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J4653-1

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

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
---------------------------------
 BH singlet state G2 calculation
---------------------------------

Molecule:
---------
Stoichiometry     = BH
Charge            = 0
Multiplicity      = 1
Alpha Electrons   = 3
Alpha Valence     = 2
Beta Electrons    = 3
Beta Valence      = 2

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

0  1
B
H        1        rbh

rbh = 1.233139
-----------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
---------------------------------
 BH triplet state G2 calculation
---------------------------------

Molecule:
---------
Stoichiometry     = BH(3)
Charge            = 0
Multiplicity      = 3
Alpha Electrons   = 4
Alpha Valence     = 3
Beta Electrons    = 2
Beta Valence      = 1

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

0  3
B
H        1        rbh

rbh = 1.186627
-----------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
------------------------
 BH2 C2V G2 calculation
------------------------

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
-----------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
------------------------
 BH3 D3H G2 calculation
------------------------

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
```

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```
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 CBS-4 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
```

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```
a1 = 119.168539
-------------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
--------------------
 BF G2 calculation
--------------------

Molecule:
---------
Stoichiometry    = BF
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 7
Alpha Valence    = 5
Beta Electrons   = 7
Beta Valence     = 5

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

0  1
B
F        1        rbf

rbf = 1.278689
-------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------------------------
 BF triplet state CBS-4 calculation
-----------------------------------

Molecule:
---------
Stoichiometry    = BF(3)
Charge           = 0
Multiplicity     = 3
Alpha Electrons  = 8
Alpha Valence    = 6
Beta Electrons   = 6
Beta Valence     = 4

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

0  3
B
F        1        rbf

rbf = 1.328698
-------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 Difluoroborane radical (BF2) C2V G2 calculation
-------------------------------------------------

Molecule:
---------
Stoichiometry    = BF2(2)
Charge           = 0
```

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```
Multiplicity     = 2
Alpha Electrons  = 12
Alpha Valence    = 9
Beta Electrons   = 11
Beta Valence     = 8

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

0  2
B
F         1         rbf
F         1         rbf       2         a

rbf = 1.319517
a = 121.103022
-----------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
----------------------------------------
 Trifluoroborane (BF3) D3H G2 calculation
----------------------------------------

Molecule:
---------
Stoichiometry    = BF3
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 16
Alpha Valence    = 12
Beta Electrons   = 16
Beta Valence     = 12

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

0  1
B
F         1         rbf
F         1         rbf       2         a
F         1         rbf       2         a         3         t         0

rbf = 1.321760
t = 180.000000
a = 120.000000
-----------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
----------------------------------------
 BHF radical Cs symmetry G-2 calculation
----------------------------------------

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

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```
Beta Valence     = 5

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

0  2
B
F         1         rbf
H         1         rbh       2         a

rbf = 1.316126
rbh = 1.199870
a = 121.233218
-----------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
----------------------------------------
 Fluoroborane (BH2F) C2V G-2 calculation
----------------------------------------

Molecule:
---------
Stoichiometry    = BFH2
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 8
Alpha Valence    = 6
Beta Electrons   = 8
Beta Valence     = 6

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

0  1
B
F         1         rbf
H         1         rbh       2         a
H         1         rbh       2         a         3         180.      0

rbf = 1.329794
rbh = 1.191995
a = 117.967387
-----------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
----------------------------------------
 Difluoroborane (BF2H) C2V G-2 calculation
----------------------------------------

Molecule:
---------
Stoichiometry    = BF2H
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 12
Alpha Valence    = 9
Beta Electrons   = 12
Beta Valence     = 9

Z-matrix: MP2
```

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

0  1
B
H         1         rbh
F         1         rbf       2         a
F         1         rbf       2         a         3         180.      0

rbh = 1.185753
rbf = 1.324278
a = 120.783318
---------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------------------------
 Methyl radical D3H G2 calculation
-----------------------------------

Molecule:
---------
Stoichiometry     = CH3(2)
Charge            = 0
Multiplicity      = 2
Alpha Electrons   = 5
Alpha Valence     = 4
Beta Electrons    = 4
Beta Valence      = 3

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

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

r = 1.078411
---------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------------------------
 Ethane radical Cs G2 calculation
-----------------------------------

Molecule:
---------
Stoichiometry     = C2H5(2)
Charge            = 0
Multiplicity      = 2
Alpha Electrons   = 9
Alpha Valence     = 7
Beta Electrons    = 8
Beta Valence      = 6

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

0  2
C
```

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```
C       1       rcc
H       1       rch1    2       a1
H       1       rch2    2       a2      3       t1      0
H       1       rch2    2       a2      3       -t1     0
H       2       rch3    1       a3      3       t2      0
H       2       rch3    1       a3      3       -t2     0

rcc = 1.489059
rch1 = 1.099468
rch2 = 1.093104
rch3 = 1.081942
a1 = 111.900218
a2 = 111.385311
a3 = 120.665542
t1 = 119.621031
t2 = 82.977567
-------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
---------------------------
 Ethane D3D G2 calculation
---------------------------

Molecule:
---------
Stoichiometry    = C2H6
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 9
Alpha Valence    = 7
Beta Electrons   = 9
Beta Valence     = 7

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

0  1
C
C       1       rcc
H       1       rch     2       a
H       1       rch     2       a       3       120.    0
H       1       rch     2       a       3       -120.   0
H       2       rch     1       a       3       180.    0
H       2       rch     1       a       6       120.    0
H       2       rch     1       a       6       -120.   0

rcc = 1.524296
rch = 1.092896
a = 111.199178
-------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-------------------------------------------------------------------
 Methylborane "borene" singlet state (CH3B) Cs symmetric G2 calculation
-------------------------------------------------------------------

Molecule:
---------
Stoichiometry    = CH3B
Charge           = 0
```

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```
Multiplicity     = 1
Alpha Electrons  = 7
Alpha Valence    = 5
Beta Electrons   = 7
Beta Valence     = 5

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

0  1
C
B         1         rbc
H         1         rch1      2         a1
H         1         rch2      2         a2        3         t1        0
H         1         rch2      2         a2        3         -t1       0

rbc = 1.551768
t1 = 119.994394
rch1 = 1.096889
rch2 = 1.096859
a1 = 110.305965
a2 = 110.326713
-----------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------------------------------------------------------
 Methylborane "borene" triplet state (CH3B) Cs symmetric G2 calculation
-----------------------------------------------------------------

Molecule:
---------
Stoichiometry    = CH3B(3)
Charge           = 0
Multiplicity     = 3
Alpha Electrons  = 8
Alpha Valence    = 6
Beta Electrons   = 6
Beta Valence     = 4

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

0  3
C
B         1         rbc
H         1         rch1      2         a1
H         1         rch2      2         a2        3         t1        0
H         1         rch2      2         a2        3         -t1       0

rbc = 1.556370
t1 = 115.966516
rch1 = 1.100403
rch2 = 1.093440
a1 = 103.627324
a2 = 114.451588
-----------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------------------------------------------------
 Methylborane radical (CH3BH) Cs symmetric G-2 calculation
```

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Molecule:

Stoichiometry = CH4B(2)
Charge = 0
Multiplicity = 2
Alpha Electrons = 8
Alpha Valence = 6
Beta Electrons = 7
Beta Valence = 5

Z-matrix: MP2
---

0 2
B
C 1 rbc
H 1 rbh 2 a1
H 2 rch1 1 a2 3 180. 0
H 2 rch2 1 a3 4 t1 0
H 2 rch2 1 a3 4 -t1 0

rbc = 1.553094
rbh = 1.194586
t1 = 122.488674
rch1 = 1.090784
rch2 = 1.097833
a1 = 126.120789
a2 = 115.285523
a3 = 109.058391

++

Methylborane radical (CH2-BH2) C2V G-2 calculation

Molecule:

Stoichiometry = CH4B(2)
Charge = 0
Multiplicity = 2
Alpha Electrons = 8
Alpha Valence = 6
Beta Electrons = 7
Beta Valence = 5

Z-matrix: MP2
---

0 2
C
B 1 rbc
H 1 rch 2 a1
H 1 rch 2 a1 3 180. 0
H 2 rbh 1 a2 3 0. 0
H 2 rbh 1 a2 5 180. 0

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```
rbc = 1.529771
rbh = 1.194742
rch = 1.085686
a1 = 122.979015
a2 = 120.403890
-------------------------------------------------------------------------
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--------------------------
 Methylborane (CH3BH2) Cs
--------------------------

Molecule:
---------
Stoichiometry    = CH5B
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 8
Alpha Valence    = 6
Beta Electrons   = 8
Beta Valence     = 6

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

0  1
C
B         1         rcb
H         1         rch1      2         a1
H         1         rch2      2         a2        3         t1        0
H         1         rch2      2         a2        3         -t1       0
H         2         rbh       1         a3        3         t2        0
H         2         rbh       1         a3        3         -t2       0

rbh = 1.196241
t1 = 116.025906
t2 = 88.200355
rcb = 1.560588
rch1 = 1.102200
rch2 = 1.091684
a1 = 104.927576
a2 = 114.293739
a3 = 120.996084
-------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------------------------------------------
 Dimethylborane radical ((CH3)2B) C2 G-2 calculation
-----------------------------------------------------

Molecule:
---------
Stoichiometry    = C2H6B(2)
Charge           = 0
Multiplicity     = 2
Alpha Electrons  = 12
Alpha Valence    = 9
Beta Electrons   = 11
Beta Valence     = 8
```

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

0  2
B
C         1         rbc
C         1         rbc       2         a1
H         2         rbh1      1         a2        3         t1        0
H         2         rbh2      1         a3        4         t2        0
H         2         rbh3      1         a4        4         t3        0
H         3         rbh1      1         a2        2         t1        0
H         3         rbh2      1         a3        7         t2        0
H         3         rbh3      1         a4        7         t3        0

rbc = 1.559139
rbh1 = 1.096515
rbh2 = 1.091522
rbh3 = 1.099996
t1 = 30.314529
t2 = 126.152650
t3 = -116.331162
a1 = 126.887819
a2 = 113.000819
a3 = 114.613427
a4 = 105.990513
-----------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-------------------------------------------------------
 Dimethylborane ((CH3)2BH) C2 symmetric G-2 calculation
-------------------------------------------------------

Molecule:
---------
Stoichiometry    = C2H7B
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 12
Alpha Valence    = 9
Beta Electrons   = 12
Beta Valence     = 9

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

0  1
B
H         1         rbh
C         1         rbc       2         a1
C         1         rbc       2         a1        3         180.      0
H         3         rch1      1         a2        2         t1        0
H         3         rch2      1         a3        5         t2        0
H         3         rch3      1         a4        5         t3        0
H         4         rch1      1         a2        2         t1        0
H         4         rch2      1         a3        8         t2        0
H         4         rch3      1         a4        8         t3        0

rbc = 1.566953
rbh = 1.201841
```

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```
t1 = 37.042618
t2 = 126.464745
t3 = -115.563671
rch1 = 1.093369
rch2 = 1.092651
rch3 = 1.100642
a1 = 118.273626
a2 = 113.153892
a3 = 114.368260
a4 = 106.321723
-------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-------------------------------------------------
 Difluoromethylborane (CH3BF2) Cs G-2 calculation
-------------------------------------------------

Molecule:
---------
Stoichiometry    = CH3BF2
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 16
Alpha Valence    = 12
Beta Electrons   = 16
Beta Valence     = 12

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

0  1
C
B        1        rcb
H        1        rch1     2        a1
H        1        rch2     2        a2       3        t1       0
H        1        rch2     2        a2       3        -t1      0
F        2        rbf      1        a3       3        t2       0
F        2        rbf      1        a3       3        -t2      0

rbf = 1.333431
t1 = 118.407923
t2 = 89.106172
rcb = 1.559988
rch1 = 1.095377
rch2 = 1.090807
a1 = 109.120141
a2 = 111.776027
a3 = 121.949452
-------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------------------------------------------
 Aminoborane radical complex (BH2NH3) Cs G-2 calculation
-----------------------------------------------------

Molecule:
---------
Stoichiometry    = BH5N(2)
Charge           = 0
Multiplicity     = 2
```

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```
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
```

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```
rbn = 1.660439
rnh = 1.019768
a1 = 104.600963
a2 = 111.060612
t1 = 120.000000
t2 = 180.000000
-----------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------------------------------------------------------
 Dihydroxyborane radical (B(OH)2) Cs symmetric UHF/6-31G* fopt
-----------------------------------------------------------------

Molecule:
---------
Stoichiometry    = BH2O2(2)
Charge           = 0
Multiplicity     = 2
Alpha Electrons  = 12
Alpha Valence    = 9
Beta Electrons   = 11
Beta Valence     = 8

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

0  2
B
O          1        rbo1
O          1        rbo2     2        a1
H          2        roh1     1        a2       3        180.     0
H          3        roh2     1        a3       2        0.       0

roh1 = 0.969040
roh2 = 0.976392
a1 = 121.955155
a2 = 111.745127
a3 = 110.780105
rbo1 = 1.368222
rbo2 = 1.355620
-----------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
-----------------------------------------------------------
 Dihydroxyborane (HB(OH)2) Cs symmetric G2 calculation
-----------------------------------------------------------

Molecule:
---------
Stoichiometry    = BH3O2
Charge           = 0
Multiplicity     = 1
Alpha Electrons  = 12
Alpha Valence    = 9
Beta Electrons   = 12
Beta Valence     = 9

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

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```
0  1
B
H         1         rbh
O         1         rbo1      2         a1
O         1         rbo2      2         a2        3         180.      0
H         3         roh1      1         a3        2         0.        0
H         4         roh2      1         a4        2         180.      0

rbh = 1.194009
roh1 = 0.968822
roh2 = 0.973071
a1 = 122.794361
a2 = 117.926790
a3 = 111.705075
rbo1 = 1.372825
a4 = 110.412307
rbo2 = 1.362663
-----------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

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

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
BH CBS-4 calculation

Molecule:
---------
Stoichiometry:     B1H1
Charge:            0
Multiplicity:      1
Electronic State:  1-SG
Point group:       C*V [C*(H1B1)]
Number of Imaginary Freqencies: 0

Calculated S**2:  0.0000
Exact S**2:       0.0000
Delta S**2:       0.0000

Alpha Electrons:   3                 Alpha Valence Electrons: 2
Beta Electrons:    3                 Beta Valence Electrons:  2


Z-matrix:(RHF/3-21G*)
------------------------------------------------------------------------------
BH singlet state

0 1
B
H,1,rbh

rbh=1.22865704
------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
BH triplet state

Molecule:
---------
Stoichiometry:     B1H1(3)
Charge:            0
Multiplicity:      3
Electronic State:  undetermined
Point group:       C*V [C*(H1B1)]
Number of Imaginary Freqencies: 0

Calculated S**2:  2.0030
Exact S**2:       2.0000
Delta S**2:       0.0030

Alpha Electrons:   4                 Alpha Valence Electrons: 3
Beta Electrons:    2                 Beta Valence Electrons:  1


Z-matrix:(UHF/3-21G*)
------------------------------------------------------------------------------
BH triplet state CBS-4 calculation

0 3
```

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```
B
H,1,rbh

rbh=1.1825774
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Borane radical (BH2) C2V

Molecule:
---------
Stoichiometry:     B1H2(2)
Charge:            0
Multiplicity:      2
Electronic State:  2-A1
Point group:       C02V [C2(B1),SGV(H2)]
Number of Imaginary Freqencies: 0

Calculated S**2:  0.7530
Exact S**2:       0.7500
Delta S**2:       0.0030

Alpha Electrons:   4                 Alpha Valence Electrons: 3
Beta Electrons:    3                 Beta Valence Electrons:  2


Z-matrix:(UHF/3-21G*)
--------------------------------------------------------------------------------
Borane radical (BH2) C2V CBS-4 calculation

0 2
B
H,1,rbh
H,1,rbh,2,a

rbh=1.18518362
a=127.71937383
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Borane (BH3) D3H

Molecule:
---------
Stoichiometry:     B1H3
Charge:            0
Multiplicity:      1
Electronic State:  1-A1'
Point group:       D03H [O(B1),3C2(H1)]
Number of Imaginary Freqencies: 0

Calculated S**2:  0.0000
Exact S**2:       0.0000
Delta S**2:       0.0000

Alpha Electrons:   4                 Alpha Valence Electrons: 3
Beta Electrons:    4                 Beta Valence Electrons:  3


Z-matrix:(RHF/3-21G*)
```

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```
--------------------------------------------------------------------------------
Borane (BH3) D3H CBS-4 calculation

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

rbh=1.18767787
a=120.
t=180.
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Diborane radical (B2H5) C2V symmetry

Molecule:
---------
Stoichiometry:      B2H5(2)
Charge:             0
Multiplicity:       2
Electronic State:   2-A1
Point group:        C02V [C2(H1),SGV(B2),X(H4)]
Number of Imaginary Freqencies: 0

Calculated S**2:  0.7560
Exact S**2:       0.7500
Delta S**2:       0.0060

Alpha Electrons:    8                 Alpha Valence Electrons: 6
Beta Electrons:     7                 Beta Valence Electrons:  5


Z-matrix:(UHF/3-21G*)
--------------------------------------------------------------------------------
Diborane radical (B2H5) C2V symmetry CBS-4 calculation

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=1.32436514
rbh2=1.18040491
a1=137.35281419
a2=111.48884678
t1=73.84902794
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Diborane (B2H6) D2H symmetry CBS-4 calculation
```

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```
Molecule:
---------
Stoichiometry:      B2H6
Charge:             0
Multiplicity:       1
Electronic State:   1-AG
Point group:        D02H [C2(B1.B1),C2"(H1.H1),SG"(H4)]
Number of Imaginary Freqencies: 0

Calculated S**2:  0.0000
Exact S**2:       0.0000
Delta S**2:       0.0000

Alpha Electrons:    8                 Alpha Valence Electrons: 6
Beta Electrons:     8                 Beta Valence Electrons:  6


Z-matrix:(RHF/3-21G*)
-------------------------------------------------------------------------
Diborane (B2H6) D2H symmetry CBS-4 calculation

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=0.89259668
rhx=0.96522213
rbh=1.18225772
a1=118.81138328
-------------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
BF CBS-4 calculation

Molecule:
---------
Stoichiometry:      B1F1
Charge:             0
Multiplicity:       1
Electronic State:   1-SG
Point group:        C*V [C*(B1F1)]
Number of Imaginary Freqencies: 0

Calculated S**2:  0.0000
Exact S**2:       0.0000
Delta S**2:       0.0000

Alpha Electrons:    7                 Alpha Valence Electrons: 5
Beta Electrons:     7                 Beta Valence Electrons:  5
```

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Z-matrix:(RHF/3-21G*)

BF CBS-4 calculation

0 1
B
F,1,rbf

rbf=1.30261208

++

BF triplet state CBS-4 calculation

Molecule:

Stoichiometry: B1F1(3)
Charge: 0
Multiplicity: 3
Electronic State: undetermined
Point group: C*V [C*(B1F1)]
Number of Imaginary Freqencies: 0

Calculated S**2: 2.0030
Exact S**2: 2.0000
Delta S**2: 0.0030

Alpha Electrons: 8 Alpha Valence Electrons: 6
Beta Electrons: 6 Beta Valence Electrons: 4

Z-matrix:(UHF/3-21G*)

BF triplet state CBS-4 calculation

0 3
B
F,1,rbf

rbf=1.34619413

++

Difluoroborane radical (BF2) C2V CBS-4 calculation

Molecule:

Stoichiometry: B1F2(2)
Charge: 0
Multiplicity: 2
Electronic State: 2-A1
Point group: C02V [C2(B1),SGV(F2)]
Number of Imaginary Freqencies: 0

Calculated S**2: 0.7520
Exact S**2: 0.7500
Delta S**2: 0.0020

Alpha Electrons: 12 Alpha Valence Electrons: 9
Beta Electrons: 11 Beta Valence Electrons: 8

J465322

Z-matrix:(UHF/3-21G*)

Difluoroborane radical (BF2) C2V CBS-4 calculation

0 2
B
F,1,rbf
F,1,rbf,2,a

rbf=1.33206307
a=119.73467126

++

Trifluoroborane (BF3) D3H CBS-4 calculation

Molecule:

Stoichiometry: B1F3
Charge: 0
Multiplicity: 1
Electronic State: 1-A1'
Point group: D03H [O(B1),3C2(F1)]
Number of Imaginary Freqencies: 0

Calculated S**2: 0.0000
Exact S**2: 0.0000
Delta S**2: 0.0000

Alpha Electrons: 16 Alpha Valence Electrons: 12
Beta Electrons: 16 Beta Valence Electrons: 12

Z-matrix:(RHF/3-21G*)

Trifluoroborane (BF3) D3H CBS-4 calculation

0 1
B
F,1,rbf
F,1,rbf,2,a
F,1,rbf,2,a,3,t,0

rbf=1.32847486
a=120.
t=180.

++

BHF radical Cs symmetry CBS-4 calculation

Molecule:

Stoichiometry: B1F1H1(2)
Charge: 0
Multiplicity: 2
Electronic State: 2-A'
Point group: CS [SG(B1F1H1)]

J465323

Number of Imaginary Freqencies: 0

Calculated S**2: 0.7530
Exact S**2: 0.7500
Delta S**2: 0.0030

Alpha Electrons: 8 Alpha Valence Electrons: 6
Beta Electrons: 7 Beta Valence Electrons: 5

Z-matrix:(UHF/3-21G*)

BHF radical Cs symmetry CBS-4 calculation

0 2
B
F,1,rbf
H,1,rbh,2,a

rbf=1.33636623
rbh=1.18769724
a=122.69017802

++

Fluoroborane (BH2F) C2V CBS-4 calculation

Molecule:

Stoichiometry: B1F1H2
Charge: 0
Multiplicity: 1
Electronic State: 1-A1
Point group: C02V [C2(B1F1),SGV(H2)]
Number of Imaginary Freqencies: 0

Calculated S**2: 0.0000
Exact S**2: 0.0000
Delta S**2: 0.0000

Alpha Electrons: 8 Alpha Valence Electrons: 6
Beta Electrons: 8 Beta Valence Electrons: 6

Z-matrix:(RHF/3-21G*)

Fluoroborane (BH2F) C2V CBS-4 calculation

0 1
B
F,1,rbf
H,1,rbh,2,a
H,1,rbh,2,a,3,180.,0

rbf=1.34727992
rbh=1.18222453
a=117.80777457

++

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Difluoroborane (BF2H) C2V CBS-4 calculation

Molecule:

Stoichiometry: B1F2H1
Charge: 0
Multiplicity: 1
Electronic State: 1-A1
Point group: C02V [C2(B1H1),SGV(F2)]
Number of Imaginary Freqencies: 0

Calculated S**2: 0.0000
Exact S**2: 0.0000
Delta S**2: 0.0000

Alpha Electrons: 12 Alpha Valence Electrons: 9
Beta Electrons: 12 Beta Valence Electrons: 9

Z-matrix:(RHF/3-21G*)

Difluoroborane (BF2H) C2V CBS-4 calculation

0 1
B
H,1,rbh
F,1,rbf,2,a
F,1,rbf,2,a,3,180.,0

rbh=1.17111182
rbf=1.33690868
a=121.54998702

++
Methyl radical D3H CBS-4 calculation

Molecule:

Stoichiometry: C1H3(2)
Charge: 0
Multiplicity: 2
Electronic State: 2-A2"
Point group: D3H [O(C),3C2(H)]
Number of Imaginary Freqencies: 0

Calculated S**2: 0.7610
Exact S**2: 0.7500
Delta S**2: 0.0110

Alpha Electrons: 5 Alpha Valence Electrons: 4
Beta Electrons: 4 Beta Valence Electrons: 3

Z-matrix:(UHF/3-21G*)

Ethyl radical Cs CBS-4 calculation

0 2

J4653-25

```
C
H,1,r
H,1,r,2,120.
H,1,r,2,120.,3,180.,0

r=1.07167469
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Ethyl radical Cs CBS-4 calculation

Molecule:
---------
Stoichiometry:      C2H5(2)
Charge:             0
Multiplicity:       2
Electronic State:   2-A'
Point group:        CS [SG(C2H1),X(H4)]
Number of Imaginary Freqencies: 0

Calculated S**2:  0.7630
Exact S**2:       0.7500
Delta S**2:       0.0130

Alpha Electrons:    9                 Alpha Valence Electrons: 7
Beta Electrons:     8                 Beta Valence Electrons:  6


Z-matrix:(UHF/3-21G*)
--------------------------------------------------------------------------------
Ethyl radical Cs CBS-4 calculation

0 2
C
C,1,rcc
H,1,rch1,2,a1
H,1,rch2,2,a2,3,t1,0
H,1,rch2,2,a2,3,-t1,0
H,2,rch3,1,a3,3,t2,0
H,2,rch3,1,a3,3,-t2,0

rcc=1.50722277
rch1=1.0894274
rch2=1.08427068
rch3=1.07335272
a1=111.31436683
a2=111.12474674
a3=120.42165258
t1=119.70461999
t2=84.12927518
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Ethane D3D CBS-4 calculation

Molecule:
---------
Stoichiometry:      C2H6
Charge:             0
Multiplicity:       1
```

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Electronic State: 1-A1G
Point group: D03D [C3(C1.C1),3SGD(H2)]
Number of Imaginary Freqencies: 0

Calculated S**2: 0.0000
Exact S**2: 0.0000
Delta S**2: 0.0000

Alpha Electrons: 9 Alpha Valence Electrons: 7
Beta Electrons: 9 Beta Valence Electrons: 7

Z-matrix:(RHF/3-21G*)

Ethane D3D CBS-4 calculation

0 1
C
C,1,rcc
H,1,rch,2,a
H,1,rch,2,a,3,120.,0
H,1,rch,2,a,3,-120.,0
H,2,rch,1,a,3,180.,0
H,2,rch,1,a,6,120.,0
H,2,rch,1,a,6,-120.,0

rcc=1.54242054
rch=1.08412062
a=110.79465213

++

Methylborane "borene" singlet state (CH3B) Cs symmetric CBS-4 calculation

Molecule:

Stoichiometry: C1H3B1
Charge: 0
Multiplicity: 1
Electronic State: 1-A'
Point group: CS [SG(C1H1B1),X(H2)]
Number of Imaginary Freqencies: 0

Calculated S**2: 0.0000
Exact S**2: 0.0000
Delta S**2: 0.0000

Alpha Electrons: 7 Alpha Valence Electrons: 5
Beta Electrons: 7 Beta Valence Electrons: 5

Z-matrix:(RHF/3-21G*)

Methylborane "borene" singlet state (CH3B) Cs symmetric CBS-4 calculation

0 1
C
B,1,rbc
H,1,rch1,2,a1

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```
H,1,rch2,2,a2,3,t1,0
H,1,rch2,2,a2,3,-t1,0

rbc=1.57212547
rch1=1.09120559
rch2=1.09120489
a1=110.83644318
a2=110.83746064
t1=119.99956253
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Methylborane "borene" triplet state (CH3B) Cs symmetric CBS-4 calculation

Molecule:
---------
Stoichiometry:     C1H3B1(3)
Charge:            0
Multiplicity:      3
Electronic State:  3-A"
Point group:       CS [SG(C1H1B1),X(H2)]
Number of Imaginary Freqencies: 0

Calculated S**2:  2.0040
Exact S**2:       2.0000
Delta S**2:       0.0040

Alpha Electrons:   8                Alpha Valence Electrons: 6
Beta Electrons:    6                Beta Valence Electrons:  4


Z-matrix:(UHF/3-21G*)
--------------------------------------------------------------------------------
Methylborane "borene" triplet state (CH3B) Cs symmetric CBS-4 calculation

0 3
C
B,1,rbc
H,1,rch1,2,a1
H,1,rch2,2,a2,3,t1,0
H,1,rch2,2,a2,3,-t1,0

rbc=1.57636226
rch1=1.0934071
rch2=1.08619823
a1=106.49177137
a2=113.43988432
t1=117.3195433
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Methylborane radical (CH3BH) Cs symmetric CBS-4 calculation

Molecule:
---------
Stoichiometry:     C1H4B1(2)
Charge:            0
Multiplicity:      2
Electronic State:  2-A'
Point group:       CS [SG(C1H2B1),X(H2)]
```

JA953628

Number of Imaginary Freqencies: 0

Calculated S**2: 0.7530
Exact S**2: 0.7500
Delta S**2: 0.0030

Alpha Electrons: 8 Alpha Valence Electrons: 6
Beta Electrons: 7 Beta Valence Electrons: 5

Z-matrix:(UHF/3-21G*)

Methylborane radical (CH3BH) Cs symmetric CBS-4 calculation

0 2
B
C,1,rbc
H,1,rbh,2,a1
H,2,rch1,1,a2,3,180.,0
H,2,rch2,1,a3,4,t1,0
H,2,rch2,1,a3,4,-t1,0

rbc=1.57043948
rbh=1.19071054
rch1=1.0839717
rch2=1.09188497
a1=126.42228462
a2=114.29457313
a3=109.87991263
t1=121.88951313

++

Methylborane radical (CH2-BH2) C2V CBS-4 calculation

Molecule:

Stoichiometry: C1H4B1(2)
Charge: 0
Multiplicity: 2
Electronic State: 2-B1
Point group: C02V [C2(B1C1),SGV(H4)]
Number of Imaginary Freqencies: 0

Calculated S**2: 0.7580
Exact S**2: 0.7500
Delta S**2: 0.0080

Alpha Electrons: 8 Alpha Valence Electrons: 6
Beta Electrons: 7 Beta Valence Electrons: 5

Z-matrix:(UHF/3-21G*)

Methylborane radical (CH2-BH2) C2V CBS-4 calculation

0 2
C
B,1,rbc

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```
H,1,rch,2,a1
H,1,rch,2,a1,3,180.,0
H,2,rbh,1,a2,3,0.,0
H,2,rbh,1,a2,5,180.,0

rbc=1.53718203
rch=1.07731411
rbh=1.19053388
a1=122.76039959
a2=120.60133421
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Methylborane (CH3BH2) Cs CBS-4 calculation

Molecule:
---------
Stoichiometry:     C1H5B1
Charge:            0
Multiplicity:      1
Electronic State:  1-A'
Point group:       CS [SG(C1H1B1),X(H4)]
Number of Imaginary Freqencies: 0

Calculated S**2:  0.0000
Exact S**2:       0.0000
Delta S**2:       0.0000

Alpha Electrons:   8                 Alpha Valence Electrons: 6
Beta Electrons:    8                 Beta Valence Electrons:  6


Z-matrix:(RHF/3-21G*)
--------------------------------------------------------------------------------
Methylborane (CH3BH2) Cs CBS-4 calculation

0 1
C
B,1,rcb
H,1,rch1,2,a1
H,1,rch2,2,a2,3,t1,0
H,1,rch2,2,a2,3,-t1,0
H,2,rbh,1,a3,3,t2,0
H,2,rbh,1,a3,3,-t2,0

rcb=1.57655113
rch1=1.09577183
rch2=1.08552467
rbh=1.19200962
a1=107.21585226
a2=113.46986414
a3=121.05998033
t1=117.23578314
t2=88.75489713
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Dimethylborane radical ((CH3)2B) C2 CBS-4 calculation

Molecule:
```

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Stoichiometry: C2H6B1(2)
Charge: 0
Multiplicity: 2
Electronic State: 2-A
Point group: C02 [C2(B1),X(C2H6)]
Number of Imaginary Freqencies: 0

Calculated S**2: 0.7540
Exact S**2: 0.7500
Delta S**2: 0.0040

Alpha Electrons: 12 Alpha Valence Electrons: 9
Beta Electrons: 11 Beta Valence Electrons: 8

Z-matrix:(UHF/3-21G*)

Dimethylborane radical ((CH3)2B) C2 CBS-4 calculation

0 2
B
C,1,rbc
C,1,rbc,2,a1
H,2,rbh1,1,a2,3,t1,0
H,2,rbh2,1,a3,4,t2,0
H,2,rbh3,1,a4,4,t3,0
H,3,rbh1,1,a2,2,t1,0
H,3,rbh2,1,a3,7,t2,0
H,3,rbh3,1,a4,7,t3,0

rbc=1.57631739
rbh1=1.08942083
rbh2=1.08551156
rbh3=1.0940432
a1=127.82249449
a2=113.14895952
a3=113.22378007
a4=107.8171932
t1=26.0480793
t2=124.494517
t3=-117.89829713

++
Dimethylborane ((CH3)2BH) C2 symmetric CBS-4 calculation

Molecule:

Stoichiometry: C2H7B1
Charge: 0
Multiplicity: 1
Electronic State: 1-A
Point group: C02 [C2(B1H1),X(C2H6)]
Number of Imaginary Freqencies: 0

Calculated S**2: 0.0000
Exact S**2: 0.0000
Delta S**2: 0.0000

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Alpha Electrons: 12 Alpha Valence Electrons: 9
Beta Electrons: 12 Beta Valence Electrons: 9

Z-matrix:(RHF/3-21G*)

Dimethylborane ((CH3)2BH) C2 symmetric CBS-4 calculation

0 1
B
H,1,rbh
C,1,rbc,2,a1
C,1,rbc,2,a1,3,180.,0
H,3,rch1,1,a2,2,t1,0
H,3,rch2,1,a3,5,t2,0
H,3,rch3,1,a4,5,t3,0
H,4,rch1,1,a2,2,t1,0
H,4,rch2,1,a3,8,t2,0
H,4,rch3,1,a4,8,t3,0

rbh=1.19750153
rbc=1.58169037
rch1=1.08858991
rch2=1.08544302
rch3=1.09393879
a1=117.8944538
a2=111.74436825
a3=114.11656788
a4=108.49010867
t1=44.83939512
t2=124.07642311
t3=-116.09110911

++
Trimethylborane ((CH3)3B) C3H CBS-4 calculation

Molecule:

Stoichiometry: C3H9B1
Charge: 0
Multiplicity: 1
Electronic State: 1-A'
Point group: C03H [O(B1),SGH(C3H3),X(H6)]
Number of Imaginary Freqencies: 0

Calculated S**2: 0.0000
Exact S**2: 0.0000
Delta S**2: 0.0000

Alpha Electrons: 16 Alpha Valence Electrons: 12
Beta Electrons: 16 Beta Valence Electrons: 12

Z-matrix:(RHF/3-21G*)

Trimethylborane ((CH3)3B) C3H CBS-4 calculation

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```
0 1
B
C,1,rbc
C,1,rbc,2,120.
C,1,rbc,2,120.,3,180.,0
H,2,rch1,1,a1,3,0.,0
H,2,rch2,1,a2,5,t1,0
H,2,rch2,1,a2,5,-t1,0
H,3,rch1,1,a1,4,0.,0
H,3,rch2,1,a2,8,t1,0
H,3,rch2,1,a2,8,-t1,0
H,4,rch1,1,a1,2,0.,0
H,4,rch2,1,a2,11,t1,0
H,4,rch2,1,a2,11,-t1,0

rbc=1.58939859
rch1=1.08550067
rch2=1.0915574
a1=114.37011668
a2=110.11084434
t1=121.98895995
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Difluoromethylborane (CH3BF2) Cs CBS-4 calculation

Molecule:
---------
Stoichiometry:      C1H3B1F2
Charge:             0
Multiplicity:       1
Electronic State:   1-A'
Point group:        CS [SG(C1H1B1),X(H2F2)]
Number of Imaginary Freqencies: 0

Calculated S**2:  0.0000
Exact S**2:       0.0000
Delta S**2:       0.0000

Alpha Electrons:    16                Alpha Valence Electrons: 12
Beta Electrons:     16                Beta Valence Electrons:  12


Z-matrix:(RHF/3-21G*)
--------------------------------------------------------------------------------
Difluoromethylborane (CH3BF2) Cs CBS-4 calculation

0 1
C
B,1,rcb
H,1,rch1,2,a1
H,1,rch2,2,a2,3,t1,0
H,1,rch2,2,a2,3,-t1,0
F,2,rbf,1,a3,3,t2,0
F,2,rbf,1,a3,3,-t2,0

rcb=1.5575503
rch1=1.0901828
rch2=1.08441702
```

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```
rbf=1.34516875
a1=109.88449437
a2=111.83260155
a3=122.83389298
t1=118.72499272
t2=89.29266456
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Aminoborane radical complex (BH2NH3) Cs CBS-4 calculation

Molecule:
---------
Stoichiometry:      B1H5N1(2)
Charge:             0
Multiplicity:       2
Electronic State:   2-A'
Point group:        CS [SG(B1H1N1),X(H4)]
Number of Imaginary Freqencies: 0

Calculated S**2:   0.7560
Exact S**2:        0.7500
Delta S**2:        0.0060

Alpha Electrons:    9                  Alpha Valence Electrons: 7
Beta Electrons:     8                  Beta Valence Electrons:  6


Z-matrix:(UHF/3-21G*)
--------------------------------------------------------------------------------
Aminoborane radical complex (BH2NH3) Cs CBS-4 calculation

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

rbn=1.69243749
rbh=1.20071816
rnh1=1.01197558
rnh2=1.00987077
a1=107.78021401
a2=110.48665523
a3=108.75801263
t1=113.74579292
t3=120.30008039
t2=180.
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Aminoborane complex (BH3NH3) C3V CBS-4 calculation

Molecule:
---------
Stoichiometry:      B1H6N1
```

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Charge: 0
Multiplicity: 1
Electronic State: 1-A1
Point group: C03V [C3(B1N1),3SGV(H2)]
Number of Imaginary Freqencies: 0

Calculated S**2: 0.0000
Exact S**2: 0.0000
Delta S**2: 0.0000

Alpha Electrons: 9 Alpha Valence Electrons: 7
Beta Electrons: 9 Beta Valence Electrons: 7

Z-matrix:(RHF/3-21G*)

Aminoborane complex (BH3NH3) C3V CBS-4 calculation

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

rbn=1.71350921
rbh=1.20855183
rnh=1.00962316
a1=104.48964365
a2=109.04149788
t1=120.
t2=180.

++

Dihydroxyborane radical (B(OH)2) Cs symmetric CBS-4 calculation

Molecule:

Stoichiometry: B1H2O2(2)
Charge: 0
Multiplicity: 2
Electronic State: 2-A'
Point group: CS [SG(B1H2O2)]
Number of Imaginary Freqencies: 0

Calculated S**2: 0.7530
Exact S**2: 0.7500
Delta S**2: 0.0030

Alpha Electrons: 12 Alpha Valence Electrons: 9
Beta Electrons: 11 Beta Valence Electrons: 8

Z-matrix:(UHF/3-21G*)

J4653-35

Dihydroxyborane radical (B(OH)2) Cs symmetric CBS-4 calculation

```
0 2
B
O,1,rbo1
O,1,rbo2,2,a1
H,2,roh1,1,a2,3,180.,0
H,3,roh2,1,a3,2,0.,0

rbo1=1.37509196
rbo2=1.36503015
roh1=0.9612261
roh2=0.96841673
a1=121.82511569
a2=119.2164278
a3=118.9544357
```

++

Dihydroxyborane (HB(OH)2) Cs symmetric CBS-4 calculation

Molecule:

Stoichiometry: B1H3O2
Charge: 0
Multiplicity: 1
Electronic State: 1-A'
Point group: CS [SG(B1H3O2)]
Number of Imaginary Freqencies: 0

Calculated S**2: 0.0000
Exact S**2: 0.0000
Delta S**2: 0.0000

Alpha Electrons: 12 Alpha Valence Electrons: 9
Beta Electrons: 12 Beta Valence Electrons: 9

Z-matrix:(RHF/3-21G*)

Dihydroxyborane (HB(OH)2) Cs symmetric CBS-4 calculation

```
0 1
B
H,1,rbh
O,1,rbo1,2,a1
O,1,rbo2,2,a2,3,180.,0
H,3,roh1,1,a3,2,0.,0
H,4,roh2,1,a4,2,180.,0

rbh=1.18359211
rbo1=1.37966592
rbo2=1.37032931
roh1=0.96112223
roh2=0.96471238
a1=123.42086588
a2=117.75673428
a3=119.85216477
a4=117.98164654
```

J4653-36

++
Methoxyhydroxyborane radical ((CH3O)B(OH)) Cs CBS-4 calculation

Molecule:

Stoichiometry: C1H4B1O2(2)
Charge: 0
Multiplicity: 2
Electronic State: 2-A'
Point group: CS [SG(C1H2B1O2),X(H2)]
Number of Imaginary Freqencies: 0

Calculated S**2: 0.7530
Exact S**2: 0.7500
Delta S**2: 0.0030

Alpha Electrons: 16 Alpha Valence Electrons: 12
Beta Electrons: 15 Beta Valence Electrons: 11

Z-matrix:(UHF/3-21G*)

Methoxyhydroxyborane radical ((CH3O)B(OH)) Cs CBS-4 calculation

0 2
O
B,1,rbo1
O,2,rbo2,1,a1
C,3,rco,2,a2,1,t1,0
H,1,roh,2,a3,3,t2,0
H,4,rch1,3,a4,2,t3,0
H,4,rch2,3,a5,6,t4,0
H,4,rch2,3,a5,6,-t4,0

rbo1=1.36745861
rbo2=1.36818982
rco=1.44069343
roh=0.96856963
rch1=1.08151457
rch2=1.07974818
a1=122.24384421
a2=125.81842743
a3=118.54780894
a4=111.34090289
a5=108.57371414
t4=120.60490578
t1=180.
t2=0.
t3=0.

++
Methoxyhydroxyborane ((CH3O)BH(OH)) Cs symmetric CBS-4 calculation

Molecule:

Stoichiometry: C1H5B1O2
Charge: 0

J4653-37

```
Multiplicity:       1
Electronic State:   1-A'
Point group:        CS [SG(C1H3B1O2),X(H2)]
Number of Imaginary Freqencies: 0

Calculated S**2:   0.0000
Exact S**2:        0.0000
Delta S**2:        0.0000

Alpha Electrons:    16                Alpha Valence Electrons:  12
Beta Electrons:     16                Beta Valence Electrons:   12


Z-matrix:(RHF/3-21G*)
---------------------------------------------------------------------------
Methoxyhydroxyborane ((CH3O)BH(OH)) Cs symmetric CBS-4 calculation

0 1
O
B,1,rbo1
O,2,rbo2,1,a1
C,3,rco,2,a2,1,t1,0
H,1,roh,2,a3,3,t2,0
H,2,rbh,3,a4,4,t3,0
H,4,rch1,3,a5,2,t4,0
H,4,rch2,3,a6,7,t5,0
H,4,rch2,3,a6,7,-t5,0

rbo1=1.37189021
rbo2=1.37349312
rco=1.43904534
roh=0.96477624
rbh=1.18576675
rch1=1.08271764
rch2=1.07999899
a1=119.55379474
a2=125.69277467
a3=117.87766016
a4=122.51783703
a5=111.2983944
a6=108.73939545
t5=120.5237283
t1=180.
t2=0.
t3=0.
t4=0.
---------------------------------------------------------------------------
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Dimethoxyborane radical ((CH3O)2B) C2V symmetric CBS-4 calculation

Molecule:
---------
Stoichiometry:      C2H6B1O2(2)
Charge:             0
Multiplicity:       2
Electronic State:   2-A1
Point group:        C02V [C2(B1),SGV(C2H2O2),X(H4)]
Number of Imaginary Freqencies: 0
```

J465338

```
Calculated S**2:  0.7540
Exact S**2:       0.7500
Delta S**2:       0.0040

Alpha Electrons:   20              Alpha Valence Electrons: 15
Beta Electrons:    19              Beta Valence Electrons:  14


Z-matrix:(UHF/3-21G*)
--------------------------------------------------------------------------
Dimethoxyborane radical ((CH3O)2B) C2V symmetric CBS-4 calculation

0 2
B
O,1,rbo
O,1,rbo,2,a1
C,2,rco,1,a2,3,t1,0
C,3,rco,1,a2,2,t1,0
H,4,rch1,2,a3,1,t2,0
H,4,rch2,2,a4,6,t3,0
H,4,rch2,2,a4,6,-t3,0
H,5,rch1,3,a3,1,t2,0
H,5,rch2,3,a4,9,t3,0
H,5,rch2,3,a4,9,-t3,0

rbo=1.36323188
rco=1.43924024
rch1=1.08234493
rch2=1.07978872
a1=122.55994922
a2=126.25969702
a3=111.61377136
a4=108.53534351
t3=120.65333749
t1=180.
t2=0.
--------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Dimethoxyborane ((CH3O)2BH) C2V symmetric CBS-4 calculation

Molecule:
---------
Stoichiometry:     C2H7B1O2
Charge:            0
Multiplicity:      1
Electronic State:  1-A1
Point group:       C02V [C2(B1H1),SGV(C2H2O2),X(H4)]
Number of Imaginary Freqencies: 0

Calculated S**2:  0.0000
Exact S**2:       0.0000
Delta S**2:       0.0000

Alpha Electrons:   20              Alpha Valence Electrons: 15
Beta Electrons:    20              Beta Valence Electrons:  15
```

J4653339

Z-matrix:(RHF/3-21G*)

Dimethoxyborane ((CH3O)2BH) C2V symmetric CBS-4 calculation

```
0 1
H
B,1,rbh
O,2,rbo,1,a1
O,2,rbo,1,a1,3,t1,0
C,3,rco,2,a2,1,t2,0
C,4,rco,2,a2,1,t2,0
H,5,rch1,3,a3,2,t3,0
H,5,rch2,3,a4,7,t4,0
H,5,rch2,3,a4,7,-t4,0
H,6,rch1,4,a3,2,t3,0
H,6,rch2,4,a4,10,t4,0
H,6,rch2,4,a4,10,-t4,0

rbh=1.19860994
rbo=1.36820228
rco=1.4373791
rch1=1.08363227
rch2=1.08005726
a1=120.43817704
a2=125.73741356
a3=111.58010313
a4=108.71415734
t4=120.58849906
t1=180.
t2=0.
t3=0.
```

++

ethanediol-bridged borane radical C2V CBS-4 calculation

Molecule:

Stoichiometry: C2H4B1O2(2)
Charge: 0
Multiplicity: 2
Electronic State: 2-A1
Point group: C02V [C2(B1),SGV(C2O2),X(H4)]
Number of Imaginary Freqencies: 0

Calculated S**2: 0.7540
Exact S**2: 0.7500
Delta S**2: 0.0040

Alpha Electrons: 19 Alpha Valence Electrons: 14
Beta Electrons: 18 Beta Valence Electrons: 13

Z-matrix:(UHF/3-21G*)

---

ethanediol-bridged borane radical C2V CBS-4 calculation

```
0 2
X
```

J4653401

```
B,1,1.
O,2,rbo,1,a1
O,2,rbo,1,a1,3,t1,0
C,3,rco,2,a2,1,t2,0
C,4,rco,2,a2,1,t2,0
H,5,rch,3,a3,2,t3,0
H,6,rch,4,a3,2,t3,0
H,5,rch,3,a3,2,-t3,0
H,6,rch,4,a3,2,-t3,0

rbo=1.38110672
rco=1.47059888
rch=1.0772877
a1=123.9301172
a2=109.52110068
a3=108.48680199
t3=120.25545847
t1=180.
t2=180.
--------------------------------------------------------------------------------
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
ethanediol-bridged borane C2V CBS-4 calculation

Molecule:
---------
Stoichiometry:     C2H5B1O2
Charge:            0
Multiplicity:      1
Electronic State:  1-A1
Point group:       C02V [C2(B1H1),SGV(C2O2),X(H4)]
Number of Imaginary Freqencies: 0

Calculated S**2:  0.0000
Exact S**2:       0.0000
Delta S**2:       0.0000

Alpha Electrons:   19                Alpha Valence Electrons: 14
Beta Electrons:    19                Beta Valence Electrons:  14


Z-matrix:(RHF/3-21G*)
--------------------------------------------------------------------------------
ethanediol-bridged borane C2V CBS-4 calculation

0 1
H
B,1,rbh
O,2,rbo,1,a1
O,2,rbo,1,a1,3,t1,0
C,3,rco,2,a2,1,t2,0
C,4,rco,2,a2,1,t2,0
H,5,rch,3,a3,2,t3,0
H,6,rch,4,a3,2,t3,0
H,5,rch,3,a3,2,-t3,0
H,6,rch,4,a3,2,-t3,0

rbh=1.17153339
rbo=1.38455388
```