0
H         4         rbh       1         a1        2         0.        0
H         4         rbh       1         a1        2         180.      0

rbh = 1.189461
rhx = 0.974465
rbx = 0.874705
a1 = 119.168539
-------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
----------------
 Ammonia C3V G2
----------------

Molecule:
---------
Stoichiometry    = H3N
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 5
Beta Electrons   = 5

Z-matrix:
-------------------------------------------------------------------------

0         1
N
H         1         r
H         1         r         2         a
H         1         r         2         a         3         a         1

r = 1.017028
a = 106.332730
-------------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
--------------
 Water C2V G2
--------------

Molecule:
---------
Stoichiometry    = H2O
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 5
Beta Electrons   = 5

Z-matrix:
-------------------------------------------------------------------------

0         1
O
H         1         r
H         1         r         2         a
```

```
r = 0.968580
a = 103.961947
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
------------------
 Phosphine C3V G2
------------------

Molecule:
---------
Stoichiometry    = H3P
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 9
Beta Electrons   = 9

Z-matrix:
--------------------------------------------------------------------------------

0        1
P
H        1         r
H        1         r         2         a
H        1         r         2         a         3         a         1

r = 1.414610
a = 94.645437
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
------------
 H2S C2V G2
------------

Molecule:
---------
Stoichiometry    = H2S
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 9
Beta Electrons   = 9

Z-matrix:
--------------------------------------------------------------------------------

0        1
S
H        1         r
H        1         r         2         a

r = 1.339462
a = 93.332139
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
------------------------
 Carbon monoxide C*V G2
------------------------

Molecule:
```

```
---------
Stoichiometry    = CO
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 7
Beta Electrons   = 7

Z-matrix:
--------------------------------------------------------------------------

0        1
C
O        1         r

r = 1.150245
--------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
----------------------
 Formaldehyde C2V G2
----------------------

Molecule:
---------
Stoichiometry    = CH2O
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 8
Beta Electrons   = 8

Z-matrix:
--------------------------------------------------------------------------

0        1
C
O        1         r1
H        1         r2        2         a1
H        1         r2        2         a1        3         180.      0

r1 = 1.219903
r2 = 1.104127
a1 = 122.193159
--------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
---------------------------------
 Hydrogen cyanide C*V MP2/6-31G*
---------------------------------

Molecule:
---------
Stoichiometry    = CHN
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 7
Beta Electrons   = 7

Z-matrix:
--------------------------------------------------------------------------
```

```
0        1
N
C        1         r1
X        2         1.        1         90.
H        2         r2        3         90.       1         180.      0

r1 = 1.177281
r2 = 1.069333
-------------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
------------------------
 HNC C*V MP2/6-31G* G2
------------------------

Molecule:
---------
Stoichiometry    = CHN
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 7
Beta Electrons   = 7

Z-matrix:
-------------------------------------------------------------------------

0        1
C
N        1         r1
X        2         1.        1         90.
H        2         r2        3         90.       1         180.      0

r1 = 1.186701
r2 = 1.002240
-------------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
------------------------------------------------------
 Aminoborane radical complex (BH2NH3) Cs G-2 calculation
------------------------------------------------------

Molecule:
---------
Stoichiometry    = BH5N(2)
Charge           = 0
Multiplicity     = 2
Alpha Electrons  = 9
Alpha Valence    = 7
Beta Electrons   = 8
Beta Valence     = 6

Z-matrix: MP2
-----------------------------------------------------------------

0  2
B
N        1        rbn
X        1        1.       2        90.
H        1        rbh      2        a1       3        t1       0
H        1        rbh      2        a1       3        -t1      0
```

```
H         2         rnh1      1         a2        3         t2        0
H         2         rnh2      1         a3        6         t3        0
H         2         rnh2      1         a3        6         -t3       0

rbh = 1.199728
rnh1 = 1.024204
rnh2 = 1.019853
rbn = 1.636639
t1 = 113.020002
t3 = 120.499437
a1 = 108.465339
a2 = 113.155903
a3 = 110.481636
t2 = 180.000000
--------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
------------------------------------------------
 Aminoborane complex (BH3NH3) C3V G-2 calculation
------------------------------------------------

Molecule:
---------
Stoichiometry    = BH6N
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 9
Alpha Valence    = 7
Beta Electrons   = 9
Beta Valence     = 7

Z-matrix: MP2
--------------------------------------------------------------------

0  1
B
N         1         rbn
H         1         rbh       2         a1
H         1         rbh       2         a1        3         t1        0
H         1         rbh       2         a1        3         -t1       0
H         2         rnh       1         a2        3         t2        0
H         2         rnh       1         a2        6         t1        0
H         2         rnh       1         a2        6         -t1       0

rbh = 1.209193
rbn = 1.660439
rnh = 1.019768
a1 = 104.600963
a2 = 111.060612
t1 = 120.000000
t2 = 180.000000
--------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-------------------------------------------
 Water-borane complex radical (BH2OH2) C1 G2
-------------------------------------------

Molecule:
---------
```

```
Stoichiometry    = BH4O(2)
Charge           = 0
Multiplicity     = 2
Alpha Electrons  = 9
Beta Electrons   = 8

Z-matrix:
--------------------------------------------------------------------------

0        2
B
O        1         rbo
H        1         rbh1      2         a1
H        1         rbh2      2         a2        3         t1        0
H        2         roh1      1         a3        3         t2        0
H        2         roh2      1         a4        4         t3        0

rbo = 1.702294
rbh1 = 1.199704
rbh2 = 1.193567
roh1 = 0.974935
roh2 = 0.976919
a1 = 105.273008
a2 = 103.815783
a3 = 106.697139
a4 = 109.290769
t1 = 130.527573
t2 = 52.739149
t3 = -291.431322
--------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-------------------------
 Water-borane complex G2
-------------------------

Molecule:
---------
Stoichiometry    = BH5O
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 9
Beta Electrons   = 9

Z-matrix:
--------------------------------------------------------------------------

0        1
B
O        1         rbo
H        1         rbh1      2         a1
H        1         rbh2      2         a2        3         t1        0
H        1         rbh2      2         a2        3         -t1       0
H        2         roh       1         a3        3         t2        0
H        2         roh       1         a3        3         -t2       0

rbo = 1.729126
rbh1 = 1.207190
rbh2 = 1.200851
```

```
roh = 0.974797
a1 = 102.698909
a2 = 101.124266
a3 = 107.175455
t1 = 119.922892
t2 = 56.779612
--------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------------------------------------------
 PH3-Borane radical complex (BH2PH3) Cs G-2 calculation
-----------------------------------------------------

Molecule:
---------
Stoichiometry    = BH5P(2)
Charge           = 0
Multiplicity     = 2
Alpha Electrons  = 13
Alpha Valence    = 7
Beta Electrons   = 12
Beta Valence     = 6

Z-matrix: MP2
-----------------------------------------------------------------

0  2
B
P         1         rbp
X         1         1.        2         90.
H         1         rbh       2         a1        3         t1        0
H         1         rbh       2         a1        3         -t1       0
H         2         rph1      1         a2        3         180.      0
H         2         rph2      1         a3        6         t3        0
H         2         rph2      1         a3        6         -t3       0

rbp = 1.860631
rbh = 1.189449
rph1 = 1.425028
rph2 = 1.404788
a1 = 115.990033
a2 = 124.957454
a3 = 114.875221
t1 = 96.401992
t3 = 120.867553
--------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------------------------------------
 PH3-Borane complex (BH3PH3) C3V G-2 calculation
-----------------------------------------------

Molecule:
---------
Stoichiometry    = BH6P
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 13
Alpha Valence    = 7
Beta Electrons   = 13
```

```
Beta Valence      = 7

Z-matrix: MP2
-----------------------------------------------------------------

0  1
B
P         1         rbp
H         1         rbh       2         a1
H         1         rbh       2         a1        3         120.      0
H         1         rbh       2         a1        3         -120.     0
H         2         rph       1         a2        3         180.      0
H         2         rph       1         a2        6         120.      0
H         2         rph       1         a2        6         -120.     0

rbp = 1.943458
rbh = 1.206313
rph = 1.403799
a1 = 103.919108
a2 = 117.723637
-----------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------------------------------------------
 H2S-Borane complex radical (BH2-SH2) Cs MP2/6-31G* fopt
-----------------------------------------------------

Molecule:
---------
Stoichiometry     = BH4S(2)
Charge            = 0
Multiplicity      = 2
Alpha Electrons   = 13
Beta Electrons    = 12

Z-matrix:
-----------------------------------------------------------------------

0         2
B
S         1          rbs
H         1          rbh1      2          a1
H         1          rbh2      2          a2        3         180.      0
H         2          rsh1      1          a3        3         0.        0
H         2          rsh2      1          a4        3         180.      0

rbs = 1.771663
rbh1 = 1.189049
rbh2 = 1.189240
rsh1 = 4.213782
rsh2 = 1.341380
a1 = 116.325009
a2 = 121.178907
a3 = 175.404365
a4 = 99.230979
-----------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-------------------------
 H2S-Borane complex Cs G2
```

```
-------------------------

Molecule:
---------
Stoichiometry    = BH5S
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 13
Beta Electrons   = 13

Z-matrix:
-------------------------------------------------------------------

0        1
B
S        1         rbc
H        1         rbh1      2         a1
H        1         rbh2      2         a2        3         t1        0
H        1         rbh2      2         a2        3         -t1       0
H        2         rsh       1         a3        3         t2        0
H        2         rsh       1         a3        3         -t2       0

rbc = 2.565319
rbh1 = 1.191423
rbh2 = 1.191076
rsh = 1.325632
a1 = 95.643804
a2 = 94.500289
a3 = 100.614505
t1 = 120.069061
t2 = 48.439348
-------------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------------------------------------------
 CO-Borane radical complex (BH2CO) C2V G-2 calculation
-----------------------------------------------------

Molecule:
---------
Stoichiometry    = CH2BO(2)
Charge           = 0
Multiplicity     = 2
Alpha Electrons  = 11
Alpha Valence    = 8
Beta Electrons   = 10
Beta Valence     = 7

Z-matrix: MP2
-------------------------------------------------------------------

0  2
B
C        1        rbc
H        1        rbh       2        a1
H        1        rbh       2        a1        3        180.      0
O        1        rbo       3        a1        2        0.        0

rbc = 1.481726
```

```
rbh = 1.187798
rbo = 2.647800
a1 = 116.890727
-------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------------------------------------
 CO-Borane complex (BH3CO) C3V G-2 calculation
-----------------------------------------------

Molecule:
---------
Stoichiometry    = CH3BO
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 11
Alpha Valence    = 8
Beta Electrons   = 11
Beta Valence     = 8

Z-matrix: MP2
-------------------------------------------------------------------

0  2
B
C        1        rbc
H        1        rbh      2        a1
H        1        rbh      2        a1       3        120.     0
H        1        rbh      2        a1       3        -120.    0
O        1        rbo      3        a1       2        0.       0

rbc = 1.546843
rbh = 1.205734
rbo = 2.694923
a1 = 104.138721
-------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
----------------
 BH2-C=OH Cs G2
----------------

Molecule:
---------
Stoichiometry    = CH3BO
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 11
Beta Electrons   = 11

Z-matrix:
-------------------------------------------------------------------

0        1
B
C        1        r1
X        2        1.       1        90.
O        2        r2       3        a1       1        180.     0
H        1        r3       2        a2       3        t1       0
H        1        r3       2        a2       3        -t1      0
```

```
H        4          r4         2          a3         3          0.         0

r1 = 1.394057
r2 = 1.275671
r3 = 1.192757
r4 = 0.985796
a1 = 93.734817
a2 = 117.530379
a3 = 111.381199
t1 = 89.257564
-------------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
------------------------------
 BH2-CH=O Cs perpendicular G2
------------------------------

Molecule:
---------
Stoichiometry    = CH3BO
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 11
Beta Electrons   = 11

Z-matrix:
-------------------------------------------------------------------------

0        1
B
C        1          r1
O        2          r2         1          a1
H        1          r3         2          a2         3          t1         0
H        1          r3         2          a2         3          -t1        0
H        2          r4         1          a3         3          180.       0

r1 = 1.590782
r2 = 1.197294
r3 = 1.186478
r4 = 1.100159
a1 = 120.196452
a2 = 119.683100
a3 = 120.373651
t1 = 89.695519
-------------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------------------------------
 OC-Borane complex radical (BH2-OC) C2V G2
-----------------------------------------

Molecule:
---------
Stoichiometry    = CH2BO(2)
Charge           = 0
Multiplicity     = 2
Alpha Electrons  = 11
Beta Electrons   = 10

Z-matrix:
```

```
---------------------------------------------------------------------

0        2
B
O        1         rbo
H        1         rbh       2         a1
H        1         rbh       2         a1        3         180.      0
C        1         rbc       3         a1        2         0.        0

rbo = 1.375479
rbh = 1.185511
rbc = 2.617132
a1 = 116.156416
---------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
----------------------------------
 OC-Borane complex (BH3CO) C3V G2
----------------------------------

Molecule:
---------
Stoichiometry    = CH3BO
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 11
Beta Electrons   = 11

Z-matrix:
---------------------------------------------------------------------

0        1
B
O        1         rbo
H        1         rbh       2         a1
H        1         rbh       2         a1        3         120.      0
H        1         rbh       2         a1        3         -120.     0
C        1         rbc       3         a1        2         0.        0

rbo = 2.585920
rbh = 1.191044
rbc = 3.736529
a1 = 90.969066
---------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
---------------------------
 BH2OCH Cs MP2/6-31G* fopt
---------------------------

Molecule:
---------
Stoichiometry    = CH3BO
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 11
Beta Electrons   = 11

Z-matrix:
---------------------------------------------------------------------
```

```
0        1
B
O        1         r1
C        2         r2        1         a1
H        1         r3        2         a2        3         180.      0
H        1         r4        2         a3        3         0.        0
H        3         r5        2         a4        1         180.      0

r1 = 1.406247
r2 = 1.347838
r3 = 1.188961
r4 = 1.186419
r5 = 1.115765
a1 = 115.954123
a2 = 114.937687
a3 = 119.842903
a4 = 101.749729
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
------------------------------------------
 H2CO-Borane radical complex (BH2OCH2) C1 G2
------------------------------------------

Molecule:
---------
Stoichiometry    = CH4BO(2)
Charge           = 0
Multiplicity     = 2
Alpha Electrons  = 12
Beta Electrons   = 11

Z-matrix:
--------------------------------------------------------------------------------

0        2
B
O        1         rbo
H        1         rbh1      2         a1
H        1         rbh2      2         a2        3         t1        0
C        2         rco       1         a3        3         t2        0
H        5         rch1      2         a4        1         t3        0
H        5         rch2      2         a5        6         t4        0

rbo = 1.361330
rbh1 = 1.197174
rbh2 = 1.190434
rco = 1.373948
rch1 = 1.082467
rch2 = 1.079019
a1 = 120.209208
a2 = 116.251945
a3 = 121.942861
a4 = 117.876713
a5 = 114.213709
t1 = 180.288919
t2 = -2.257247
t3 = 10.757934
```

```
t4 = 154.954996
-------------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------------------------
 H2CO-Borane complex (BH3OCH2) Cs G2
-----------------------------------

Molecule:
---------
Stoichiometry    = CH5BO
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 12
Beta Electrons   = 12

Z-matrix:
-------------------------------------------------------------------------

0        1
B
O        1         rbo
H        1         rbh1      2         a1
H        1         rbh2      2         a2        3         t1        0
H        1         rbh2      2         a2        3         -t1       0
C        2         rco       1         a3        3         0.        0
H        6         rch1      2         a4        1         0.        0
H        6         rch2      2         a5        7         180.      0

rbo = 1.686060
rbh1 = 1.208547
rbh2 = 1.201164
rco = 1.233081
rch1 = 1.092875
rch2 = 1.091981
a1 = 102.766828
a2 = 101.256954
a3 = 120.533239
a4 = 120.851363
a5 = 118.829924
t1 = 120.333538
-------------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------
 BH2-O-CH3 Cs G2
-----------------

Molecule:
---------
Stoichiometry    = CH5BO
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 12
Beta Electrons   = 12

Z-matrix:
-------------------------------------------------------------------------

0        1
```

```
B
O         1         r1
C         2         r2         1         a1
H         1         r3         2         a2         3         0.         0
H         1         r4         2         a3         3         180.       0
H         3         r5         2         a4         1         0.         0
H         3         r6         2         a5         6         t1         0
H         3         r6         2         a5         6         -t1        0

r1 = 1.349328
r2 = 1.430177
r3 = 1.200052
r4 = 1.192901
r5 = 1.092744
r6 = 1.091139
a1 = 121.373824
a2 = 120.804315
a3 = 116.462314
a4 = 111.205616
a5 = 108.308888
t1 = 120.853995
--------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
------------------------------------------------------
 HCN-borane radical complex (BH2NCH) Cs MP2/6-31G* fopt
------------------------------------------------------

Molecule:
---------
Stoichiometry    = CH3BN(2)
Charge           = 0
Multiplicity     = 2
Alpha Electrons  = 11
Beta Electrons   = 10

Z-matrix:
--------------------------------------------------------------------------

0         2
B
N         1         r1
C         2         r2         1         a1
H         1         r3         2         a2         3         t1         0
H         1         r3         2         a2         3         -t1        0
H         3         r4         2         a3         1         180.       0

r1 = 1.402691
r2 = 1.194101
r3 = 1.191373
r4 = 1.096865
a1 = 173.674751
a2 = 118.288569
a3 = 131.041125
t1 = 90.496568
--------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------------------------
 HCN-borane complex (BH3NCH) C3V G2
```

```
-----------------------------------

Molecule:
---------
Stoichiometry    = CH4BN
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 11
Beta Electrons   = 11

Z-matrix:
--------------------------------------------------------------------------

0        1
B
N        1         rbn
H        1         rbh       2         a1
H        1         rbh       2         a1        3         120.      0
H        1         rbh       2         a1        3         -120.     0
C        1         r3        3         a1        2         0.        0
H        1         r4        3         a1        2         0.        0

rbn = 1.587458
rbh = 1.205276
r3 = 2.752305
r4 = 3.821607
a1 = 103.841613
--------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
------------------
 BH2-N=CH2 C2V G2
------------------

Molecule:
---------
Stoichiometry    = CH4BN
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 11
Beta Electrons   = 11

Z-matrix:
--------------------------------------------------------------------------

0        1
B
N        1         r1
X        2         1.        1         90.
C        2         r2        3         90.       1         180.      0
H        1         r3        2         a1        3         0.        0
H        1         r3        2         a1        3         180.      0
H        4         r4        2         a2        3         90.       0
H        4         r4        2         a2        3         -90.      0

r1 = 1.363306
r2 = 1.256382
r3 = 1.193875
r4 = 1.093109
```

```
a1 = 118.445843
a2 = 121.544017
--------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
--------------------------------------------------------
 HNC-borane radical complex (BH2CNH) Cs MP2/6-31G* fopt
--------------------------------------------------------

Molecule:
---------
Stoichiometry     = CH3BN(2)
Charge            = 0
Multiplicity      = 2
Alpha Electrons   = 11
Beta Electrons    = 10

Z-matrix:
--------------------------------------------------------------------------

0         2
B
C         1          r1
N         2          r2         1          a1
H         1          r3         2          a2         3          t1         0
H         1          r3         2          a2         3          -t1        0
H         3          r4         2          a3         1          180.       0

r1 = 1.479150
r2 = 1.210232
r3 = 1.191248
r4 = 1.017850
a1 = 174.172882
a2 = 118.134240
a3 = 132.026488
t1 = 90.486908
--------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------------------------
 HNC-borane complex (BH3CNH) C3V G2
-----------------------------------

Molecule:
---------
Stoichiometry     = CH4BN
Charge            = 0
Multiplicity      = 1
Alpha Electrons   = 11
Beta Electrons    = 11

Z-matrix:
--------------------------------------------------------------------------

0         1
B
C         1          rbc
H         1          rbh        2          a1
H         1          rbh        2          a1         3          120.       0
H         1          rbh        2          a1         3          -120.      0
```

```
N         1         r3        3         a1        2         0.        0
H         1         r4        3         a1        2         0.        0

rbc = 1.559977
rbh = 1.208515
r3 = 2.731762
r4 = 3.733346
a1 = 105.264468
-------------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
------------------
 BH2-C=NH2 C2V G2
------------------

Molecule:
---------
Stoichiometry    = CH4BN
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 11
Beta Electrons   = 11

Z-matrix:
-------------------------------------------------------------------------

0         1
B
C         1         r1
X         2         1.        1         90.
N         2         r2        3         90.       1         180.      0
H         1         r3        2         a1        3         0.        0
H         1         r3        2         a1        3         180.      0
H         4         r4        2         a2        3         90.       0
H         4         r4        2         a2        3         -90.      0

r1 = 1.406795
r2 = 1.280770
r3 = 1.194755
r4 = 1.020366
a1 = 118.571237
a2 = 122.719371
-------------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-------------------
 BH2-CH=NH Z Cs G2
-------------------

Molecule:
---------
Stoichiometry    = CH4BN
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 11
Beta Electrons   = 11

Z-matrix:
-------------------------------------------------------------------------
```

```
0         1
B
C         1         r1
N         2         r2        1         a1
H         1         r3        2         a2        3         0.        0
H         1         r4        2         a3        4         180.      0
H         2         r5        1         a4        3         180.      0
H         3         r6        2         a5        1         0.        0

r1 = 1.578997
r2 = 1.264137
r3 = 1.190826
r4 = 1.188045
r5 = 1.083451
r6 = 1.008108
a1 = 124.176655
a2 = 118.716346
a3 = 121.437692
a4 = 120.361189
a5 = 111.049915
--------------------------------------------------------------------------
```

HF/3-21G* Optimized Geometries (CBS-4 calculations):

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
----------------------------------------
 Borane radical (BH2) C2V HF/3-21G* fopt
----------------------------------------

Molecule:
---------
Stoichiometry    = BH2(2)
Charge           = 0
Multiplicity     = 2
Alpha Electrons  = 4
Beta Electrons   = 3

Z-matrix:
--------------------------------------------------------------------------

0        2
B
H        1         r
H        1         r         2         a

r = 1.185003
a = 127.640240
--------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
---------------------------
 Borane D3H HF/3-21G* fopt
---------------------------

Molecule:
---------
Stoichiometry    = BH3
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 4
Beta Electrons   = 4

Z-matrix:
--------------------------------------------------------------------------

0        1
B
H        1         r
H        1         r         2         120.
H        1         r         2         120.      3         180.      0

r = 1.187676
--------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-------------------------------------------
 Diborane radical (B2H5) C2V HF/3-21G* fopt
-------------------------------------------

Molecule:
---------
```

```
Stoichiometry    = B2H5(2)
Charge           = 0
Multiplicity     = 2
Alpha Electrons  = 8
Beta Electrons   = 7

Z-matrix:
-----------------------------------------------------------------------

0        2
X
H        1          1.
B        2          rbh1      1          a1
B        2          rbh1      1          a1         3          180.       0
X        3          1.        2          90.        1          0.         0
H        3          rbh2      2          a2         5          t1         0
H        3          rbh2      2          a2         5          -t1        0
X        4          1.        2          90.        1          0.         0
H        4          rbh2      2          a2         8          t1         0
H        4          rbh2      2          a2         8          -t1        0

rbh1 = 1.324365
rbh2 = 1.180405
a1 = 137.352814
a2 = 111.488847
t1 = 73.849028
-----------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------------------------
 Diborane (B2H6) D2H HF/3-21G* fopt
-----------------------------------

Molecule:
---------
Stoichiometry    = B2H6
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 8
Beta Electrons   = 8

Z-matrix:
-----------------------------------------------------------------------

0        1
X
X        1          1.
B        1          rbx       2          90.
B        1          rbx       2          90.        3          180.       0
H        1          rhx       2          90.        3          90.        0
H        1          rhx       2          90.        3          -90.       0
H        3          rbh       1          a1         2          0.         0
H        3          rbh       1          a1         2          180.       0
H        4          rbh       1          a1         2          0.         0
H        4          rbh       1          a1         2          180.       0

rbx = 0.892423
rhx = 0.965080
rbh = 1.182257
```

```
a1 = 118.832591
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
------------------
 Ammonia C3V CBS-4
------------------

Molecule:
---------
Stoichiometry    = H3N
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 5
Beta Electrons   = 5

Z-matrix:
--------------------------------------------------------------------------------

0        1
N
H        1         r
H        1         r         2         a
H        1         r         2         a         3         a         1

r = 1.002587
a = 112.396114
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------
 Water C2V CBS-4
-----------------

Molecule:
---------
Stoichiometry    = H2O
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 5
Beta Electrons   = 5

Z-matrix:
--------------------------------------------------------------------------------

0        1
O
H        1         r
H        1         r         2         a

r = 0.966599
a = 107.691109
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
---------------------
 Phosphine C3V CBS-4
---------------------

Molecule:
---------
```

```
Stoichiometry    = H3P
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 9
Beta Electrons   = 9

Z-matrix:
--------------------------------------------------------------------------

0        1
P
H        1         r
H        1         r         2         a
H        1         r         2         a         3         a         1

r = 1.402456
a = 95.051350
--------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
---------------
 H2S C2V CBS-4
---------------

Molecule:
---------
Stoichiometry    = H2S
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 9
Beta Electrons   = 9

Z-matrix:
--------------------------------------------------------------------------

0        1
S
H        1         r
H        1         r         2         a

r = 1.326863
a = 94.202796
--------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
---------------------------
 Carbon monoxide C*V CBS-4
---------------------------

Molecule:
---------
Stoichiometry    = CO
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 7
Beta Electrons   = 7

Z-matrix:
--------------------------------------------------------------------------
```