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Supporting Information available for

Arylpentazoles with surprisingly high kinetic stability: A co-stabilization method

Xiao-xu Bo,[a,b] Zhi-yong Dong,[a] and Yi-hong Ding*[b,a]

[a] Laboratory of Theoretical and Computational Chemistry, Institute of Theoretical Chemistry, Jilin University, Changchun 130023, P. R. China.

[b] Key Laboratory of Carbon Materials of Zhejiang Province, College of Chemistry and Materials Engineering, Wenzhou University, Wenzhou 325035, P. R. China.

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Table S1 The N_2-leaving barrier (kcal/mol), NPA (e) of N_5-ring and EA (eV) of R for the parent ArN_5.

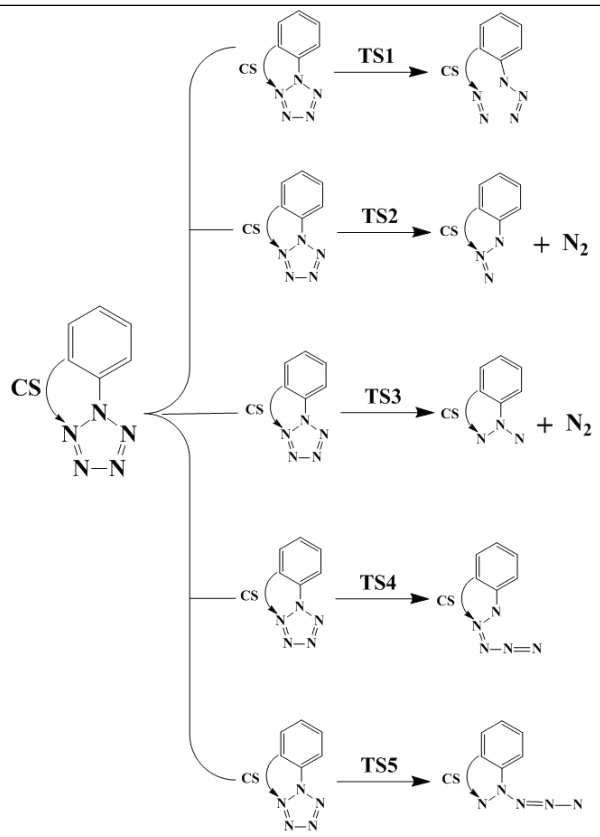
ArN_5	N_2-leaving barrier	NPA	EA
01	15.84(20.04)[16.5][a][20.66][c]	-0.28615	1.21
02	16.79(20.71)[17.7][a]	-0.29857	1.31
03	16.85(20.81)	-0.30118	1.27
04	17.06(20.89)	-0.30336	1.23
05	16.92(20.88)[19.2][b]	-0.29947	1.24
06	16.55(20.35)[18.3][a][19.6][b]	-0.31968	1.23
07	15.51(19.62)[17.5][b]	-0.27769	1.6
08	14.56(18.92)	-0.26765	1.73
09	13.73(17.71)	-0.24554	2.63
10	14.23(18.63)[15.8][a]	-0.26273	1.94

a. Carlqvist, P.; Östmark, H.;Brinck, T. *J. Phys. Chem. A*, 2004, **108**, 7463-7467

b. Ren, G.;Liu, R.;Zhou, P.;Zhang, C.; Liu, J.;Han, K. Chem. Commun., 2019, 55, 2628-2631.

c. Bo, X. X.; Zheng, H. F.;Xin, J. F.Ding, Y. H. *Chem. Commun.*, **2019**, *55*, 2597-2600.

Table S2 The kinetic process of co-stabilized arylpentazoles (ArN_5-nCS) with elementary substituent R=H (n=1,2).

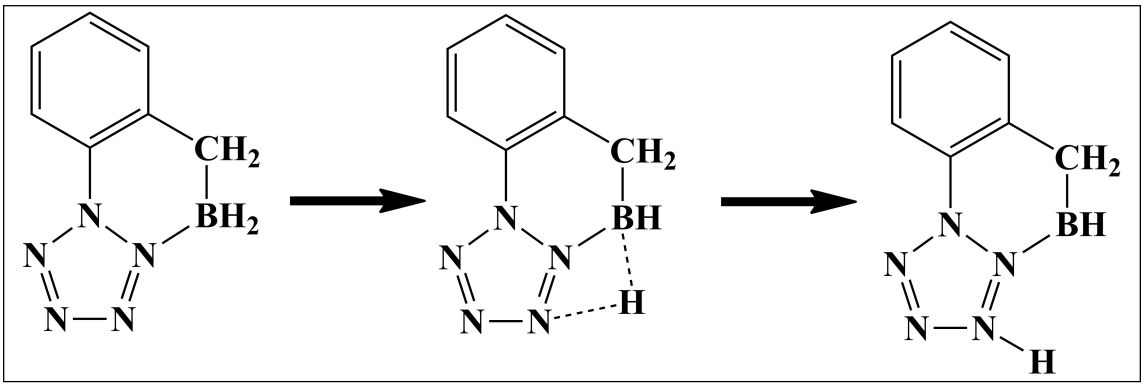


		N_2-leaving		Ring-opening		
ArN_5-nCS	**TS1**	**TS2**	**TS3**	**TS4**	**TS5**	**Rate-determining barrier**
01 (n=0)	15.84(20.04)	—	—	—	—	15.84(20.04)
01-1BH_2	25.19(29.28)	28.88(34.26)	26.15(32.33)	27.03(35.33)	35.53(43.82)	25.19(29.28)
01-2BH_2	22.48(27.13)	28.34(33.39)	—	25.88(33.95)	37.46(45.52)	22.48(27.13)
01-1CH_2BH_2	22.75(27.00)	27.48(31.8)	61.26(62.34)	36.76(45.87)	27.83(36.58)	22.75(27.00)
01-2CH_2BH_2	32.96(38.03)	—	52.9(61.00)	—	—	32.96(38.03)
02 (n=0)	16.79(20.71)	—	—	—	—	16.79(20.71)
02-1BH_2	26.29(30.13)	31.6(37.44)	62.58(65.31)	35.26(43.35)	26.53(34.94)	26.29(30.13)
02-2BH_2	23.71(27.77)	30.34(36.07)	62.08(66.25)	37.18(45.08)	25.46(33.69)	23.71(27.77)
02-1CH_2BH_2	23.66(27.73)	28.55(32.86)	61.87(64.62)	36.24(45.21)	27.17(36.15)	23.66(27.73)

02-2CH_2BH_2	34.33(39.04)	—	53.86(62.4)	—	—	34.33(39.04)
03 (n=0)	16.85(20.81)	—	—	—	—	16.85(20.81)
03-1BH_2	26.27(30.11)	31.29(36.91)	—	26.69(35.13)	35.47(43.56)	26.27(30.11)
03-2BH_2	24.26(28.19)	30.78(36.59)	61.74(65.89)	37.15(45.12)	25.58(33.93)	24.26(28.19)
03-1CH_2BH_2	23.82(27.88)	28.41(32.66)	61.91(64.48)	27.28(36.29)	36.17(45.07)	23.82(27.88)
03-2CH_2BH_2	32.62(36.22)	—	50.45(55.44)	—	—	32.62(36.22)
04 (n=0)	17.06(20.89)	—	—	—	—	17.06(20.89)
04-1BH_2	26.87(30.56)	32.24(38.07)	62.39(65.04)	35.35(43.49)	26.81(35.34)	26.87(30.56)
04-2BH_2	24.43(28.41)	31.22(37.13)	62.26(67.11)	36.61(42.42)	25.92(34.24)	24.43(28.41)
04-1CH_2BH_2	24.23(28.18)	29.24(33.58)	62.08(64.94)	36.06(44.86)	27.1(36.1)	24.23(28.18)
04-2CH_2BH_2	36.25(40.46)	—	54.01(62.38)	—	—	36.25(40.46)
05 (n=0)	16.92(20.88)	—	—	—	—	16.92(20.88)
05-1BH_2	26.14(30.03)	26.87(32.23)	62.67(65.31)	26.63(35.05)	35.5(43.6)	26.14(30.03)
05-2BH_2	23.85(27.95)	30.56(36.27)	62.09(66.16)	25.58(33.83)	37.2(45.08)	23.85(27.95)
05-1CH_2BH_2	23.74(27.87)	28.38(32.7)	—	36.17(45.16)	27.2(36.19)	23.74(27.87)
05-2CH_2BH_2	32.3(36.56)	—	51.15(59.26)	—	—	32.3(36.56)
06(n=0)	16.55(20.35)	—	—	—	—	16.55(20.35)
06-1BH_2	27.44(31.18)	27.55(32.8)	62.91(67.62)	26.54(35.09)	35.47(43.49)	27.44(31.18)
06-2BH_2	25.48(29.31)	31.45(37.18)	62.85(66.46)	25.63(34.04)	37.42(45.26)	25.48(29.31)
06-1CH_2BH_2	24.95(28.90)	29.45(33.84)	62.08(65.98)	27.04(36.13)	35.82(44.40)	24.95(28.90)
06-2CH_2BH_2	36.53(40.83)	—	54.12(62.2)	—	—	36.53(40.83)
07(n=0)	14.23(18.63)	—	—	—	—	14.23(18.63)
07-1BH_2	23.89(28.33)	29.13(35.06)	62.13(65.63)	26.09(34.21)	35.07(43.27)	23.89(28.33)
07-2BH_2	21.68(26.42)	28.00(34.01)	61.86(66.44)	24.94(32.93)	37.01(44.89)	21.68(26.42)
07-1CH_2BH_2	21.45(25.93)	25.96(30.55)	61.43(62.27)	36.68(45.97)	27.06(35.64)	21.45(25.93)
07-2CH_2BH_2	31.25(36.37)	—	53.27(62.34)	—	—	31.25(36.37)
08(n=0)	13.73(17.71)	—	—	—	—	13.73(17.71)

08-1BH_2	23.79(27.53)	—	61.86(65.63)	24.71(32.29)	34.18(41.95)	23.79(27.53)
08-2BH_2	23.74(27.31)	29.01(33.81)	—	25.09(33.14)	34.76(42.62)	23.74(27.31)
08-1CH_2BH_2	21.14(25.14)	25.57(29.89)	61.78(63.04)	25.88(34.08)	36.01(45.32)	21.14(25.14)
08-2CH_2BH_2	31.78(36.61)	—	—	—	—	31.78(36.61)
09(n=0)	13.73(17.71)	—	—	—	—	15.51(19.62)
09-1BH_2	25.00(29.07)	26.65(32.54)	—	26.41(34.64)	35.17(43.37)	25.00(29.07)
09-2BH_2	22.39(27.04)	29.05(35.09)	61.86(66.44)	25.28(33.35)	37.1(45.11)	22.39(27.04)
09-1CH_2BH_2	22.49(26.78)	27.15(31.57)	61.63(63.22)	27.26(36.00)	36.54(45.69)	22.49(26.78)
09-2CH_2BH_2	32.7(37.67)	53.48(62.24)	—	—	—	32.7(37.67)
10(n=0)	14.56(18.92)	—	—	—	—	14.56(18.92)
10-1BH_2	24.28(28.66)	28.52(33.92)	—	26.47(34.6)	34.92(43.14)	24.28(28.66)
10-2BH_2	21.69(26.46)	27.96(33.84)	61.62(66.46)	25.24(33.2)	37.00(44.99)	21.69(26.46)
10-1CH_2BH_2	21.81(26.03)	26.35(30.65)	60.85(61.63)	27.42(35.98)	36.78(45.97)	21.81(26.03)
10-2CH_2BH_2	31.51(36.63)	—	52.95(61.78)	—	—	31.51(36.63)

Scheme S1 The kinetic process of 1,3-R-transfer from B to N_5 for ArN_5-1CH_2BH_2.



ISO	Barrier (kcal/mol)
R=H	82.04 (83.92)

Table S4 The N_2-leaving barrier (kcal/mol), NPA (e) of N_5-ring and EA (eV) of R for the parent ArN_5-1CS.

Name	N_2-leaving	NPA	EA
01-1BH_2	25.19(29.28)	-0.08854	2.27
01-1CH_2BH_2	22.75(27)	-0.07037	3.27
02-1BH_2	26.29(30.13)	-0.10416	2.36
02-1CH_2BH_2	23.66(27.73)	-0.0859	3.31
03-1BH_2	26.27(30.11)	-0.109	2.28
03-1CH2BH_2	23.82(27.88)	-0.09041	3.24
04-1BH_2	26.87(30.56)	-0.10945	2.33
04-1CH_2BH_2	24.23(28.18)	-0.09021	3.35
05-1BH_2	26.14(30.03)	-0.10539	2.31
05-1CH_2BH_2	23.74(27.87)	-0.08877	3.23
06-1BH_2	27.44(31.18)	-0.13123	2.24
06-1CH_2BH_2	24.95(28.9)	-0.1119	3.22
07-1BH_2	23.79(27.53)	-0.06761	2.95
07-1CH_2BH_2	21.45(25.93)	-0.0541	3.82
08-1BH_2	23.79(27.53)	-0.049	2.76
08-1CH_2BH_2	21.14(25.14)	-0.03733	3.96
09-1BH_2	25.00(29.07)	-0.08201	2.63
09-1CH_2BH_2	22.49(26.78)	-0.06662	3.56
10-1BH_2	24.28(28.66)	-0.07193	2.75
10-1CH_2BH_2	21.81(26.03)	-0.05689	3.64

Table S5 The N_2-leaving barrier (kcal/mol) of R for the parent ArN_5-2CS.

Name	N_2-leaving
01-2BH_2	22.48(27.13)
01-2CH_2BH_2	32.96(38.03)
02-2BH_2	23.71(27.77)
02-2CH_2BH_2	34.33(39.04)
03-2BH_2	24.26(28.19)
03-2CH_2BH_2	32.62(36.22)
04-2BH_2	24.43(28.41)
04-2CH_2BH_2	36.25(40.46)
05-2-BH_2	23.85(27.95)
05-2CH_2BH_2	32.3(36.56)
06-2BH_2	25.48(29.31)
06-2CH_2BH_2	36.53(40.83)
07-2BH_2	21.69(26.46)
07-2CH_2BH_2	31.51(36.63)

08-2BH_2	23.74(27.31)
08-2CH_2BH_2	31.78(36.61)
09-2BH_2	22.39(27.04)
09-2CH_2BH_2	32.7(37.67)
10-2BH_2	21.69(26.46)
10-2CH_2BH_2	31.51(36.63)

Fig. S1 Structure of ArN_5-nCS (CS=-BH_2 and -CH_2BH_2; n=1,2).

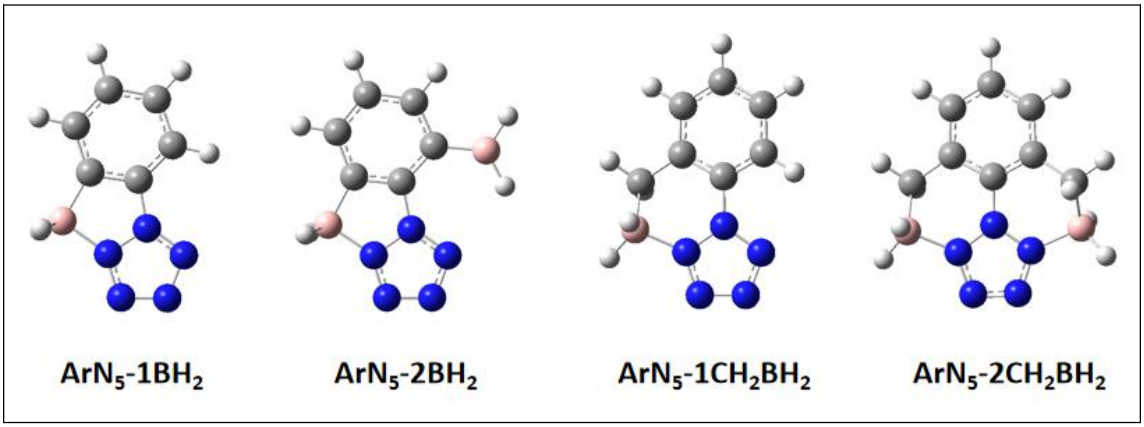


Table S6 Cartesian coordinates of the optimized isomeric structures and transitional structure**.**

"mol"----"Stoichiometry"

"lf"----"lowest frequency(cm-1)"

"te_zpe"----"total energy with zero-point energy (a.u.)"

"te_gfe"----"total energy with Gibbs free energy (a.u.)"

"bh_zpe"----"barrier height with zero-point energy correction (kcal/mol)"

"bh_gfe"----"barrier height with Gibbs free energy correction (kcal/mol)"

##
#

01-2BH2-b3-iso-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H7B2N5 01-2BH2-b3-iso-b3-2d-d-p-cbs-qb3 CBS-QB3

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6 1.381679 1.172095 -0.000004

6 0.417203 0.144539 0.000002

6 0.665769 -1.232685 0.000005

6 2.011733 -1.618225 0.000010

6 3.021454 -0.660567 0.000001

1 3.508158 1.432157 -0.000021

1 2.266135 -2.672512 0.000018

1 4.060042 -0.971530 0.000002

7 -1.004994 0.316045 -0.000010

7 -1.850927 1.320908 -0.000009

7 -3.045255 0.770250 -0.000037

7 -2.942053 -0.554420 -0.000000

7 -1.676395 -0.838441 -0.000015

5 -0.682783 -2.100195 -0.000003

1 -0.890426 -2.733124 1.002044

1 -0.890395 -2.733116 -1.002063

5 1.127654 2.694870 0.000031

1 2.079653 3.410885 0.000120

1 0.038601 3.160656 0.000226

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6 1.441246 1.164380 -0.000036

6 0.425820 0.181214 -0.000018

6 0.635952 -1.209524 -0.000024

6 1.967663 -1.629268 -0.000049

6 3.021338 -0.713166 -0.000066

1 3.577811 1.359064 -0.000073

1 2.184874 -2.692477 -0.000054

1 4.045562 -1.067740 -0.000085

7 -0.957632 0.412720 0.000005

7 -1.825055 1.324016 0.000055

7 -3.009318 1.141739 0.000100

7 -2.999314 -0.736156 0.000085

7 -1.862750 -1.000576 0.000039

5 -0.673927 -2.136720 -0.000002

1 -0.864565 -2.769951 1.004038

1 -0.864612 -2.769927 -1.004049

5 1.215500 2.681174 -0.000035

1 2.166462 3.398572 -0.000050

1 0.127868 3.162424 -0.000022

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6 -0.336334 1.524117 -0.111974

6 0.040178 0.162647 -0.087916

6 -0.864171 -0.926867 -0.102013

6 -2.226214 -0.620043 -0.004905

6 -2.611698 0.733269 0.106236

1 -2.059158 2.795936 0.025716

7 1.432580 -0.120749 -0.070174

7 2.411007 0.775440 -0.004048

7 3.549123 0.121243 0.062853

7 3.293177 -1.158682 0.062675

7 1.990264 -1.321848 -0.005936

8 -3.908046 1.096991 0.254349

1 -4.468810 0.316534 0.318457

6 -3.310026 -1.672882 -0.029257

1 -3.740630 -1.839953 0.965654

1 -4.125082 -1.388207 -0.705313

1 -2.939512 -2.630627 -0.384717

6 0.674374 2.615861 -0.359191

1 0.754989 2.730234 -1.450295

1 0.274438 3.563776 0.008911

5 2.126832 2.345949 0.291826

1 3.042735 2.949257 -0.192195

1 2.137417 2.360655 1.503938

6 -0.343572 -2.330949 -0.323549

1 -1.035313 -3.059789 0.100091

1 -0.353235 -2.506648 -1.409612

5 1.115835 -2.642569 0.296735

1 1.701826 -3.564724 -0.196895

1 1.134728 -2.666799 1.508808

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6 -0.075210 0.228279 0.131157

6 0.781584 -0.884030 0.295904

6 2.162373 -0.675367 0.153653

6 2.616970 0.620222 -0.154165

1 2.158469 2.662265 -0.562888

7 -1.440356 -0.074541 0.260113

7 -2.461706 0.670499 0.342080

7 -3.590999 0.347599 0.056204

7 -3.321658 -1.338604 -0.468802

7 -2.176632 -1.536962 -0.398651

8 3.940301 0.905452 -0.311932

1 4.462498 0.102705 -0.217517

6 3.187072 -1.774267 0.319690

1 3.586583 -2.113196 -0.643711

1 4.031924 -1.439959 0.934139

1 2.776218 -2.645838 0.823155

6 0.141063 -2.228708 0.542925

1 0.888281 -3.021765 0.547543

1 -0.310188 -2.233713 1.544719

5 -0.984670 -2.651668 -0.555039

1 -1.532925 -3.698753 -0.343150

1 -0.650474 -2.498516 -1.704818

6 -0.595569 2.661004 -0.414391

1 -0.022382 3.592971 -0.545895

1 -1.133105 2.538502 -1.363749

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1 -2.571396 3.639566 0.523271

1 -1.328624 2.723958 1.881498

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6 0.017155 0.173265 -0.036685

6 0.856249 -0.929594 0.151916

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6 2.671403 0.653027 -0.089570

1 2.177733 2.701776 -0.451920

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7 -3.960365 0.032162 0.227762

7 -3.783237 -1.026714 -0.132979

7 -1.874907 -1.172418 -0.546299

8 3.992545 0.972849 -0.136636

1 4.528883 0.181347 -0.025702

6 3.272856 -1.738170 0.391243

1 3.809555 -2.009709 -0.526125

1 4.014430 -1.409280 1.129351

1 2.829992 -2.648408 0.787750

6 0.232987 -2.286426 0.354968

1 0.948626 -3.086651 0.168045

1 -0.088667 -2.385475 1.400203

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04-2-BH2-iso-gas-cbs-qb3 charge=0 spin=1 mol=C8H11B2N5O1
04-2-BH2-iso-gas-cbs-qb3 CBS-QB3

lf=13.8 te_zpe=-710.042957 te_gfe=-710.085295 te_ms_zpe=-708.896951 te_ms_gfe=0.154966

6 1.354965 -1.329830 0.003917

6 -0.012076 -1.035876 0.006623

6 -0.379402 0.312241 0.006077

6 0.495997 1.425854 0.005631

6 1.873260 1.090245 -0.007995

6 2.266071 -0.267352 -0.006105

7 -1.813313 0.351467 0.000336

7 -2.373611 -0.862137 0.008114

7 -3.662566 -0.703529 -0.007260

7 -3.893446 0.600415 -0.025696

7 -2.756742 1.267136 -0.023418

8 3.612014 -0.492879 -0.012881

1 3.784948 -1.439941 -0.015088

6 2.990316 2.101710 -0.018126

1 3.617417 1.983509 0.870655

1 3.645868 1.929995 -0.876435

1 2.624030 3.121968 -0.053860

6 1.850423 -2.753820 0.009147

1 2.454908 -2.974891 -0.879404

1 2.464951 -2.964538 0.893222

1 1.018062 -3.455294 0.017618

5 -1.278506 -2.021457 0.013862

1 -1.421086 -2.669825 1.018915

1 -1.427830 -2.680409 -0.983231

5 -0.001765 2.887556 0.048497

1 -1.155498 3.132958 0.132660

1 0.759905 3.796521 0.006654

04-2-BH2-ts-01-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H11B2N5O1 04-2-BH2-ts-01-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-532.7 te_zpe=-710.002499 te_gfe=-710.046363 te_ms_zpe=-708.850146 te_ms_gfe=0.149290

6 1.323888 -1.320295 0.002039

6 -0.037895 -1.002308 0.010223

6 -0.372863 0.359405 0.011958

6 0.546223 1.440735 0.009478

6 1.919897 1.071300 -0.003746

6 2.272854 -0.286837 -0.005967

7 -1.777474 0.457481 0.024623

7 -2.541492 -1.044740 0.007220

7 -3.698233 -0.895162 -0.018212

7 -3.896778 0.967148 -0.036418

7 -2.734672 1.266414 -0.014315

8 3.615267 -0.558505 -0.016273

1 3.754905 -1.510406 -0.018156

6 3.055797 2.061708 -0.014451

1 3.695927 1.914067 0.860439

1 3.693402 1.896310 -0.887781

1 2.708137 3.089538 -0.024006

6 1.788648 -2.755934 0.000405

1 2.390840 -2.982862 -0.888292

1 2.398577 -2.982023 0.883974

1 0.946018 -3.444697 0.004181

5 -1.258378 -2.048489 0.020006

1 -1.383569 -2.691820 1.029695

1 -1.383851 -2.715670 -0.973713

5 0.072412 2.900178 0.031737

1 -1.085925 3.162344 0.059617

1 0.834477 3.810189 0.025585

04-2-BH2-ts-02-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H11B2N5O1 04-2-BH2-ts-02-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-509.7 te_zpe=-709.992668 te_gfe=-710.035549 te_ms_zpe=-708.837223 te_ms_gfe=0.148598

6 -1.515596 -1.284368 0.000030

6 -0.138266 -1.073039 -0.000012

6 0.325811 0.248000 -0.000028

6 -0.497681 1.398303 -0.000014

6 -1.897699 1.155031 0.000033

6 -2.369894 -0.167550 0.000056

7 1.741775 0.318433 -0.000063

7 2.319353 -0.806479 -0.000065

7 3.541987 -1.064359 -0.000047

7 4.224258 0.435052 -0.000022

7 3.569488 1.363953 -0.000002

8 -3.730952 -0.320309 0.000101

1 -3.954998 -1.256006 0.000121

6 -2.938456 2.245218 0.000059

1 -3.589360 2.151167 -0.874295

1 -3.589307 2.151174 0.874454

1 -2.494052 3.235672 0.000041

6 -2.096837 -2.677199 0.000048

1 -2.718207 -2.856351 0.886276

1 -2.718331 -2.856322 -0.886099

1 -1.311576 -3.432449 -0.000020

5 1.046028 -2.133553 -0.000064

1 1.290432 -2.718221 -1.015327

1 1.290480 -2.718284 1.015151

5 0.126849 2.803646 -0.000054

1 1.307701 2.928886 -0.000110

1 -0.535871 3.790174 -0.000035

04-2-BH2-ts-03-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H11B2N5O1 04-2-BH2-ts-03-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-357.4 te_zpe=-709.942195 te_gfe=-709.986085 te_ms_zpe=-708.788435 te_ms_gfe=0.144540

6 -1.527967 -1.300194 0.009516

6 -0.135029 -1.102220 0.016703

6 0.254603 0.214885 0.037843

6 -0.497771 1.394856 0.020491

6 -1.900964 1.140374 -0.021202

6 -2.374668 -0.188035 -0.016032

7 1.928231 0.082065 0.018918

7 2.270004 -1.107401 0.002580

7 4.548934 -0.434992 -0.050767

7 4.353429 0.659480 -0.061393

7 2.463315 1.223187 0.008138

8 -3.733687 -0.332048 -0.033403

1 -3.961181 -1.267248 -0.049387

6 -2.947173 2.225745 -0.051303

1 -3.649160 2.045256 -0.869144

1 -3.539234 2.208021 0.869316

1 -2.515903 3.214753 -0.165293

6 -2.100124 -2.695205 0.029703

1 -2.748882 -2.851016 0.900532

1 -2.691266 -2.898940 -0.872137

1 -1.305383 -3.437213 0.074004

5 1.087686 -2.135095 0.010440

1 1.150152 -2.816171 -0.988563

1 1.159051 -2.825908 1.002498

5 0.069396 2.821028 0.092911

1 1.205199 2.977405 0.400376

1 -0.592141 3.780163 -0.128368

04-2-BH2-ts-04-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H11B2N5O1 04-2-BH2-ts-04-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-207.6 te_zpe=-709.986272 te_gfe=-710.026955 te_ms_zpe=-708.831005 te_ms_gfe=0.153588

6 -1.737237 -1.197031 0.000000

6 -0.349569 -1.329247 0.000000

6 0.304921 -0.102937 0.000000

6 -0.118919 1.219641 0.000000

6 -1.506806 1.328896 0.000000

6 -2.268588 0.122367 0.000000

7 1.664012 -0.308161 0.000000

7 2.194648 -1.409719 0.000000

7 4.196366 -0.330884 0.000000

7 3.588266 0.656202 0.000000

7 2.353299 0.958806 0.000000

8 -3.617468 0.309989 0.000000

1 -4.067341 -0.541569 0.000000

6 -2.224846 2.652655 0.000000

1 -2.870756 2.753397 -0.877129

1 -2.870754 2.753398 0.877131

1 -1.509554 3.475489 -0.000001

6 -2.666193 -2.386963 0.000000

1 -3.312326 -2.407012 0.886871

1 -3.312326 -2.407012 -0.886871

1 -2.093240 -3.313754 0.000000

5 0.825494 -2.456693 0.000000

1 0.951404 -3.108616 -1.004164

1 0.951404 -3.108616 1.004163

5 1.140702 2.239326 0.000000

1 1.334770 2.851617 -1.012426

1 1.334770 2.851617 1.012427

04-2-BH2-ts-05-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H11B2N5O1 04-2-BH2-ts-05-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-237.5 te_zpe=-710.002946 te_gfe=-710.043991 te_ms_zpe=-708.843680 te_ms_gfe=0.152891

6	1.474242	-1.310502	-0.000021
6	0.103099	-1.060701	-0.000008
6	-0.320733	0.281231	0.000001
6	0.529836	1.417804	-0.000011
6	1.913954	1.134356	-0.000026
6	2.349310	-0.212142	-0.000018
7	-1.719391	0.356779	0.000014
7	-2.242965	-0.788378	0.000016
7	-3.621779	-0.915637	0.000034
7	-4.057457	0.311703	0.000046
7	-3.586072	1.371097	0.000044
8	3.701520	-0.393012	-0.000009
1	3.905590	-1.334013	-0.000014
6	2.989882	2.189087	-0.000033
1	3.637062	2.074340	0.874490
1	3.637237	2.074147	-0.874399
1	2.575984	3.192665	-0.000179
6	2.020734	-2.716396	-0.000020
1	2.636924	-2.912895	-0.886389
1	2.636634	-2.913002	0.886526
1	1.210910	-3.444282	-0.000199

5 -1.186200 -1.998263 -0.000001

1 -1.381612 -2.646480 0.997793

1 -1.381625 -2.646460 -0.997806

5 -0.062675 2.840887 -0.000003

1 -1.239893 2.992762 0.000070

1 0.626715 3.808825 -0.000066

##
#

05-2-BH2-iso-gas-cbs-qb3 charge=0 spin=1 mol=C7H9B2N5O1
05-2-BH2-iso-gas-cbs-qb3 CBS-QB3

lf=54.6 te_zpe=-670.727300 te_gfe=-670.766062 te_ms_zpe=-669.645256
te_ms_gfe=0.131775

7 -1.809013 0.165613 0.000088

6 -0.393571 0.338209 0.000021

6 0.184047 -0.935409 0.000033

6 0.310855 1.561971 -0.000038

6 1.580452 -1.006098 -0.000034

6 1.703083 1.421609 -0.000123

6 2.340203 0.166380 -0.000121

1 2.058619 -1.976843 -0.000015

1 2.330499 2.304126 -0.000186

7 -2.869272 0.940444 0.000110

7 -3.900293 0.117958 0.000037

7 -3.485725 -1.140523 0.000264

7 -2.186198 -1.115733 0.000163

8 3.694095 0.209735 -0.000191

6 4.421830 -1.015932 -0.000304

1 4.203798 -1.607781 -0.895127

1 5.472435 -0.733115 -0.000443

1 4.204043 -1.607804 0.894564

5 -0.288361 2.987098 0.000042

1 0.471085 3.904453 -0.000179

1 -1.456291 3.185226 0.000159

5 -0.918925 -2.101716 0.000168

1 -0.964267 -2.765960 -1.002295

1 -0.964149 -2.765777 1.002762

05-2-BH2-ts-01-gas-cbs-qb3 charge=0 spin=1 mol=C7H9B2N5O1 05-2-BH2-ts-01-gas-cbs-qb3 CBS-QB3

lf=-510.9 te_zpe=-670.676748 te_gfe=-670.717369 te_ms_zpe=-669.585591 te_ms_gfe=0.124051

7 1.735030 0.192770 -0.000170

6 0.324598 0.292537 -0.000050

6 -0.310451 -0.956662 0.000096

6 -0.361828 1.525945 -0.000076

6 -1.704280 -0.984566 0.000224

6 -1.763168 1.439829 0.000057

6 -2.435265 0.212262 0.000205

1 -2.215767 -1.939034 0.000338

1 -2.358606 2.344614 0.000046

7 3.639796 1.031275 -0.000403

7 4.197020 0.038056 -0.000382

7 3.367400 -1.374488 -0.000206

7 2.178376 -0.991535 -0.000126

8 -3.793509 0.284888 0.000322

6 -4.545150 -0.922777 0.000475

1 -4.342200 -1.521470 0.895090

1 -5.590380 -0.619336 0.000548

1 -4.342361 -1.521596 -0.894091

5 0.321356 2.904704 -0.000236

1 -0.359863 3.882848 -0.000244

1 1.504888 3.014860 -0.000351

5 0.720432 -2.164494 0.000090

1 0.896748 -2.766424 1.017987

1 0.896565 -2.766569 -1.017754

05-2-BH2-ts-02-gas-cbs-qb3 charge=0 spin=1 mol=C7H9B2N5O1 05-2-BH2-ts-02-gas-cbs-qb3 CBS-QB3

lf=-532.0 te_zpe=-670.686970 te_gfe=-670.728051 te_ms_zpe=-669.598388 te_ms_gfe=0.125173

7 1.792456 0.263571 0.000006

6 0.395519 0.392025 -0.000001

6 -0.167455 -0.893140 0.000001

6 -0.346476 1.596235 -0.000008

6 -1.562146 -0.975287 -0.000005

6 -1.742399 1.437903 -0.000014

6 -2.353034 0.179515 -0.000013

1 -2.023129 -1.954906 -0.000004

1 -2.379215 2.313847 -0.000020

7 2.865555 0.912871 0.000013

7 3.965269 0.431600 0.000023

7 3.467464 -1.379848 0.000026

7 2.301635 -1.342292 0.000017

8 -3.713118 0.185723 -0.000019

6 -4.403085 -1.058730 -0.000018

1 -4.169927 -1.646302 0.894512

1 -5.462189 -0.808184 -0.000024

1 -4.169918 -1.646309 -0.894542

5 0.250982 3.011159 -0.000011

1 -0.489003 3.944165 -0.000018

1 1.425027 3.201426 -0.000007

5 0.859146 -2.127837 0.000010

1 0.875230 -2.789282 1.004073

1 0.875241 -2.789287 -1.004049

05-2-BH2-ts-03-gas-cbs-qb3 charge=0 spin=1 mol=C7H9B2N5O1 05-2-BH2-ts-03-gas-cbs-qb3 CBS-QB3

lf=-370.1 te_zpe=-670.626100 te_gfe=-670.667120 te_ms_zpe=-669.537548 te_ms_gfe=0.120899

7 1.886193 -0.069008 0.000125

6 0.252676 0.267579 0.000094

6 -0.304338 -0.992457 0.000122

6 -0.368040 1.518826 0.000070

6 -1.710025 -1.011650 0.000100

6 -1.772054 1.412031 0.000059

6 -2.441282 0.176193 0.000064

1 -2.206335 -1.973951 0.000127

1 -2.369146 2.314934 0.000043

7 2.515319 1.019505 -0.000140

7 4.353125 0.278028 -0.000547

7 4.447366 -0.829046 -0.000532

7 2.086553 -1.286734 0.000262

8 -3.795194 0.254642 0.000042

6 -4.549311 -0.954455 0.000050

1 -4.344295 -1.551136 0.894885

1 -5.593761 -0.649369 0.000025

1 -4.344261 -1.551168 -0.894756

5 0.240606 2.934108 0.000035

1 -0.501704 3.864322 0.000053

1 1.414185 3.105840 -0.000011

5 0.781742 -2.169159 0.000224

1 0.764670 -2.853461 0.997231

1 0.764813 -2.853504 -0.996759

05-2-BH2-ts-04-gas-cbs-qb3 charge=0 spin=1 mol=C7H9B2N5O1 05-2-BH2-ts-04-gas-cbs-qb3 CBS-QB3

lf=-237.8 te_zpe=-670.686385 te_gfe=-670.725303 te_ms_zpe=-669.591184 te_ms_gfe=0.128065

7 1.715245 0.230905 -0.000072

6 0.321299 0.332256 -0.000020

6 -0.280237 -0.942131 0.000030

6 -0.389316 1.557230 -0.000016

6 -1.673056 -1.005295 0.000087

6 -1.780303 1.432251 0.000042

6 -2.422671 0.177826 0.000093

1 -2.164717 -1.969710 0.000127

1 -2.406301 2.316289 0.000048

7 3.689879 1.000851 -0.000167

7 4.025603 -0.109230 -0.000154

7 3.437867 -1.272623 -0.000107

7 2.087533 -0.972449 -0.000062

8 -3.776647 0.229213 0.000146

6 -4.514157 -0.990128 0.000188

1 -4.301243 -1.583937 0.894908

1 -5.562516 -0.698706 0.000215

1 -4.301298 -1.583965 -0.894527

5 0.265262 2.953386 -0.000070

1 -0.439050 3.914705 -0.000064

1 1.445815 3.087168 -0.000116

5 0.876430 -2.038124 0.000010

1 0.985931 -2.703019 0.998917

1 0.985854 -2.703070 -0.998871

05-2-BH2-ts-05-gas-cbs-qb3 charge=0 spin=1 mol=C7H9B2N5O1 05-2-BH2-ts-05-gas-cbs-qb3 CBS-QB3

lf=-239.3 te_zpe=-670.667484 te_gfe=-670.706781 te_ms_zpe=-669.572873 te_ms_gfe=0.127289

7 -1.757884 -0.110309 0.017329

6 -0.358979 0.194535 0.037626

6 0.304764 -1.037079 0.063096

6 0.263607 1.464500 0.002429

6 1.703161 -1.026227 0.044271

6 1.658943 1.406221 -0.058863

6 2.378659 0.192145 -0.026047

1 2.243498 -1.963506 0.072664

1 2.233578 2.322777 -0.110663

7 -2.746437 0.962021 -0.106758

7 -3.838505 0.314194 -0.124062

7 -4.265284 -0.756365 -0.081622

7 -2.093566 -1.296764 0.061405

8 3.725820 0.330171 -0.071583

6 4.536292 -0.841776 -0.050116

1 4.329936 -1.483557 -0.912703

1 5.564428 -0.488856 -0.098526

1 4.389055 -1.409965 0.874004

5 -0.357312 2.871353 0.187496

1 0.313909 3.808353 -0.116523

1 -1.420402 3.046224 0.677248

5 -0.800063 -2.191684 0.108185

1 -0.845607 -2.925730 -0.853114

1 -0.835027 -2.848799 1.123444

##
###

01-2BH2-b3-ts-03-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H7B2N5
01-2BH2-b3-ts-03-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-452.7 te_zpe=-556.156593 te_gfe=-556.194165 te_ms_zpe=-555.227706 te_ms_gfe=0.096831

6 -2.780710 0.560002 0.000075

6 -1.499154 1.131530 -0.000024

6 -0.438972 0.189250 -0.000037

6 -0.576071 -1.200531 -0.000001

6 -1.893580 -1.690056 0.000071

6 -2.978330 -0.825512 0.000119

1 -3.637548 1.223320 0.000098

1 -2.055670 -2.762434 0.000092

1 -3.987144 -1.223027 0.000186

7 0.936972 0.590580 -0.000015

7 1.641520 1.530518 0.000286

7 3.369419 0.645317 0.000261

7 2.934431 -0.463704 -0.000062

7 1.782892 -0.897675 -0.000421

5 0.764899 -2.091163 -0.000025

1 0.888240 -2.744842 -1.006687

1 0.888564 -2.744396 1.006893

5 -1.373710 2.670114 -0.000256

1 -2.380817 3.305710 -0.000093

1 -0.327305 3.227560 -0.000637

01-2BH2-b3-ts-04-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H7B2N5 01-2BH2-b3-ts-04-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-239.4 te_zpe=-556.162589 te_gfe=-556.198085 te_ms_zpe=-555.228898 te_ms_gfe=0.099189

6	2.769388	0.825134	-0.000010
6	1.418943	1.217864	-0.000008
6	0.498113	0.145692	-0.000002
6	0.835354	-1.222189	0.000000
6	2.196505	-1.535665	-0.000004
6	3.151946	-0.519324	-0.000009
1	3.531460	1.596203	-0.000013
1	2.515215	-2.572806	-0.000003
1	4.206073	-0.774069	-0.000013
7	-0.897632	0.318621	0.000003
7	-2.708580	1.450118	0.000001
7	-3.232674	0.419339	0.000008
7	-2.869278	-0.835858	0.000012
7	-1.490047	-0.790653	0.000009
5	-0.508381	-2.073377	0.000016
1	-0.753665	-2.702266	0.998126
1	-0.753682	-2.702299	-0.998068
5	1.032532	2.707851	-0.000019
1	1.902364	3.522967	-0.000008
1	-0.102529	3.059851	-0.000039

01-2BH2-b3-ts-05-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H7B2N5 01-2BH2-b3-ts-05-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-244.7 te_zpe=-556.143671 te_gfe=-556.179627 te_ms_zpe=-555.210005 te_ms_gfe=0.098332

6	2.622012	0.927540	-0.088880
6	1.246221	1.216673	-0.011316
6	0.435685	0.060508	0.021564
6	0.881474	-1.266212	0.033042
6	2.267359	-1.468247	-0.004693
6	3.125859	-0.378584	-0.075583
1	3.313753	1.760228	-0.140081
1	2.667076	-2.476485	0.010167
1	4.197918	-0.534971	-0.122720
7	-1.005087	-0.013531	0.018551
7	-1.813035	1.196995	-0.084973
7	-2.994630	0.727112	-0.091419
7	-3.575840	-0.268299	-0.049115
7	-1.519820	-1.133619	0.060546
5	-0.393101	-2.224613	0.085049
1	-0.528443	-2.878057	1.094570
1	-0.575521	-2.935622	-0.877738
5	0.855265	2.702045	0.172769
1	1.686596	3.516104	-0.088175
1	-0.184977	3.050979	0.614948

##
#

01-2BH2CH3-iso-gas-cbs-qb3 charge=0 spin=1 mol=C8H11B2N5
01-2BH2CH3-iso-gas-cbs-qb3 CBS-QB3

lf=80.9 te_zpe=-634.808621 te_gfe=-634.844973 te_ms_zpe=-633.755964 te_ms_gfe=0.160260

7 2.899327 0.648877 -0.103972

7 1.655214 1.056028 -0.175186

7 0.878064 0.000015 0.000011

7 1.655257 -1.055971 0.175270

7 2.899370 -0.648853 0.103966

6 -0.546877 -0.000002 -0.000010

6 -1.184458 -1.243486 -0.162389

6 -2.577952 -1.205722 -0.152105

6 -3.261057 -0.000042 -0.000070

6 -2.577994 1.205657 0.152002

6 -1.184502 1.243463 0.162351

1 -3.127115 -2.132124 -0.271785

1 -4.345472 -0.000059 -0.000093

1 -3.127190 2.132042 0.271667

6 -0.371965 2.498075 0.367530

1 -0.171118 2.599919 1.444140

1 -0.979256 3.365296 0.096293

6 -0.371877 -2.498076 -0.367504

1 -0.979160 -3.365305 -0.096273

1 -0.170984 -2.599944 -1.444103

5 1.008772 2.516408 -0.483588

5 1.008816 -2.516375 0.483683

1 0.844991 2.477355 -1.683146

1 1.835888 3.312343 -0.141426

1 0.844979 -2.477282 1.683231

1 1.835965 -3.312292 0.141571

01-2BH2CH3-ts-01-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H11B2N5 01-2BH2CH3-ts-01-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-526.9 te_zpe=-634.753548 te_gfe=-634.792440 te_ms_zpe=-633.692796 te_ms_gfe=0.150737

7 -3.107341 -0.300533 -0.384748

7 -2.118094 -0.910528 -0.311723

7 -0.872874 0.206888 0.233028

7 -1.536800 1.284746 0.274202

7 -2.714975 1.387771 0.031375

6 0.508507 -0.040060 0.110316

6 1.425522 0.975063 -0.226628

6 2.763347 0.593474 -0.327910

6 3.154056 -0.731000 -0.145582

6 2.213072 -1.711811 0.149896

6 0.862993 -1.391586 0.297776

1 3.505019 1.347197 -0.567870

1 4.200233 -0.998830 -0.240755

1 2.522914 -2.742624 0.277888

6 -0.202034 -2.415701 0.588345

1 -0.578730 -2.264937 1.609716

1 0.246475 -3.412757 0.576861

6 0.979805 2.396867 -0.462570

1 1.871734 3.030459 -0.597465

1 0.446460 2.479889 -1.418850

5 -1.446505 -2.409610 -0.455222

5 0.176526 3.115918 0.681327

1 -1.130534 -2.412554 -1.620400

1 -2.349989 -3.154831 -0.192386

1 0.293438 2.775599 1.817582

1 -0.458151 4.091967 0.428356

01-2BH2CH3-ts-03-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H11B2N5 01-2BH2CH3-ts-03-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-421.2 te_zpe=-634.722583 te_gfe=-634.760675 te_ms_zpe=-633.656997 te_ms_gfe=0.150816

7 3.458683 0.552880 -0.044117

7 1.464261 1.206885 -0.129080

7 0.916658 0.096390 -0.049793

7 1.556084 -1.092337 -0.099061

7 3.311698 -0.551605 0.133973

6 -0.593142 -0.000126 -0.037347

6 -1.171808 -1.267283 -0.173426

6 -2.571264 -1.315845 -0.137218

6 -3.320390 -0.155354 0.004677

6 -2.694353 1.079410 0.141796

6 -1.300417 1.197475 0.134031

1 -3.060793 -2.276139 -0.242338

1 -4.402927 -0.212818 0.017413

1 -3.284027 1.976345 0.288126

6 -0.610304 2.504207 0.372633

1 -0.430345 2.621003 1.449061

1 -1.247090 3.335652 0.062671

6 -0.342628 -2.488335 -0.333526

1 -0.855863 -3.380480 0.031477

1 -0.053744 -2.647712 -1.375839

5 0.807706 2.556458 -0.449531

5 1.048309 -2.320268 0.621694

1 0.638155 2.532487 -1.656762

1 1.545652 3.436796 -0.093918

1 0.769450 -2.134411 1.779699

1 1.775610 -3.242058 0.366416

##
##

01-BH2-b3-iso-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H6B1N5
01-BH2-b3-iso-2d-d-p-cbs-qb3 CBS-QB3

lf=116.3 te_zpe=-530.772125 te_gfe=-530.805462 te_ms_zpe=-529.916126
te_ms_gfe=0.094072

6 2.670817 -1.190590 -0.000010

6 1.310347 -1.473454 -0.000027

6 0.459685 -0.375736 -0.000022

6 0.843794 0.972719 0.000010

6 2.221274 1.206334 0.000017

6 3.116604 0.137647 0.000008

1 3.387601 -2.002523 -0.000012

1 0.929940 -2.486818 -0.000040

1 2.597349 2.223130 0.000027

1 4.182727 0.335043 0.000013

7 -0.958344 -0.432769 -0.000015

7 -1.862065 -1.381366 0.000041

7 -3.020265 -0.749589 0.000018

7 -2.827248 0.562986 -0.000097

7 -1.541364 0.763455 0.000004

5 -0.434742 1.948748 0.000050

1 -0.597030 2.593539 -1.002371

1 -0.596999 2.593339 1.002617

01-BH2-b3-ts-01-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H6B1N5 01-BH2-b3-ts-01-2d-d-p-cbs-qb3 CBS-QB3

lf=-562.2 te_zpe=-530.727452 te_gfe=-530.763793 te_ms_zpe=-529.861591 te_ms_gfe=0.085501

6 -2.371914 -1.521583 -0.131041

6 -0.985904 -1.416999 -0.191867

6 -0.381610 -0.163378 -0.092273

6 -1.144517 1.020168 0.087103

6 -2.546318 0.864481 0.088367

6 -3.159870 -0.379229 -0.004149

1 -2.835230 -2.498654 -0.206639

1 -0.367184 -2.295343 -0.323254

1 -3.155809 1.755207 0.190698

1 -4.240025 -0.460553 0.020044

7 1.025493 -0.157067 -0.148535

7 2.106591 -1.196658 0.672331

7 3.162398 -0.738630 0.450081

7 3.004735 0.660761 -0.506526

7 1.800253 0.730231 -0.656315

5 -0.564632 2.412766 0.401219

1 0.575392 2.581362 0.685266

1 -1.309475 3.342919 0.413701

01-BH2-b3-ts-02-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H6B1N5 01-BH2-b3-ts-02-2d-d-p-cbs-qb3 CBS-QB3

lf=-238.0 te_zpe=-530.728657 te_gfe=-530.762386 te_ms_zpe=-529.859431 te_ms_gfe=0.090027

6 -2.748850 -1.251382 -0.000017

6 -1.383716 -1.500289 -0.000033

6 -0.540363 -0.388909 -0.000007

6 -0.979861 0.953183 0.000034

6 -2.358898 1.159050 0.000048

6 -3.227454 0.067197 0.000023

1 -3.448918 -2.078245 -0.000035

1 -0.982129 -2.506221 -0.000064

1 -2.761847 2.165998 0.000079

1 -4.298583 0.237556 0.000035

7 0.858403 -0.473394 -0.000020

7 2.720951 -1.494344 -0.000057

7 3.190510 -0.435220 -0.000033

7 2.756917 0.795067 0.000004

7 1.379884 0.670163 0.000009

5 0.309294 1.889881 0.000049

1 0.516612 2.531234 0.998805

1 0.516595 2.531279 -0.998681

01-BH2-b3-ts-03-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H6B1N5 01-BH2-b3-ts-03-2d-d-p-cbs-qb3 CBS-QB3

lf=-238.6 te_zpe=-530.715037 te_gfe=-530.748837 te_ms_zpe=-529.845824 te_ms_gfe=0.089784

6 2.562311 -1.346874 -0.000165

6 1.179192 -1.466057 -0.000178

6 0.470680 -0.268882 -0.000016

6 1.017631 1.021071 0.000147

6 2.414124 1.090999 0.000152

6 3.168320 -0.080084 0.000000

1 3.177995 -2.238257 -0.000285

1 0.678569 -2.425033 -0.000305

1 2.912939 2.053840 0.000277

1 4.251151 -0.017903 0.000008

7 -0.948612 -0.120148 -0.000008

7 -1.791759 -1.307295 -0.000159

7 -2.958853 -0.797935 -0.000106

7 -3.492085 0.226096 0.000013

7 -1.409055 1.022553 0.000128

5 -0.205698 2.056221 0.000223

1 -0.331574 2.741186 -0.988898

1 -0.331593 2.741134 0.989370

01-BH2-b3-ts-04-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H6B1N5 01-BH2-b3-ts-04-2d-d-p-cbs-qb3 CBS-QB3

lf=-441.8 te_zpe=-530.724921 te_gfe=-530.759441 te_ms_zpe=-529.860334 te_ms_gfe=0.089101

6 2.762793 -1.103569 -0.000049

6 1.426915 -1.466169 -0.000095

6 0.489252 -0.430399 -0.000054

6 0.787267 0.937329 0.000038

6 2.151780 1.254762 0.000080

6 3.117610 0.254318 0.000038

1 3.530546 -1.867513 -0.000082

1 1.109979 -2.501656 -0.000161

1 2.455792 2.295443 0.000147

1 4.167680 0.525428 0.000072

7 -0.907705 -0.700050 -0.000065

7 -1.679762 -1.586280 0.000046

7 -3.340716 -0.527404 0.000118

7 -2.792542 0.527146 0.000001

7 -1.601075 0.844963 -0.000198

5 -0.468118 1.949242 0.000103

1 -0.542163 2.608111 -1.007240

1 -0.542352 2.607721 1.007692

01-BH2-b3-ts-05-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H6B1N5
01-BH2-b3-ts-05-2d-d-p-cbs-qb3 CBS-QB3

lf=-535.6 te_zpe=-530.730712 te_gfe=-530.765322 te_ms_zpe=-529.868191 te_ms_gfe=0.088430

6 -2.720616 -1.162559 -0.037972

6 -1.368600 -1.480406 0.055371

6 -0.466363 -0.422632 0.079515

6 -0.822293 0.937280 0.028026

6 -2.189381 1.204350 -0.059845

6 -3.127103 0.171454 -0.092906

1 -3.455072 -1.958605 -0.066799

1 -1.028073 -2.507283 0.105320

1 -2.527666 2.233856 -0.108315

1 -4.182951 0.406261 -0.164580

7 0.930699 -0.534746 0.198491

7 1.853610 -1.369401 -0.001846

7 3.010598 -1.094664 -0.145947

7 2.840510 0.787489 -0.113162

7 1.694726 0.950189 0.031324

5 0.395031 1.983464 0.077523

1 0.531439 2.569193 1.119477

1 0.542305 2.682269 -0.887871

###
#

01-CH3BH2-iso-gas-cbs-qb3 charge=0 spin=1 mol=C7H8B1N5
01-CH3BH2-iso-gas-cbs-qb3 CBS-QB3

lf=95.9 te_zpe=-570.067758 te_gfe=-570.102478 te_ms_zpe=-569.144371
te_ms_gfe=0.121199

7 -2.960838 0.050545 0.099870

7 -1.750754 0.522571 0.161874

7 -0.921744 -0.494158 -0.059135

7 -1.617983 -1.598759 -0.256874

7 -2.871673 -1.251854 -0.151514

6 0.505195 -0.383584 -0.031784

6 1.255590 -1.547064 0.131779

6 2.638268 -1.440108 0.171485

6 3.236262 -0.184181 0.058291

6 2.459429 0.958731 -0.105271

6 1.063054 0.897748 -0.161636

1 0.757866 -2.502565 0.229014

1 3.243267 -2.328918 0.299898

1 4.315944 -0.096632 0.098631

1 2.936664 1.927860 -0.195333

6 0.176296 2.099611 -0.362890

1 -0.041184 2.188396 -1.437572

1 0.727939 3.003795 -0.093792

5 -1.198372 2.012913 0.495606

1 -1.020174 1.972865 1.692765

1 -2.072063 2.765298 0.168963

01-CH3BH2-ts-01-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H8B1N5 01-CH3BH2-ts-01-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-536.6 te_zpe=-570.030795 te_gfe=-570.066229 te_ms_zpe=-569.100620 te_ms_gfe=0.116218

7 -2.996290 0.157938 0.387027

7 -1.948219 0.662522 0.277977

7 -0.866902 -0.535300 -0.344270

7 -1.618054 -1.559664 -0.360020

7 -2.787527 -1.543652 -0.070482

6 0.531113 -0.443266 -0.174141

6 1.318042 -1.563198 0.101319

6 2.684906 -1.391190 0.276318

6 3.236891 -0.112170 0.208056

6 2.427710 0.991794 -0.047568

6 1.052546 0.860727 -0.259453

1 0.862178 -2.543636 0.163326

1 3.312886 -2.251338 0.474687

1 4.302010 0.024632 0.354867

1 2.866257 1.982391 -0.093367

6 0.129357 2.021074 -0.515361

1 -0.220601 1.977704 -1.556278

1 0.688144 2.956266 -0.422833

5 -1.147184 2.089525 0.485569

1 -0.871344 2.025066 1.659531

1 -1.968061 2.925753 0.225568

01-CH3BH2-ts-02-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H8B1N5 01-CH3BH2-ts-02-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-508.8 te_zpe=-570.021886 te_gfe=-570.058681 te_ms_zpe=-569.091599 te_ms_gfe=0.113349

7 -2.907809 0.455156 0.108046

7 -1.683822 0.512476 0.222698

7 -0.892291 -0.470071 0.085667

7 -2.172563 -1.781696 -0.350061

7 -3.145178 -1.165583 -0.258463

6 0.512702 -0.387963 0.045560

6 1.221346 -1.573923 0.253150

6 2.608881 -1.556649 0.208126

6 3.276301 -0.355847 -0.025441

6 2.555153 0.819399 -0.225181

6 1.159209 0.839899 -0.209193

1 0.676228 -2.489433 0.445946

1 3.164404 -2.473370 0.364586

1 4.359580 -0.332818 -0.051639

1 3.083589 1.749043 -0.406450

6 0.346757 2.088124 -0.428492

1 -0.011852 2.118146 -1.466408

1 0.992401 2.967717 -0.314325

5 -0.864710 2.262417 0.597470

1 -0.655484 2.056621 1.757913

1 -1.755767 3.001802 0.316653

01-CH3BH2-ts-03-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H8B1N5 01-CH3BH2-ts-03-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-283.8 te_zpe=-569.968416 te_gfe=-570.004861 te_ms_zpe=-569.043286 te_ms_gfe=0.111193

7 -3.611321 -0.151927 0.158488

7 -1.530712 0.727999 0.496727

7 -1.015838 -0.295224 0.006555

7 -1.368891 -1.358321 -0.566346

7 -3.345684 -1.135531 -0.297612

6 0.548591 -0.400753 -0.064330

6 1.192307 -1.583327 0.270247

6 2.580196 -1.553130 0.325519

6 3.258710 -0.364801 0.049575

6 2.562619 0.795892 -0.263239

6 1.158582 0.824081 -0.335248

1 0.629495 -2.480210 0.480356

1 3.122705 -2.452985 0.587228

1 4.341757 -0.342692 0.087132

1 3.099120 1.717863 -0.454440

6 0.351328 2.062063 -0.513883

1 -0.168592 2.060197 -1.478681

1 0.988172 2.947188 -0.473329

5 -0.778790 2.060900 0.701037

1 -0.342229 2.105776 1.831104

1 -1.583361 2.951239 0.518908

01-CH3BH2-ts-04-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H8B1N5 01-CH3BH2-ts-04-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-187.1 te_zpe=-570.008272 te_gfe=-570.043890 te_ms_zpe=-569.070363 te_ms_gfe=0.115825

7 -3.586397 -0.237410 0.054128

7 -1.576039 0.828467 0.151893

7 -0.942326 -0.173312 -0.030663

7 -1.719068 -1.543681 -0.230221

7 -2.892994 -1.145357 -0.118246

6 0.488173 -0.319621 -0.035870

6 1.062014 -1.582741 0.101180

6 2.445824 -1.678658 0.151405

6 3.221023 -0.521937 0.066431

6 2.621287 0.726411 -0.077089

6 1.232179 0.871395 -0.136359

1 0.431498 -2.456194 0.177000

1 2.914318 -2.648655 0.262290

1 4.301919 -0.593930 0.110780

1 3.236508 1.616114 -0.148847

6 0.533239 2.190630 -0.331047

1 0.406901 2.349406 -1.411937

1 1.178592 3.002129 0.016600

5 -0.909044 2.240700 0.418419

1 -0.857081 2.223015 1.638188

1 -1.672094 3.090791 0.043687

01-CH3BH2-ts-05-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H8B1N5 01-CH3BH2-ts-05-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-231.2 te_zpe=-570.022859 te_gfe=-570.058123 te_ms_zpe=-569.085530 te_ms_gfe=0.116745

7 -2.955232 0.388373 0.096585

7 -1.547754 0.554700 0.104342

7 -0.841846 -0.450442 -0.051421

7 -2.535642 -1.851250 -0.223595

7 -3.135627 -0.879976 -0.069956

6 0.559132 -0.378626 -0.030476

6 1.239717 -1.596238 0.088916

6 2.624991 -1.598631 0.139813

6 3.313815 -0.387011 0.057249

6 2.624708 0.816609 -0.085227

6 1.230759 0.859799 -0.137111

1 0.666353 -2.512763 0.154935

1 3.164658 -2.531834 0.243843

1 4.397332 -0.380536 0.097862

1 3.176835 1.746856 -0.161229

6 0.427040 2.114948 -0.336967

1 0.278503 2.255141 -1.418081

1 1.003146 2.981595 -0.000051

5 -0.991856 2.059315 0.438994

1 -0.901891 2.002496 1.648225

1 -1.833930 2.827534 0.070652

##
#

01-iso-gas charge=0 spin=1 mol=C6H5N5 01-iso-gas CBS-QB3

lf=23.1 te_zpe=-505.322800 te_gfe=-505.357051 te_ms_zpe=-504.528288 te_ms_gfe=0.080626

7 -3.017569 0.674794 -0.000436

7 -1.795181 1.098151 0.001067

7 -1.043743 0.000081 -0.000023

7 -1.795341 -1.097938 -0.000348

7 -3.017827 -0.674919 -0.000080

6 0.384736 0.000034 -0.000050

6 1.064011 -1.216953 0.000312

6 2.454755 -1.206395 0.000316

6 3.152654 -0.000088 -0.000021

6 2.454863 1.206282 -0.000364

6 1.064120 1.216962 -0.000387

1 0.507914 -2.144153 0.000584

1 2.992217 -2.147066 0.000599

1 4.236153 -0.000137 -0.000007

1 2.992410 2.146905 -0.000623

1 0.508099 2.144207 -0.000646

01-ts-01-gas charge=0 spin=1 mol=C6H5N5 01-ts-01-gas CBS-QB3

lf=-555.8 te_zpe=-505.296580 te_gfe=-505.331805 te_ms_zpe=-504.495376 te_ms_gfe=0.075590

7 -2.964224 -0.937677 -0.131491

7 -1.761816 -1.041531 -0.279056

7 -0.989601 -0.028499 -0.149888

7 -2.069850 1.229325 0.290194

7 -3.123165 0.717565 0.265529

6 0.417617 -0.034581 -0.079764

6 1.079225 1.190333 -0.201463

6 2.466376 1.225764 -0.114282

6 3.194360 0.052448 0.074124

6 2.524167 -1.164706 0.185833

6 1.136432 -1.217722 0.120964

1 0.505335 2.094487 -0.356890

1 2.979484 2.176105 -0.203383

1 4.275674 0.085616 0.132540

1 3.082552 -2.081952 0.332700

1 0.608477 -2.157763 0.215547

##
#

02-2BH2-iso-gas-cbs-qb3 charge=0 spin=1 mol=C6H7B2N5O1 02-2BH2-iso-gas-cbs-qb3 CBS-QB3

lf=59.4 te_zpe=-631.444761 te_gfe=-631.481509 te_ms_zpe=-630.433891 te_ms_gfe=0.105662

6 -1.794631 -1.343979 0.000036

6 -0.421791 -1.098180 0.000070

6 -0.019395 0.243840 -0.000011

6 -0.878166 1.362366 -0.000100

6 -2.243337 1.043227 -0.000125

6 -2.701535 -0.283024 -0.000061

1 -2.160768 -2.367264 0.000087

1 -2.978799 1.837847 -0.000193

7 1.407006 0.260086 0.000019

7 1.950581 -0.960020 0.000152

7 3.241554 -0.812706 -0.000147

7 3.485980 0.490022 0.000208

7 2.355463 1.168338 -0.000125

8 -4.047492 -0.464128 -0.000108

1 -4.250277 -1.406185 -0.000026

5 0.826803 -2.107078 0.000184

1 0.960090 -2.758701 -1.002439

1 0.959965 -2.758531 1.002942

5 -0.468025 2.853968 -0.000072

1 0.664468 3.200600 0.000335

1 -1.339593 3.665267 -0.000014

02-2BH2-ts-01-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H7B2N5O1 02-2BH2-ts-01-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-532.2 te_zpe=-631.404809 te_gfe=-631.443726 te_ms_zpe=-630.387461 te_ms_gfe=0.099179

6 -1.769320 -1.325776 -0.000012

6 -0.401658 -1.059905 0.000005

6 -0.023905 0.294653 0.000007

6 -0.924653 1.382905 -0.000004

6 -2.289190 1.036000 -0.000022

6 -2.712060 -0.292599 -0.000025

1 -2.110263 -2.358402 -0.000015

1 -3.038278 1.817983 -0.000032

7 1.377361 0.359780 0.000028

7 2.104400 -1.158974 0.000022

7 3.264237 -1.034355 0.000013

7 3.505499 0.827404 0.000003

7 2.350110 1.152246 0.000009

8 -4.055455 -0.522689 -0.000043

1 -4.220989 -1.471418 -0.000044

5 0.787238 -2.139144 0.000022

1 0.894865 -2.791418 -1.004122

1 0.894851 -2.791397 1.004181

5 -0.525205 2.866599 0.000005

1 0.611961 3.214469 0.000025

1 -1.385212 3.690052 -0.000008

02-2BH2-ts-02-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H7B2N5O1 02-2BH2-ts-02-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-509.2 te_zpe=-631.394621 te_gfe=-631.433153 te_ms_zpe=-630.374618 te_ms_gfe=0.098003

6 -1.964036 -1.283313 -0.000029

6 -0.583994 -1.114188 -0.000006

6 -0.088590 0.200012 0.000002

6 -0.902785 1.350974 -0.000011

6 -2.290343 1.118320 -0.000033

6 -2.818839 -0.172788 -0.000043

1 -2.389987 -2.284106 -0.000036

1 -2.976570 1.956256 -0.000043

7 1.324227 0.252227 0.000025

7 1.890873 -0.878389 0.000032

7 3.113957 -1.133765 0.000044

7 3.790296 0.357085 0.000046

7 3.134335 1.287520 0.000036

8 -4.176345 -0.294583 -0.000065

1 -4.417790 -1.226885 -0.000068

5 0.573608 -2.201268 0.000015

1 0.812393 -2.780827 -1.017925

1 0.812361 -2.780821 1.017966

5 -0.366910 2.794111 -0.000004

1 0.798716 3.026041 0.000008

1 -1.146135 3.695944 -0.000011

02-2BH2-ts-03-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H7B2N5O1 02-2BH2-ts-03-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-369.1 te_zpe=-631.343549 te_gfe=-631.382573 te_ms_zpe=-630.326011 te_ms_gfe=0.094741

6 1.971602 -1.308107 0.000339

6 0.578215 -1.150130 0.000230

6 0.156530 0.163908 -0.000020

6 0.903755 1.341941 -0.000176

6 2.292467 1.092949 -0.000050

6 2.821994 -0.204238 0.000202

1 2.384084 -2.314117 0.000535

1 2.977335 1.931095 -0.000151

7 -1.503893 -0.002580 -0.000089

7 -1.830116 -1.192281 0.000094

7 -4.135953 -0.486272 -0.000159

7 -3.921780 0.603625 -0.000332

7 -2.015525 1.146460 -0.000315

8 4.177470 -0.311920 0.000301

1 4.429965 -1.241563 0.000473

5 -0.625277 -2.206553 0.000338

1 -0.679692 -2.888156 0.997507

1 -0.679574 -2.888495 -0.996607

5 0.442179 2.812758 -0.000456

1 -0.707838 3.102308 -0.000580

1 1.274947 3.662657 -0.000548

02-2BH2-ts-04-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H7B2N5O1 02-2BH2-ts-04-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-240.3 te_zpe=-631.384997 te_gfe=-631.422261 te_ms_zpe=-630.361522 te_ms_gfe=0.101202

6 -1.965207 -1.309052 0.028141

6 -0.575791 -1.185882 0.053256

6 -0.043727 0.110644 0.034830

6 -0.791045 1.308932 0.001138

6 -2.176011 1.113534 -0.068315

6 -2.760087 -0.166621 -0.041831

1 -2.428243 -2.292217 0.050779

1 -2.838012 1.969017 -0.121182

7 1.379656 -0.047278 0.018737

7 1.836086 -1.192605 0.061129

7 3.938057 -0.430691 -0.074852

7 3.404688 0.591027 -0.116632

7 2.250542 1.121564 -0.101122

8 -4.116882 -0.212147 -0.091949

1 -4.411223 -1.129574 -0.075999

5 0.643711 -2.219134 0.100492

1 0.769970 -2.941186 -0.862339

1 0.742621 -2.870929 1.114656

5 -0.312684 2.770183 0.196836

1 0.712976 3.044603 0.719532

1 -1.060165 3.638772 -0.130626

02-2BH2-ts-05-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H7B2N5O1 02-2BH2-ts-05-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-238.3 te_zpe=-631.404055 te_gfe=-631.440938 te_ms_zpe=-630.380057 te_ms_gfe=0.102000

6 -1.918681 -1.319746 0.000012

6 -0.544253 -1.107052 0.000021

6 -0.094264 0.230931 -0.000010

6 -0.938667 1.365653 -0.000050

6 -2.310033 1.086895 -0.000057

6 -2.797221 -0.230514 -0.000026

1 -2.318165 -2.331071 0.000033

1 -3.029601 1.896491 -0.000087

7 1.302642 0.290316 0.000005

7 1.810635 -0.862238 0.000041

7 3.185133 -1.005963 0.000071

7 3.636385 0.217917 0.000048

7 3.173942 1.281247 0.000015

8 -4.147115 -0.380963 -0.000032

1 -4.370266 -1.318418 -0.000016

5 0.731232 -2.062215 0.000046

1 0.917032 -2.708899 -0.999168

1 0.917023 -2.708902 0.999258

5 -0.441563 2.826278 -0.000081

1 0.717158 3.087948 -0.000078

1 -1.247041 3.704294 -0.000107

##########
#

02-2CH3BH2-iso-gas-cbs-qb3 charge=0 spin=1 mol=C8H11B2N5O1 02-2CH3BH2-iso-gas-cbs-qb3 CBS-QB3

lf=66.5 te_zpe=-710.051720 te_gfe=-710.089384 te_ms_zpe=-708.908171 te_ms_gfe=0.163188

6 -2.243791 1.194942 0.148519

6 -0.855955 1.234373 0.158165

6 -0.202598 -0.003378 -0.000358

6 -0.846248 -1.249743 -0.158761

6 -2.231847 -1.227390 -0.150370

6 -2.925863 -0.019695 -0.001576

1 -2.800658 2.118844 0.269839

1 -2.797508 -2.142637 -0.270095

7 1.211359 0.004040 0.000114

7 1.984688 1.065279 -0.171374

7 3.233291 0.661785 -0.100501

7 3.239857 -0.632983 0.099834

7 1.995210 -1.049153 0.171586

8 -4.277201 -0.089017 -0.011121

1 -4.652247 0.792269 0.097005

6 -0.052926 2.494100 0.366725

1 0.147886 2.589916 1.443885

1 -0.663353 3.360203 0.099108

6 -0.027670 -2.499767 -0.365533

1 0.175107 -2.593483 -1.442501

1 -0.629748 -3.371742 -0.099115

5 1.330372 2.517369 -0.483453

5 1.355220 -2.508089 0.484910

1 2.146937 3.324045 -0.140727

1 1.163505 2.479633 -1.682727

1 2.181436 -3.305784 0.144191

1 1.188848 -2.468965 1.684357

02-2CH3BH2-ts-01-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H11B2N5O1 02-2CH3BH2-ts-01-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-523.4 te_zpe=-709.994348 te_gfe=-710.034668 te_ms_zpe=-708.843280 te_ms_gfe=0.153394

6 2.114190 -1.314079 0.217518

6 0.732551 -1.202247 0.347450

6 0.166647 0.072921 0.145136

6 0.925796 1.211140 -0.198489

6 2.303560 1.052386 -0.280550

6 2.896655 -0.196916 -0.077483

1 2.582229 -2.284226 0.355003

1 2.940874 1.894476 -0.521118

7 -1.233204 0.095930 0.242030

7 -2.270732 -1.204859 -0.348761

7 -3.343322 -0.760893 -0.440594

7 -3.238916 0.962823 -0.003671

7 -2.065930 1.048363 0.278511

8 4.251115 -0.261075 -0.190116

1 4.543713 -1.166256 -0.039379

6 -0.163347 -2.380582 0.619764

1 -0.592865 -2.281471 1.626147

1 0.434009 -3.296174 0.633466

6 0.265520 2.542602 -0.454979

1 -0.274934 2.524564 -1.410525

1 1.045886 3.306760 -0.601806

5 -1.362110 -2.572868 -0.463680

5 -0.643126 3.140789 0.679977

1 -2.137123 -3.457037 -0.221795

1 -1.009913 -2.530850 -1.617457

1 -1.414746 4.008909 0.414855

1 -0.484558 2.829402 1.819245

02-2CH3BH2-ts-03-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H11B2N5O1 02-2CH3BH2-ts-03-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-438.1 te_zpe=-709.964337 te_gfe=-710.003558 te_ms_zpe=-708.807167 te_ms_gfe=0.154037

6 -2.332141 1.136272 0.135585

6 -0.943199 1.228740 0.125054

6 -0.239694 0.024063 -0.045127

6 -0.855253 -1.232490 -0.175898

6 -2.245809 -1.270167 -0.139917

6 -2.982459 -0.094018 -0.001109

1 -2.912138 2.041783 0.283430

1 -2.771096 -2.211162 -0.237983

7 1.246748 0.097201 -0.056143

7 1.826418 1.189808 -0.137774

7 3.820100 0.480256 -0.026912

7 3.627290 -0.617168 0.141566

7 1.877319 -1.121840 -0.129192

8 -4.332232 -0.206160 0.004077

1 -4.733159 0.664027 0.106855

6 -0.236084 2.527717 0.367770

1 -0.070458 2.638521 1.447587

1 -0.860789 3.367612 0.055212

6 -0.043900 -2.466775 -0.325655

1 0.240787 -2.641425 -1.366115

1 -0.564106 -3.348363 0.054582

5 1.188125 2.556081 -0.434785

5 1.354232 -2.312938 0.631862

1 1.944128 3.420269 -0.076673

1 1.033220 2.541555 -1.646307

1 2.054180 -3.259510 0.393009

1 1.071616 -2.097589 1.783355

##
#

02-BH2-iso-gas-cbs-qb3 charge=0 spin=1 mol=C6H6B1N5O1
02-BH2-iso-gas-cbs-qb3 CBS-QB3

lf=86.8 te_zpe=-606.013707 te_gfe=-606.048434 te_ms_zpe=-605.067117
te_ms_gfe=0.096872

6 1.855987 1.101763 0.000023

6 0.477453 0.912117 0.000023

6 0.036007 -0.420119 -0.000037

6 0.856749 -1.542764 -0.000093

6 2.221934 -1.317090 -0.000108

6 2.718108 -0.000545 -0.000049

1 2.269836 2.106371 0.000079

1 0.447501 -2.544934 -0.000132

1 2.927610 -2.137438 -0.000160

7 -1.377454 -0.422373 -0.000026

7 -1.914782 0.796048 0.000023

7 -3.209175 0.644481 0.000416

7 -3.451660 -0.656637 -0.000404

7 -2.316822 -1.335446 0.000112

8 4.069627 0.132708 -0.000070

1 4.302477 1.067640 -0.000022

5 -0.764260 1.937661 0.000164

1 -0.895669 2.588042 -1.002992

1 -0.895658 2.587666 1.003572

02-BH2-ts-01-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H6B1N5O1 02-BH2-ts-01-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-537.8 te_zpe=-605.970459 te_gfe=-606.006533 te_ms_zpe=-605.017752 te_ms_gfe=0.091075

6 -1.834050 1.077014 -0.016356

6 -0.459773 0.861957 0.047078

6 -0.039122 -0.479539 0.084865

6 -0.905025 -1.568272 0.072239

6 -2.267855 -1.315321 0.003261

6 -2.731939 0.004662 -0.038906

1 -2.217308 2.093550 -0.054250

1 -0.528423 -2.582951 0.111480

1 -2.986181 -2.124695 -0.017594

7 1.362244 -0.529214 0.181742

7 2.054083 0.998531 0.028070

7 3.205754 0.891778 -0.118693

7 3.469922 -0.978347 -0.163643

7 2.325410 -1.310077 -0.022040

8 -4.082065 0.181549 -0.104998

1 -4.279901 1.123785 -0.126647

5 0.708794 1.963925 0.086105

1 0.820076 2.557660 1.126327

1 0.808969 2.668931 -0.881003

02-BH2-ts-02-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H6B1N5O1 02-BH2-ts-02-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-518.0 te_zpe=-605.961033 te_gfe=-605.998075 te_ms_zpe=-605.005120 te_ms_gfe=0.088503

6 2.013240 1.053176 0.000032

6 0.628905 0.927662 0.000038

6 0.096606 -0.373056 -0.000019

6 0.885388 -1.519205 -0.000080

6 2.265141 -1.368675 -0.000085

6 2.827872 -0.086982 -0.000029

1 2.475128 2.037458 0.000075

1 0.432006 -2.502850 -0.000123

1 2.924250 -2.227262 -0.000132

7 -1.314215 -0.415470 -0.000009

7 -1.884039 0.709424 0.000050

7 -3.111736 0.947746 0.000072

7 -3.761654 -0.546013 0.000008

7 -3.088677 -1.467914 -0.000041

8 4.188705 -0.009880 -0.000037

1 4.456684 0.915078 0.000004

5 -0.497771 2.045947 0.000101

1 -0.744767 2.617525 -1.019683

1 -0.744749 2.617429 1.019942

02-BH2-ts-03-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H6B1N5O1 02-BH2-ts-03-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-384.9 te_zpe=-605.911387 te_gfe=-605.948700 te_ms_zpe=-604.960438 te_ms_gfe=0.085705

6 2.027962 1.065519 -0.000001

6 0.632233 0.976946 0.000004

6 0.155995 -0.324307 0.000011

6 0.866278 -1.509674 0.000012

6 2.247760 -1.363271 0.000007

6 2.823771 -0.082278 0.000000

1 2.494092 2.047725 -0.000003

1 0.400837 -2.483496 0.000018

1 2.894548 -2.231091 0.000009

7 -1.471418 -0.129517 0.000013

7 -1.789480 1.056420 0.000024

7 -4.117735 0.272898 -0.000033

7 -3.871678 -0.809002 -0.000030

7 -1.928812 -1.297575 -0.000012

8 4.182910 -0.029813 -0.000005

1 4.469074 0.889997 -0.000009

5 -0.554937 2.061346 0.000013

1 -0.608654 2.739226 -0.998294

1 -0.608633 2.739228 0.998319

02-BH2-ts-04-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H6B1N5O1 02-BH2-ts-04-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-234.8 te_zpe=-605.957057 te_gfe=-605.992241 te_ms_zpe=-604.997571 te_ms_gfe=0.092661

6 2.005542 1.082597 0.000081

6 0.615275 1.013035 0.000050

6 0.053628 -0.272723 -0.000010

6 0.767465 -1.469390 -0.000044

6 2.145668 -1.363971 -0.000016

6 2.759884 -0.094718 0.000046

1 2.511193 2.044670 0.000132

1 0.269143 -2.429651 -0.000090

1 2.777852 -2.242475 -0.000041

7 -1.356158 -0.115297 -0.000027

7 -1.815761 1.028482 0.000010

7 -3.905221 0.233150 -0.000056

7 -3.369803 -0.789542 -0.000090

7 -2.205965 -1.302719 -0.000089

8 4.118566 -0.088590 0.000076

1 4.435362 0.821383 0.000072

5 -0.604068 2.057294 0.000061

1 -0.718069 2.740427 -0.991139

1 -0.718102 2.740398 0.991274

02-BH2-ts-05-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H6B1N5O1 02-BH2-ts-05-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-237.7 te_zpe=-605.971067 te_gfe=-606.006161 te_ms_zpe=-605.011070 te_ms_gfe=0.092975

6 1.967335 1.083020 0.000050

6 0.590437 0.906951 0.000067

6 0.108931 -0.423461 -0.000060

6 0.933823 -1.551464 -0.000213

6 2.299867 -1.344965 -0.000233

6 2.813229 -0.033428 -0.000100

1 2.398398 2.080964 0.000155

1 0.513987 -2.549896 -0.000309

1 2.998199 -2.171903 -0.000350

7 -1.283030 -0.467229 -0.000006

7 -1.778497 0.690353 0.000142

7 -3.154973 0.841678 0.000228

7 -3.611221 -0.377796 0.000116

7 -3.149361 -1.443837 -0.000017

8 4.166160 0.082084 -0.000125

1 4.409778 1.014426 -0.000019

5 -0.676116 1.878958 0.000172

1 -0.855638 2.526430 -0.999632

1 -0.855583 2.526422 0.999984

##
#

02-CH3BH2-iso-gas-cbs-qb3 charge=0 spin=1 mol=C7H8B1N5O1 02-CH3BH2-iso-gas-cbs-qb3 CBS-QB3

lf=77.8 te_zpe=-645.309336 te_gfe=-645.345419 te_ms_zpe=-644.295421 te_ms_gfe=0.124035

6 2.071469 0.969494 -0.126492

6 0.680028 0.898877 -0.172650

6 0.118137 -0.382218 -0.042861

6 0.883813 -1.539574 0.110966

6 2.261233 -1.437235 0.142966

6 2.858205 -0.174633 0.030397

1 2.547131 1.941266 -0.220019

1 0.395678 -2.500070 0.208415

1 2.888416 -2.310117 0.266198

7 -1.302383 -0.495250 -0.058333

7 -2.131105 0.521123 0.166408

7 -3.343267 0.046583 0.112619

7 -3.254311 -1.253288 -0.133606

7 -1.999073 -1.601078 -0.249138

8 4.212709 -0.127849 0.079657

1 4.511335 0.784775 0.000276

6 -0.208053 2.100020 -0.370060

1 -0.434114 2.182681 -1.443381

1 0.342145 3.007084 -0.107926

5 -1.578023 2.009111 0.497917

1 -2.451124 2.764697 0.176828

1 -1.389050 1.971907 1.693534

02-CH3BH2-ts-01-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H8B1N5O1 02-CH3BH2-ts-01-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-534.3 te_zpe=-645.270899 te_gfe=-645.307722 te_ms_zpe=-644.250485 te_ms_gfe=0.118956

6 2.052147 0.961437 -0.146565

6 0.675129 0.835675 -0.325704

6 0.136732 -0.460172 -0.218803

6 0.927064 -1.578932 0.056674

6 2.295736 -1.427127 0.197445

6 2.860172 -0.150517 0.101614

1 2.500406 1.948956 -0.208242

1 0.469519 -2.556772 0.143149

1 2.938357 -2.275909 0.392087

7 -1.263082 -0.532449 -0.347535

7 -2.308116 0.679373 0.326064

7 -3.360495 0.189920 0.458270

7 -3.195266 -1.507062 -0.026677

7 -2.035293 -1.538586 -0.358718

8 4.208260 -0.055112 0.261668

1 4.477848 0.866065 0.181907

6 -0.243038 2.004911 -0.554055

1 -0.638983 1.954408 -1.577714

1 0.326336 2.936243 -0.493160

5 -1.477259 2.089977 0.501779

1 -2.291307 2.942241 0.274045

1 -1.149850 2.025758 1.662215

02-CH3BH2-ts-02-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H8B1N5O1 02-CH3BH2-ts-02-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-501.4 te_zpe=-645.261914 te_gfe=-645.299917 te_ms_zpe=-644.241121 te_ms_gfe=0.116330

6 2.144665 0.901032 -0.232384

6 0.752287 0.869595 -0.209006

6 0.140381 -0.371582 0.067531

6 0.897513 -1.525541 0.294064

6 2.278999 -1.472331 0.241640

6 2.907355 -0.250576 -0.017361

1 2.644370 1.845717 -0.428364

1 0.388992 -2.457770 0.506157

1 2.884697 -2.353437 0.408872

7 -1.256868 -0.494675 0.112780

7 -2.062370 0.475997 0.247645

7 -3.288647 0.421344 0.099010

7 -3.524732 -1.184997 -0.295752

7 -2.565434 -1.813651 -0.401057

8 4.267603 -0.242402 -0.046400

1 4.581377 0.649955 -0.227670

6 -0.104148 2.087237 -0.424186

1 -0.474253 2.100442 -1.458347

1 0.504092 2.992648 -0.313131

5 -1.318179 2.194472 0.617689

1 -2.221787 2.927346 0.359789

1 -1.073360 2.006835 1.775285

02-CH3BH2-ts-03-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H8B1N5O1 02-CH3BH2-ts-03-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-321.0 te_zpe=-645.209166 te_gfe=-645.246823 te_ms_zpe=-644.190846 te_ms_gfe=0.114576

6 2.152060 0.869730 -0.291855

6 0.754305 0.869504 -0.350628

6 0.146416 -0.361952 -0.068196

6 0.830983 -1.526342 0.272327

6 2.211687 -1.484179 0.313484

6 2.873760 -0.283274 0.020789

1 2.676669 1.800594 -0.484000

1 0.290737 -2.432751 0.501113

1 2.791101 -2.358491 0.578555

7 -1.385217 -0.272333 0.018554

7 -1.946525 0.736841 0.479951

7 -3.992350 -0.267472 0.159142

7 -3.653583 -1.227536 -0.298696

7 -1.709910 -1.353866 -0.566673

8 4.228681 -0.302543 0.069533

1 4.575293 0.574653 -0.127519

6 -0.072686 2.095554 -0.509005

1 -0.612323 2.091170 -1.463007

1 0.549570 2.991377 -0.473883

5 -1.190315 2.067235 0.723331

1 -1.987774 2.968548 0.583897

1 -0.727205 2.065382 1.844480

02-CH3BH2-ts-04-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H8B1N5O1 02-CH3BH2-ts-04-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-182.6 te_zpe=-645.250620 te_gfe=-645.287660 te_ms_zpe=-644.222409 te_ms_gfe=0.118631

6 2.195147 0.890333 -0.098393

6 0.805482 0.960116 -0.145081

6 0.113537 -0.265041 -0.046286

6 0.762623 -1.496139 0.075345

6 2.143050 -1.531031 0.116205

6 2.862427 -0.331626 0.035205

1 2.767705 1.810186 -0.174030

1 0.182206 -2.403999 0.148760

1 2.680938 -2.464230 0.218231

7 -1.310750 -0.188085 -0.029032

7 -1.998404 0.777523 0.147774

7 -3.951196 -0.388532 0.069679

7 -3.214614 -1.262932 -0.101542

7 -2.028273 -1.611231 -0.218802

8 4.213687 -0.419038 0.086954

1 4.600429 0.461604 0.027553

6 0.042608 2.243708 -0.335446

1 -0.098021 2.391422 -1.416189

1 0.647914 3.087925 0.006541

5 -1.397785 2.223340 0.422951

1 -2.196854 3.040783 0.051918

1 -1.331476 2.202800 1.641002

02-CH3BH2-ts-05-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H8B1N5O1 02-CH3BH2-ts-05-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-228.9 te_zpe=-645.265525 te_gfe=-645.302121 te_ms_zpe=-644.237297 te_ms_gfe=0.119724

6 2.205109 0.912372 -0.102305

6 0.815861 0.910127 -0.144869

6 0.172085 -0.346551 -0.041573

6 0.899431 -1.541646 0.061948

6 2.278298 -1.512683 0.105385

6 2.934182 -0.276017 0.030139

1 2.733110 1.858773 -0.180577

1 0.359035 -2.478179 0.124508

1 2.865298 -2.416746 0.199528

7 -1.217071 -0.453778 -0.049297

7 -1.955039 0.531312 0.102752

7 -3.358485 0.315206 0.102592

7 -3.493823 -0.957934 -0.052199

7 -2.848128 -1.903207 -0.203100

8 4.288196 -0.292755 0.081064

1 4.627530 0.607436 0.024250

6 -0.022034 2.142649 -0.341730

1 -0.179689 2.271840 -1.422980

1 0.529871 3.027200 -0.011050

5 -1.438994 2.045478 0.438428

1 -2.296482 2.797356 0.071292

1 -1.339046 1.996265 1.647160

##
#

03-2BH2-iso-gas-cbs-qb3 charge=0 spin=1 mol=C7H9B2N5O1
03-2BH2-iso-gas-cbs-qb3 CBS-QB3

lf=58.4 te_zpe=-670.746813 te_gfe=-670.785815 te_ms_zpe=-669.668481
te_ms_gfe=0.130736

6 1.823499 1.582546 0.000009

6 0.424887 1.685236 -0.000003

6 -0.236473 0.440880 -0.000004

6 0.377963 -0.817777 -0.000005

6 1.777487 -0.863184 -0.000009

6 2.486513 0.349965 0.000012

1 2.425948 2.482389 0.000018

7 -1.647262 0.227053 -0.000004

7 -2.729376 0.971069 0.000009

7 -3.735764 0.119142 0.000010

7 -3.285831 -1.126790 -0.000018

7 -1.987605 -1.063658 -0.000009

8 3.846403 0.395987 0.000035

1 4.207878 -0.496294 0.000070

6 2.521385 -2.174112 -0.000006

1 3.160777 -2.274705 -0.885744

1 3.160228 -2.275002 0.886094

1 1.830765 -3.015533 -0.000366

5 -0.217673 3.089203 -0.000036

1 -1.391081 3.251247 -0.000067

1 0.512737 4.029985 0.000013

5 -0.697580 -2.012674 -0.000002

1 -0.726448 -2.680845 -1.001160

1 -0.726456 -2.680820 1.001174

03-2BH2-ts-01-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H9B2N5O1 03-2BH2-ts-01-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-529.4 te_zpe=-670.706122 te_gfe=-670.747156 te_ms_zpe=-669.621509 te_ms_gfe=0.124417

6 -1.873409 1.581388 -0.000063

6 -0.471458 1.710335 -0.000026

6 0.234235 0.487731 0.000004

6 -0.357061 -0.787537 0.000001

6 -1.755639 -0.852339 -0.000036

6 -2.503156 0.341560 -0.000068

1 -2.490898 2.471099 -0.000089

7 1.628826 0.329364 0.000045

7 2.713640 0.959287 0.000057

7 3.804684 0.461588 0.000084

7 3.271215 -1.347048 0.000091

7 2.106685 -1.283064 0.000067

8 -3.868702 0.343533 -0.000105

1 -4.198965 -0.560295 -0.000105

6 -2.476187 -2.177562 -0.000042

1 -3.114146 -2.287298 0.885761

1 -3.114097 -2.287317 -0.885879

1 -1.775785 -3.010634 -0.000014

5 0.160946 3.107488 -0.000021

1 1.339425 3.269021 0.000011

1 -0.555010 4.059322 -0.000050

5 0.654567 -2.038773 0.000040

1 0.661086 -2.704021 1.002430

1 0.661135 -2.704045 -1.002333

03-2BH2-ts-02-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H9B2N5O1 03-2BH2-ts-02-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-507.8 te_zpe=-670.696009 te_gfe=-670.736762 te_ms_zpe=-669.608410 te_ms_gfe=0.123063

6 1.871401 1.620161 0.000000

6 0.464863 1.661132 0.000002

6 -0.171226 0.404072 0.000003

6 0.506908 -0.824969 0.000003

6 1.902065 -0.820424 -0.000001

6 2.575489 0.419341 -0.000001

1 2.436726 2.544150 0.000000

7 -1.576906 0.252880 0.000001

7 -3.527440 1.014318 -0.000001

7 -4.039092 -0.001480 -0.000004

7 -3.145484 -1.382869 -0.000006

7 -1.974706 -0.947574 -0.000002

8 3.938554 0.501876 -0.000004

1 4.321861 -0.380743 -0.000004

6 2.693765 -2.105024 -0.000002

1 3.336164 -2.183196 -0.885850

1 3.336141 -2.183212 0.885861

1 2.038391 -2.975430 -0.000019

5 -0.269181 3.011038 0.000002

1 -1.456261 3.075917 0.000002

1 0.373538 4.015151 0.000003

5 -0.494034 -2.061367 0.000010

1 -0.646546 -2.674347 -1.015981

1 -0.646556 -2.674320 1.016016

03-2BH2-ts-03-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H9B2N5O1 03-2BH2-ts-03-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-370.8 te_zpe=-670.646158 te_gfe=-670.687433 te_ms_zpe=-669.561188 te_ms_gfe=0.119825

6 -1.884925 1.585893 -0.000015

6 -0.474346 1.650620 -0.000001

6 0.095501 0.379237 0.000017

6 -0.501023 -0.863628 0.000028

6 -1.909470 -0.853239 0.000012

6 -2.584349 0.376628 -0.000008

1 -2.452467 2.507743 -0.000031

7 1.722192 -0.008147 0.000038

7 2.392228 1.054814 -0.000015

7 4.196538 0.247856 -0.000098

7 4.249601 -0.862309 -0.000085

7 1.882348 -1.232630 0.000067

8 -3.943974 0.462694 -0.000021

1 -4.329077 -0.419712 -0.000012

6 -2.684154 -2.146326 0.000024

1 -3.324917 -2.228509 0.886807

1 -3.324980 -2.228488 -0.886715

1 -2.011597 -3.001758 -0.000010

5 0.183234 3.040724 -0.000001

1 1.362673 3.169065 0.000027

1 -0.523643 3.998293 -0.000028

5 0.552987 -2.071600 0.000060

1 0.515456 -2.757993 0.996011

1 0.515489 -2.758013 -0.995878

03-2BH2-ts-04-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H9B2N5O1 03-2BH2-ts-04-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-240.4 te_zpe=-670.686997 te_gfe=-670.726614 te_ms_zpe=-669.595951 te_ms_gfe=0.126170

6 -1.743114 1.613043 -0.060339

6 -0.343252 1.608881 0.004674

6 0.212359 0.309867 0.028872

6 -0.511157 -0.890175 0.038449

6 -1.909639 -0.828256 0.013530

6 -2.509649 0.437353 -0.046347

1 -2.273976 2.556125 -0.102134

7 1.596189 -0.065945 0.015679

7 2.641438 0.952916 -0.085582

7 3.697760 0.248025 -0.099816

7 4.066377 -0.844248 -0.065993

7 1.870576 -1.268438 0.049549

8 -3.859711 0.602477 -0.094908

1 -4.296051 -0.255999 -0.086075

6 -2.755431 -2.075781 0.034301

1 -3.437883 -2.087979 0.893214

1 -3.361667 -2.169457 -0.875383

1 -2.130435 -2.964771 0.101625

5 0.343683 2.983722 0.184131

1 1.439174 3.110674 0.612226

1 -0.306334 3.950972 -0.067675

5 0.537912 -2.097912 0.078132

1 0.535309 -2.768413 1.085947

1 0.554504 -2.825779 -0.889491

03-2BH2-ts-05-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H9B2N5O1 03-2BH2-ts-05-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-236.9 te_zpe=-670.705961 te_gfe=-670.745046 te_ms_zpe=-669.614320 te_ms_gfe=0.127143

6 1.897036 1.600438 -0.000010

6 0.500154 1.685976 0.000004

6 -0.165702 0.438894 0.000004

6 0.474587 -0.818219 -0.000018

6 1.869599 -0.854539 -0.000046

6 2.567117 0.369264 -0.000023

1 2.497034 2.502417 -0.000007

7 -1.556281 0.294305 0.000020

7 -3.554896 1.003108 0.000055

7 -3.855480 -0.116751 0.000047

7 -3.232292 -1.261533 0.000028

7 -1.891767 -0.919435 0.000011

8 3.926576 0.423848 -0.000015

1 4.292167 -0.467039 -0.000006

6 2.627589 -2.158174 -0.000057

1 3.267702 -2.254821 -0.885913

1 3.266961 -2.255248 0.886287

1 1.942390 -3.004438 -0.000556

5 -0.200311 3.057611 0.000021

1 -1.384797 3.151407 0.000038

1 0.470627 4.042695 0.000017

5 -0.652678 -1.947625 -0.000012

1 -0.743511 -2.617681 -0.998020

1 -0.743491 -2.617696 0.997986

##
#

03-BH2-iso-gas-cbs-qb3 charge=0 spin=1 mol=C7H8B1N5O1 03-BH2-iso-gas-cbs-qb3 CBS-QB3

lf=86.2 te_zpe=-645.313334 te_gfe=-645.350076 te_ms_zpe=-644.298414 te_ms_gfe=0.122188

6 1.360694 1.550009 0.000101

6 0.027408 1.159023 0.000065

6 -0.202815 -0.225531 -0.000017

6 0.777044 -1.208706 -0.000100

6 2.105230 -0.798903 -0.000056

6 2.377554 0.590898 0.000052

1 1.645330 2.595406 0.000148

1 0.517227 -2.260358 -0.000178

7 -1.598376 -0.447979 -0.000039

7 -2.318625 0.672171 -0.000012

7 -3.573531 0.320489 -0.000003

7 -3.611248 -1.002696 0.000323

7 -2.384498 -1.496294 -0.000272

8 3.654634 1.060916 0.000082

1 4.279646 0.328971 0.000034

6 3.236792 -1.796362 -0.000124

1 3.874570 -1.690519 -0.886019

1 3.874553 -1.690661 0.885800

1 2.855382 -2.817725 -0.000209

5 -1.357507 1.980595 0.000031

1 -1.591846 2.601135 -1.003289

1 -1.591897 2.601037 1.003404

03-BH2-ts-01-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H8B1N5O1 03-BH2-ts-01-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-517.5 te_zpe=-645.260923 te_gfe=-645.300208 te_ms_zpe=-644.237037 te_ms_gfe=0.113593

6 1.541277 1.522211 -0.000002

6 0.188452 1.213027 -0.000003

6 -0.155835 -0.149910 0.000000

6 0.782711 -1.173524 0.000005

6 2.140208 -0.854681 0.000006

6 2.503034 0.505670 0.000002

1 1.889706 2.548849 -0.000004

1 0.463001 -2.209224 0.000007

7 -1.545966 -0.395762 -0.000001

7 -2.282103 0.628084 -0.000004

7 -3.530626 0.660911 -0.000006

7 -3.924772 -0.915748 -0.000004

7 -3.097578 -1.706865 -0.000002

8 3.809402 0.903412 0.000003

1 4.386853 0.133747 0.000006

6 3.200280 -1.928631 0.000010

1 3.844793 -1.868259 -0.885553

1 3.844798 -1.868247 0.885570

1 2.748826 -2.921237 0.000018

5 -1.073739 2.173422 -0.000008

1 -1.408971 2.695322 -1.020819

1 -1.408973 2.695330 1.020798

03-BH2-ts-02-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H8B1N5O1 03-BH2-ts-02-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-537.1 te_zpe=-645.270043 te_gfe=-645.308211 te_ms_zpe=-644.248991 te_ms_gfe=0.116282

6 1.334622 1.521488 -0.017069

6 0.010459 1.103652 0.045428

6 -0.195823 -0.287565 0.087151

6 0.825527 -1.228237 0.079200

6 2.147036 -0.788136 0.010870

6 2.383981 0.599130 -0.034852

1 1.585028 2.575276 -0.058757

1 0.603080 -2.288135 0.121939

7 -1.571770 -0.556193 0.181986

7 -2.495392 0.844870 0.023738

7 -3.615614 0.557057 -0.121770

7 -3.583433 -1.331530 -0.159646

7 -2.400797 -1.479247 -0.017379

8 3.648438 1.111846 -0.101656

1 4.293223 0.397884 -0.111136

6 3.297235 -1.764290 -0.012727

1 3.893255 -1.671971 -0.928861

1 3.972453 -1.620877 0.839669

1 2.937908 -2.792868 0.033105

5 -1.314548 2.011156 0.079077

1 -1.526087 2.686314 -0.891321

1 -1.522809 2.582884 1.116727

03-BH2-ts-04-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H8B1N5O1 03-BH2-ts-04-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-237.2 te_zpe=-645.270444 te_gfe=-645.307539 te_ms_zpe=-644.242079 te_ms_gfe=0.118298

6 1.485472 -1.534956 -0.000017

6 0.147763 -1.171979 -0.000017

6 -0.137918 0.213647 0.000003

6 0.836120 1.212319 0.000022

6 2.171565 0.836083 0.000022

6 2.477680 -0.548616 0.000002

1 1.798804 -2.572519 -0.000031

1 0.553875 2.258897 0.000037

7 -1.508711 0.458636 0.000001

7 -2.165455 -0.615668 -0.000018

7 -3.550248 -0.566865 -0.000023

7 -3.826345 0.704840 -0.000005

7 -3.219092 1.695201 0.000012

8 3.766245 -0.984840 0.000001

1 4.370846 -0.235794 0.000014

6 3.281956 1.857794 0.000042

1 3.922416 1.767550 0.885977

1 3.922423 1.767577 -0.885891

1 2.877188 2.870202 0.000056

5 -1.244794 -1.952627 -0.000035

1 -1.519213 -2.566427 0.999621

1 -1.519205 -2.566397 -0.999712

03-BH2-ts-05-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H8B1N5O1 03-BH2-ts-05-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-233.4 te_zpe=-645.256367 te_gfe=-645.293549 te_ms_zpe=-644.228554 te_ms_gfe=0.117974

6 -1.534566 1.560646 0.000042

6 -0.170417 1.292726 0.000026

6 0.193096 -0.062254 -0.000002

6 -0.687127 -1.138990 -0.000016

6 -2.045780 -0.853814 0.000000

6 -2.451241 0.506922 0.000031

1 -1.919063 2.573808 0.000064

1 -0.328296 -2.160403 -0.000039

7 1.610377 -0.117960 -0.000017

7 2.236149 0.943528 -0.000003

7 4.186519 -0.160541 -0.000042

7 3.500640 -1.088921 -0.000053

7 2.273871 -1.421774 -0.000047

8 -3.769557 0.846010 0.000052

1 -4.316578 0.054114 0.000041

6 -3.079661 -1.952737 -0.000006

1 -3.724953 -1.908311 0.885934

1 -3.725070 -1.908192 -0.885855

1 -2.603263 -2.933459 -0.000106

5 1.190965 2.143456 0.000029

1 1.410083 2.800862 0.991087

1 1.410064 2.800898 -0.991010

##
#

03-CH3BH2-iso-gas-b3-cbs-qb3 charge=0 spin=1 mol=C8H10B1N5O1 03-CH3BH2-iso-gas-b3-cbs-qb3 CBS-QB3

lf=74.2 te_zpe=-684.609623 te_gfe=-684.647728 te_ms_zpe=-683.527287 te_ms_gfe=0.149377

6 -1.589915 1.488955 -0.135134

6 -0.231903 1.188365 -0.166847

6 0.097696 -0.174209 -0.069959

6 -0.855411 -1.185511 0.040486

6 -2.206622 -0.870548 0.061800

6 -2.559709 0.491900 -0.022456

1 -1.918762 2.518802 -0.201991

7 1.476882 -0.533285 -0.075350

7 2.466137 0.317698 0.183194

7 3.578594 -0.358706 0.125526

7 3.269015 -1.616555 -0.156736

7 1.973861 -1.738316 -0.290775

8 -3.855244 0.901277 0.000627

1 -4.442568 0.142658 0.081399

6 -3.267048 -1.935827 0.184905

1 -3.876071 -1.803474 1.087246

1 -3.943615 -1.939734 -0.678090

1 -2.817629 -2.927276 0.244047

6 0.852683 2.224220 -0.315873

1 1.101199 2.305275 -1.384358

1 0.462092 3.202017 -0.023819

5 2.175590 1.869972 0.555940

1 3.172177 2.469324 0.265181

1 1.970455 1.828788 1.749087

1 -0.533333 -2.216372 0.114038

03-CH3BH2-ts-01-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H10B1N5O1 03-CH3BH2-ts-01-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-505.1 te_zpe=-684.562307 te_gfe=-684.602449 te_ms_zpe=-683.473184 te_ms_gfe=0.141507

6 -1.673878 1.436776 -0.252068

6 -0.309072 1.178247 -0.206503

6 0.078235 -0.159040 0.027066

6 -0.863828 -1.176169 0.191933

6 -2.226371 -0.911388 0.120624

6 -2.619149 0.420684 -0.099954

1 -2.032134 2.446403 -0.414757

1 -0.516186 -2.186473 0.372981

7 1.433268 -0.520292 0.089942

7 2.390632 0.291134 0.277293

7 3.589781 0.029799 0.137636

7 3.547172 -1.575035 -0.331767

7 2.490396 -2.014594 -0.472192

8 -3.929761 0.788348 -0.174759

1 -4.494359 0.018471 -0.052883

6 -3.255834 -2.001618 0.286057

1 -3.915721 -1.814907 1.142053

1 -3.886807 -2.106758 -0.604848

1 -2.777112 -2.966506 0.455309

6 0.742635 2.243936 -0.354124

1 1.134123 2.238673 -1.380434

1 0.287193 3.231527 -0.214483

5 1.930977 2.112736 0.711471

1 2.954070 2.685292 0.497515

1 1.634962 1.918154 1.855697

03-CH3BH2-ts-02-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H10B1N5O1 03-CH3BH2-ts-02-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-533.2 te_zpe=-684.570878 te_gfe=-684.609773 te_ms_zpe=-683.482058 te_ms_gfe=0.144211

6 -1.567115 1.476065 -0.159469

6 -0.229234 1.129300 -0.319409

6 0.074332 -0.244140 -0.261924

6 -0.900386 -1.219284 -0.050619

6 -2.238120 -0.860774 0.075347

6 -2.556099 0.509296 0.023135

1 -1.866319 2.517036 -0.180920

1 -0.612377 -2.262969 -0.001006

7 1.442551 -0.555082 -0.371521

7 2.670678 0.430465 0.363551

7 3.620091 -0.238928 0.483870

7 3.172504 -1.861950 -0.075903

7 2.030221 -1.677607 -0.420029

8 -3.837221 0.959406 0.148226

1 -4.435979 0.217136 0.277210

6 -3.317580 -1.895892 0.273809

1 -3.855994 -1.749172 1.218047

1 -4.055463 -1.877648 -0.537376

1 -2.894681 -2.900627 0.299523

6 0.881179 2.132026 -0.478275

1 1.282647 2.063882 -1.498898

1 0.476636 3.142547 -0.377496

5 2.089508 1.955931 0.594675

1 3.044216 2.662416 0.419388

1 1.733374 1.894623 1.747004

03-CH3BH2-ts-03-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H10B1N5O1 03-CH3BH2-ts-03-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-316.8 te_zpe=-684.509376 te_gfe=-684.549068 te_ms_zpe=-683.422924 te_ms_gfe=0.139869

6	-1.705896	1.405306	-0.306591
6	-0.326105	1.192966	-0.336033
6	0.067459	-0.136530	-0.130721
6	-0.800362	-1.196506	0.108944
6	-2.167830	-0.959209	0.129522
6	-2.606631	0.362820	-0.095133
1	-2.097855	2.406094	-0.438558
1	-0.409817	-2.189000	0.280846
7	1.591946	-0.305372	-0.010977
7	2.292705	0.568602	0.529406
7	4.160573	-0.721648	0.180903
7	3.692730	-1.586225	-0.348467
7	1.758282	-1.384328	-0.662438
8	-3.925603	0.688807	-0.099735
1	-4.462713	-0.096866	0.045803
6	-3.157053	-2.066374	0.394751
1	-3.764123	-1.866159	1.285625
1	-3.839901	-2.214730	-0.450655
1	-2.644810	-3.014239	0.560971
6	0.689078	2.280006	-0.385814
1	1.244157	2.263091	-1.330910
1	0.213504	3.257245	-0.288451

5 1.754840 1.984419 0.855624

1 2.692256 2.750083 0.794586

1 1.270326 1.979858 1.967978

03-CH3BH2-ts-04-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H10B1N5O1 03-CH3BH2-ts-04-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-228.7 te_zpe=-684.565629 te_gfe=-684.604248 te_ms_zpe=-683.468942 te_ms_gfe=0.145062

6 -1.745681 1.452139 -0.109784

6 -0.376805 1.228907 -0.140361

6 0.048516 -0.119205 -0.060584

6 -0.864044 -1.179577 0.010562

6 -2.229475 -0.947433 0.044591

6 -2.657136 0.395902 -0.010760

1 -2.137697 2.460599 -0.167751

1 -0.477790 -2.191285 0.056351

7 1.400105 -0.457167 -0.061541

7 2.289968 0.388303 0.113873

7 3.639196 -0.059881 0.115111

7 3.561438 -1.333424 -0.065532

7 2.769581 -2.156126 -0.238936

8 -3.972384 0.730703 0.018733

1 -4.515203 -0.061704 0.088595

6 -3.231017 -2.071341 0.139950

1 -3.842499 -1.999404 1.047642

1 -3.910526 -2.088980 -0.720758

1 -2.727177 -3.037736 0.169745

6 0.655238 2.310643 -0.300710

1 0.838852 2.443101 -1.377429

1 0.253251 3.263967 0.053809

5 2.030975 1.961242 0.480191

1 3.005994 2.565250 0.133121

1 1.917398 1.902225 1.687609

03-CH3BH2-ts-05-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H10B1N5O1 03-CH3BH2-ts-05-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-182.9 te_zpe=-684.550934 te_gfe=-684.590095 te_ms_zpe=-683.454396 te_ms_gfe=0.143809

6 -1.740552 1.454069 -0.106408

6 -0.361415 1.287948 -0.138742

6 0.102689 -0.042485 -0.064519

6 -0.749996 -1.142848 0.021282

6 -2.124797 -0.959849 0.050536

6 -2.607865 0.363331 -0.009547

1 -2.170382 2.446823 -0.161505

1 -0.329525 -2.136903 0.077046

7 1.516579 -0.218503 -0.036193

7 2.362046 0.604708 0.161367

7 4.081246 -0.876484 0.071694

7 3.208499 -1.611472 -0.120204

7 1.984308 -1.756225 -0.250943

8 -3.935794 0.643873 0.018273

1 -4.445992 -0.170029 0.086323

6 -3.078491 -2.124102 0.152169

1 -3.694592 -2.070650 1.057952

1 -3.754317 -2.175618 -0.710033

1 -2.534904 -3.068301 0.189617

6 0.616985 2.422452 -0.290571

1 0.785839 2.576515 -1.366334

1 0.166032 3.348446 0.076866

5 2.027774 2.132004 0.467677

1 2.962785 2.799734 0.115390

1 1.954449 2.093720 1.684864

##
#

03-iso-gas charge=0 spin=1 mol=C7H7N5O1 03-iso-gas CBS-QB3

lf=16.2 te_zpe=-619.863614 te_gfe=-619.901590 te_ms_zpe=-618.910587 te_ms_gfe=0.108412

6 -1.566186 -1.658358 -0.001072

6 -0.190161 -1.495460 -0.001104

6 0.334772 -0.204693 -0.000213

6 -0.499373 0.910800 0.000594

6 -1.883030 0.757685 0.000526

6 -2.410291 -0.546433 -0.000257

1 -2.009048 -2.646192 -0.001742

1 0.471919 -2.350066 -0.001784

1 -0.062678 1.900734 0.001271

7 1.749323 -0.019396 -0.000105

7 2.635298 -1.010770 0.003004

7 3.795049 -0.431148 0.002123

7 3.621268 0.903119 -0.001607

7 2.351693 1.166065 -0.003196

8 -3.749731 -0.790383 -0.000258

1 -4.237587 0.039426 0.000211

6 -2.802707 1.953474 0.001241

1 -3.448429 1.970248 -0.884890

1 -3.449236 1.968637 0.886813

1 -2.233647 2.883105 0.002365

03-ts-01-gas charge=0 spin=1 mol=C7H7N5O1 03-ts-01-gas CBS-QB3

lf=-559.3 te_zpe=-619.836340 te_gfe=-619.874732 te_ms_zpe=-618.877005 te_ms_gfe=0.103949

6 1.573738 -1.639716 0.220538

6 0.202640 -1.470527 0.116187

6 -0.313528 -0.195650 -0.134331

6 0.545894 0.896985 -0.255244

6 1.923894 0.746877 -0.120793

6 2.431482 -0.543303 0.111482

1 2.003379 -2.617311 0.400469

1 -0.466815 -2.315609 0.214226

1 0.125377 1.876375 -0.449344

7 -1.700517 0.043100 -0.229773

7 -2.593180 -0.800360 -0.607670

7 -3.768365 -0.626828 -0.348255

7 -3.716934 0.820891 0.559137

7 -2.606215 1.176847 0.676804

8 3.766538 -0.790380 0.240514

1 4.262832 0.029437 0.152172

6 2.857723 1.926280 -0.236352

1 3.434643 2.079821 0.683571

1 3.570427 1.803329 -1.060855

1 2.303266 2.845772 -0.424964

##
#

04-2BH2CH3-iso-gas-cbs-qb3 charge=0 spin=1 mol=C10H15B2N5O1 04-2BH2CH3-iso-gas-cbs-qb3 CBS-QB3

lf=57.5 te_zpe=-788.647311 te_gfe=-788.689393 te_ms_zpe=-787.369239 te_ms_gfe=0.213931

6 1.861566 -1.221032 -0.126393

6 0.466085 -1.255035 -0.106820

6 -0.183589 -0.006152 0.000920

6 0.450782 1.249027 0.109097

6 1.845953 1.250773 0.129542

6 2.519319 0.021495 0.006159

7 -1.602200 -0.010716 -0.000714

7 -2.382228 -1.054581 0.237589

7 -3.629588 -0.655284 0.138222

7 -3.632371 0.623234 -0.144891

7 -2.387009 1.029811 -0.240813

8 3.877640 0.077904 0.016354

1 4.245043 -0.809314 -0.051867

6 2.629956 2.531477 0.283250

1 3.686072 2.324935 0.439540

1 2.539317 3.158947 -0.609264

1 2.263239 3.116174 1.129989

6 2.707641 -2.461969 -0.295074

1 3.431915 -2.341656 -1.110208

1 3.264660 -2.706086 0.618195

1 2.106986 -3.331935 -0.546106

6 -0.363747 -2.514508 -0.234732

1 0.210727 -3.378534 0.100907

1 -0.569096 -2.686578 -1.301726

6 -0.381682 2.503287 0.239624

1 0.203838 3.366944 -0.078465

1 -0.591439 2.665965 1.307765

5 -1.736550 -2.477105 0.627691

5 -1.751250 2.461921 -0.626163

1 -2.556523 -3.303864 0.344588

1 -1.550379 -2.373519 1.820883

1 -2.581783 3.277830 -0.342146

1 -1.564631 2.361961 -1.819746

04-2BH2CH3-ts-01-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C10H15B2N5O1 04-2BH2CH3-ts-01-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-516.8 te_zpe=-788.587242 te_gfe=-788.631622 te_ms_zpe=-787.302444 te_ms_gfe=0.204785

6 -1.776655 -1.280587 0.187891

6 -0.383519 -1.205373 0.308028

6 0.204175 0.071733 0.177118

6 -0.509874 1.255688 -0.092797

6 -1.901305 1.163560 -0.195075

6 -2.502288 -0.098912 -0.053649

7 1.604518 0.060144 0.267557

7 2.627920 -1.192888 -0.468397

7 3.698439 -0.746271 -0.551141

7 3.611780 0.943366 0.031430

7 2.447298 1.001472 0.352955

8 -3.864360 -0.135121 -0.168299

1 -4.172467 -1.043029 -0.090977

6 -2.762577 2.375994 -0.465183

1 -3.798010 2.085159 -0.624105

1 -2.740202 3.077888 0.374983

1 -2.422461 2.915520 -1.353486

6 -2.551973 -2.572457 0.316115

1 -3.357200 -2.481943 1.056109

1 -3.003539 -2.873903 -0.637308

1 -1.927368 -3.397846 0.646275

6 0.535966 -2.388367 0.494385

1 -0.023292 -3.323485 0.489701

1 1.005466 -2.325685 1.485713

6 0.231663 2.562120 -0.256117

1 -0.482017 3.397954 -0.251519

1 0.699454 2.611689 -1.248525

5 1.695457 -2.530091 -0.639631

5 1.256527 2.960494 0.871826

1 2.460105 -3.441421 -0.474561

1 1.307343 -2.417725 -1.777143

1 2.103736 3.764853 0.639181

1 1.074050 2.619778 1.999964

04-2BH2CH3-ts-03-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C10H15B2N5O1 04-2BH2CH3-ts-03-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-452.2 te_zpe=-788.559591 te_gfe=-788.603326 te_ms_zpe=-787.268169 te_ms_gfe=0.204671

6 1.942087 1.176526 0.114962

6 0.544598 1.261482 0.068349

6 -0.151428 0.042690 -0.053484

6 0.456235 -1.220634 -0.139593

6 1.856126 -1.278252 -0.131640

6 2.569023 -0.079220 -0.012106

7 -1.643193 0.103802 -0.066856

7 -2.235141 1.183523 -0.215698

7 -4.212867 0.488871 -0.030441

7 -4.018145 -0.595479 0.212019

7 -2.279456 -1.114714 -0.054767

8 3.926777 -0.176901 -0.007225

1 4.319916 0.699571 0.051607

6 2.591331 -2.590319 -0.260792

1 3.660268 -2.425325 -0.372966

1 2.439960 -3.216234 0.624968

1 2.238320 -3.157930 -1.125067

6 2.824942 2.384799 0.329459

1 3.506763 2.231709 1.174841

1 3.432272 2.605731 -0.557883

1 2.250055 3.278038 0.554491

6 -0.195680 2.561486 0.218966

1 0.388752 3.396880 -0.166892

1 -0.368755 2.757796 1.285551

6 -0.368253 -2.454628 -0.212739

1 0.141262 -3.320954 0.210934

1 -0.669335 -2.691240 -1.236879

5 -1.607767 2.523737 -0.601049

5 -1.744930 -2.257694 0.762785

1 -2.369597 3.409128 -0.312773

1 -1.427728 2.431349 -1.805782

1 -2.444590 -3.218881 0.591121

1 -1.440562 -1.980256 1.895754

##
#

04-BH2-iso-gas-cbs-qb3 charge=0 spin=1 mol=C8H10B1N5O1 04-BH2-iso-gas-cbs-qb3 CBS-QB3

lf=84.4 te_zpe=-684.615986 te_gfe=-684.654842 te_ms_zpe=-683.533252 te_ms_gfe=0.147619

6 -1.370493 1.171132 0.000021

6 0.001118 0.911109 0.000002

6 0.385601 -0.436006 -0.000008

6 -0.474263 -1.527300 -0.000020

6 -1.837210 -1.267408 -0.000021

6 -2.260071 0.081891 0.000003

1 -0.097815 -2.542794 -0.000034

7 1.797469 -0.497972 -0.000024

7 2.386662 0.696088 -0.000024

7 3.674160 0.489384 0.000293

7 3.860578 -0.820005 -0.000263

7 2.697214 -1.450282 -0.000042

8 -3.610649 0.268554 0.000005

1 -3.810459 1.210492 0.000022

6 -2.860975 -2.371073 -0.000039

1 -3.511097 -2.305007 0.876842

1 -3.511133 -2.304947 -0.876888

1 -2.377835 -3.349252 -0.000081

6 -1.905815 2.582804 0.000055

1 -2.518882 2.787312 -0.886589

1 -2.518843 2.787285 0.886732

1 -1.089758 3.303871 0.000047

5 1.288107 1.882687 0.000040

1 1.450280 2.529822 1.002124

1 1.450272 2.529967 -1.001949

04-BH2-ts-01-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H10B1N5O1 04-BH2-ts-01-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-534.0 te_zpe=-684.571740 te_gfe=-684.612029 te_ms_zpe=-683.483113 te_ms_gfe=0.141705

6 1.344601 1.154249 -0.000876

6 -0.021902 0.863078 0.053399

6 -0.377380 -0.495003 0.083426

6 0.530483 -1.547134 0.070527

6 1.888836 -1.252888 0.009742

6 2.273088 0.099145 -0.022370

1 0.191395 -2.575777 0.103998

7 -1.775058 -0.614994 0.174011

7 -2.543667 0.877517 0.031653

7 -3.689104 0.716318 -0.110865

7 -3.859586 -1.172943 -0.162079

7 -2.698362 -1.441841 -0.026420

8 3.620878 0.331959 -0.078891

1 3.785174 1.280019 -0.093137

6 2.936872 -2.333545 -0.019424

1 3.545326 -2.267689 -0.925931

1 3.624491 -2.237641 0.825635

1 2.478513 -3.323177 0.017997

6 1.840605 2.581193 -0.039185

1 2.460968 2.819688 0.833910

1 2.437139 2.781188 -0.938280

1 1.009817 3.285050 -0.044184

5 -1.249245 1.903520 0.089696

1 -1.389198 2.602602 -0.878379

1 -1.395207 2.499496 1.125494

04-BH2-ts-02-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H10B1N5O1 04-BH2-ts-02-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-519.3 te_zpe=-684.562210 te_gfe=-684.603470 te_ms_zpe=-683.470165 te_ms_gfe=0.139066

6 -1.523329 1.130140 0.000019

6 -0.141816 0.944313 0.000128

6 0.344217 -0.371956 -0.000012

6 -0.476016 -1.493931 -0.000248

6 -1.856353 -1.317746 -0.000352

6 -2.357693 -0.003878 -0.000215

1 -0.048370 -2.489685 -0.000351

7 1.752861 -0.461511 0.000106

7 2.360267 0.643479 0.000271

7 3.593676 0.847080 0.000399

7 4.201247 -0.673614 0.000293

7 3.499107 -1.572549 0.000132

8 -3.721316 0.112995 -0.000331

1 -3.968043 1.043129 -0.000206

6 -2.810363 -2.483082 -0.000606

1 -3.463894 -2.458559 0.876155

1 -3.463776 -2.458271 -0.877445

1 -2.267910 -3.429903 -0.000724

6 -2.134909 2.512218 0.000151

1 -2.758418 2.683560 -0.886263

1 -2.758507 2.683351 0.886543

1 -1.364100 3.282914 0.000282

5 1.030647 2.018163 0.000402

1 1.298811 2.585828 1.018354

1 1.298943 2.586208 -1.017304

04-BH2-ts-03-gas-cbs-qb3 charge=0 spin=1 mol=C8H10B1N5O1 04-BH2-ts-03-gas-cbs-qb3 CBS-QB3

lf=-388.7 te_zpe=-684.513925 te_gfe=-684.555415 te_ms_zpe=-683.426956 te_ms_gfe=0.136434

6 -1.542310 1.137711 0.000369

6 -0.145779 0.992587 0.000155

6 0.285609 -0.320068 -0.000086

6 -0.450892 -1.487215 -0.000143

6 -1.834300 -1.319210 0.000069

6 -2.353178 -0.007177 0.000318

1 -0.006470 -2.471113 -0.000334

7 1.923387 -0.182619 -0.000288

7 2.278241 0.994337 -0.000177

7 4.564474 0.161564 -0.000588

7 4.299711 -0.916876 -0.000699

7 2.353537 -1.359385 -0.000503

8 -3.716072 0.083034 0.000508

1 -3.979799 1.008925 0.000680

6 -2.771101 -2.498523 0.000029

1 -3.423659 -2.480141 0.877412

1 -3.423680 -2.480069 -0.877339

1 -2.216752 -3.438133 -0.000019

6 -2.168054 2.512975 0.000643

1 -2.792617 2.674440 -0.886870

1 -2.792559 2.674112 0.888256

1 -1.399000 3.283555 0.000763

5 1.078636 2.037206 0.000128

1 1.157397 2.716114 0.997537

1 1.157123 2.716380 -0.997121

04-BH2-ts-04-gas-cbs-qb3 charge=0 spin=1 mol=C8H10B1N5O1 04-BH2-ts-04-gas-cbs-qb3 CBS-QB3

lf=-233.2 te_zpe=-684.559207 te_gfe=-684.598501 te_ms_zpe=-683.463501 te_ms_gfe=0.143413

6 -1.532992 1.148880 0.000135

6 -0.142162 1.030861 0.000018

6 0.385922 -0.266374 -0.000030

6 -0.351407 -1.447263 0.000036

6 -1.732310 -1.329467 0.000175

6 -2.297672 -0.029612 0.000234

1 0.130679 -2.416304 -0.000015

7 1.798735 -0.143998 -0.000181

7 2.289511 0.987114 -0.000239

7 4.360886 0.134614 -0.000463

7 3.795125 -0.871530 -0.000394

7 2.619240 -1.354156 -0.000261

8 -3.660913 0.009188 0.000410

1 -3.959024 0.924838 0.000513

6 -2.637797 -2.532554 0.000276

1 -3.291271 -2.533987 0.877252

1 -3.291543 -2.533930 -0.876496

1 -2.056103 -3.455524 0.000158

6 -2.213169 2.496900 0.000196

1 -2.844681 2.637985 -0.886080

1 -2.843472 2.638477 0.887256

1 -1.473472 3.296332 -0.000551

5 1.104757 2.044444 -0.000110

1 1.238839 2.726917 0.990283

1 1.238623 2.726950 -0.990508

04-BH2-ts-05-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H10B1N5O1 04-BH2-ts-05-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-235.7 te_zpe=-684.572926 te_gfe=-684.612125 te_ms_zpe=-683.476594 te_ms_gfe=0.143756

6 1.473364 1.153152 0.000048

6 0.102413 0.913723 -0.000061

6 -0.329731 -0.430956 0.000007

6 0.529508 -1.531619 0.000177

6 1.894582 -1.297869 0.000290

6 2.342256 0.045417 0.000227

1 0.137429 -2.541911 0.000222

7 -1.718305 -0.525183 -0.000124

7 -2.256695 0.613311 -0.000272

7 -3.640298 0.713106 -0.000418

7 -4.049984 -0.520837 -0.000356

7 -3.553114 -1.571235 -0.000217

8 3.695175 0.207818 0.000348

1 3.910340 1.146606 0.000306

6 2.901619 -2.417470 0.000472

1 3.552986 -2.363464 -0.876452

1 3.552937 -2.363223 0.877416

1 2.401885 -3.387404 0.000589

6 2.035565 2.554961 -0.000009

1 2.651644 2.750047 0.886882

1 2.652074 2.749803 -0.886656

1 1.231107 3.289225 -0.000309

5 -1.201415 1.838560 -0.000262

1 -1.406604 2.482332 -0.998869

1 -1.406804 2.482479 0.998209

##
#

04-CH3-BH2-iso-gas-cbs-qb3 charge=0 spin=1 mol=C9H12B1N5O1 04-CH3-BH2-iso-gas-cbs-qb3 CBS-QB3

lf=67.1 te_zpe=-723.908120 te_gfe=-723.948453 te_ms_zpe=-722.758273 te_ms_gfe=0.174851

6 1.618882 1.087631 -0.099431

6 0.218498 0.965822 -0.112999

6 -0.293835 -0.340785 -0.048608

6 0.499936 -1.484170 0.040306

6 1.877429 -1.364281 0.076675

6 2.415170 -0.066070 0.014973

1 0.032155 -2.458754 0.088513

7 -1.709229 -0.520031 -0.080561

7 -2.591752 0.432946 0.198599

7 -3.778448 -0.097503 0.099785

7 -3.619302 -1.371373 -0.229490

7 -2.346702 -1.645932 -0.351939

8 3.774247 0.006584 0.065026

1 4.057252 0.926483 0.046345

6 2.786933 -2.558009 0.188437

1 3.473692 -2.610180 -0.660972

1 3.405203 -2.498274 1.088416

1 2.210302 -3.483305 0.224567

6 2.312431 2.426274 -0.208960

1 2.740680 2.746073 0.748895

1 3.123371 2.394529 -0.946650

1 1.631997 3.208312 -0.535855

6 -0.741666 2.130189 -0.217742

1 -0.957950 2.306890 -1.281989

1 -0.270394 3.043576 0.147288

5 -2.110344 1.909852 0.627390

1 -3.012461 2.650779 0.353956

1 -1.920734 1.805586 1.819676

04-CH3-BH2-ts-01-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C9H12B1N5O1 04-CH3-BH2-ts-01-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-533.3 te_zpe=-723.868640 te_gfe=-723.909842 te_ms_zpe=-722.712488 te_ms_gfe=0.169558

6 1.598668 1.084835 -0.130884

6 0.212638 0.916145 -0.298705

6 -0.275342 -0.403726 -0.269634

6 0.539838 -1.517957 -0.068637

6 1.907773 -1.356681 0.081140

6 2.413097 -0.046523 0.056060

1 0.101312 -2.508502 -0.042979

7 -1.673045 -0.529052 -0.398726

7 -2.763958 0.555148 0.401536

7 -3.786304 0.001566 0.514323

7 -3.540411 -1.638971 -0.125628

7 -2.390288 -1.572682 -0.483418

8 3.764768 0.063814 0.225048

1 4.020774 0.991238 0.225293

6 2.837349 -2.524313 0.278306

1 3.587260 -2.569754 -0.516569

1 3.385074 -2.436253 1.220685

1 2.284427 -3.465005 0.285349

6 2.267558 2.440729 -0.148978

1 1.600175 3.223438 -0.499747

1 2.617340 2.736640 0.847624

1 3.131898 2.448733 -0.824573

6 -0.793395 2.032833 -0.437930

1 -1.217898 2.007180 -1.451167

1 -0.316550 3.007800 -0.338754

5 -1.998634 1.983030 0.654005

1 -2.855963 2.810687 0.504231

1 -1.633886 1.864035 1.799158

04-CH3-BH2-ts-02-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C9H12B1N5O1 04-CH3-BH2-ts-02-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-497.6 te_zpe=-723.859791 te_gfe=-723.901853 te_ms_zpe=-722.703014 te_ms_gfe=0.167362

6 1.686317 1.045293 -0.167113

6 0.286239 0.956928 -0.115381

6 -0.274583 -0.327412 0.056778

6 0.512193 -1.474589 0.186653

6 1.893870 -1.394164 0.142233

6 2.461107 -0.121465 -0.027520

1 0.024303 -2.432665 0.320232

7 -1.663638 -0.520885 0.078945

7 -2.518816 0.389405 0.295747

7 -3.741545 0.300332 0.122712

7 -3.905078 -1.271633 -0.435241

7 -2.922592 -1.846617 -0.596411

8 3.826328 -0.082560 -0.054069

1 4.127898 0.827014 -0.140173

6 2.776680 -2.605837 0.278276

1 3.411853 -2.732106 -0.603093

1 3.447707 -2.510026 1.136521

1 2.178611 -3.509473 0.405560

6 2.407771 2.358194 -0.376645

1 2.887681 2.715437 0.542825

1 3.184046 2.266607 -1.146091

1 1.735444 3.142273 -0.716376

6 -0.650374 2.137590 -0.192821

1 -1.007897 2.267617 -1.223715

1 -0.128227 3.065028 0.060279

5 -1.877215 2.045001 0.838413

1 -2.804739 2.773780 0.663872

1 -1.614856 1.760546 1.973616

04-CH3-BH2-ts-03-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C9H12B1N5O1 04-CH3-BH2-ts-03-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-326.3 te_zpe=-723.807813 te_gfe=-723.849525 te_ms_zpe=-722.653391 te_ms_gfe=0.165684

6 1.703093 1.017735 -0.218999

6 0.294289 0.975951 -0.247529

6 -0.270949 -0.298984 -0.107679

6 0.436644 -1.480188 0.091741

6 1.818423 -1.427330 0.143637

6 2.429268 -0.169351 -0.020427

1 -0.087926 -2.416646 0.211936

7 -1.803565 -0.283813 -0.013498

7 -2.407908 0.622967 0.586212

7 -4.403665 -0.405773 0.122500

7 -4.027093 -1.274271 -0.470268

7 -2.089053 -1.281079 -0.750918

8 3.789554 -0.173724 0.034900

1 4.126079 0.725733 -0.030837

6 2.658459 -2.654820 0.374590

1 3.343240 -2.825500 -0.460856

1 3.275789 -2.545963 1.270477

1 2.029766 -3.538617 0.491390

6 2.460099 2.316146 -0.381135

1 2.801853 2.718775 0.579638

1 3.337967 2.188858 -1.025828

1 1.845606 3.079085 -0.853808

6 -0.603068 2.170183 -0.233683

1 -1.156225 2.265115 -1.175756

1 -0.048894 3.093905 -0.076645

5 -1.696578 1.935978 0.995990

1 -2.527583 2.817837 0.988737

1 -1.211771 1.805047 2.101112

04-CH3-BH2-ts-04-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C9H12B1N5O1 04-CH3-BH2-ts-04-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-179.2 te_zpe=-723.849536 te_gfe=-723.890991 te_ms_zpe=-722.685649 te_ms_gfe=0.169186

6 1.754396 1.016512 -0.084045

6 0.351655 1.048245 -0.089116

6 -0.304194 -0.200412 -0.035025

6 0.364917 -1.422965 0.034103

6 1.747264 -1.452360 0.069796

6 2.421458 -0.219540 0.017484

1 -0.204047 -2.340345 0.074506

7 -1.729946 -0.177094 -0.025929

7 -2.461422 0.745679 0.179671

7 -4.365814 -0.474849 0.016358

7 -3.599505 -1.319042 -0.182947

7 -2.407715 -1.634041 -0.297661

8 3.779241 -0.291792 0.059179

1 4.158439 0.592986 0.038562

6 2.523732 -2.738308 0.164943

1 3.200140 -2.854345 -0.686498

1 3.145270 -2.757672 1.064550

1 1.850088 -3.595876 0.190970

6 2.590556 2.271530 -0.190318

1 3.081346 2.518488 0.759225

1 3.369944 2.167230 -0.955134

1 1.990796 3.131307 -0.477025

6 -0.471582 2.310997 -0.199275

1 -0.589199 2.550536 -1.266483

1 0.064336 3.155268 0.239262

5 -1.922082 2.195430 0.530466

1 -2.743842 3.002792 0.187810

1 -1.865192 2.120054 1.746788

04-CH3-BH2-ts-05-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C9H12B1N5O1 04-CH3-BH2-ts-05-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-226.6 te_zpe=-723.864411 te_gfe=-723.905262 te_ms_zpe=-722.700223 te_ms_gfe=0.170502

6 1.747677 1.039105 -0.080689

6 0.348061 0.993733 -0.089523

6 -0.254275 -0.286731 -0.035572

6 0.495674 -1.469584 0.016356

6 1.875751 -1.431321 0.058951

6 2.480935 -0.161495 0.018540

1 -0.031577 -2.415916 0.041742

7 -1.637799 -0.449920 -0.057965

7 -2.424254 0.489523 0.125025

7 -3.818658 0.204968 0.094321

7 -3.887864 -1.063136 -0.118511

7 -3.195521 -1.969616 -0.301293

8 3.840313 -0.158160 0.063642

1 4.169340 0.746609 0.044826

6 2.722073 -2.673147 0.144051

1 3.409481 -2.741850 -0.703696

1 3.337732 -2.669725 1.047953

1 2.096710 -3.567016 0.155613

6 2.517823 2.336204 -0.180503

1 3.023087 2.585587 0.760957

1 3.279147 2.289029 -0.968997

1 1.867767 3.171399 -0.427695

6 -0.553586 2.197886 -0.213027

1 -0.689997 2.415088 -1.283275

1 -0.076937 3.083485 0.212834

5 -1.978410 1.996425 0.532006

1 -2.857889 2.734850 0.188462

1 -1.889442 1.900972 1.739558

##
#

04-iso-gas charge=0 spin=1 mol=C8H9N5O1 04-iso-gas CBS-QB3

lf=17.0 te_zpe=-659.165120 te_gfe=-659.205057 te_ms_zpe=-658.143319 te_ms_gfe=0.133998

6 -1.559889 -1.218033 0.000520

6 -0.167430 -1.208383 0.000485

6 0.516715 0.002221 -0.000046

6 -0.164945 1.217498 -0.000537

6 -1.554783 1.237176 -0.000556

6 -2.239399 0.010467 -0.000018

1 0.386243 -2.137632 0.000895

1 0.393033 2.144231 -0.000927

7 1.943817 -0.001234 -0.000045

7 2.691318 -1.100911 -0.004043

7 3.917606 -0.679499 -0.002326

7 3.921330 0.665808 0.002405

7 2.697280 1.094061 0.004029

8 -3.602625 0.080982 -0.000039

1 -3.978581 -0.804991 0.000297

6 -2.329397 2.528002 -0.001278

1 -2.978945 2.594945 -0.878511

1 -2.979539 2.595599 0.875457

1 -1.656220 3.386125 -0.001375

6 -2.329793 -2.516002 0.001357

1 -2.968933 -2.610252 0.887579

1 -2.969541 -2.611107 -0.884331

1 -1.652452 -3.370031 0.001530

04-ts-01-gas charge=0 spin=1 mol=C8H9N5O1 04-ts-01-gas CBS-QB3

lf=-558.6 te_zpe=-659.137528 te_gfe=-659.177871 te_ms_zpe=-658.109613 te_ms_gfe=0.129555

6 -1.556752 1.220654 0.083293

6 -0.167380 1.185215 -0.001539

6 0.497812 -0.029767 -0.167358

6 -0.221543 -1.224535 -0.225458

6 -1.607245 -1.225752 -0.111780

6 -2.262108 0.007508 0.034613

1 0.402490 2.105205 0.047589

1 0.312838 -2.157835 -0.354570

7 1.905557 -0.100113 -0.238749

7 2.691292 0.821426 -0.668274

7 3.874247 0.818913 -0.386956

7 3.990426 -0.556487 0.623500

7 2.931770 -1.041733 0.756557

8 -3.625681 -0.038935 0.125479

1 -3.978816 0.851253 0.219512

6 -2.409091 -2.499215 -0.159645

1 -2.986648 -2.633828 0.759315

1 -3.129817 -2.479469 -0.981928

1 -1.758009 -3.364806 -0.289069

6 -2.297051 2.526848 0.239594

1 -2.991586 2.703691 -0.590630

1 -2.874643 2.560008 1.171414

1 -1.603263 3.367484 0.261668

##
#

05-2CH3BH2-iso-gas-cbs-qb3 charge=0 spin=1 mol=C9H13B2N5O1 05-2CH3BH2-iso-gas-cbs-qb3 CBS-QB3

lf=54.5 te_zpe=-749.330005 te_gfe=-749.369952 te_ms_zpe=-748.113996 te_ms_gfe=0.188871

7 -1.563769 -0.075935 -0.071701

6 -0.154589 0.066261 -0.117075

6 0.623678 -1.107233 -0.154070

6 0.376370 1.378370 -0.134950

6 2.001940 -0.942665 -0.056039

6 1.751713 1.481031 -0.037345

6 2.565004 0.337645 0.034302

1 2.625212 -1.825772 -0.071436

1 2.229566 2.452550 -0.033082

7 -2.444699 0.911166 0.024923

7 -3.639920 0.370518 0.123357

7 -3.509816 -0.928656 0.111380

7 -2.231828 -1.219752 0.004358

8 3.886950 0.578036 0.151262

6 4.794678 -0.521397 0.221654

1 4.769081 -1.115393 -0.696992

1 5.780941 -0.077621 0.338590

1 4.576472 -1.159924 1.082758

6 -0.523419 2.569901 -0.351398

1 -0.025465 3.468973 0.019911

1 -0.610411 2.705527 -1.439420

6 -0.017130 -2.452362 -0.391012

1 -0.072035 -2.586607 -1.481465

1 0.649702 -3.239331 -0.029382

5 -1.988096 2.443590 0.321976

5 -1.479045 -2.634179 0.277301

1 -1.978322 2.450601 1.533915

1 -2.842477 3.143895 -0.143675

1 -1.468681 -2.662647 1.488823

1 -2.172738 -3.484276 -0.205648

05-2CH3BH2-ts-01-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C9H13B2N5O1
05-2CH3BH2-ts-01-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-531.5 te_zpe=-749.275676 te_gfe=-749.318483 te_ms_zpe=-748.052857 te_ms_gfe=0.178658

7 -1.585444 -0.051212 -0.439335

6 -0.195369 0.135987 -0.336437

6 0.537574 -1.066963 -0.314459

6 0.409173 1.403901 -0.181255

6 1.919333 -0.987568 -0.137583

6 1.789539 1.430049 -0.043687

6 2.547581 0.252314 -0.011556

1 2.486831 -1.907284 -0.104847

1 2.312885 2.373608 0.053002

7 -2.544816 0.749582 -0.632573

7 -3.694559 0.533270 -0.314711

7 -3.556677 -1.058800 0.409287

7 -2.429081 -1.358462 0.379137

8 3.884872 0.426764 0.144892

6 4.724712 -0.721707 0.193937

1 4.670723 -1.296028 -0.736832

1 5.735991 -0.341383 0.325093

1 4.467598 -1.368564 1.039150

6 -0.377164 2.690889 -0.170056

1 0.322632 3.539575 -0.144480

1 -0.916644 2.841674 -1.116722

6 -0.185604 -2.383891 -0.401109

1 -0.610924 -2.498714 -1.407597

1 0.530133 -3.200699 -0.277045

5 -1.396436 2.948910 0.992390

5 -1.364656 -2.560161 0.706136

1 -1.562185 2.173360 1.881478

1 -2.006216 3.973189 0.991746

1 -1.033975 -2.300302 1.837669

1 -2.014985 -3.565001 0.608216

05-2CH3BH2-ts-03-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C9H13B2N5O1 05-2CH3BH2-ts-03-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-436.9 te_zpe=-749.247363 te_gfe=-749.288436 te_ms_zpe=-748.018425 te_ms_gfe=0.180353

7 1.580776 0.176745 -0.047356

6 0.108513 -0.039097 -0.113651

6 -0.695182 1.110335 -0.192804

6 -0.396013 -1.350074 -0.056251

6 -2.073875 0.916397 -0.116693

6 -1.774749 -1.487034 0.028288

6 -2.615072 -0.367344 0.014918

1 -2.711104 1.788181 -0.163000

1 -2.224148 -2.469804 0.089338

7 2.297801 -0.963909 -0.400800

7 4.005261 -0.362910 -0.189429

7 4.126934 0.725252 0.069099

7 2.065438 1.277586 0.216661

8 -3.936946 -0.631272 0.110550

6 -4.864858 0.451985 0.098315

1 -4.815933 1.006275 -0.844161

1 -5.847434 -0.004208 0.198949

1 -4.691287 1.132569 0.937434

6 0.504492 -2.536099 -0.121537

1 0.132801 -3.360610 0.491707

1 0.583849 -2.882274 -1.156355

6 -0.088165 2.471941 -0.362786

1 0.113798 2.633440 -1.430400

1 -0.799787 3.242929 -0.058476

5 2.040701 -2.193859 0.466262

5 1.289376 2.576569 0.493596

1 2.000791 -1.933925 1.644685

1 2.786361 -3.066861 0.113458

1 1.151880 2.553428 1.705702

1 2.001385 3.502083 0.183404

##
#

05-BH2-iso-gas-cbs-qb3 charge=0 spin=1 mol=C7H8B1N5O1
05-BH2-iso-gas-cbs-qb3 CBS-QB3

lf=63.1 te_zpe=-645.294865 te_gfe=-645.331657 te_ms_zpe=-644.277210
te_ms_gfe=0.122892

7 1.776563 -0.452120 -0.000013

6 0.365303 -0.369539 -0.000007

6 -0.515285 -1.438760 -0.000036

6 -0.001336 0.989446 0.000029

6 -1.872380 -1.138305 -0.000019

1 -0.165102 -2.463185 -0.000062

6 -1.361789 1.255622 0.000034

6 -2.293877 0.204928 0.000014

1 -2.590525 -1.945597 -0.000033

1 -1.741391 2.270353 0.000052

7 2.382067 0.733744 0.000013

7 3.665294 0.508806 -0.000123

7 3.833688 -0.804554 0.000120

7 2.662722 -1.417234 -0.000043

8 -3.594910 0.584876 0.000029

6 -4.611972 -0.411640 -0.000024

1 -4.556026 -1.039729 0.895158

1 -5.554786 0.131626 -0.000028

1 -4.555986 -1.039673 -0.895243

5 1.297676 1.942345 0.000036

1 1.470196 2.582201 1.003573

1 1.470201 2.582256 -1.003461

05-BH2-ts-01-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H8B1N5O1 05-BH2-ts-01-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-237.2 te_zpe=-645.252061 te_gfe=-645.289222 te_ms_zpe=-644.220987 te_ms_gfe=0.118950

7 -1.686623 -0.486963 0.000024

6 -0.299165 -0.363088 0.000054

6 0.585889 -1.437829 0.000204

6 0.107713 0.995618 -0.000100

6 1.944611 -1.156788 0.000195

1 0.224611 -2.459048 0.000321

6 1.467623 1.248239 -0.000108

6 2.384088 0.182514 0.000038

1 2.655012 -1.971223 0.000308

1 1.864181 2.256877 -0.000225

7 -2.246039 0.640548 -0.000136

7 -3.629009 0.714637 -0.000217

7 -4.016909 -0.528299 -0.000083

7 -3.500193 -1.568313 0.000062

8 3.690420 0.543511 0.000011

6 4.694345 -0.465902 0.000168

1 4.630315 -1.093580 -0.894744

1 5.644216 0.065136 0.000130

1 4.630260 -1.093355 0.895234

5 -1.212772 1.894416 -0.000194

1 -1.433643 2.528582 -1.000258

1 -1.433661 2.528592 0.999868

05-BH2-ts-02-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H8B1N5O1 05-BH2-ts-02-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-536.9 te_zpe=-645.251849 te_gfe=-645.290006 te_ms_zpe=-644.227985 te_ms_gfe=0.117097

7 1.760568 -0.554506 0.178864

6 0.363502 -0.433280 0.095070

6 -0.555595 -1.470077 0.092905

6 0.011554 0.933040 0.054351

6 -1.911065 -1.148200 0.033295

1 -0.234162 -2.503583 0.133468

6 -1.344428 1.217951 0.000571

6 -2.305512 0.194710 -0.010716

1 -2.639300 -1.946715 0.022805

1 -1.697961 2.241784 -0.039448

7 2.531610 0.933760 0.013668

7 3.675041 0.764832 -0.138039

7 3.839744 -1.117645 -0.172377

7 2.680271 -1.387354 -0.022156

8 -3.599917 0.610274 -0.068901

6 -4.632694 -0.365929 -0.085978

1 -4.622859 -0.976809 0.823516

1 -5.566230 0.191768 -0.133645

1 -4.555491 -1.016785 -0.963999

5 1.237404 1.971773 0.078125

1 1.393068 2.561667 1.114702

1 1.370039 2.664717 -0.893528

05-BH2-ts-03-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H8B1N5O1 05-BH2-ts-03-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-233.3 te_zpe=-645.237819 te_gfe=-645.275084 te_ms_zpe=-644.207253 te_ms_gfe=0.118609

7 1.767627 -0.147819 -0.000106

6 0.349529 -0.200107 -0.000015

6 -0.448187 -1.335787 0.000077

6 -0.116974 1.126818 -0.000034

6 -1.821211 -1.131279 0.000156

1 -0.023650 -2.330950 0.000086

6 -1.493467 1.298386 0.000046

6 -2.341539 0.180501 0.000140

1 -2.481317 -1.986868 0.000228

1 -1.948140 2.281996 0.000039

7 2.309926 0.958072 -0.000180

7 4.338152 0.007220 -0.000272

7 3.725993 -0.971382 -0.000198

7 2.527942 -1.396866 -0.000108

8 -3.669136 0.458164 0.000214

6 -4.606693 -0.612775 0.000311

1 -4.503410 -1.235187 0.895354

1 -5.588434 -0.143165 0.000356

1 -4.503522 -1.235252 -0.894699

5 1.177941 2.077436 -0.000150

1 1.347873 2.748945 0.991008

1 1.347749 2.748873 -0.991377

05-BH2-ts-04-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H8B1N5O1 05-BH2-ts-04-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-563.3 te_zpe=-645.248872 te_gfe=-645.288836 te_ms_zpe=-644.222650 te_ms_gfe=0.114112

7 -1.819742 -0.295806 -0.197516

6 -0.425485 -0.087668 -0.138224

6 0.374564 -1.218259 -0.253706

6 0.149408 1.193491 0.084128

6 1.762435 -1.121698 -0.164262

1 -0.091939 -2.181561 -0.417531

6 1.547666 1.263836 0.121092

6 2.360744 0.128442 0.012431

1 2.358089 -2.020004 -0.253189

1 2.034127 2.221669 0.261299

7 -2.693067 0.403104 -0.830642

7 -3.880387 0.260178 -0.613648

7 -3.875057 -0.921224 0.616714

7 -2.772078 -1.216770 0.882083

8 3.697608 0.346104 0.090054

6 4.579040 -0.767286 -0.011682

1 5.583019 -0.357689 0.078849

1 4.407241 -1.487523 0.795387

1 4.478342 -1.269137 -0.979976

5 -0.653912 2.479424 0.375609

1 -0.062953 3.510944 0.451436

1 -1.825153 2.465837 0.567646

05-BH2-ts-05-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H8B1N5O1 05-BH2-ts-05-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-383.5 te_zpe=-645.192393 te_gfe=-645.231792 te_ms_zpe=-644.170497 te_ms_gfe=0.111683

7 1.889841 -0.164553 -0.000022

6 0.253274 -0.250619 -0.000010

6 -0.529422 -1.382449 -0.000036

6 -0.138196 1.083513 0.000033

6 -1.905485 -1.149083 -0.000017

1 -0.129331 -2.384865 -0.000069

6 -1.519938 1.260659 0.000050

6 -2.397234 0.167434 0.000026

1 -2.573355 -1.998670 -0.000036

1 -1.944247 2.258477 0.000083

7 2.283843 0.998305 0.000009

7 4.550073 0.072212 -0.000038

7 4.240710 -0.993662 -0.000066

7 2.271851 -1.359432 -0.000060

8 -3.718315 0.479769 0.000047

6 -4.676932 -0.571472 0.000025

1 -4.586194 -1.196172 0.895155

1 -5.649444 -0.083040 0.000048

1 -4.586210 -1.196119 -0.895144

5 1.119955 2.085840 0.000051

1 1.222454 2.757499 0.998534

1 1.222436 2.757557 -0.998395

##
#

05-CH3BH2-iso-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H10B1N5O1
05-CH3BH2-iso-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=61.7 te_zpe=-684.591251 te_gfe=-684.629373 te_ms_zpe=-683.506273 te_ms_gfe=0.150090

7 -3.734846 -0.166937 0.141190

7 -2.564190 0.403385 0.186392

7 -1.659306 -0.540327 -0.059697

7 -2.267080 -1.697049 -0.254775

7 -3.544519 -1.452947 -0.120887

6 -0.252512 -0.311853 -0.060474

6 0.603983 -1.398857 0.075885

6 1.975290 -1.187955 0.092471

6 2.467004 0.120550 -0.018912

6 1.579745 1.197439 -0.157853

6 0.203984 1.015797 -0.187276

1 0.198293 -2.397077 0.173219

1 2.639193 -2.033055 0.202812

1 1.997342 2.192773 -0.247364

6 -0.785083 2.139726 -0.361137

1 -1.034904 2.210761 -1.429999

1 -0.306918 3.086889 -0.100528

5 -2.128514 1.928977 0.526198

1 -1.918785 1.893965 1.718582

1 -3.067102 2.612167 0.227726

8 3.780111 0.446199 -0.004750

6 4.748633 -0.589933 0.135196

1 5.715465 -0.091185 0.121109

1 4.628057 -1.121688 1.084457

1 4.694364 -1.300387 -0.695957

05-CH3BH2-ts-01-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H10B1N5O1 05-CH3BH2-ts-01-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-504.4 te_zpe=-684.544046 te_gfe=-684.584145 te_ms_zpe=-683.452164 te_ms_gfe=0.142348

7 -3.718500 0.190418 0.118071

7 -2.502731 0.357577 0.259926

7 -1.614052 -0.535934 0.113138

7 -2.788636 -1.960673 -0.400601

7 -3.805440 -1.428933 -0.288889

6 -0.233054 -0.291140 0.059073

6 0.621326 -1.370188 0.273935

6 1.999162 -1.199581 0.210041

6 2.516506 0.073690 -0.050428

6 1.646461 1.154800 -0.254464

6 0.268481 1.003778 -0.218686

1 0.199594 -2.344612 0.487022

1 2.646836 -2.049198 0.373088

1 2.083547 2.126923 -0.449380

6 -0.694276 2.142202 -0.421673

1 -1.075819 2.124311 -1.451566

1 -0.163217 3.095669 -0.317282

5 -1.899670 2.148209 0.632746

1 -1.631779 1.973718 1.787073

1 -2.869472 2.794891 0.384698

8 3.839815 0.367887 -0.125166

6 4.785432 -0.676262 0.075654

1 5.764203 -0.212097 -0.029095

1 4.695239 -1.109874 1.077303

1 4.675988 -1.464867 -0.676494

05-CH3BH2-ts-02-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H10B1N5O1 05-CH3BH2-ts-02-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-534.5 te_zpe=-684.552667 te_gfe=-684.591546 te_ms_zpe=-683.461094 te_ms_gfe=0.145001

7 -3.756479 -0.014917 0.515533

7 -2.746704 0.553456 0.369229

7 -1.629924 -0.566457 -0.347146

7 -2.324803 -1.627486 -0.358848

7 -3.475937 -1.689156 -0.002221

6 -0.236373 -0.390802 -0.252526

6 0.640249 -1.446745 -0.022397

6 2.004482 -1.197974 0.081427

6 2.469682 0.119378 -0.007695

6 1.566085 1.171148 -0.211538

6 0.203141 0.947558 -0.350744

1 0.261144 -2.458075 0.059111

1 2.681223 -2.025661 0.239288

1 1.961330 2.178329 -0.264978

6 -0.807891 2.047152 -0.531964

1 -1.224368 1.986472 -1.547028

1 -0.307171 3.016575 -0.465787

5 -2.016775 2.020300 0.554134

1 -1.657044 1.955473 1.705073

1 -2.899208 2.812200 0.365965

8 3.775037 0.481059 0.091268

6 4.751765 -0.530184 0.308556

1 5.707687 -0.011993 0.354745

1 4.579290 -1.056612 1.253422

1 4.770793 -1.251940 -0.515169

05-CH3BH2-ts-04-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H10B1N5O1 05-CH3BH2-ts-04-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-183.0 te_zpe=-684.532590 te_gfe=-684.571737 te_ms_zpe=-683.433273 te_ms_gfe=0.144569

7 -4.281335 -0.723655 0.095817

7 -2.463066 0.636810 0.163182

7 -1.678493 -0.246925 -0.028544

7 -2.249604 -1.745818 -0.223785

7 -3.461737 -1.518464 -0.090682

6 -0.255512 -0.170857 -0.062569

6 0.519640 -1.321916 0.039528

6 1.902328 -1.213418 0.066691

6 2.490108 0.057560 -0.009136

6 1.687119 1.203026 -0.123072

6 0.303188 1.126056 -0.155318

1 0.040672 -2.287481 0.110153

1 2.502177 -2.107744 0.153950

1 2.180359 2.164895 -0.192060

6 -0.598155 2.320556 -0.323566

1 -0.765433 2.463420 -1.401081

1 -0.083467 3.221327 0.021817

5 -2.020665 2.139421 0.446620

1 -1.942413 2.113876 1.663835

1 -2.908883 2.866311 0.090017

8 3.822560 0.283798 0.014265

6 4.712577 -0.824504 0.124071

1 5.713278 -0.397560 0.122894

1 4.551879 -1.372023 1.058138

1 4.606571 -1.505164 -0.726579

05-CH3BH2-ts-05-gas-b3-cbs-qb3 charge=0 spin=1 mol=C8H10B1N5O1 05-CH3BH2-ts-05-gas-b3-cbs-qb3 CBS-QB3

lf=-228.9 te_zpe=-684.547393 te_gfe=-684.586034 te_ms_zpe=-683.448072 te_ms_gfe=0.145752

7 -3.776636 0.079809 0.128020

7 -2.397684 0.422880 0.116731

7 -1.575816 -0.490228 -0.052032

7 -3.071768 -2.080892 -0.204801

7 -3.797720 -1.198341 -0.038273

6 -0.202306 -0.256456 -0.059115

6 0.628697 -1.376920 0.026526

6 2.005693 -1.227139 0.057644

6 2.547629 0.065416 -0.012846

6 1.704792 1.183944 -0.127784

6 0.326545 1.057709 -0.157172

1 0.176938 -2.359564 0.086414

1 2.637959 -2.099587 0.138531

1 2.167070 2.161226 -0.199553

6 -0.624832 2.209135 -0.332378

1 -0.806503 2.333569 -1.410308

1 -0.151705 3.136950 0.001130

5 -2.018041 1.976171 0.460799

1 -1.901919 1.925243 1.668200

1 -2.946494 2.647532 0.109875

8 3.871213 0.338795 0.011891

6 4.800344 -0.736525 0.122929

1 5.784982 -0.273682 0.126612

1 4.655774 -1.291675 1.055124

1 4.722399 -1.418803 -0.729489

##
#

05-iso-gas charge=0 spin=1 mol=C7H7N5O1 05-iso-gas CBS-QB3

lf=16.3 te_zpe=-619.845118 te_gfe=-619.883164 te_ms_zpe=-618.889305 te_ms_gfe=0.109119

7 -1.920426 -0.031935 -0.000041

6 -0.497742 0.069637 -0.000234

6 0.273500 -1.086651 0.003079

6 0.102541 1.331756 -0.003794

6 1.661859 -0.989681 0.002722

1 -0.208604 -2.054615 0.005789

6 1.481804 1.424700 -0.003837

1 -0.513036 2.220744 -0.006373

6 2.275511 0.267839 -0.000642

1 2.248240 -1.897703 0.005272

1 1.974662 2.388522 -0.006553

7 -2.746420 1.009778 0.007518

7 -3.938160 0.499084 0.004860

7 -3.842796 -0.842770 -0.004334

7 -2.591058 -1.180086 -0.007493

8 3.615219 0.473439 -0.001140

6 4.482725 -0.656187 0.002344

1 4.337828 -1.272545 -0.890989

1 5.492728 -0.251446 0.001501

1 4.337259 -1.267441 0.899081

05-ts-01-gas charge=0 spin=1 mol=C7H7N5O1 05-ts-01-gas CBS-QB3

lf=-559.0 te_zpe=-619.817842 te_gfe=-619.856200 te_ms_zpe=-618.855705 te_ms_gfe=0.104766

7 -1.886956 0.034016 -0.234642

6 -0.478203 0.074476 -0.182907

6 0.284188 -1.061988 0.084759

6 0.152659 1.310070 -0.371139

6 1.672186 -0.976300 0.141501

1 -0.207709 -2.014902 0.234872

6 1.529737 1.401914 -0.284739

1 -0.446631 2.187749 -0.577427

6 2.303774 0.259661 -0.035407

1 2.244284 -1.873228 0.334433

1 2.037115 2.348636 -0.420835

7 -2.971454 1.019467 0.650740

7 -3.993303 0.448099 0.593366

7 -3.786703 -1.028927 -0.241067

7 -2.608029 -0.985352 -0.537081

8 3.646734 0.456199 0.013669

6 4.492355 -0.659806 0.266353

1 4.395336 -1.420769 -0.515557

1 5.507531 -0.267634 0.262576

1 4.281132 -1.108734 1.242856

05-ts-02-gas charge=0 spin=1 mol=C7H7N5O1 05-ts-02-gas CBS-QB3

lf=-559.0 te_zpe=-619.817842 te_gfe=-619.856200 te_ms_zpe=-618.855705 te_ms_gfe=0.104766

7 1.886959 0.034036 -0.234671

6 0.478207 0.074489 -0.182929

6 -0.284176 -1.061979 0.084745

6 -0.152664 1.310078 -0.371159

6 -1.672174 -0.976299 0.141498

1 0.207728 -2.014890 0.234856

6 -1.529742 1.401915 -0.284750

1 0.446620 2.187760 -0.577453

6 -2.303770 0.259659 -0.035408

1 -2.244266 -1.873230 0.334435

1 -2.037126 2.348633 -0.420844

7 2.608033 -0.985330 -0.537118

7 3.786698 -1.028920 -0.241069

7 3.993280 0.448073 0.593418

7 2.971433 1.019445 0.650782

8 -3.646731 0.456189 0.013677

6 -4.492343 -0.659819 0.266376

1 -4.281106 -1.108742 1.242880

1 -5.507521 -0.267653 0.262610

1 -4.395330 -1.420787 -0.515530

##
#

06-2BH2-gas-b3-iso-cbs-qb3 charge=0 spin=1 mol=C8H12B2N6
06-2BH2-gas-b3-iso-cbs-qb3 CBS-QB3

lf=33.3 te_zpe=-690.137568 te_gfe=-690.179731 te_ms_zpe=-688.998659
te_ms_gfe=0.168480

7 2.140431 0.223955 -0.000093

6 0.721498 0.301567 -0.000220

6 0.223346 -1.009753 -0.000086

6 -0.070542 1.465873 -0.000307

6 -1.156480 -1.172553 -0.000084

6 -1.453407 1.236275 -0.000330

6 -2.031733 -0.060822 -0.000321

1 -1.556817 -2.177252 0.000226

1 -2.092965 2.106911 -0.000468

7 3.147433 1.068228 -0.000068

7 4.232039 0.314652 -0.000085

7 3.902856 -0.966611 0.000351

7 2.603158 -1.029897 0.000118

7 -3.395897 -0.224212 -0.000580

6 -3.970839 -1.561039 -0.000608

1 -5.056146 -1.481986 -0.002980

1 -3.671483 -2.132469 -0.887053

1 -3.675076 -2.131442 0.887789

6 -4.280085 0.932091 0.001823

1 -5.312655 0.588692 0.002616

1 -4.132653 1.557170 0.890231

1 -4.134735 1.559245 -0.885458

5 1.404206 -2.100071 0.000187

1 1.495427 -2.759663 1.003043

1 1.495587 -2.759940 -1.002475

5 0.427105 2.927444 -0.000495

1 -0.393730 3.792195 -0.000226

1 1.578011 3.209031 -0.000402

06-2BH2-gas-b3-ts-01-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H12B2N6 06-2BH2-gas-b3-ts-01-2d-d-p-cbs-qb3 CBS-QB3

lf=-518.5 te_zpe=-690.086118 te_gfe=-690.129606 te_ms_zpe=-688.938076 te_ms_gfe=0.161236

7 -2.070599 0.236612 0.002008

6 -0.660217 0.243720 -0.011766

6 -0.102762 -1.045811 -0.017109

6 0.113332 1.419594 -0.011041

6 1.278482 -1.164873 -0.029204

6 1.509316 1.243907 -0.024747

6 2.124843 -0.026127 -0.045185

1 1.713571 -2.155832 -0.025921

1 2.116988 2.137462 -0.018071

7 -3.927220 1.199461 0.009148

7 -4.543993 0.242381 0.016089

7 -3.804774 -1.221664 0.013826

7 -2.592477 -0.914617 0.006854

7 3.499558 -0.158884 -0.083976

6 4.107550 -1.472321 0.053522

1 5.188628 -1.373242 -0.029350

1 3.880303 -1.944176 1.019713

1 3.777065 -2.149244 -0.740757

6 4.345046 1.016736 0.046821

1 5.387564 0.716283 -0.044690

1 4.139843 1.742939 -0.745931

1 4.217414 1.523204 1.013692

5 -1.209799 -2.185476 -0.002493

1 -1.437276 -2.777973 -1.015919

1 -1.417146 -2.770366 1.019745

5 -0.472638 2.840209 0.007231

1 0.273825 3.771244 0.013284

1 -1.645605 3.034055 0.015132

06-2BH2-gas-b3-ts-02-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H12B2N6 06-2BH2-gas-b3-ts-02-2d-d-p-cbs-qb3 CBS-QB3

lf=-532.8 te_zpe=-690.095992 te_gfe=-690.139125 te_ms_zpe=-688.950970 te_ms_gfe=0.163269

7 -2.122511 0.324361 0.010698

6 -0.721966 0.360564 -0.009290

6 -0.239540 -0.960334 -0.015619

6 0.104726 1.502700 -0.008808

6 1.139289 -1.133320 -0.031670

6 1.491010 1.254604 -0.027595

6 2.042545 -0.043091 -0.051844

1 1.521549 -2.145515 -0.028891

1 2.139707 2.118611 -0.021639

7 -3.152722 1.037361 0.004854

7 -4.282390 0.626918 0.007978

7 -3.900522 -1.211306 0.012388

7 -2.734993 -1.250260 0.010971

7 3.409768 -0.243852 -0.098832

6 3.949619 -1.585306 0.054223

1 5.033586 -1.543880 -0.040025

1 3.706826 -2.031431 1.029060

1 3.577027 -2.254534 -0.727395

6 4.311609 0.886785 0.050224

1 5.337905 0.537692 -0.051950

1 4.139949 1.635461 -0.729266

1 4.213118 1.382330 1.026507

5 -1.344757 -2.126176 0.002030

1 -1.416304 -2.791709 -0.997173

1 -1.394683 -2.779333 1.010873

5 -0.393944 2.952910 0.015234

1 0.406837 3.835990 0.019644

1 -1.552167 3.224477 0.029804

06-2BH2-gas-b3-ts-03-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H12B2N6 06-2BH2-gas-b3-ts-03-2d-d-p-cbs-qb3 CBS-QB3

lf=-371.9 te_zpe=-690.035567 te_gfe=-690.079578 te_ms_zpe=-688.890878 te_ms_gfe=0.157849

7 -2.240102 -0.013880 -0.000579

6 -0.592218 0.216160 -0.016967

6 -0.109914 -1.078083 -0.015503

6 0.112589 1.416453 -0.011411

6 1.283848 -1.184646 -0.023820

6 1.511505 1.223510 -0.019159

6 2.127132 -0.052552 -0.036473

1 1.705625 -2.181191 -0.020335

1 2.118157 2.116754 -0.011493

7 -2.802409 1.109447 0.004449

7 -4.683379 0.473337 0.019862

7 -4.831728 -0.628322 0.021501

7 -2.516006 -1.217802 0.004573

7 3.499293 -0.176796 -0.066797

6 4.108518 -1.493671 0.038131

1 5.189739 -1.391823 -0.036293

1 3.875384 -1.988248 0.990630

1 3.779956 -2.149420 -0.774634

6 4.344690 1.001137 0.049756

1 5.387304 0.697610 -0.026111

1 4.149309 1.714546 -0.757513

1 4.210132 1.522386 1.007153

5 -1.270218 -2.183697 -0.003250

1 -1.308370 -2.870727 -0.998113

1 -1.292287 -2.864221 0.996695

5 -0.400367 2.866873 -0.003718

1 0.400974 3.748207 0.012597

1 -1.559575 3.118528 -0.016132

06-2BH2-gas-b3-ts-04-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H12B2N6 06-2BH2-gas-b3-ts-04-2d-d-p-cbs-qb3 CBS-QB3

lf=-236.7 te_zpe=-690.096820 te_gfe=-690.138881 te_ms_zpe=-688.944515 te_ms_gfe=0.165089

7 2.047430 0.271634 -0.000032

6 0.656703 0.285475 -0.000015

6 0.129463 -1.026512 0.000021

6 -0.136852 1.454623 -0.000032

6 -1.247650 -1.175335 0.000041

6 -1.519651 1.246481 -0.000011

6 -2.108982 -0.047897 0.000025

1 -1.666339 -2.172944 0.000070

1 -2.153634 2.121741 -0.000023

7 3.967788 1.168450 -0.000076

7 4.376337 0.081221 -0.000056

7 3.867711 -1.115992 -0.000022

7 2.497550 -0.907118 -0.000010

7 -3.474354 -0.197214 0.000044

6 -4.066166 -1.527128 0.000090

1 -5.150392 -1.434281 0.000099

1 -3.775413 -2.101362 -0.887213

1 -3.775394 -2.101311 0.887420

6 -4.347526 0.967778 0.000033

1 -5.383455 0.634590 0.000044

1 -4.194214 1.592267 0.887691

1 -4.194226 1.592239 -0.887647

5 1.355839 -2.049047 0.000030

1 1.505550 -2.705878 0.999577

1 1.505526 -2.705924 -0.999491

5 0.423861 2.889362 -0.000071

1 -0.342345 3.804000 -0.000082

1 1.592568 3.103520 -0.000090

06-2BH2-gas-b3-ts-05-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H12B2N6 06-2BH2-gas-b3-ts-05-2d-d-p-cbs-qb3 CBS-QB3

lf=-236.6 te_zpe=-690.077321 te_gfe=-690.120094 te_ms_zpe=-688.925917 te_ms_gfe=0.163896

7 2.105248 -0.064249 0.014261

6 0.694317 0.143780 0.045715

6 0.110907 -1.132804 0.064368

6 -0.024367 1.358443 0.027306

6 -1.275818 -1.219204 0.054910

6 -1.415920 1.205779 -0.022439

6 -2.075555 -0.055817 0.002410

1 -1.737128 -2.197364 0.076060

1 -2.005951 2.110039 -0.060656

7 3.021833 1.079677 -0.102845

7 4.153345 0.509281 -0.131834

7 4.664072 -0.524158 -0.103863

7 2.525836 -1.223922 0.043984

7 -3.447593 -0.128212 -0.027195

6 -4.107420 -1.425168 -0.021214

1 -5.185328 -1.277016 -0.043317

1 -3.829209 -2.028598 -0.893646

1 -3.863465 -1.998937 0.880169

6 -4.255074 1.079985 -0.110946

1 -5.307383 0.802650 -0.119981

1 -4.089940 1.740563 0.747834

1 -4.048640 1.649503 -1.024920

5 1.295739 -2.209980 0.091940

1 1.385558 -2.868050 1.103727

1 1.384982 -2.931871 -0.875741

5 0.491685 2.805283 0.211183

1 -0.263835 3.691531 -0.049864

1 1.557610 3.062143 0.656501

##
#

06-2CH3BH2-gas-b3-b3-iso charge=0 spin=1 mol=C10H16B2N6 06-2CH3BH2-gas-b3-b3-iso CBS-QB3

lf=49.3 te_zpe=-768.746549 te_gfe=-768.789011 te_ms_zpe=-767.474734 te_ms_gfe=0.226763

7 -1.866286 0.000006 -0.000041

6 -0.461958 -0.000009 -0.000061

6 0.197263 1.240422 -0.139175

6 0.197237 -1.240451 0.139079

6 1.579096 1.213283 -0.130132

6 1.579069 -1.213346 0.130007

6 2.305896 -0.000044 -0.000126

1 2.101206 2.152417 -0.242153

1 2.101152 -2.152480 0.242138

7 -2.647453 -1.057264 -0.177858

7 -3.896477 -0.644901 -0.103324

7 -3.896464 0.644958 0.103255

7 -2.647430 1.057290 0.177795

7 3.673131 -0.000044 -0.000250

6 4.413401 1.250320 -0.119064

1 5.479394 1.036689 -0.079998

1 4.203292 1.756807 -1.067547

1 4.175642 1.938827 0.698792

6 4.413467 -1.250269 0.119614

1 5.479433 -1.036710 0.079421

1 4.204066 -1.755670 1.068854

1 4.175086 -1.939697 -0.697258

6 -0.612625 2.499111 -0.336336

1 -0.813657 2.603164 -1.412836

1 -0.007123 3.366246 -0.060519

6 -0.612683 -2.499107 0.336322

1 -0.007205 -3.366277 0.060562

1 -0.813729 -2.603084 1.412826

5 -1.999720 2.505769 0.509158

5 -1.999776 -2.505769 -0.509176

1 -1.834268 2.458255 1.709026

1 -2.816768 3.316429 0.173829

1 -2.816842 -3.316397 -0.173815

1 -1.834323 -2.458304 -1.709045

06-2CH3BH2-gas-b3-b3-ts-01-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C10H16B2N6 06-2CH3BH2-gas-b3-b3-ts-01-2d-d-p-cbs-qb3 CBS-QB3

lf=-518.6 te_zpe=-768.685788 te_gfe=-768.730790 te_ms_zpe=-767.407117 te_ms_gfe=0.216996

7 -1.892342 0.054739 0.245178

6 -0.496664 0.101122 0.187164

6 0.219767 1.272802 -0.124833

6 0.134292 -1.146365 0.377326

6 1.603771 1.185492 -0.174422

6 1.517382 -1.193804 0.280595

6 2.289035 -0.035975 0.032086

1 2.157830 2.087061 -0.394378

1 1.997858 -2.153765 0.404214

7 -2.853129 -1.283323 -0.417195

7 -3.942120 -0.887624 -0.527655

7 -3.932241 0.831666 -0.049013

7 -2.773842 0.962088 0.280603

7 3.664775 -0.092795 -0.012209

6 4.434566 1.079462 -0.396327

1 5.495575 0.844044 -0.333563

1 4.217467 1.406571 -1.422138

1 4.241970 1.920765 0.277373

6 4.345147 -1.374818 0.086291

1 5.420888 -1.207963 0.074643

1 4.097985 -1.884245 1.022965

1 4.093733 -2.047379 -0.744620

6 -0.502666 2.572489 -0.383547

1 -0.993519 2.547693 -1.365361

1 0.237015 3.385184 -0.469640

6 -0.713038 -2.372972 0.593585

1 -0.072846 -3.259441 0.605765

1 -1.177610 -2.319059 1.587936

5 -1.499382 3.084137 0.720815

5 -1.869010 -2.598853 -0.530105

1 -1.349132 2.782071 1.864022

1 -2.323834 3.896681 0.437845

1 -2.603678 -3.528337 -0.332277

1 -1.484999 -2.514155 -1.671796

06-2CH3BH2-gas-b3-b3-ts-02-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C10H16B2N6 06-2CH3BH2-gas-b3-b3-ts-02-2d-d-p-cbs-qb3 CBS-QB3

lf=-429.4 te_zpe=-768.658646 te_gfe=-768.702758 te_ms_zpe=-767.373955 te_ms_gfe=0.217475

7 1.907906 0.080643 -0.071546

6 0.434081 0.037624 -0.055831

6 -0.217544 -1.202144 -0.175536

6 -0.256732 1.254800 0.101977

6 -1.605329 -1.214525 -0.131124

6 -1.641399 1.195111 0.120099

6 -2.354841 -0.023665 -0.002727

1 -2.102560 -2.168951 -0.220678

1 -2.174006 2.122848 0.270982

7 2.512856 1.161403 -0.173233

7 4.490547 0.424455 0.025099

7 4.279059 -0.668724 0.196995

7 2.522399 -1.152863 -0.134921

7 -3.723300 -0.043549 0.008292

6 -4.440492 -1.308177 -0.082514

1 -5.510297 -1.114317 -0.041535

1 -4.226128 -1.828296 -1.022895

1 -4.185712 -1.978349 0.746196

6 -4.480976 1.195127 0.132470

1 -5.543392 0.968460 0.071270

1 -4.295157 1.693853 1.090757

1 -4.238989 1.896552 -0.672802

6 0.567729 -2.454098 -0.319639

1 0.854290 -2.637767 -1.358125

1 0.029717 -3.324739 0.061714

6 0.479496 2.540058 0.336035

1 -0.129782 3.393564 0.029802

1 0.662745 2.648036 1.413329

5 1.966902 -2.319438 0.639215

5 1.895515 2.533513 -0.484768

1 1.681755 -2.085404 1.787355

1 2.646213 -3.286612 0.419489

1 2.669215 3.391574 -0.147316

1 1.719763 2.508952 -1.693839

##
#

06-BH2-iso-gas-cbs-qb3 charge=0 spin=1 mol=C8H11B1N6
06-BH2-iso-gas-cbs-qb3 CBS-QB3

lf=41.3 te_zpe=-664.705798 te_gfe=-664.745729 te_ms_zpe=-663.630931
te_ms_gfe=0.159905

7 2.147818 -0.420323 -0.000032

6 0.740315 -0.455314 -0.000089

6 0.255649 0.864139 -0.000035

6 -0.059826 -1.590462 -0.000133

6 -1.120957 1.025217 -0.000052

6 -1.429036 -1.400889 -0.000157

1 0.367724 -2.585302 -0.000149

6 -1.994122 -0.093086 -0.000153

1 -1.527861 2.026731 0.000049

1 -2.069468 -2.270289 -0.000208

7 3.112185 -1.308839 -0.000026

7 4.229849 -0.597322 0.000006

7 3.953568 0.694431 0.000105

7 2.653673 0.812810 0.000057

7 -3.357884 0.074805 -0.000267

6 -3.931344 1.412597 -0.000073

1 -5.016812 1.334370 -0.000801

1 -3.633447 1.982517 0.887596

1 -3.632369 1.983079 -0.886989

6 -4.245955 -1.077604 0.000500

1 -5.277621 -0.731377 0.000581

1 -4.101996 -1.704845 -0.887241

1 -4.101559 -1.704050 0.888740

5 1.471353 1.923375 0.000082

1 1.586960 2.577955 -1.003189

1 1.586880 2.577823 1.003449

06-BH2-ts-01-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H11B1N6
06-BH2-ts-01-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-266.5 te_zpe=-664.602857 te_gfe=-664.645478 te_ms_zpe=-663.520467 te_ms_gfe=0.148499

7 2.200624 -0.127384 0.041742

6 0.655934 -0.318482 0.082159

6 0.130325 0.974394 0.000936

6 -0.066336 -1.501472 0.109258

6 -1.255868 1.054021 -0.016641

6 -1.445591 -1.379253 0.077996

1 0.406176 -2.471064 0.166917

6 -2.073383 -0.104513 -0.002735

1 -1.709214 2.036224 0.003940

1 -2.038923 -2.280208 0.130208

7 2.669391 -1.277971 -0.226688

7 4.638674 -0.820033 -0.090572

7 4.913019 0.250925 -0.018203

7 2.553256 1.062094 0.109877

7 -3.443583 -0.003326 -0.032317

6 -4.079585 1.301584 -0.141497

1 -5.158677 1.168716 -0.188338

1 -3.853290 1.938299 0.722042

1 -3.762594 1.830648 -1.046783

6 -4.275714 -1.194780 0.034050

1 -5.322734 -0.898279 0.031905

1 -4.110684 -1.858185 -0.823369

1 -4.090537 -1.767666 0.950101

5 1.325139 2.048830 0.095673

1 1.446333 2.763207 -0.878340

1 1.310097 2.715020 1.105319

06-BH2-ts-02-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H11B1N6 06-BH2-ts-02-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-535.3 te_zpe=-664.660936 te_gfe=-664.702006 te_ms_zpe=-663.580091 te_ms_gfe=0.154254

7 2.139981 -0.530719 0.140287

6 0.740352 -0.525951 0.060243

6 0.270439 0.800651 0.033051

6 -0.099741 -1.631558 0.055874

6 -1.105297 0.980447 -0.015995

6 -1.469648 -1.419992 0.001510

1 0.300280 -2.637672 0.094165

6 -2.007879 -0.110814 -0.044801

1 -1.486861 1.992136 -0.036122

1 -2.120623 -2.281898 -0.003648

7 3.136773 -1.272173 -0.022783

7 4.275745 -0.902143 -0.128368

7 3.942829 0.960712 -0.085377

7 2.785162 1.029076 0.027532

7 -3.373311 0.092409 -0.123798

6 -3.913193 1.437476 -0.008041

1 -4.995028 1.396812 -0.125436

1 -3.690037 1.900681 0.963275

1 -3.520502 2.090978 -0.793039

6 -4.282850 -1.032715 0.011379

1 -5.305792 -0.679528 -0.109003

1 -4.101799 -1.784812 -0.763282

1 -4.204100 -1.526516 0.990497

5 1.401555 1.942323 0.072415

1 1.484657 2.644305 -0.899506

1 1.488684 2.548516 1.108248

06-BH2-ts-03-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H11B1N6 06-BH2-ts-03-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-452.1 te_zpe=-664.660795 te_gfe=-664.701828 te_ms_zpe=-663.577553 te_ms_gfe=0.155160

7 -2.128139 -0.686624 -0.000036

6 -0.731792 -0.548035 -0.000017

6 -0.286471 0.786213 -0.000018

6 0.127877 -1.651102 0.000006

6 1.085896 0.987958 0.000004

6 1.484753 -1.422916 0.000028

1 -0.268209 -2.659445 0.000009

6 2.002245 -0.092631 0.000024

1 1.453692 2.004536 0.000008

1 2.154036 -2.270399 0.000047

7 -2.994066 -1.487572 -0.000039

7 -4.530112 -0.283962 -0.000066

7 -3.891197 0.721868 -0.000068

7 -2.677453 0.929547 -0.000058

7 3.355446 0.124277 0.000040

6 3.880423 1.483421 0.000063

1 4.967879 1.444396 0.000038

1 3.560026 2.040878 -0.887074

1 3.560061 2.040843 0.887237

6 4.287891 -0.994353 0.000115

1 5.305211 -0.608250 0.000112

1 4.167136 -1.625100 0.888286

1 4.167167 -1.625187 -0.887997

5 -1.442260 1.916461 -0.000042

1 -1.451009 2.580684 1.007586

1 -1.450976 2.580677 -1.007674

06-BH2-ts-04-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H11B1N6
06-BH2-ts-04-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-235.9 te_zpe=-664.663249 te_gfe=-664.703428 te_ms_zpe=-663.574757 te_ms_gfe=0.156153

7 -2.064761 -0.469652 0.000008

6 -0.679709 -0.454024 0.000008

6 -0.163802 0.866301 -0.000014

6 0.132417 -1.589607 0.000026

6 1.209585 1.022900 -0.000017

6 1.500306 -1.410140 0.000023

1 -0.299349 -2.583405 0.000043

6 2.074220 -0.104000 0.000002

1 1.626314 2.020823 -0.000033

1 2.138466 -2.281525 0.000038

7 -3.950378 -1.413878 0.000023

7 -4.393071 -0.337557 0.000005

7 -3.918419 0.870912 -0.000015

7 -2.540238 0.698959 -0.000012

7 3.438220 0.053281 -0.000001

6 4.023767 1.386476 -0.000022

1 5.108487 1.298671 -0.000019

1 3.729585 1.958661 -0.887173

1 3.729582 1.958690 0.887110

6 4.319259 -1.105147 0.000017

1 5.353122 -0.765561 0.000010

1 4.170211 -1.730652 0.887874

1 4.170208 -1.730682 -0.887818

5 -1.413380 1.865591 -0.000031

1 -1.577727 2.518025 1.000110

1 -1.577727 2.517992 -1.000193

06-BH2-ts-05-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H11B1N6 06-BH2-ts-05-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-230.1 te_zpe=-664.648703 te_gfe=-664.689198 te_ms_zpe=-663.561050 te_ms_gfe=0.155529

7 -2.122762 -0.114806 -0.000258

6 -0.720077 -0.275611 -0.000085

6 -0.147817 1.007774 -0.000023

6 0.001085 -1.465653 0.000009

6 1.236391 1.083108 0.000145

6 1.378085 -1.362565 0.000176

1 -0.491212 -2.429388 -0.000043

6 2.029655 -0.092184 0.000248

1 1.710103 2.055080 0.000195

1 1.963154 -2.270425 0.000256

7 -2.977698 -1.309171 -0.000353

7 -4.138614 -0.796898 -0.000497

7 -4.688127 0.217979 -0.000570

7 -2.585845 1.027778 -0.000321

7 3.402198 -0.019970 0.000413

6 4.066221 1.275160 0.000520

1 5.143899 1.122999 0.000689

1 3.807090 1.864748 -0.886501

1 3.806813 1.864737 0.887467

6 4.210134 -1.229936 0.000480

1 5.262907 -0.954282 0.000562

1 4.023947 -1.845611 0.888383

1 4.024086 -1.845608 -0.887454

5 -1.367106 2.056865 -0.000178

1 -1.480817 2.739243 0.992250

1 -1.480573 2.739237 -0.992637

##
#

06-CH3-BH2-iso-gas-cbs-qb3 charge=0 spin=1 mol=C9H13B1N6
06-CH3-BH2-iso-gas-cbs-qb3 CBS-QB3

lf=42.3 te_zpe=-704.002650 te_gfe=-704.043883 te_ms_zpe=-702.860488 te_ms_gfe=0.187152

7 -2.028416 -0.502551 -0.061812

6 -0.613796 -0.384929 -0.060449

6 -0.046685 0.898079 -0.170568

6 0.164991 -1.535843 0.060273

6 1.339110 0.978158 -0.138038

6 1.540361 -1.431354 0.081128

1 -0.313479 -2.502804 0.143999

6 2.168662 -0.162331 -0.011310

1 1.780586 1.961153 -0.221078

1 2.126999 -2.332125 0.183164

7 -2.725399 -1.608911 -0.258096

7 -3.982307 -1.263171 -0.127475

7 -4.072138 0.030822 0.132335

7 -2.858264 0.509408 0.180976

7 3.534992 -0.046578 0.020088

6 4.163874 1.264751 -0.047100

1 5.244097 1.144010 0.004510

1 3.926081 1.781031 -0.984136

1 3.854224 1.907058 0.785322

6 4.370875 -1.230463 0.156299

1 5.416845 -0.930658 0.143580

1 4.181676 -1.758436 1.098554

1 4.213060 -1.934551 -0.668511

6 -0.940786 2.100775 -0.340965

1 -0.391363 3.005176 -0.067496

1 -1.174504 2.200625 -1.411361

5 -2.306135 1.991116 0.531995

1 -2.109738 1.938063 1.726702

1 -3.182732 2.751704 0.229042

06-CH3-BH2-ts-01-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C9H13B1N6 06-CH3-BH2-ts-01-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-500.0 te_zpe=-703.953915 te_gfe=-703.996955 te_ms_zpe=-702.804742 te_ms_gfe=0.179534

7 -1.980796 -0.521416 0.121475

6 -0.591967 -0.373862 0.075886

6 0.005471 0.881843 -0.176684

6 0.195513 -1.509528 0.281968

6 1.391462 0.946457 -0.206716

6 1.573581 -1.430944 0.222716

1 -0.288889 -2.457228 0.483893

6 2.213001 -0.192549 -0.026576

1 1.842187 1.914444 -0.376426

1 2.152677 -2.328774 0.381668

7 -3.291590 -1.817625 -0.507999

7 -4.250867 -1.195215 -0.376753

7 -4.021503 0.392065 0.096986

7 -2.797304 0.438619 0.283982

7 3.584979 -0.098682 -0.090616

6 4.224068 1.196481 -0.261012

1 5.302188 1.056616 -0.316039

1 3.903267 1.681837 -1.188830

1 4.010632 1.878913 0.572095

6 4.410383 -1.261256 0.195143

1 5.457899 -0.994367 0.067360

1 4.274232 -1.626380 1.221585

1 4.191154 -2.086186 -0.491270

6 -0.878390 2.088642 -0.341355

1 -0.289398 3.002397 -0.200545

1 -1.259657 2.132217 -1.370775

5 -2.087598 2.121497 0.715915

1 -1.819294 1.901141 1.863698

1 -2.998171 2.861950 0.504272

06-CH3-BH2-ts-02-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C9H13B1N6 06-CH3-BH2-ts-02-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-531.8 te_zpe=-703.962482 te_gfe=-704.004123 te_ms_zpe=-702.814015 te_ms_gfe=0.182379

7 -2.003424 -0.530917 -0.346905

6 -0.603284 -0.472318 -0.274908

6 -0.051068 0.819497 -0.375897

6 0.194891 -1.591945 -0.038206

6 1.327506 0.939329 -0.246922

6 1.567725 -1.452835 0.052724

1 -0.261135 -2.570079 0.057962

6 2.173852 -0.177173 -0.053292

1 1.747929 1.933626 -0.300845

1 2.166276 -2.336683 0.217701

7 -2.793167 -1.521226 -0.371192

7 -3.941374 -1.487635 0.005623

7 -4.068381 0.195709 0.548868

7 -3.014584 0.676755 0.400719

7 3.542412 -0.030868 0.028288

6 4.132967 1.298049 0.046512

1 5.217287 1.204459 0.074977

1 3.872388 1.860101 -0.855778

1 3.816445 1.886596 0.918322

6 4.377315 -1.170839 0.371108

1 5.421959 -0.864993 0.351441

1 4.156161 -1.568930 1.370895

1 4.257637 -1.983336 -0.352852

6 -0.971019 2.000585 -0.535449

1 -0.391960 2.926452 -0.478934

1 -1.413111 1.977438 -1.541238

5 -2.157081 2.070899 0.575955

1 -1.778868 1.974307 1.719034

1 -2.969294 2.939712 0.407704

06-CH3-BH2-ts-03-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C9H13B1N6 06-CH3-BH2-ts-03-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-351.9 te_zpe=-703.902385 te_gfe=-703.944945 te_ms_zpe=-702.754003 te_ms_gfe=0.178291

7 -2.103716 -0.274011 0.008312

6 -0.592147 -0.323781 -0.068391

6 0.007871 0.925731 -0.307567

6 0.126957 -1.481601 0.219825

6 1.398981 0.952558 -0.267837

6 1.504747 -1.421064 0.246959

1 -0.390913 -2.406894 0.425064

6 2.180631 -0.199629 -0.014110

1 1.876921 1.910064 -0.416595

1 2.055345 -2.318116 0.487815

7 -2.403425 -1.347706 -0.625806

7 -4.311295 -1.311264 -0.349103

7 -4.703107 -0.388345 0.144840

7 -2.714210 0.702208 0.480338

7 3.549927 -0.136987 -0.004537

6 4.230628 1.130996 -0.227708

1 5.305803 0.970260 -0.181402

1 3.992971 1.549046 -1.212109

1 3.965540 1.874092 0.533209

6 4.340328 -1.329472 0.266119

1 5.396864 -1.079382 0.194522

1 4.153499 -1.724888 1.271704

1 4.132689 -2.123835 -0.459059

6 -0.846114 2.143408 -0.397979

1 -0.240232 3.047101 -0.306601

1 -1.374146 2.185591 -1.358367

5 -1.976977 2.028944 0.815264

1 -1.515120 1.954602 1.936408

1 -2.784861 2.927488 0.734928

06-CH3-BH2-ts-04-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C9H13B1N6 06-CH3-BH2-ts-04-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-225.9 te_zpe=-703.959281 te_gfe=-704.000792 te_ms_zpe=-702.802624 te_ms_gfe=0.183156

7 -1.945313 -0.462485 -0.050767

6 -0.566838 -0.328706 -0.058153

6 0.060065 0.941021 -0.146505

6 0.195478 -1.503476 0.013325

6 1.443157 0.978617 -0.113771

6 1.570902 -1.447244 0.046770

1 -0.318911 -2.455881 0.060837

6 2.236559 -0.193140 -0.002048

1 1.919429 1.946423 -0.187723

1 2.132402 -2.367124 0.116083

7 -3.538464 -1.950520 -0.198111

7 -4.210313 -1.022194 -0.037684

7 -4.109203 0.249725 0.119133

7 -2.706410 0.506067 0.110166

7 3.603110 -0.118207 0.047935

6 4.275755 1.172406 -0.019236

1 5.348875 1.018957 0.075112

1 4.087161 1.682730 -0.971015

1 3.956439 1.833650 0.792971

6 4.405699 -1.331483 0.119502

1 5.458521 -1.059713 0.159393

1 4.173991 -1.915675 1.016817

1 4.253997 -1.973084 -0.756325

6 -0.806833 2.157952 -0.325229

1 -0.271939 3.051504 0.009661

1 -0.974793 2.292741 -1.404417

5 -2.219906 2.023315 0.459210

1 -2.111476 1.971217 1.667850

1 -3.091678 2.765302 0.102087

06-CH3-BH2-ts-05-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C9H13B1N6 06-CH3-BH2-ts-05-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-184.1 te_zpe=-703.944441 te_gfe=-703.986796 te_ms_zpe=-702.788595 te_ms_gfe=0.181489

7 -2.024057 -0.204643 -0.026687

6 -0.610899 -0.232018 -0.058071

6 0.044818 1.017973 -0.142540

6 0.092153 -1.434967 0.029233

6 1.430472 1.004914 -0.109125

6 1.470445 -1.420839 0.057753

1 -0.449934 -2.367720 0.088368

6 2.181103 -0.193113 -0.000242

1 1.938869 1.956060 -0.180041

1 1.997632 -2.360073 0.134792

7 -2.725726 -1.694425 -0.216350

7 -3.905106 -1.353043 -0.089035

7 -4.655754 -0.487279 0.088051

7 -2.753077 0.724983 0.149099

7 3.549828 -0.167949 0.042720

6 4.267257 1.098272 -0.021244

1 5.335358 0.905743 0.056700

1 4.084755 1.623387 -0.966025

1 3.983038 1.763803 0.800860

6 4.307474 -1.409229 0.122852

1 5.370101 -1.176389 0.144971

1 4.066503 -1.972469 1.031339

1 4.120830 -2.056456 -0.741817

6 -0.769645 2.274242 -0.314915

1 -0.195988 3.137850 0.034059

1 -0.919082 2.427684 -1.393828

5 -2.208391 2.200808 0.446486

1 -2.136415 2.168306 1.662831

1 -3.035531 2.991311 0.078577

06-CH3-BH2-ts-05-gas-2d-d-p charge=0 spin=1 mol=C9H13B1N6 RB3LYP/6-311G(2d,d,p)

lf=-184.1 te_zpe=-703.944441 te_gfe=-703.986796

7 -2.024057 -0.204643 -0.026687

6 -0.610899 -0.232018 -0.058071

6 0.044818 1.017973 -0.142540

6 0.092153 -1.434967 0.029233

6 1.430472 1.004914 -0.109125

6 1.470445 -1.420839 0.057753

1 -0.449934 -2.367720 0.088368

6 2.181103 -0.193113 -0.000242

1 1.938869 1.956060 -0.180041

1 1.997632 -2.360073 0.134792

7 -2.725726 -1.694425 -0.216350

7 -3.905106 -1.353043 -0.089035

7 -4.655754 -0.487279 0.088051

7 -2.753077 0.724983 0.149099

7 3.549828 -0.167949 0.042720

6 4.267257 1.098272 -0.021244

1 5.335358 0.905743 0.056700

1 4.084755 1.623387 -0.966025

1 3.983038 1.763803 0.800860

6 4.307474 -1.409229 0.122852

1 5.370101 -1.176389 0.144971

1 4.066503 -1.972469 1.031339

1 4.120830 -2.056456 -0.741817

6 -0.769645 2.274242 -0.314915

1 -0.195988 3.137850 0.034059

1 -0.919082 2.427684 -1.393828

5 -2.208391 2.200808 0.446486

1 -2.136415 2.168306 1.662831

1 -3.035531 2.991311 0.078577

##
#

07-2BH2-b3-iso-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H6B2N6 07-2BH2-b3-iso-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=52.0 te_zpe=-648.465372 te_gfe=-648.503393 te_ms_zpe=-647.403902 te_ms_gfe=0.098673

6 -1.948444 1.159922 0.000029

6 -0.568979 1.422943 -0.000029

6 0.232913 0.265426 -0.000025

6 -0.215879 -1.061312 -0.000011

6 -1.598211 -1.250742 0.000025

6 -2.461752 -0.147577 0.000055

1 -2.636698 1.995631 0.000042

1 -2.011932 -2.252182 0.000034

7 1.662556 0.225621 -0.000043

7 2.647963 1.095541 0.000036

7 3.745999 0.375978 0.000011

7 3.448796 -0.921469 -0.000024

7 2.157036 -1.016079 -0.000072

5 0.990339 -2.118953 -0.000048

1 1.099423 -2.773915 -1.002307

1 1.099505 -2.773923 1.002195

5 -0.092769 2.897016 -0.000162

1 1.053272 3.192267 -0.000312

1 -0.929983 3.742195 -0.000063

6 -3.879397 -0.349386 0.000115

7 -5.022769 -0.510453 0.000165

07-2BH2-b3-ts-01-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H6B2N6 07-2BH2-b3-ts-01-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-492.5 te_zpe=-648.419171 te_gfe=-648.458773 te_ms_zpe=-647.348113 te_ms_gfe=0.091616

6 -1.998682 1.192654 -0.000169

6 -0.605582 1.391052 -0.000071

6 0.170293 0.214327 0.000010

6 -0.352753 -1.091531 0.000002

6 -1.734134 -1.225689 -0.000099

6 -2.562849 -0.087079 -0.000185

1 -2.650008 2.057891 -0.000235

1 -2.191582 -2.208661 -0.000113

7 1.581831 0.232302 0.000112

7 3.373058 1.226244 0.000211

7 4.025963 0.290743 0.000278

7 3.338683 -1.180825 0.000263

7 2.121017 -0.918099 0.000174

5 0.780142 -2.205063 0.000119

1 1.005195 -2.788237 -1.018083

1 1.005051 -2.788160 1.018398

5 -0.031411 2.821101 -0.000063

1 1.139065 3.021545 0.000009

1 -0.789362 3.739339 -0.000132

6 -3.985089 -0.241669 -0.000287

7 -5.133301 -0.368407 -0.000370

07-2BH2-b3-ts-02-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H6B2N6 07-2BH2-b3-ts-02-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-529.7 te_zpe=-648.429072 te_gfe=-648.468839 te_ms_zpe=-647.360051 te_ms_gfe=0.092863

6 1.982692 1.170288 -0.000010

6 0.603317 1.451810 0.000009

6 -0.235759 0.315022 0.000021

6 0.202343 -1.024367 0.000019

6 1.578414 -1.224033 0.000005

6 2.472312 -0.138634 -0.000009

1 2.680468 1.998277 -0.000024

1 1.976090 -2.232468 0.000005

7 -1.633606 0.312735 0.000052

7 -2.639163 1.075121 -0.000013

7 -3.774534 0.695257 -0.000060

7 -3.458420 -1.149826 -0.000045

7 -2.293587 -1.225381 0.000007

5 -0.938357 -2.154810 0.000041

1 -1.019682 -2.808144 1.004598

1 -1.019669 -2.808209 -1.004472

5 0.131159 2.915978 0.000030

1 -1.020597 3.207437 0.000070

1 0.952794 3.776229 0.000008

6 3.883643 -0.373992 -0.000022

7 5.022854 -0.564410 -0.000031

07-2BH2-b3-ts-03-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H6B2N6 07-2BH2-b3-ts-03-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-379.9 te_zpe=-648.364765 te_gfe=-648.405107 te_ms_zpe=-647.295683 te_ms_gfe=0.087772

6 -2.010012 1.170147 -0.000016

6 -0.613528 1.381470 -0.000009

6 0.091663 0.179567 -0.000002

6 -0.354649 -1.124900 -0.000001

6 -1.752742 -1.246911 -0.000011

6 -2.573397 -0.114698 -0.000018

1 -2.658971 2.036352 -0.000019

1 -2.197884 -2.235523 -0.000014

7 1.756269 -0.036907 0.000012

7 2.293485 1.104231 0.000024

7 4.177915 0.536574 0.000035

7 4.399893 -0.550702 0.000039

7 2.050768 -1.231789 0.000014

5 0.820365 -2.212632 0.000004

1 0.854282 -2.894868 -0.996276

1 0.854272 -2.894874 0.996280

5 -0.107006 2.840605 -0.000019

1 1.050521 3.093342 -0.000045

1 -0.916644 3.711259 -0.000003

6 -3.998727 -0.259552 -0.000026

7 -5.147475 -0.373734 -0.000032

07-2BH2-b3-ts-04-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H6B2N6 07-2BH2-b3-ts-04-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-237.1 te_zpe=-648.425508 te_gfe=-648.463649 te_ms_zpe=-647.351299 te_ms_gfe=0.095000

6 -2.022283 1.180737 -0.000028

6 -0.640294 1.417102 -0.000027

6 0.158428 0.252756 -0.000003

6 -0.324484 -1.071268 0.000018

6 -1.705744 -1.242641 0.000012

6 -2.552064 -0.121732 -0.000011

1 -2.701803 2.024055 -0.000044

1 -2.140972 -2.235275 0.000026

7 1.564030 0.275494 0.000004

7 3.476208 1.199400 0.000000

7 3.893848 0.122012 0.000019

7 3.390599 -1.090264 0.000038

7 2.032941 -0.894024 0.000026

5 0.918549 -2.064085 0.000036

1 1.093026 -2.714212 -0.998171

1 1.093019 -2.714198 0.998253

5 -0.093723 2.861134 -0.000054

1 1.072910 3.081613 -0.000078

1 -0.870234 3.763459 -0.000053

6 -3.971869 -0.303680 -0.000015

7 -5.117659 -0.449521 -0.000019

07-2BH2-b3-ts-05-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H6B2N6 07-2BH2-b3-ts-05-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-245.4 te_zpe=-648.405896 te_gfe=-648.444412 te_ms_zpe=-647.331872 te_ms_gfe=0.094215

6 1.905183 1.164664 -0.050192

6 0.514479 1.338200 0.014188

6 -0.203539 0.124876 0.042144

6 0.339301 -1.164968 0.066661

6 1.732157 -1.267049 0.048630

6 2.510297 -0.107371 -0.021189

1 2.538473 2.041391 -0.102570

1 2.215052 -2.236671 0.076144

7 -1.632905 -0.051864 0.017166

7 -2.517908 1.092312 -0.112245

7 -3.665424 0.538303 -0.136340

7 -4.160226 -0.503157 -0.094439

7 -2.062820 -1.208786 0.059442

5 -0.863004 -2.214893 0.108133

1 -0.960799 -2.870346 1.119716

1 -0.976840 -2.943361 -0.851139

5 0.003783 2.791676 0.203006

1 -1.032868 3.043601 0.712879

1 0.739848 3.671425 -0.116536

6 3.938393 -0.204312 -0.067157

7 5.090086 -0.280264 -0.103969

###
#

07-2BH2CH3-iso-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C9H10B2N6 07-2BH2CH3-iso-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=54.2 te_zpe=-727.069969 te_gfe=-727.108963 te_ms_zpe=-725.876766 te_ms_gfe=0.156044

7 -3.455991 -0.649924 -0.104762

7 -2.213911 -1.056457 -0.176920

7 -1.436817 -0.000004 0.000028

7 -2.213915 1.056445 0.177019

7 -3.456003 0.649939 0.104877

6 -0.011026 -0.000002 -0.000000

6 0.624933 1.243034 -0.164409

6 2.016350 1.211668 -0.154518

6 2.704400 0.000004 -0.000057

6 2.016362 -1.211664 0.154435

6 0.624947 -1.243036 0.164384

1 2.571308 2.133111 -0.275553

1 2.571330 -2.133104 0.275448

6 -0.186876 -2.497289 0.369251

1 -0.390470 -2.595475 1.445376

1 0.420657 -3.364962 0.101361

6 -0.186904 2.497283 -0.369237

1 0.420637 3.364957 -0.101371

1 -0.390548 2.595471 -1.445352

5 -1.565446 -2.516227 -0.486680

5 -1.565434 2.516214 0.486760

1 -1.398482 -2.472077 -1.684964

1 -2.391216 -3.313315 -0.147649

1 -1.398416 2.472054 1.685036

1 -2.391220 3.313304 0.147773

6 4.136216 0.000007 -0.000087

7 5.290981 0.000011 -0.000111

07-2BH2CH3-ts-01-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C9H10B2N6 07-2BH2CH3-ts-01-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-531.0 te_zpe=-727.017583 te_gfe=-727.059166 te_ms_zpe=-725.816195 te_ms_gfe=0.146621

7 -3.542998 -0.834608 -0.438178

7 -2.461698 -1.255750 -0.333031

7 -1.457999 0.071802 0.219529

7 -2.306636 1.015993 0.227504

7 -3.476436 0.891420 -0.041589

6 -0.053996 0.081585 0.136526

6 0.672270 1.247769 -0.179398

6 2.056613 1.122189 -0.240170

6 2.682254 -0.114396 -0.035040

6 1.922233 -1.256128 0.242094

6 0.536126 -1.182673 0.345162

1 2.661160 1.992115 -0.464878

1 2.417935 -2.207389 0.389038

6 -0.328627 -2.383491 0.619380

1 -0.750170 -2.297586 1.630376

1 0.294661 -3.281196 0.627164

6 -0.013748 2.565629 -0.437281

1 0.752413 3.346253 -0.569431

1 -0.539341 2.542427 -1.400845

5 -1.527117 -2.607814 -0.453419

5 -0.951721 3.137867 0.688070

1 -1.188650 -2.551265 -1.610432

1 -2.284134 -3.504565 -0.206749

1 -0.812450 2.811737 1.825423

1 -1.732492 3.994495 0.416006

6 4.107656 -0.207281 -0.115566

7 5.258707 -0.279500 -0.180402

07-2BH2CH3-ts-02-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C9H10B2N6 07-2BH2CH3-ts-02-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-447.8 te_zpe=-726.983431 te_gfe=-727.024071 te_ms_zpe=-725.775757 te_ms_gfe=0.146790

7 3.834305 -0.667124 0.109248

7 2.088967 -1.135722 -0.123751

7 1.477691 0.092118 -0.047066

7 2.064838 1.176421 -0.132995

7 4.056234 0.424430 -0.061342

6 -0.025829 0.034590 -0.032334

6 -0.703668 1.251849 0.133339

6 -2.096966 1.178763 0.131375

6 -2.761130 -0.044608 -0.010557

6 -2.038252 -1.232036 -0.143909

6 -0.641639 -1.215694 -0.166668

1 -2.669019 2.087236 0.268673

1 -2.560275 -2.174251 -0.245825

6 0.153176 -2.462567 -0.305619

1 0.425677 -2.653614 -1.346550

1 -0.379853 -3.331352 0.086462

6 0.018668 2.541926 0.375593

1 -0.594588 3.386291 0.053954

1 0.175311 2.656119 1.456097

5 1.555107 -2.322411 0.643337

5 1.451852 2.554956 -0.409544

1 1.283770 -2.097934 1.795001

1 2.244828 -3.274702 0.402213

1 1.319601 2.554858 -1.624039

1 2.220544 3.399356 -0.035188

6 -4.192455 -0.080916 -0.006967

7 -5.346638 -0.110490 -0.004847

##
#

078-iso-gas charge=0 spin=1 mol=C8H10N6 078-iso-gas CBS-QB3

lf=20.2 te_zpe=-639.255344 te_gfe=-639.296128 te_ms_zpe=-638.242462 te_ms_gfe=0.146541

7 -2.293006 0.000000 0.001150

6 -0.868965 0.000000 -0.006788

6 -0.173498 1.207689 -0.008101

6 -0.173498 -1.207688 -0.008104

6 1.210745 1.208293 -0.015706

1 -0.719461 2.141356 -0.000831

6 1.210744 -1.208293 -0.015710

1 -0.719462 -2.141355 -0.000837

6 1.948008 0.000000 -0.027856

1 1.721353 2.160302 -0.011481

1 1.721352 -2.160303 -0.011486

7 -3.043279 -1.097653 0.004832

7 -4.269914 -0.671483 0.011012

7 -4.269912 0.671481 0.011005

7 -3.043278 1.097655 0.004810

7 3.323742 0.000000 -0.054108

6 4.055915 1.253775 0.031240

1 5.122438 1.048064 -0.039037

1 3.792483 1.927064 -0.791321

1 3.871847 1.781106 0.976625

6 4.055916 -1.253775 0.031230

1 5.122438 -1.048064 -0.039053

1 3.871854 -1.781111 0.976614

1 3.792478 -1.927060 -0.791333

078-ts-01-gas charge=0 spin=1 mol=C8H10N6 078-ts-01-gas CBS-QB3

lf=20.2 te_zpe=-639.255344 te_gfe=-639.296128 te_ms_zpe=-638.242462 te_ms_gfe=0.146541

7 -2.293006 0.000000 0.001150

6 -0.868965 0.000000 -0.006788

6 -0.173498 1.207689 -0.008101

6 -0.173498 -1.207688 -0.008104

6 1.210745 1.208293 -0.015706

1 -0.719461 2.141356 -0.000831

6 1.210744 -1.208293 -0.015710

1 -0.719462 -2.141355 -0.000837

6 1.948008 0.000000 -0.027856

1 1.721353 2.160302 -0.011481

1 1.721352 -2.160303 -0.011486

7 -3.043279 -1.097653 0.004832

7 -4.269914 -0.671483 0.011012

7 -4.269912 0.671481 0.011005

7 -3.043278 1.097655 0.004810

7 3.323742 0.000000 -0.054108

6 4.055915 1.253775 0.031240

1 5.122438 1.048064 -0.039037

1 3.792483 1.927064 -0.791321

1 3.871847 1.781106 0.976625

6 4.055916 -1.253775 0.031230

1 5.122438 -1.048064 -0.039053

1 3.871854 -1.781111 0.976614

1 3.792478 -1.927060 -0.791333

##
#

07-BH2-b3-iso-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H5B1N6 07-BH2-b3-iso-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=65.8 te_zpe=-623.034492 te_gfe=-623.070504 te_ms_zpe=-622.037788 te_ms_gfe=0.089853

6 1.929741 -1.372629 -0.000039

6 0.558274 -1.573443 -0.000055

6 -0.230794 -0.430921 -0.000015

6 0.225957 0.894253 0.000030

6 1.609803 1.058912 0.000038

6 2.451780 -0.063540 0.000008

1 2.605978 -2.217220 -0.000065

1 0.125693 -2.565406 -0.000090

1 2.046784 2.049929 0.000064

7 -1.648777 -0.410275 -0.000016

7 -2.603952 -1.307668 -0.000103

7 -3.722744 -0.613580 0.000133

7 -3.457566 0.689087 -0.000069

7 -2.165050 0.817572 0.000022

5 -0.996239 1.941193 0.000035

1 -1.118645 2.591755 -1.002925

1 -1.118646 2.591733 1.003009

6 3.872182 0.117950 0.000017

7 5.017857 0.261971 0.000024

07-BH2-b3-ts-01-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H5B1N6 07-BH2-b3-ts-01-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-499.3 te_zpe=-622.985881 te_gfe=-623.024089 te_ms_zpe=-621.979699 te_ms_gfe=0.081983

6 -1.972591 -1.391737 -0.000151

6 -0.591557 -1.531736 -0.000167

6 0.178523 -0.373528 -0.000041

6 -0.358003 0.926591 0.000102

6 -1.742063 1.040210 0.000115

6 -2.549633 -0.111634 -0.000011

1 -2.610653 -2.265887 -0.000247

1 -0.125590 -2.508946 -0.000274

1 -2.216849 2.014402 0.000221

7 1.588160 -0.406205 -0.000045

7 3.310526 -1.453764 -0.000161

7 4.007098 -0.545510 -0.000062

7 3.379281 0.946367 0.000102

7 2.152783 0.727868 0.000079

5 0.760671 2.053901 0.000224

1 1.004739 2.623577 1.020770

1 1.004739 2.623800 -1.020197

6 -3.973846 0.020487 0.000004

7 -5.124237 0.127191 0.000016

07-BH2-b3-ts-02-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H5B1N6 07-BH2-b3-ts-02-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-534.2 te_zpe=-622.995151 te_gfe=-623.032438 te_ms_zpe=-621.991358 te_ms_gfe=0.084354

6 -1.963159 -1.384662 0.021844

6 -0.594394 -1.604472 0.083935

6 0.235477 -0.488109 0.099843

6 -0.212589 0.846190 0.066931

6 -1.590620 1.026994 0.009464

6 -2.463699 -0.073411 -0.013310

1 -2.648162 -2.222267 0.001376

1 -0.187294 -2.607004 0.117231

1 -2.005208 2.027525 -0.023843

7 1.634261 -0.504282 0.187494

7 2.607115 -1.281402 -0.029405

7 3.737893 -0.924904 -0.191354

7 3.445888 0.937533 -0.146084

7 2.294171 1.024076 0.018108

5 0.934102 1.971697 0.098006

1 1.049777 2.556755 1.141409

1 1.009813 2.681539 -0.865974

6 -3.877004 0.139861 -0.076122

7 -5.018401 0.310497 -0.126721

07-BH2-b3-ts-03-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H5B1N6 07-BH2-b3-ts-03-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-397.4 te_zpe=-622.932945 te_gfe=-622.971501 te_ms_zpe=-621.930629 te_ms_gfe=0.078884

6 1.966077 -1.383734 0.000008

6 0.581582 -1.518237 0.000003

6 -0.107850 -0.322282 -0.000002

6 0.368202 0.976397 -0.000001

6 1.767106 1.054439 0.000004

6 2.552956 -0.104633 0.000008

1 2.591922 -2.266626 0.000011

1 0.103113 -2.485433 0.000003

1 2.246086 2.026778 0.000006

7 -1.742933 -0.108727 -0.000004

7 -2.200361 -1.280047 -0.000014

7 -4.131942 -0.809800 -0.000018

7 -4.411230 0.262944 -0.000014

7 -2.051765 1.076371 -0.000000

5 -0.809628 2.070481 0.000002

1 -0.855270 2.747635 -0.997702

1 -0.855266 2.747631 0.997708

6 3.981324 0.006002 0.000013

7 5.132686 0.092102 0.000017

07-BH2-b3-ts-04-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H5B1N6
07-BH2-b3-ts-04-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-236.1 te_zpe=-622.992563 te_gfe=-623.028929 te_ms_zpe=-621.982907 te_ms_gfe=0.085914

6 2.011926 -1.388287 -0.000020

6 0.640657 -1.577527 -0.000034

6 -0.159198 -0.435077 -0.000025

6 0.330592 0.888413 -0.000013

6 1.712039 1.048359 0.000004

6 2.544964 -0.082101 0.000003

1 2.684506 -2.236081 -0.000023

1 0.203911 -2.568215 -0.000048

1 2.158802 2.035362 0.000020

7 -1.560505 -0.467494 -0.000015

7 -3.449910 -1.409289 0.000019

7 -3.886322 -0.337108 0.000032

7 -3.398688 0.879337 0.000043

7 -2.036657 0.698201 0.000010

5 -0.919900 1.875939 -0.000050

1 -1.100109 2.523350 -0.998912

1 -1.100115 2.523581 0.998651

6 3.966140 0.087164 0.000025

7 5.113480 0.221590 0.000043

07-BH2-b3-ts-05-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H5B1N6 07-BH2-b3-ts-05-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-240.5 te_zpe=-622.978195 te_gfe=-623.014618 te_ms_zpe=-621.968414 te_ms_gfe=0.085688

6 1.877306 -1.366550 -0.000003

6 0.496690 -1.474674 -0.000010

6 -0.208231 -0.275826 -0.000022

6 0.341043 1.012099 -0.000030

6 1.734063 1.085509 -0.000016

6 2.490899 -0.094295 -0.000003

1 2.495927 -2.254406 0.000008

1 -0.004430 -2.433104 -0.000005

1 2.240978 2.042827 -0.000013

7 -1.627392 -0.125237 0.000015

7 -2.470996 -1.302562 -0.000034

7 -3.638658 -0.786591 -0.000005

7 -4.151572 0.248235 0.000046

7 -2.079917 1.022632 0.000057

5 -0.878830 2.051808 -0.000026

1 -0.998188 2.737783 -0.988290

1 -0.998082 2.738043 0.988056

6 3.921041 -0.017106 0.000016

7 5.074403 0.042790 0.000032

##
#

07-CH3BH2-iso-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H7B1N6
07-CH3BH2-iso-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=60.5 te_zpe=-662.329367 te_gfe=-662.366758 te_ms_zpe=-661.265285
te_ms_gfe=0.116978

7 -3.588185 0.047479 0.128953

7 -2.380828 0.522482 0.172991

7 -1.551893 -0.493267 -0.059661

7 -2.248494 -1.601014 -0.245387

7 -3.499067 -1.257510 -0.123445

6 -0.126680 -0.380895 -0.049632

6 0.626721 -1.543363 0.104420

6 2.006936 -1.441915 0.130737

6 2.606588 -0.178594 0.012911

6 1.821212 0.970043 -0.142480

6 0.427642 0.901848 -0.184613

1 0.133416 -2.500510 0.205266

1 2.619578 -2.325233 0.251346

1 2.302989 1.935259 -0.236557

6 -0.462164 2.101742 -0.375635

1 -0.694644 2.185559 -1.447240

1 0.091032 3.007399 -0.116532

5 -1.825084 2.013269 0.502631

1 -1.630481 1.967840 1.696254

1 -2.701569 2.765894 0.188588

6 4.032860 -0.064167 0.050311

7 5.183668 0.026009 0.079349

07-CH3BH2-ts-01-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H7B1N6 07-CH3BH2-ts-01-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-506.6 te_zpe=-662.285907 te_gfe=-662.325388 te_ms_zpe=-661.214503 te_ms_gfe=0.109258

7 -3.560026 0.364691 0.091117

7 -2.339367 0.478672 0.194925

7 -1.513348 -0.479366 0.065407

7 -2.741437 -1.843835 -0.326818

7 -3.734487 -1.258812 -0.244003

6 -0.115108 -0.350621 0.040364

6 0.628257 -1.517508 0.239451

6 2.011183 -1.463550 0.213920

6 2.649017 -0.233333 0.003148

6 1.888287 0.927937 -0.193741

6 0.496352 0.900745 -0.192995

1 0.111997 -2.452711 0.413816

1 2.598334 -2.359691 0.365749

1 2.396801 1.869953 -0.359717

6 -0.349067 2.125156 -0.417365

1 -0.689855 2.147292 -1.461185

1 0.267354 3.023002 -0.288947

5 -1.582811 2.255349 0.588362

1 -1.388360 2.045590 1.750180

1 -2.492269 2.964891 0.293712

6 4.077056 -0.160458 -0.013593

7 5.230693 -0.102104 -0.027850

07-CH3BH2-ts-02-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H7B1N6 07-CH3BH2-ts-02-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-538.9 te_zpe=-662.294490 te_gfe=-662.332569 te_ms_zpe=-661.223271 te_ms_gfe=0.112151

7 -3.603164 0.198776 0.470569

7 -2.553871 0.689655 0.314920

7 -1.518157 -0.526482 -0.334786

7 -2.281665 -1.545855 -0.306835

7 -3.437845 -1.502361 0.027568

6 -0.116257 -0.457377 -0.224028

6 0.663519 -1.591826 0.011663

6 2.036144 -1.450852 0.128687

6 2.611311 -0.174676 0.039542

6 1.804962 0.950232 -0.180496

6 0.423944 0.838817 -0.330825

1 0.196694 -2.565336 0.090522

1 2.662381 -2.316939 0.298032

1 2.265622 1.928304 -0.245017

6 -0.486592 2.014843 -0.552532

1 -0.874036 1.974930 -1.579917

1 0.090679 2.940101 -0.481560

5 -1.723829 2.103620 0.494990

1 -1.406874 2.028231 1.657360

1 -2.538092 2.953513 0.265757

6 4.027460 -0.021742 0.171285

7 5.171248 0.099778 0.277148

07-CH3BH2-ts-03-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H7B1N6 07-CH3BH2-ts-03-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-275.3 te_zpe=-662.229734 te_gfe=-662.268865 te_ms_zpe=-661.164301 te_ms_gfe=0.106925

7 -4.244566 -0.258833 0.190892

7 -2.173469 0.695737 0.519703

7 -1.636399 -0.305509 0.007600

7 -1.959627 -1.373557 -0.577544

7 -3.945730 -1.225660 -0.277445

6 -0.080025 -0.363515 -0.082460

6 0.605841 -1.523058 0.251000

6 1.989125 -1.456575 0.295474

6 2.632110 -0.241384 0.009560

6 1.892257 0.903051 -0.300579

6 0.491044 0.880554 -0.358384

1 0.075365 -2.437979 0.467279

1 2.568212 -2.333581 0.551684

1 2.405242 1.835909 -0.497273

6 -0.356730 2.090694 -0.528133

1 -0.898295 2.064125 -1.480054

1 0.250081 2.996654 -0.504949

5 -1.459798 2.048916 0.712766

1 -1.005708 2.106374 1.834573

1 -2.293803 2.915124 0.548617

6 4.061808 -0.171444 0.043563

7 5.214836 -0.118058 0.070515

07-CH3BH2-ts-04-gas-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H7B1N6 07-CH3BH2-ts-04-gas-2d-d-p-cbs-qb3 CBS-QB3

lf=-232.6 te_zpe=-662.285708 te_gfe=-662.323630 te_ms_zpe=-661.207957 te_ms_gfe=0.112574

7 -3.599126 0.302314 0.126589

7 -2.208922 0.511658 0.119321

7 -1.467546 -0.468346 -0.054308

7 -3.111759 -1.921341 -0.218161

7 -3.744498 -0.975665 -0.049847

6 -0.070172 -0.338710 -0.047204

6 0.659044 -1.527466 0.068527

6 2.040972 -1.482315 0.104688

6 2.685950 -0.238953 0.011010

6 1.942821 0.942617 -0.128088

6 0.550790 0.924812 -0.164462

1 0.125968 -2.466858 0.143406

1 2.622936 -2.388746 0.205526

1 2.463039 1.889096 -0.211409

6 -0.303048 2.147185 -0.352149

1 -0.480112 2.276293 -1.429948

1 0.244862 3.036663 -0.029362

5 -1.700242 2.034799 0.455590

1 -1.580645 1.966873 1.661027

1 -2.577886 2.772881 0.113478

6 4.114799 -0.176991 0.049172

7 5.268439 -0.128801 0.079317

07-CH3BH2-ts-05-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H7B1N6 07-CH3BH2-ts-05-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-189.9 te_zpe=-662.270131 te_gfe=-662.308304 te_ms_zpe=-661.191233 te_ms_gfe=0.111808

7 -4.187842 -0.466970 0.099526

7 -2.263431 0.747105 0.170085

7 -1.565133 -0.211344 -0.036147

7 -2.226940 -1.614300 -0.228879

7 -3.432886 -1.318353 -0.092837

6 -0.126145 -0.250603 -0.060626

6 0.538986 -1.468740 0.065569

6 1.923564 -1.471760 0.102117

6 2.617176 -0.255716 0.015630

6 1.922242 0.953110 -0.116658

6 0.528293 0.991197 -0.162891

1 -0.023609 -2.387006 0.143424

1 2.467373 -2.401435 0.203284

1 2.476563 1.880599 -0.188767

6 -0.264572 2.257028 -0.342419

1 -0.419852 2.406171 -1.420538

1 0.325553 3.112060 -0.002654

5 -1.696095 2.194585 0.427347

1 -1.628891 2.179686 1.647045

1 -2.523373 2.990107 0.070758

6 4.047971 -0.250176 0.059873

7 5.202179 -0.247444 0.094987

##
#

07-iso-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H4N6
07-iso-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=31.9 te_zpe=-597.584800 te_gfe=-597.621472 te_ms_zpe=-596.648802 te_ms_gfe=0.076676

7 -3.734230 0.676546 -0.000957

7 -2.514556 1.099451 -0.002071

7 -1.762078 -0.000046 0.000001

7 -2.514480 -1.099552 0.001912

7 -3.734093 -0.676425 0.001076

6 -0.338058 -0.000032 0.000009

6 0.341898 -1.217521 -0.000921

6 1.728629 -1.213204 -0.000879

6 2.431655 0.000012 0.000005

6 1.728589 1.213205 0.000889

6 0.341858 1.217478 0.000933

1 2.272156 -2.149142 -0.001590

1 2.272086 2.149161 0.001597

1 -0.212560 2.145501 0.001640

1 -0.212493 -2.145559 -0.001632

6 3.862054 0.000036 0.000003

7 5.016730 0.000054 0.000002

07-ts-01-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H4N6 07-ts-01-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-550.0 te_zpe=-597.560668 te_gfe=-597.598796 te_ms_zpe=-596.617643 te_ms_gfe=0.071265

7 -3.849434 0.776948 0.000244

7 -2.790296 1.277496 0.000258

7 -1.713161 -0.053058 -0.000110

7 -2.496949 -1.068439 -0.000214

7 -3.703208 -0.919937 -0.000086

6 -0.311222 -0.061579 -0.000076

6 0.414923 -1.259327 -0.000033

6 1.799667 -1.216209 0.000001

6 2.473972 0.013650 0.000004

6 1.734487 1.205289 -0.000034

6 0.349563 1.172171 -0.000079

1 2.366922 -2.138400 0.000031

1 2.251216 2.156523 -0.000033

1 -0.224687 2.088618 -0.000114

1 -0.107600 -2.206430 -0.000030

6 3.902547 0.051599 0.000044

7 5.057409 0.082151 0.000077

##
##

08-2BH2-b3-iso-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H7B2N7O4
08-2BH2-b3-iso-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=48.9 te_zpe=-1004.623800 te_gfe=-1004.667169 te_ms_zpe=-1003.118271
te_ms_gfe=0.128069

6 -1.406602 -0.948865 -0.033798

6 -0.084461 -1.406294 -0.007612

6 0.847471 -0.385678 -0.009067

6 0.559778 0.983840 -0.040107

6 -0.800334 1.327158 -0.021805

6 -1.846470 0.399049 -0.040324

7 2.257323 -0.547518 0.024447

7 3.093725 -1.555813 0.057189

7 4.288300 -1.003912 0.078293

7 4.185663 0.322392 0.057739

7 2.919717 0.606296 0.025973

5 1.905859 1.866685 -0.062925

1 2.077453 2.569875 0.893764

1 2.124933 2.416663 -1.104958

5 -0.080368 -2.986904 0.008130

1 0.336421 -3.483547 1.022144

1 0.370802 -3.503026 -0.980928

6 -3.303857 0.768768 -0.100214

1 -3.804264 0.205129 -0.887770

1 -3.800321 0.505753 0.837787

1 -3.443476 1.832045 -0.263042

7 -1.105963 2.779043 0.032527

7 -2.275403 -2.083664 -0.032922

8 -1.942424 3.144680 0.846665

8 -0.483373 3.504659 -0.722300

8 -1.635108 -3.212534 -0.014259

8 -3.479805 -2.060232 -0.038628

08-2BH2-b3-ts-02-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H7B2N7O4
08-2BH2-b3-ts-02-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-538.5 te_zpe=-1004.585141 te_gfe=-1004.629338 te_ms_zpe=-1003.073910 te_ms_gfe=0.123298

6 -1.459403 -0.898742 -0.039406

6 -0.160090 -1.414306 -0.100116

6 0.836802 -0.456005 -0.137320

6 0.604840 0.927380 -0.135632

6 -0.737335 1.330452 -0.041597

6 -1.834997 0.463988 -0.009719

7 2.219546 -0.709709 -0.227741

7 3.023028 -1.633659 0.108069

7 4.177658 -1.458870 0.357049

7 4.199790 0.422706 0.255802

7 3.090689 0.678344 -0.007087

5 1.925473 1.843291 -0.221785

1 2.095926 2.631894 0.661230

1 2.159803 2.265686 -1.318612

5 -0.228441 -2.994547 -0.111217

1 0.227156 -3.531058 0.867156

1 0.140399 -3.512067 -1.134805

6 -3.272971 0.909176 0.013931

1 -3.849646 0.365453 -0.734223

1 -3.725057 0.686057 0.984196

1 -3.366813 1.976562 -0.156459

7 -0.965896 2.794747 0.042159

7 -2.375917 -1.992827 -0.002461

8 -1.742998 3.195024 0.897647

8 -0.343583 3.499004 -0.734806

8 -1.788361 -3.151650 -0.041067

8 -3.576347 -1.917756 0.067620

08-2BH2-b3-ts-03-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H7B2N7O4 08-2BH2-b3-ts-03-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-443.4 te_zpe=-1004.576652 te_gfe=-1004.620941 te_ms_zpe=-1003.063471 te_ms_gfe=0.123368

6 -1.497746 -0.871490 -0.027206

6 -0.220634 -1.433842 -0.003119

6 0.809333 -0.503475 0.003454

6 0.641438 0.886058 -0.034707

6 -0.690260 1.337085 -0.023007

6 -1.813626 0.511030 -0.029010

7 2.176844 -0.902316 0.034715

7 2.854506 -1.861059 -0.014512

7 4.608384 -0.957835 0.016701

7 4.161370 0.138988 0.078890

7 2.997968 0.554093 0.154198

5 1.996192 1.759483 -0.060680

1 2.065553 2.540618 0.850915

1 2.193039 2.257588 -1.136642

5 -0.349540 -3.007795 0.007134

1 0.031282 -3.540713 1.017481

1 0.057730 -3.554502 -0.985158

6 -3.229032 1.017181 -0.061491

1 -3.781227 0.544517 -0.874721

1 -3.746535 0.750256 0.863630

1 -3.270650 2.096279 -0.169534

7 -0.887724 2.809437 0.008964

7 -2.458827 -1.925165 -0.029138

8 -1.560462 3.257263 0.926546

8 -0.359300 3.458904 -0.874249

8 -1.916565 -3.105823 -0.012837

8 -3.657040 -1.797940 -0.039016

08-2BH2-b3-ts-04-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H7B2N7O4 08-2BH2-b3-ts-04-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-231.6 te_zpe=-1004.583477 te_gfe=-1004.627188 te_ms_zpe=-1003.065117 te_ms_gfe=0.124223

6 -1.437876 -0.990058 -0.032145

6 -0.102049 -1.404008 -0.005554

6 0.815421 -0.361120 -0.007540

6 0.459643 0.999601 -0.037859

6 -0.907170 1.305607 -0.020490

6 -1.923773 0.343862 -0.043581

7 2.207635 -0.536247 0.021369

7 3.980822 -1.654776 0.073820

7 4.530426 -0.636280 0.068280

7 4.163040 0.625987 0.042704

7 2.795199 0.576318 0.015692

5 1.800697 1.859239 -0.065378

1 2.020460 2.562733 0.882767

1 2.050151 2.399932 -1.108284

5 -0.047848 -2.981645 0.010730

1 0.384968 -3.466709 1.024745

1 0.418499 -3.485117 -0.978996

6 -3.392510 0.662037 -0.117172

1 -3.871115 0.059238 -0.888792

1 -3.883149 0.409705 0.827113

1 -3.566961 1.715109 -0.309325

7 -1.250456 2.748594 0.037503

7 -2.270050 -2.151356 -0.028746

8 -2.147300 3.085821 0.798999

8 -0.593036 3.503238 -0.658401

8 -1.594803 -3.260683 -0.010016

8 -3.475303 -2.168885 -0.031121

08-2BH2-b3-ts-05-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H7B2N7O4 08-2BH2-b3-ts-05-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-245.1 te_zpe=-1004.568058 te_gfe=-1004.611768 te_ms_zpe=-1003.050010 te_ms_gfe=0.124038

6 -1.237510 -1.104937 -0.031853

6 0.146490 -1.317423 -0.007861

6 0.872852 -0.137123 -0.005129

6 0.335105 1.152828 -0.030591

6 -1.064431 1.246985 -0.016130

6 -1.918862 0.142639 -0.036829

7 2.295460 0.000094 0.022590

7 3.129277 -1.174582 0.048157

7 4.300188 -0.660063 0.066061

7 4.803631 0.380093 0.066127

7 2.750869 1.147135 0.021494

5 1.562412 2.183883 -0.043915

1 1.643056 2.931515 0.898808

1 1.700362 2.802349 -1.070392

5 0.430281 -2.873127 0.001727

1 0.926120 -3.295127 1.013385

1 0.959583 -3.300364 -0.990487

6 -3.419472 0.236713 -0.098530

1 -3.805933 -0.402057 -0.892887

1 -3.860516 -0.123127 0.834888

1 -3.751940 1.257744 -0.251641

7 -1.626221 2.620088 0.031562

7 -1.890293 -2.375654 -0.033591

8 -2.523500 2.833273 0.836078

8 -1.135468 3.444311 -0.719254

8 -1.060545 -3.372819 -0.019625

8 -3.080438 -2.567588 -0.037947

##
##

08-2BH2CH3-iso-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C9H11B2N7O4 08-2BH2CH3-iso-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=32.1 te_zpe=-1083.186291 te_gfe=-1083.233669 te_ms_zpe=-1081.554950 te_ms_gfe=0.180835

7 4.156422 -0.647816 0.090832

7 2.916822 -1.042337 0.226037

7 2.136528 -0.004390 -0.029645

7 2.910745 1.028906 -0.318910

7 4.152984 0.628056 -0.236296

6 0.710837 -0.000081 0.001444

6 0.079306 1.251651 0.083242

6 -1.314296 1.189586 0.092780

6 -2.057831 0.005180 0.024305

6 -1.317541 -1.180287 -0.036190

6 0.072925 -1.250721 -0.044572

6 0.881188 -2.517709 -0.161853

1 1.063068 -2.697036 -1.231194

1 0.296564 -3.365039 0.195397

6 0.901827 2.513327 0.159461

1 0.308054 3.369390 -0.162296

1 1.124621 2.699403 1.218753

5 2.273152 -2.462355 0.671695

5 2.252631 2.448271 -0.737394

1 2.121040 -2.315032 1.862551

1 3.086684 -3.291633 0.388413

1 2.045278 2.297659 -1.920260

1 3.080645 3.276692 -0.496519

6 -3.564318 -0.012325 0.025288

1 -3.977171 0.852005 0.542127

1 -3.938299 0.003736 -1.001174

1 -3.943897 -0.912479 0.508618

7 -2.075564 -2.453616 -0.123942

7 -2.058570 2.467924 0.186077

8 -2.659844 -2.668674 -1.172600

8 -2.064518 -3.179499 0.856193

8 -2.814900 2.735356 -0.734348

8 -1.863695 3.153307 1.175954

08-2BH2CH3-ts-01-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C9H11B2N7O4 08-2BH2CH3-ts-01-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-531.5 te_zpe=-1083.133588 te_gfe=-1083.183017 te_ms_zpe=-1081.494547 te_ms_gfe=0.172340

7 4.270330 0.547192 -0.455948

7 3.208543 1.026314 -0.435946

7 2.135504 -0.164542 0.270002

7 2.938995 -1.134779 0.433211

7 4.117543 -1.098537 0.176351

6 0.734363 -0.124424 0.155829

6 -0.031061 -1.285122 -0.059369

6 -1.411941 -1.080363 -0.123986

6 -2.037629 0.169181 -0.049275

6 -1.182518 1.263891 0.094757

6 0.203763 1.180140 0.211423

6 1.134004 2.350596 0.369199

1 1.561971 2.318298 1.379937

1 0.590775 3.290831 0.289855

6 0.638038 -2.631441 -0.170063

1 -0.107319 -3.426666 -0.295357

1 1.210811 -2.678927 -1.104575

5 2.333231 2.388822 -0.730040

5 1.516873 -3.098235 1.048581

1 1.983321 2.206780 -1.868538

1 3.124991 3.276813 -0.588830

1 1.330605 -2.663877 2.141698

1 2.289485 -3.989004 0.891820

6 -3.533769 0.336716 -0.145683

1 -3.982896 0.306544 0.849262

1 -3.792368 1.291787 -0.601808

1 -3.987997 -0.454252 -0.740504

7 -1.805794 2.608477 0.159223

7 -2.287273 -2.265748 -0.288364

8 -2.504275 2.844820 1.131781

8 -1.581653 3.374144 -0.764230

8 -3.113488 -2.468749 0.586592

8 -2.125126 -2.954582 -1.285688

##
#

08-BH2-b3-iso-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H6B1N7O4 08-BH2-b3-iso-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=25.9 te_zpe=-979.154794 te_gfe=-979.199073 te_ms_zpe=-977.715232 te_ms_gfe=0.114960

6 -1.421424 -1.097287 -0.013723

6 -0.101677 -1.533832 0.020188

6 0.862196 -0.549508 -0.001230

6 0.617603 0.828791 -0.038756

6 -0.726181 1.178732 0.003722

6 -1.794989 0.262046 0.005120

1 0.130873 -2.588769 0.057177

7 2.263106 -0.758410 0.010590

7 3.062854 -1.796493 0.038529

7 4.276274 -1.288714 0.035980

7 4.220659 0.040846 0.005283

7 2.965740 0.371311 -0.009131

5 1.992276 1.670636 -0.089236

1 2.209930 2.365738 0.863461

1 2.217838 2.204733 -1.137729

6 -3.225955 0.736442 0.067165

1 -3.408557 1.212504 1.031197

1 -3.409472 1.491988 -0.700325

1 -3.927984 -0.073933 -0.085562

7 -1.018487 2.636272 0.055769

7 -2.423654 -2.193253 -0.068707

8 -0.465746 3.336522 -0.773700

8 -1.769317 3.027800 0.936131

8 -3.391719 -2.051380 -0.799313

8 -2.180329 -3.187774 0.597491

08-BH2-b3-ts-02-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H6B1N7O4 08-BH2-b3-ts-02-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-540.6 te_zpe=-979.116747 te_gfe=-979.161164 te_ms_zpe=-977.671222 te_ms_gfe=0.111022

6 -1.479643 -1.058663 -0.042230

6 -0.178228 -1.550354 -0.106412

6 0.844533 -0.626645 -0.153945

6 0.646741 0.763980 -0.142526

6 -0.677086 1.168750 -0.021423

6 -1.793604 0.311885 0.015009

1 -0.006487 -2.616998 -0.111948

7 2.217565 -0.910537 -0.267188

7 3.004582 -1.851111 0.064414

7 4.165681 -1.698089 0.302664

7 4.229650 0.174261 0.201224

7 3.126111 0.462087 -0.049922

5 1.984924 1.654142 -0.243482

1 2.184860 2.431318 0.643616

1 2.214632 2.079219 -1.340401

6 -3.207245 0.835818 0.085931

1 -3.787072 0.297434 0.835992

1 -3.225195 1.891172 0.336714

1 -3.711169 0.676867 -0.868575

7 -0.877261 2.639323 0.092709

7 -2.534242 -2.102279 -0.031340

8 -0.426625 3.326784 -0.807075

8 -1.447930 3.052200 1.090698

8 -3.635847 -1.815044 -0.474578

8 -2.221048 -3.200682 0.406913

08-BH2-b3-ts-03-b3-cbs-qb3 charge=0 spin=1 mol=C7H6B1N7O4
08-BH2-b3-ts-03-b3-cbs-qb3 CBS-QB3

lf=-382.7 te_zpe=-979.053775 te_gfe=-979.100492 te_ms_zpe=-977.608185 te_ms_gfe=0.104127

6 -1.330996 -1.212471 -0.008880

6 0.039497 -1.468902 0.008288

6 0.826522 -0.347047 -0.006660

6 0.440069 0.980255 -0.028904

6 -0.946510 1.130675 0.007618

6 -1.882817 0.087219 0.007451

1 0.402711 -2.483764 0.036775

7 2.465738 -0.246926 -0.002059

7 2.816589 -1.457012 0.000675

7 4.802569 -1.166553 0.016173

7 5.209647 -0.138255 0.007793

7 2.860547 0.909622 -0.006891

5 1.695687 1.989246 -0.047794

1 1.765715 2.691980 0.928395

1 1.797200 2.624563 -1.064399

6 -3.366463 0.359774 0.011648

1 -3.574435 1.391717 0.278397

1 -3.788476 0.145279 -0.971583

1 -3.882483 -0.287771 0.719920

7 -1.430644 2.541812 0.051618

7 -2.183736 -2.427631 -0.040498

8 -1.221032 3.222535 -0.933751

8 -1.987448 2.901301 1.076646

8 -3.299102 -2.331224 -0.528638

8 -1.699849 -3.456444 0.408296

08-BH2-b3-ts-04-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H6B1N7O4 08-BH2-b3-ts-04-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-241.8 te_zpe=-979.100903 te_gfe=-979.144596 te_ms_zpe=-977.648972 te_ms_gfe=0.112086

6 1.258505 -1.203078 -0.037934

6 -0.108787 -1.440358 -0.017060

6 -0.910974 -0.317019 -0.000129

6 -0.461934 1.005579 -0.028268

6 0.921228 1.158106 -0.036082

6 1.834679 0.089857 -0.056496

1 -0.496988 -2.448468 -0.021404

7 -2.335340 -0.285367 0.043552

7 -3.078041 -1.520866 0.076218

7 -4.284708 -1.096478 0.105380

7 -4.859864 -0.093839 0.111134

7 -2.872995 0.825116 0.048141

5 -1.761630 1.949977 -0.025916

1 -1.963299 2.556619 -1.048538

1 -1.896432 2.681233 0.922973

6 3.322840 0.313852 -0.155978

1 3.544126 1.280108 -0.602609

1 3.776100 0.294225 0.836893

1 3.797551 -0.469241 -0.743375

7 1.425161 2.555730 -0.004875

7 2.101199 -2.424780 -0.019536

8 0.890299 3.354347 -0.753882

8 2.320671 2.809619 0.788041

8 3.182720 -2.364399 0.545379

8 1.637043 -3.424892 -0.547385

08-BH2-b3-ts-05-b3-cbs-qb3 charge=0 spin=1 mol=C7H6B1N7O4 08-BH2-b3-ts-05-b3-cbs-qb3 CBS-QB3

lf=-231.2 te_zpe=-979.116127 te_gfe=-979.159693 te_ms_zpe=-977.664494 te_ms_gfe=0.112418

6 1.440999 -1.140615 -0.034187

6 0.108837 -1.530891 -0.011135

6 -0.837548 -0.521666 -0.002489

6 -0.523053 0.849670 -0.039004

6 0.829566 1.162477 -0.041804

6 1.865083 0.206888 -0.060526

1 -0.153766 -2.579298 -0.007656

7 -2.221573 -0.742767 0.042262

7 -3.944448 -1.916887 0.114763

7 -4.536456 -0.921434 0.112371

7 -4.211208 0.353747 0.079889

7 -2.845415 0.351202 0.039546

5 -1.890435 1.670918 -0.054867

1 -2.175160 2.195831 -1.096454

1 -2.130251 2.363040 0.896325

6 3.316923 0.599245 -0.172214

1 3.423558 1.573191 -0.643541

1 3.771991 0.659223 0.818301

1 3.877634 -0.138667 -0.741751

7 1.162306 2.610496 -0.001507

7 2.417739 -2.257096 -0.010578

8 0.485485 3.355341 -0.690066

8 2.068182 2.958762 0.742381

8 3.485377 -2.072334 0.554338

8 2.071796 -3.306692 -0.534147

##
##

08-CH3BH2-iso-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H8B1N7O4 08-CH3BH2-iso-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=28.6 te_zpe=-1018.449054 te_gfe=-1018.494510 te_ms_zpe=-1016.943473 te_ms_gfe=0.142266

7 -4.297636 -0.317854 0.065748

7 -3.144583 0.266970 0.177531

7 -2.216393 -0.641875 -0.111254

7 -2.795252 -1.794393 -0.400880

7 -4.074694 -1.584512 -0.284173

6 -0.811860 -0.391315 -0.062947

6 0.051029 -1.470662 0.009581

6 1.415515 -1.224257 0.041824

6 1.954101 0.074179 0.042936

6 1.004886 1.100880 -0.026240

6 -0.379644 0.944113 -0.084147

1 -0.313688 -2.486876 0.045495

6 -1.373212 2.067253 -0.189929

1 -1.582241 2.227574 -1.257069

1 -0.933294 2.995826 0.176369

5 -2.740244 1.767112 0.639336

1 -2.560642 1.642312 1.828267

1 -3.673075 2.462320 0.362329

6 3.425017 0.393777 0.112175

1 3.879700 0.293322 -0.875882

1 3.585195 1.408957 0.471180

1 3.949878 -0.294265 0.771670

7 1.511584 2.498285 -0.065140

7 2.279395 -2.428861 0.078254

8 1.633098 3.075226 1.001834

8 1.765001 2.950515 -1.167333

8 1.788628 -3.450898 0.532951

8 3.412955 -2.328952 -0.367348

08-CH3BH2-ts-01-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H8B1N7O4
08-CH3BH2-ts-01-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-494.4 te_zpe=-1018.406355 te_gfe=-1018.453764 te_ms_zpe=-1016.893875 te_ms_gfe=0.134884

7 -4.304394 -0.123014 -0.073078

7 -3.089814 -0.300631 -0.212708

7 -2.200565 0.577490 0.012687

7 -3.372084 1.974380 0.590787

7 -4.381960 1.438995 0.444788

6 -0.817564 0.336866 -0.015749

6 0.012570 1.446201 -0.094631

6 1.388914 1.270883 -0.078382

6 1.993603 0.005853 -0.024899

6 1.090801 -1.063969 0.041728

6 -0.299014 -0.974121 0.056087

1 -0.398046 2.442763 -0.169553

6 -1.235478 -2.144518 0.150515

1 -1.544249 -2.269777 1.196663

1 -0.725292 -3.070781 -0.128745

5 -2.502873 -2.017105 -0.821312

1 -2.300658 -1.693387 -1.955200

1 -3.450493 -2.700769 -0.597644

6 3.480345 -0.243207 -0.051799

1 3.902696 -0.136669 0.949790

1 3.699098 -1.246701 -0.414688

1 3.991187 0.474604 -0.689721

7 1.671209 -2.430396 0.132162

7 2.192248 2.515401 -0.122399

8 1.691305 -3.097065 -0.889550

8 2.082484 -2.775894 1.226026

8 1.671540 3.497908 -0.629817

8 3.311245 2.489641 0.369938

08-CH3BH2-ts-02-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H8B1N7O4 08-CH3BH2-ts-02-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-540.0 te_zpe=-1018.414627 te_gfe=-1018.460823 te_ms_zpe=-1016.902657 te_ms_gfe=0.137489

7 -4.315587 -0.289297 0.433775

7 -3.332250 0.334477 0.327868

7 -2.170397 -0.677032 -0.432830

7 -2.802539 -1.783465 -0.499557

7 -3.952270 -1.907791 -0.166420

6 -0.787140 -0.460638 -0.278292

6 0.112895 -1.501414 -0.118604

6 1.462231 -1.202414 0.022233

6 1.950218 0.113240 0.069560

6 0.969767 1.104162 -0.071264

6 -0.394857 0.892013 -0.259438

1 -0.206664 -2.533559 -0.108700

6 -1.433940 1.964257 -0.403520

1 -1.813992 1.938252 -1.433418

1 -0.999874 2.953181 -0.257326

5 -2.672466 1.810061 0.641487

1 -2.343299 1.671412 1.792647

1 -3.574335 2.580674 0.475505

6 3.396478 0.488284 0.273906

1 3.937490 0.449409 -0.674005

1 3.482431 1.495333 0.679713

1 3.893135 -0.202183 0.951886

7 1.427471 2.517861 -0.046913

7 2.364284 -2.373456 0.123045

8 1.250531 3.141543 0.985982

8 1.945226 2.941370 -1.066035

8 1.876628 -3.419800 0.526441

8 3.527932 -2.230219 -0.223138

08-CH3BH2-ts-03-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H8B1N7O4 08-CH3BH2-ts-03-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-272.2 te_zpe=-1018.349112 te_gfe=-1018.396051 te_ms_zpe=-1016.841522 te_ms_gfe=0.132544

7 4.962002 0.495233 0.198137

7 2.910807 -0.517437 0.695868

7 2.341193 0.327002 -0.018720

7 2.621607 1.268812 -0.815601

7 4.602619 1.315692 -0.463195

6 0.802300 0.293785 -0.154750

6 0.053379 1.446517 -0.051773

6 -1.326786 1.310602 0.004061

6 -1.972687 0.061267 -0.065315

6 -1.118318 -1.042338 -0.149217

6 0.282719 -1.005752 -0.191528

1 0.502944 2.426329 -0.017167

6 1.185866 -2.177453 -0.095893

1 1.774891 -2.291649 -1.011415

1 0.643987 -3.105023 0.075511

5 2.227588 -1.819545 1.156879

1 1.718373 -1.647509 2.241400

1 3.082065 -2.677026 1.214986

6 -3.469101 -0.119535 -0.085839

1 -3.956228 0.691459 -0.622188

1 -3.741835 -1.064244 -0.553212

1 -3.863692 -0.113846 0.932345

7 -1.740083 -2.392081 -0.210053

7 -2.079468 2.578123 0.156853

8 -2.302622 -2.782877 0.798378

8 -1.638816 -2.999040 -1.262329

8 -1.527611 3.601770 -0.218703

8 -3.187629 2.523805 0.669385

08-CH3BH2-ts-04-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H8B1N7O4 08-CH3BH2-ts-04-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-230.8 te_zpe=-1018.407333 te_gfe=-1018.453274 te_ms_zpe=-1016.888681 te_ms_gfe=0.137944

7 4.348493 -0.111694 0.179325

7 2.981054 -0.397274 0.191838

7 2.182958 0.521432 -0.059950

7 3.719863 2.038301 -0.343316

7 4.421747 1.159537 -0.101948

6 0.797122 0.305323 -0.048551

6 -0.005859 1.439273 -0.034594

6 -1.384176 1.296211 0.001087

6 -2.015593 0.040160 -0.023589

6 -1.140059 -1.054167 -0.069832

6 0.250469 -0.996306 -0.074422

1 0.433639 2.426579 -0.040872

6 1.168993 -2.180302 -0.143118

1 1.345666 -2.405310 -1.204056

1 0.685220 -3.067165 0.272455

5 2.554079 -1.909578 0.651815

1 2.417437 -1.746600 1.845158

1 3.469576 -2.626764 0.375624

6 -3.507257 -0.169287 -0.035153

1 -4.014338 0.613597 -0.594515

1 -3.762414 -1.133759 -0.471767

1 -3.899523 -0.137598 0.984032

7 -1.746122 -2.410601 -0.125951

7 -2.158942 2.556600 0.074674

8 -2.197347 -2.855141 0.915755

8 -1.744179 -2.969499 -1.209342

8 -1.629591 3.562054 -0.375496

8 -3.262740 2.518255 0.599231

08-CH3BH2-ts-05-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H8B1N7O4
08-CH3BH2-ts-05-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-194.1 te_zpe=-1018.391043 te_gfe=-1018.437125 te_ms_zpe=-1016.870623 te_ms_gfe=0.137293

7	4.885496	0.505394	0.095700
7	3.005309	-0.747405	0.237917
7	2.284797	0.182971	-0.030024
7	2.895721	1.572847	-0.302957
7	4.115119	1.328545	-0.149368
6	0.847049	0.179980	-0.062994
6	0.149977	1.375510	-0.036770
6	-1.236258	1.334700	-0.000308
6	-1.963243	0.132112	-0.020984
6	-1.176468	-1.025516	-0.063378
6	0.216553	-1.077399	-0.076210
1	0.660116	2.326086	-0.039468
6	1.026667	-2.340222	-0.142051
1	1.153474	-2.594794	-1.203090
1	0.471586	-3.170175	0.300174
5	2.472538	-2.178097	0.591027
1	2.422618	-2.088138	1.807985
1	3.307534	-2.981751	0.275809
6	-3.466745	0.038033	-0.025409
1	-3.913983	0.850621	-0.593443
1	-3.796712	-0.908969	-0.449813
1	-3.850775	0.113533	0.994463
7	-1.885891	-2.331278	-0.109800
7	-1.910088	2.652535	0.076288

8 -2.323711 -2.756007 0.945390

8 -1.975643 -2.868787 -1.199924

8 -1.303636 3.614089 -0.370992

8 -3.013883 2.697658 0.600098

##
#

08-iso-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H5N7O4
08-iso-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=30.5 te_zpe=-953.704226 te_gfe=-953.748326 te_ms_zpe=-952.324643
te_ms_gfe=0.102733

7 4.446493 -0.674326 0.031317

7 3.227760 -1.097273 0.052631

7 2.476466 0.001959 -0.000834

7 3.227511 1.101321 -0.054631

7 4.446319 0.678508 -0.034051

6 1.055942 0.001514 -0.000681

6 0.366909 1.205528 0.023976

6 -1.019556 1.177038 -0.005814

6 -1.789755 -0.001187 -0.006168

6 -1.019151 -1.176411 0.006151

6 0.368168 -1.203064 -0.024670

1 0.893613 -2.146459 -0.061023

1 0.887787 2.150889 0.065184

6 -3.296900 0.004094 -0.052435

1 -3.704425 0.705737 0.676757

1 -3.632753 0.344540 -1.032912

1 -3.702662 -0.978886 0.156291

7 -1.650972 -2.524239 0.049139

7 -1.665501 2.518018 -0.030651

8 -2.555043 -2.703229 0.849473

8 -1.184559 -3.367104 -0.699087

8 -1.093040 3.413788 0.568625

8 -2.703863 2.637962 -0.661122

08-ts-01-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H5N7O4 08-ts-01-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-548.1 te_zpe=-953.680716 te_gfe=-953.726442 te_ms_zpe=-952.294784 te_ms_gfe=0.097252

7 -4.591201 0.637816 0.148445

7 -3.549718 1.174451 0.164807

7 -2.439751 -0.107949 -0.068631

7 -3.193249 -1.144315 -0.143470

7 -4.401789 -1.030219 -0.065532

6 -1.038874 -0.086155 -0.046246

6 -0.397812 1.149361 -0.069258

6 0.986965 1.193096 -0.010320

6 1.819412 0.058570 0.012667

6 1.107211 -1.152178 -0.005251

6 -0.277506 -1.251038 0.003036

1 -0.745424 -2.224338 0.039455

1 -0.959227 2.070204 -0.130037

6 3.324086 0.140664 0.087382

1 3.710625 0.857071 -0.638892

1 3.626225 0.501282 1.071544

1 3.781984 -0.822010 -0.108495

7 1.806019 -2.466809 -0.029626

7 1.561154 2.565801 0.017948

8 2.732550 -2.605643 -0.812521

8 1.369754 -3.330837 0.713886

8 0.951188 3.431215 -0.590415

8 2.584594 2.743070 0.659897

##
##

09-2BH2-b3-iso-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H6B2Cl1N5
09-2BH2-b3-iso-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=54.1 te_zpe=-1015.835402 te_gfe=-1015.872909 te_ms_zpe=-1014.445540
te_ms_gfe=0.091038

6 -1.826827 1.174840 -0.000079

6 -0.444153 1.433388 -0.000026

6 0.357040 0.275652 0.000035

6 -0.099596 -1.048199 0.000053

6 -1.484196 -1.235268 -0.000010

6 -2.326193 -0.128219 -0.000069

1 -2.516370 2.008667 -0.000123

1 -1.905295 -2.233031 -0.000020

7 1.785703 0.229771 0.000078

7 2.773781 1.095514 -0.000162

7 3.870729 0.370218 0.000631

7 3.568554 -0.923755 -0.000286

7 2.274725 -1.013371 0.000160

5 1.102457 -2.111348 0.000072

1 1.208634 -2.766972 -1.002426

1 1.208497 -2.766980 1.002588

5 0.033449 2.905203 0.000105

1 1.180385 3.198521 -0.000103

1 -0.801172 3.753658 -0.000560

17 -4.060300 -0.370879 -0.000153

09-2BH2-b3-ts-01-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H6B2Cl1N5 09-2BH2-b3-ts-01-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-530.8 te_zpe=-1015.797504 te_gfe=-1015.837230 te_ms_zpe=-1014.400222 te_ms_gfe=0.084660

6 1.862929 1.186504 -0.000066

6 0.478792 1.463809 -0.000229

6 -0.359043 0.327758 -0.000262

6 0.084609 -1.008262 -0.000210

6 1.464117 -1.206433 -0.000078

6 2.336010 -0.117427 -0.000001

1 2.561989 2.012565 -0.000003

1 1.868519 -2.211612 -0.000015

7 -1.759725 0.320916 -0.000478

7 -2.769081 1.072938 0.000256

7 -3.904640 0.690430 0.000765

7 -3.576738 -1.156099 0.000539

7 -2.411839 -1.224735 -0.000001

5 -1.050022 -2.144792 -0.000312

1 -1.127475 -2.799662 1.004021

1 -1.127650 -2.799208 -1.004935

5 0.004602 2.925617 -0.000439

1 -1.148316 3.214477 -0.000731

1 0.823046 3.789668 -0.000332

17 4.066274 -0.406481 0.000191

09-2BH2-b3-ts-02-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H6B2Cl1N5 09-2BH2-b3-ts-02-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-499.3 te_zpe=-1015.787451 te_gfe=-1015.826622 te_ms_zpe=-1014.387951 te_ms_gfe=0.083767

6 -1.877022 1.203057 -0.000116

6 -0.479627 1.397648 -0.000154

6 0.296071 0.222103 -0.000044

6 -0.232123 -1.080334 0.000088

6 -1.616676 -1.213606 0.000122

6 -2.423427 -0.072751 0.000019

1 -2.530176 2.066056 -0.000193

1 -2.080462 -2.192951 0.000226

7 1.709687 0.235884 -0.000049

7 3.515345 1.225220 -0.000085

7 4.161370 0.285681 0.000006

7 3.462666 -1.186086 0.000126

7 2.246044 -0.912729 0.000071

5 0.894872 -2.199522 0.000169

1 1.119202 -2.783110 -1.018174

1 1.119193 -2.782992 1.018580

5 0.095081 2.825895 -0.000315

1 1.266194 3.025060 -0.000370

1 -0.660651 3.746723 -0.000388

17 -4.167766 -0.263715 0.000064

09-2BH2-b3-ts-03-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H6B2Cl1N5 09-2BH2-b3-ts-03-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-373.7 te_zpe=-1015.734550 te_gfe=-1015.774329 te_ms_zpe=-1014.337364 te_ms_gfe=0.080185

6 1.884558 1.180194 -0.000005

6 0.485358 1.390088 -0.000014

6 -0.221493 0.189421 -0.000005

6 0.230997 -1.113525 0.000010

6 1.630682 -1.235254 0.000018

6 2.432461 -0.101597 0.000011

1 2.536259 2.043501 -0.000010

1 2.080914 -2.220907 0.000030

7 -1.881871 -0.026762 -0.000008

7 -2.423145 1.110615 -0.000021

7 -4.309901 0.527303 -0.000018

7 -4.511607 -0.564457 -0.000007

7 -2.174135 -1.223556 0.000004

5 -0.942210 -2.203552 0.000015

1 -0.976420 -2.885852 0.996695

1 -0.976414 -2.885864 -0.996658

5 -0.019381 2.847729 -0.000033

1 -1.177237 3.101279 -0.000044

1 0.789273 3.719953 -0.000037

17 4.175342 -0.277115 0.000022

09-2BH2-b3-ts-04-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H6B2Cl1N5 09-2BH2-b3-ts-04-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-237.8 te_zpe=-1015.794974 te_gfe=-1015.832620 te_ms_zpe=-1014.392245 te_ms_gfe=0.087340

6 1.897393 1.193237 -0.000006

6 0.512467 1.426022 -0.000010

6 -0.286130 0.261728 -0.000004

6 0.203782 -1.060066 0.000004

6 1.587179 -1.229793 0.000006

6 2.411357 -0.105389 0.000002

1 2.579009 2.033975 -0.000009

1 2.029505 -2.218620 0.000012

7 -1.689772 0.277491 -0.000004

7 -3.601365 1.198775 -0.000003

7 -4.019113 0.119750 0.000005

7 -3.517977 -1.089355 0.000009

7 -2.155582 -0.892308 0.000001

5 -1.036778 -2.057776 0.000002

1 -1.206291 -2.708876 0.998690

1 -1.206284 -2.708860 -0.998700

5 -0.034391 2.868623 -0.000020

1 -1.201469 3.088368 -0.000025

1 0.740614 3.772941 -0.000024

17 4.150067 -0.325180 0.000008

09-2BH2-b3-ts-05-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H6B2Cl1N5 09-2BH2-b3-ts-05-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-242.9 te_zpe=-1015.775722 te_gfe=-1015.813787 te_ms_zpe=-1014.373084 te_ms_gfe=0.086511

6 -1.783390 1.173659 -0.045627

6 -0.389885 1.345212 0.013582

6 0.329636 0.132068 0.040679

6 -0.220906 -1.155076 0.063853

6 -1.615441 -1.256751 0.047423

6 -2.372866 -0.095487 -0.017005

1 -2.419497 2.047755 -0.093651

1 -2.103801 -2.223075 0.073105

7 1.756050 -0.052280 0.017281

7 2.649464 1.091822 -0.105666

7 3.792951 0.533654 -0.127502

7 4.292477 -0.505327 -0.087959

7 2.183554 -1.209289 0.057635

5 0.977047 -2.211102 0.103754

1 1.086219 -2.936909 -0.858134

1 1.071423 -2.867207 1.115324

5 0.118184 2.799206 0.192798

1 1.170677 3.057815 0.665885

1 -0.632924 3.676421 -0.099651

17 -4.120742 -0.209831 -0.069388

##
##

09-2BH2CH3-iso-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H10B2Cl1N5
09-2BH2CH3-iso-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=56.8 te_zpe=-1094.440856 te_gfe=-1094.479327 te_ms_zpe=-1092.918663
te_ms_gfe=0.148430

7 3.570320 0.648941 -0.102366

7 2.326257 1.056745 -0.173722

7 1.549039 0.000001 0.000030

7 2.326253 -1.056741 0.173823

7 3.570319 -0.648948 0.102486

6 0.127497 0.000001 0.000001

6 -0.513300 -1.241927 -0.161172

6 -1.905335 -1.211951 -0.152416

6 -2.575841 -0.000001 -0.000053

6 -1.905343 1.211950 0.152338

6 -0.513308 1.241928 0.161151

1 -2.464783 -2.130038 -0.272978

1 -2.464797 2.130036 0.272879

6 0.296600 2.497615 0.366977

1 0.496550 2.596301 1.443882

1 -0.310592 3.364822 0.096611

6 0.296618 -2.497613 -0.366957

1 -0.310584 -3.364820 -0.096615

1 0.496615 -2.596304 -1.443854

5 1.678622 2.515135 -0.484158

5 1.678603 -2.515131 0.484239

1 1.514064 2.474350 -1.683207

1 2.502238 3.313884 -0.141888

1 1.513993 -2.474339 1.683281

1 2.502234 -3.313880 0.142008

17 -4.323641 -0.000002 -0.000088

09-2BH2CH3-ts-01-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H10B2Cl1N5
09-2BH2CH3-ts-01-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-527.8 te_zpe=-1094.386127 te_gfe=-1094.427210 te_ms_zpe=-1092.856001 te_ms_gfe=0.138875

7 -3.650034 -0.847409 -0.450297

7 -2.566502 -1.261113 -0.343653

7 -1.572092 0.071407 0.229049

7 -2.427744 1.006351 0.241778

7 -3.595834 0.881698 -0.038152

6 -0.168153 0.088837 0.146651

6 0.554669 1.253663 -0.176196

6 1.942229 1.136027 -0.238584

6 2.553449 -0.096082 -0.029353

6 1.818550 -1.241244 0.250400

6 0.430114 -1.170560 0.356234

1 2.547032 2.004196 -0.466386

1 2.322622 -2.187645 0.395797

6 -0.429916 -2.375998 0.625986

1 -0.859907 -2.291277 1.633556

1 0.197091 -3.271144 0.638653

6 -0.137490 2.567641 -0.438550

1 0.624134 3.353281 -0.568315

1 -0.659536 2.539540 -1.403976

5 -1.620611 -2.606005 -0.455969

5 -1.082382 3.135377 0.683040

1 -1.272829 -2.551033 -1.610336

1 -2.372908 -3.508572 -0.213514

1 -0.937573 2.819850 1.822779

1 -1.872123 3.982963 0.406985

17 4.300218 -0.203956 -0.130659

09-2BH2CH3-ts-02-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H10B2Cl1N5 09-2BH2CH3-ts-02-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-439.6 te_zpe=-1094.354026 te_gfe=-1094.394108 te_ms_zpe=-1092.817857 te_ms_gfe=0.139211

7 4.168785 0.427269 -0.042323

7 2.181864 1.173244 -0.132971

7 1.591421 0.088812 -0.050857

7 2.200547 -1.137865 -0.124743

7 3.954179 -0.666112 0.126280

6 0.092966 0.035802 -0.038765

6 -0.530279 -1.211635 -0.171770

6 -1.927777 -1.227426 -0.142924

6 -2.630427 -0.038388 -0.006898

6 -1.980726 1.183601 0.132045

6 -0.586563 1.252791 0.127731

1 -2.456253 -2.165489 -0.243929

1 -2.555127 2.089389 0.272863

6 0.137761 2.541947 0.369512

1 0.297325 2.655450 1.449732

1 -0.473728 3.388073 0.048907

6 0.260334 -2.460088 -0.317430

1 -0.275150 -3.330518 0.067401

1 0.536945 -2.644298 -1.358535

5 1.568980 2.550729 -0.421395

5 1.661503 -2.325753 0.634819

1 1.428070 2.544844 -1.634566

1 2.337268 3.398347 -0.052100

1 1.387495 -2.106869 1.787289

1 2.349547 -3.279483 0.392011

17 -4.377536 -0.078317 0.003947

##
#

09-BH2-b3-iso-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H5B1Cl1N5
09-BH2-b3-iso-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=71.3 te_zpe=-990.404095 te_gfe=-990.439611 te_ms_zpe=-989.078589 te_ms_gfe=0.082205

6 1.807027 -1.369482 -0.000043

6 0.434096 -1.573149 -0.000066

6 -0.360491 -0.434879 -0.000017

6 0.098425 0.890017 0.000028

6 1.482941 1.059826 0.000049

6 2.308563 -0.062179 0.000019

1 2.489215 -2.208367 -0.000073

1 0.007350 -2.567756 -0.000111

1 1.922059 2.049173 0.000076

7 -1.777267 -0.414567 -0.000028

7 -2.731475 -1.312204 -0.000201

7 -3.852399 -0.617316 0.000187

7 -3.587999 0.682812 0.000010

7 -2.293801 0.812402 -0.000005

5 -1.125008 1.936316 0.000003

1 -1.247276 2.587325 -1.002980

1 -1.247306 2.587317 1.002988

17 4.045778 0.161877 0.000032

09-BH2-b3-ts-01-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H5B1Cl1N5 09-BH2-b3-ts-01-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-536.9 te_zpe=-990.363016 te_gfe=-990.399774 te_ms_zpe=-989.031010 te_ms_gfe=0.076664

6 -1.841903 -1.382028 0.026938

6 -0.470399 -1.605106 0.092098

6 0.364482 -0.494261 0.105555

6 -0.083093 0.839069 0.070134

6 -1.463012 1.026474 0.010507

6 -2.319060 -0.073081 -0.010663

1 -2.533109 -2.213718 0.006755

1 -0.070073 -2.610504 0.128669

1 -1.878701 2.025835 -0.025337

7 1.766273 -0.513387 0.198354

7 2.737750 -1.284098 -0.031931

7 3.869161 -0.928843 -0.200478

7 3.574727 0.934039 -0.149663

7 2.424291 1.019140 0.022763

5 1.063357 1.964662 0.103516

1 1.177492 2.549123 1.147946

1 1.140102 2.676996 -0.859097

17 -4.051765 0.193800 -0.091602

09-BH2-b3-ts-02-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H5B1Cl1N5 09-BH2-b3-ts-02-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-561.2 te_zpe=-990.358606 te_gfe=-990.397147 te_ms_zpe=-989.023695 te_ms_gfe=0.073599

6 -1.647691 -1.350264 -0.144107

6 -0.259954 -1.319995 -0.201537

6 0.419947 -0.105111 -0.098934

6 -0.275104 1.118290 0.080080

6 -1.682384 1.054362 0.078418

6 -2.353734 -0.156922 -0.017386

1 -2.178444 -2.290361 -0.221348

1 0.301655 -2.235891 -0.331973

1 -2.248848 1.971273 0.180062

7 1.822899 -0.182072 -0.151701

7 2.840321 -1.282418 0.672649

7 3.920203 -0.880723 0.456639

7 3.846835 0.524514 -0.491939

7 2.649126 0.663892 -0.651168

5 0.382572 2.479161 0.396373

1 1.526645 2.575807 0.694246

1 -0.305668 3.450731 0.394938

17 -4.104140 -0.188934 0.016567

09-BH2-b3-ts-04-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H5B1Cl1N5 09-BH2-b3-ts-04-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-237.0 te_zpe=-990.361650 te_gfe=-990.397529 te_ms_zpe=-989.023023 te_ms_gfe=0.078246

6 -1.884952 -1.383859 0.000028

6 -0.512198 -1.575886 0.000025

6 0.292764 -0.437146 0.000004

6 -0.199003 0.886640 -0.000016

6 -1.581236 1.051571 -0.000013

6 -2.396495 -0.079025 0.000009

1 -2.563876 -2.225728 0.000044

1 -0.081015 -2.569248 0.000039

1 -2.030751 2.036646 -0.000028

7 1.691441 -0.468356 0.000000

7 3.576710 -1.416309 0.000019

7 4.017607 -0.344187 0.000003

7 3.537739 0.871072 -0.000020

7 2.169767 0.695585 -0.000022

5 1.053670 1.873600 -0.000048

1 1.231509 2.521472 0.999219

1 1.231494 2.521398 -0.999366

17 -4.136580 0.129945 0.000015

09-BH2-b3-ts-05-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H5B1Cl1N5 09-BH2-b3-ts-05-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-237.2 te_zpe=-990.347625 te_gfe=-990.383571 te_ms_zpe=-989.009034 te_ms_gfe=0.077993

6 -1.752229 -1.359240 0.000008

6 -0.370152 -1.469546 0.000013

6 0.339823 -0.273696 0.000010

6 -0.212587 1.013810 0.000005

6 -1.606490 1.091638 -0.000002

6 -2.345590 -0.087329 -0.000000

1 -2.377152 -2.241938 0.000010

1 0.125973 -2.430777 0.000018

1 -2.116229 2.046838 -0.000009

7 1.755951 -0.122164 0.000005

7 2.600384 -1.305190 -0.000002

7 3.767124 -0.792200 -0.000010

7 4.291566 0.236465 -0.000018

7 2.212558 1.023073 0.000000

5 1.008416 2.054077 0.000011

1 1.127140 2.738361 0.989570

1 1.127136 2.738414 -0.989508

17 -4.096393 0.006178 -0.000010

##
##

09-CH3BH2-iso-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H7B1Cl1N5 09-CH3BH2-iso-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=64.7 te_zpe=-1029.699450 te_gfe=-1029.736330 te_ms_zpe=-1028.306656 te_ms_gfe=0.109340

7 -3.714515 0.038160 0.125206

7 -2.506462 0.516531 0.172245

7 -1.675124 -0.496594 -0.058737

7 -2.368182 -1.605415 -0.246410

7 -3.621729 -1.264242 -0.125287

6 -0.251451 -0.378960 -0.048822

6 0.510596 -1.535458 0.104413

6 1.892272 -1.428749 0.129676

6 2.468532 -0.164618 0.010020

6 1.695635 0.981278 -0.143977

6 0.301134 0.904835 -0.183480

1 0.024954 -2.496606 0.206324

1 2.512984 -2.305672 0.250811

1 2.177136 1.945906 -0.238888

6 -0.591973 2.102774 -0.374579

1 -0.823194 2.186660 -1.446568

1 -0.042104 3.010112 -0.113998

5 -1.955988 2.008261 0.501637

1 -1.761920 1.966793 1.695776

1 -2.834491 2.758788 0.185995

17 4.210599 -0.018410 0.054338

09-CH3BH2-ts-01-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H7B1Cl1N5 09-CH3BH2-ts-01-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-505.3 te_zpe=-1029.654139 te_gfe=-1029.693069 te_ms_zpe=-1028.254292 te_ms_gfe=0.101595

7 -3.682755 0.368777 0.092671

7 -2.460344 0.467631 0.216514

7 -1.635590 -0.488455 0.085521

7 -2.883781 -1.844462 -0.359551

7 -3.868687 -1.249587 -0.270204

6 -0.236974 -0.351484 0.055065

6 0.519318 -1.505998 0.267868

6 1.904749 -1.442252 0.232825

6 2.510970 -0.211322 0.001084

6 1.759474 0.941831 -0.205712

6 0.365395 0.899823 -0.196487

1 0.015002 -2.444803 0.458676

1 2.504719 -2.327693 0.392999

1 2.263356 1.883341 -0.384218

6 -0.492406 2.115456 -0.420518

1 -0.843424 2.129759 -1.461182

1 0.114994 3.020390 -0.300134

5 -1.719818 2.231249 0.597937

1 -1.506282 2.033870 1.759044

1 -2.633218 2.941070 0.314399

17 4.259935 -0.108578 -0.031099

09-CH3BH2-ts-02-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H7B1Cl1N5 09-CH3BH2-ts-02-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-537.1 te_zpe=-1029.662891 te_gfe=-1029.700485 te_ms_zpe=-1028.263263 te_ms_gfe=0.104412

7 -3.726804 0.192849 0.481646

7 -2.677765 0.683451 0.326336

7 -1.643261 -0.529938 -0.342473

7 -2.408884 -1.544583 -0.323032

7 -3.563800 -1.508307 0.019401

6 -0.240206 -0.458641 -0.232623

6 0.545616 -1.585101 0.013229

6 1.920795 -1.438811 0.130134

6 2.471460 -0.163394 0.031959

6 1.680027 0.958447 -0.191682

6 0.297459 0.837570 -0.343175

1 0.086044 -2.561758 0.098940

1 2.554532 -2.297621 0.304860

1 2.140505 1.935849 -0.257568

6 -0.617918 2.010814 -0.560995

1 -1.015334 1.966795 -1.584439

1 -0.043409 2.938411 -0.497472

5 -1.846815 2.097117 0.498115

1 -1.518047 2.026985 1.657594

1 -2.663628 2.946876 0.274526

17 4.205506 0.031721 0.194044

09-CH3BH2-ts-03-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H7B1Cl1N5 09-CH3BH2-ts-03-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-290.2 te_zpe=-1029.599562 te_gfe=-1029.638122 te_ms_zpe=-1028.204208 te_ms_gfe=0.099488

7 -4.369559 -0.287588 0.179625

7 -2.314247 0.703832 0.503017

7 -1.760358 -0.297181 0.013155

7 -2.073488 -1.375579 -0.566929

7 -4.048415 -1.250937 -0.281871

6 -0.210350 -0.354304 -0.079731

6 0.485829 -1.508545 0.253773

6 1.870448 -1.438328 0.295515

6 2.491535 -0.222624 0.006438

6 1.764720 0.919398 -0.302417

6 0.362583 0.890410 -0.357876

1 -0.037377 -2.426590 0.475034

1 2.457208 -2.309125 0.553067

1 2.278416 1.851472 -0.497663

6 -0.486699 2.100175 -0.522148

1 -1.027195 2.078842 -1.475065

1 0.119113 3.006821 -0.493135

5 -1.595437 2.054764 0.715444

1 -1.138092 2.093261 1.837183

1 -2.422369 2.927956 0.559083

17 4.237738 -0.133022 0.045528

09-CH3BH2-ts-04-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H7B1Cl1N5 09-CH3BH2-ts-04-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-230.9 te_zpe=-1029.655481 te_gfe=-1029.692890 te_ms_zpe=-1028.248760 te_ms_gfe=0.104949

7 -3.734864 0.285151 0.119498

7 -2.340199 0.509933 0.113320

7 -1.592380 -0.465114 -0.052558

7 -3.218183 -1.931575 -0.210117

7 -3.864281 -0.991577 -0.047985

6 -0.198447 -0.331914 -0.047269

6 0.540119 -1.515534 0.061706

6 1.923529 -1.464622 0.097836

6 2.543409 -0.218301 0.008869

6 1.813133 0.960796 -0.124423

6 0.420024 0.934222 -0.159254

1 0.014719 -2.459768 0.132925

1 2.514742 -2.364773 0.194833

1 2.333227 1.906823 -0.205743

6 -0.437835 2.153921 -0.348294

1 -0.607310 2.283962 -1.427401

1 0.104420 3.045079 -0.020380

5 -1.842168 2.034512 0.448055

1 -1.730724 1.975676 1.654947

1 -2.718841 2.769625 0.095037

17 4.289786 -0.134607 0.055611

09-CH3BH2-ts-05-gas-b3-cbs-qb3 charge=0 spin=1 mol=C7H7B1Cl1N5 09-CH3BH2-ts-05-gas-b3-cbs-qb3 CBS-QB3

lf=-186.2 te_zpe=-1029.640377 te_gfe=-1029.678097 te_ms_zpe=-1028.233003 te_ms_gfe=0.104078

7 -4.313447 -0.479367 0.090328

7 -2.392733 0.744070 0.162287

7 -1.686147 -0.207639 -0.032844

7 -2.349618 -1.627267 -0.223557

7 -3.552606 -1.328184 -0.094038

6 -0.251562 -0.242129 -0.056870

6 0.423676 -1.455133 0.065728

6 1.809749 -1.452113 0.100452

6 2.479018 -0.232570 0.012732

6 1.795830 0.972668 -0.117196

6 0.400603 1.001991 -0.158880

1 -0.131278 -2.378255 0.143692

1 2.363089 -2.375576 0.200838

1 2.349775 1.899513 -0.191613

6 -0.397260 2.264953 -0.339948

1 -0.548302 2.414004 -1.418866

1 0.187962 3.122513 0.002431

5 -1.831254 2.198964 0.426086

1 -1.763278 2.181994 1.645034

1 -2.658862 2.991863 0.064345

17 4.226982 -0.218127 0.063081

##
###

09-ts-01-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C6H4Cl1N5
09-ts-01-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-554.9 te_zpe=-964.928269 te_gfe=-964.965687 te_ms_zpe=-963.657620
te_ms_gfe=0.063746

7 3.974146 0.740404 0.298188

7 2.916687 1.244401 0.305518

7 1.856237 -0.024903 -0.151136

7 2.640723 -1.031324 -0.265541

7 3.839368 -0.911371 -0.096929

6 0.450478 -0.047912 -0.102879

6 -0.260889 -1.236996 0.087914

6 -1.648987 -1.207566 0.131749

6 -2.316912 0.007393 0.006930

6 -1.613589 1.195089 -0.171309

6 -0.226330 1.167481 -0.235863

1 -2.209285 -2.122814 0.270718

1 -2.146284 2.131778 -0.268456

1 0.334604 2.080859 -0.383403

1 0.270795 -2.173678 0.192154

17 -4.067210 0.041086 0.074061

##
#

10-2BH2-b3-iso-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H6B2F3N5
10-2BH2-b3-iso-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=10.5 te_zpe=-893.335081 te_gfe=-893.377313 te_ms_zpe=-892.037015
te_ms_gfe=0.100441

6 -1.199096 1.260102 -0.026592

6 0.189115 1.482428 -0.014469

6 0.953691 0.299938 -0.009027

6 0.462145 -1.010013 -0.018335

6 -0.928645 -1.151196 -0.030741

6 -1.747996 -0.024943 -0.033882

1 -1.857678 2.119107 -0.039782

1 -1.372602 -2.139047 -0.045091

7 2.382366 0.213559 0.002075

7 3.395350 1.050399 0.015738

7 4.469652 0.294903 0.021884

7 4.129951 -0.991638 0.012363

7 2.835381 -1.043429 -0.000034

5 1.631792 -2.106806 -0.015426

1 1.727822 -2.759396 -1.020954

1 1.712946 -2.771671 0.983256

5 0.711731 2.938827 -0.010925

1 1.866625 3.198253 0.002612

1 -0.097398 3.811347 -0.021797

6 -3.247507 -0.184260 0.004981

9 -3.644175 -1.365016 -0.509952

9 -3.713618 -0.127668 1.272337

9 -3.872926 0.790729 -0.687084

############################

10-2BH2-b3-ts-01-b3-cbs-qb3 charge=0 spin=1 mol= 0/

lf=0.0

6 -1.190204 1.290843 0.080078

6 0.195822 1.508467 -0.063250

6 0.976517 0.341861 -0.198733

6 0.477651 -0.969835 -0.205323

6 -0.903883 -1.102474 -0.072203

6 -1.735949 0.014572 0.043150

1 -1.836672 2.148714 0.212220

1 -1.340028 -2.093995 -0.025125

7 2.383987 0.335792 -0.418783

7 3.370416 0.995162 0.056258

7 4.406526 0.497770 0.404606

7 4.027340 -1.185094 0.272364

7 2.901993 -1.217559 -0.054048

5 1.561648 -2.143759 -0.141131

1 1.700219 -2.890918 -1.067460

1 1.559691 -2.685430 0.934608

5 0.728969 2.951129 -0.114114

1 1.820359 3.209778 -0.505923

1 0.005812 3.834023 0.224064

6 -3.227432 -0.182818 0.068033

9 -3.878876 0.867674 0.604732

9 -3.717504 -0.356761 -1.181051

9 -3.575780 -1.282602 0.773046

##
###

10-2BH2-b3-ts-02-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H6B2F3N5
10-2BH2-b3-ts-02-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-493.4 te_zpe=-893.288294 te_gfe=-893.332761 te_ms_zpe=-891.980843
te_ms_gfe=0.092646

6 1.238852 1.282120 -0.013813

6 -0.163041 1.444354 -0.008365

6 -0.905127 0.248117 -0.005157

6 -0.345193 -1.042366 -0.009189

6 1.040554 -1.132979 -0.015532

6 1.830464 0.025739 -0.017347

1 1.862774 2.166283 -0.018885

1 1.522660 -2.104546 -0.024439

7 -2.318447 0.224782 0.000118

7 -4.125668 1.171957 0.010580

7 -4.760895 0.223508 0.011383

7 -4.036023 -1.233478 0.004838

7 -2.826467 -0.938898 -0.000045

5 -1.442357 -2.190256 -0.008163

1 -1.649759 -2.781439 1.009284

1 -1.656855 -2.776060 -1.027285

5 -0.776135 2.856206 -0.006963

1 -1.951814 3.025509 -0.000788

1 -0.044618 3.796146 -0.011928

6 3.327664 -0.124232 0.003091

9 3.966474 1.046330 -0.193427

9 3.760649 -0.620262 1.185446

9 3.754826 -0.981096 -0.952082

10-2BH2-b3-ts-03-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H6B2F3N5 10-2BH2-b3-ts-03-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-380.1 te_zpe=-893.234634 te_gfe=-893.279117 te_ms_zpe=-891.928834 te_ms_gfe=0.089657

6 1.254093 1.240214 -0.027167

6 -0.147580 1.426462 -0.015772

6 -0.827149 0.209998 -0.010131

6 -0.353984 -1.083643 -0.018015

6 1.049194 -1.172450 -0.028586

6 1.838207 -0.027587 -0.032598

1 1.882151 2.121397 -0.041486

1 1.512977 -2.151972 -0.041199

7 -2.487651 -0.038950 0.000756

7 -3.052099 1.088181 0.009334

7 -4.917615 0.474210 0.020699

7 -5.106368 -0.619952 0.018473

7 -2.756404 -1.240491 -0.001894

5 -1.505057 -2.195686 -0.015319

1 -1.518933 -2.884260 0.977360

1 -1.532539 -2.873435 -1.015223

5 -0.683181 2.873350 -0.011369

1 -1.845294 3.104493 0.008260

1 0.108594 3.760615 -0.026557

6 3.341928 -0.143519 0.006189

9 3.937487 0.845135 -0.693622

9 3.807073 -0.063695 1.272221

9 3.771766 -1.315107 -0.501135

10-2BH2-b3-ts-04-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H6B2F3N5 10-2BH2-b3-ts-04-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-237.1 te_zpe=-893.294619 te_gfe=-893.337097 te_ms_zpe=-891.983855 te_ms_gfe=0.096614

6 -1.263722 1.271591 -0.028433

6 0.125939 1.473668 -0.016324

6 0.892556 0.288486 -0.010821

6 0.372973 -1.020270 -0.019772

6 -1.015286 -1.149841 -0.032319

6 -1.822648 -0.010140 -0.035923

1 -1.917131 2.134775 -0.040829

1 -1.475382 -2.130765 -0.047088

7 2.299589 0.271321 0.000279

7 4.242677 1.140763 0.022250

7 4.624590 0.050264 0.020907

7 4.088037 -1.145745 0.010576

7 2.734158 -0.910096 -0.001042

5 1.586592 -2.047859 -0.016045

1 1.750844 -2.696757 -1.017206

1 1.736528 -2.709651 0.978736

5 0.710317 2.901092 -0.011971

1 1.882406 3.092083 0.001922

1 -0.041467 3.824557 -0.022149

6 -3.321939 -0.162956 0.005845

9 -3.776851 -0.209125 1.278799

9 -3.952737 0.865830 -0.598272

9 -3.731625 -1.297726 -0.598041

10-2BH2-b3-ts-05-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H6B2F3N5 10-2BH2-b3-ts-05-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-243.8 te_zpe=-893.275384 te_gfe=-893.318346 te_ms_zpe=-891.964591 te_ms_gfe=0.095703

6 -1.169147 1.204746 -0.048462

6 0.224114 1.365070 0.013291

6 0.927745 0.142011 0.041880

6 0.366947 -1.138208 0.064086

6 -1.030986 -1.219254 0.046586

6 -1.785463 -0.054998 -0.019599

1 -1.787566 2.092008 -0.105997

1 -1.523745 -2.183217 0.068953

7 2.355482 -0.056483 0.018028

7 3.259776 1.075273 -0.104426

7 4.397901 0.503741 -0.127430

7 4.880408 -0.543433 -0.088396

7 2.768038 -1.219294 0.057392

5 1.551679 -2.206192 0.101417

1 1.655011 -2.931658 -0.861739

1 1.640560 -2.868763 1.109407

5 0.750703 2.812209 0.193449

1 1.802572 3.057888 0.674698

1 0.013120 3.698274 -0.106020

6 -3.292236 -0.113574 -0.033797

9 -3.755291 -1.359872 -0.249148

9 -3.810986 0.308068 1.141445

9 -3.810271 0.682026 -0.994931

##
#

10-2BH2CH3-iso-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C9H10B2F3N5
10-2BH2CH3-iso-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=10.5 te_zpe=-971.939587 te_gfe=-971.982765 te_ms_zpe=-970.509613 te_ms_gfe=0.157818

7 4.123535 0.645297 -0.087279

7 2.882327 1.054124 -0.167721

7 2.102525 -0.000863 0.001996

7 2.875855 -1.058686 0.183341

7 4.119613 -0.654317 0.121924

6 0.676097 0.001409 -0.009246

6 0.039288 -1.239543 -0.179649

6 -1.353550 -1.202163 -0.183613

6 -2.033903 0.006122 -0.036699

6 -1.352513 1.212067 0.123156

6 0.040359 1.244688 0.146869

1 -1.907030 -2.122269 -0.318529

1 -1.905141 2.136441 0.229138

6 0.850997 2.499029 0.356183

1 1.041955 2.601636 1.434292

1 0.246679 3.365896 0.078226

6 0.849756 -2.495323 -0.379809

1 0.238405 -3.361676 -0.116052

1 1.060227 -2.594384 -1.454624

5 2.239179 2.515332 -0.483496

5 2.222408 -2.518195 0.485209

1 2.086287 2.472074 -1.683872

1 3.063071 3.310768 -0.135176

1 2.047416 -2.476741 1.682565

1 3.049872 -3.315681 0.150345

6 -3.543080 0.000780 0.004399

9 -4.063906 -0.998408 -0.736006

9 -4.064028 1.157205 -0.452305

9 -3.993997 -0.165801 1.267171

10-2BH2CH3-ts-01-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C9H10B2F3N5 10-2BH2CH3-ts-01-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-530.1 te_zpe=-971.886650 te_gfe=-971.932549 te_ms_zpe=-970.448505 te_ms_gfe=0.148175

7 4.174658 -0.904490 0.476118

7 3.085069 -1.296732 0.349015

7 2.125340 0.057757 -0.217455

7 2.997059 0.979323 -0.206655

7 4.158505 0.827529 0.083131

6 0.719261 0.101466 -0.159808

6 0.015609 1.283677 0.143374

6 -1.373748 1.188745 0.176846

6 -2.018433 -0.027224 -0.042330

6 -1.289033 -1.182526 -0.306366

6 0.102295 -1.145834 -0.383644

1 -1.959497 2.075882 0.382460

1 -1.803399 -2.120236 -0.472825

6 0.941253 -2.366977 -0.647963

1 1.382944 -2.288716 -1.651066

1 0.295592 -3.248609 -0.670321

6 0.727189 2.585450 0.413553

1 -0.023468 3.383899 0.528432

1 1.231730 2.552487 1.388144

5 2.114570 -2.626220 0.444446

5 1.701181 3.134946 -0.691710

1 1.756985 -2.568253 1.595706

1 2.854268 -3.539934 0.206270

1 1.577372 2.812963 -1.832174

1 2.497028 3.972746 -0.403978

6 -3.517937 -0.097865 0.072023

9 -4.109640 1.050934 -0.322637

9 -3.908453 -0.317358 1.348939

9 -4.038735 -1.095024 -0.672693

10-2BH2CH3-ts-02-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C9H10B2F3N5 10-2BH2CH3-ts-02-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-440.6 te_zpe=-971.853285 te_gfe=-971.898383 te_ms_zpe=-970.409231 te_ms_gfe=0.148251

7 4.727257 0.413594 -0.033675

7 2.746331 1.168094 -0.125058

7 2.153984 0.084988 -0.046877

7 2.755321 -1.140799 -0.112605

7 4.508177 -0.679248 0.135520

6 0.647092 0.038303 -0.044613

6 0.025117 -1.206246 -0.185738

6 -1.374581 -1.210138 -0.171039

6 -2.082316 -0.023064 -0.041451

6 -1.417581 1.192186 0.104318

6 -0.023160 1.259960 0.115454

1 -1.900314 -2.148303 -0.284874

1 -1.982455 2.107011 0.229864

6 0.705731 2.545291 0.360302

1 0.858049 2.661257 1.441191

1 0.100997 3.393523 0.032557

6 0.810976 -2.457941 -0.327091

1 0.266818 -3.325795 0.051471

1 1.093830 -2.642551 -1.366581

5 2.144096 2.548270 -0.418598

5 2.204711 -2.332959 0.634806

1 2.015024 2.543972 -1.632790

1 2.913081 3.391100 -0.040751

1 1.925563 -2.117807 1.786659

1 2.892729 -3.286618 0.392496

6 -3.590612 -0.041408 0.003763

9 -4.040743 0.041124 1.274711

9 -4.101666 -1.169921 -0.526572

9 -4.120796 0.999863 -0.669786

##
#

10-BH2-b3-iso-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H5B1F3N5 10-BH2-b3-iso-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=10.7 te_zpe=-867.903842 te_gfe=-867.944119 te_ms_zpe=-866.670409 te_ms_gfe=0.091545

6 -1.172308 -1.400281 -0.027154

6 0.200999 -1.594477 -0.015714

6 0.981943 -0.446379 -0.008528

6 0.514499 0.873429 -0.014624

6 -0.873810 1.024385 -0.026556

6 -1.698479 -0.099898 -0.032543

1 -1.840116 -2.251462 -0.041724

1 0.640370 -2.583415 -0.015389

1 -1.315962 2.012388 -0.037910

7 2.400596 -0.414334 0.000811

7 3.362962 -1.303472 0.009982

7 4.476669 -0.600260 0.016973

7 4.200353 0.699857 0.011305

7 2.906424 0.817528 0.001633

5 1.726413 1.930960 -0.009527

1 1.838298 2.586412 0.991841

1 1.851130 2.579427 -1.014022

6 -3.197174 0.065798 0.003633

9 -3.587754 1.282514 -0.422218

9 -3.819565 -0.851830 -0.768105

9 -3.678107 -0.089445 1.257970

10-BH2-b3-ts-01-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H5B1F3N5 10-BH2-b3-ts-01-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-535.0 te_zpe=-867.864000 te_gfe=-867.905427 te_ms_zpe=-866.623577 te_ms_gfe=0.086143

6 -1.198217 -1.432936 -0.078315

6 0.175771 -1.637833 -0.122882

6 0.990813 -0.511819 -0.126193

6 0.524081 0.815194 -0.102124

6 -0.859268 0.974304 -0.063929

6 -1.709935 -0.134104 -0.051959

1 -1.870963 -2.280214 -0.074431

1 0.595511 -2.635220 -0.154589

1 -1.285448 1.970182 -0.046352

7 2.392877 -0.509835 -0.198967

7 3.370686 -1.270757 0.048875

7 4.492635 -0.898709 0.235725

7 4.175326 0.959704 0.175028

7 3.026632 1.028538 -0.016704

5 1.654133 1.956596 -0.123874

1 1.707190 2.674952 0.835622

1 1.778328 2.536191 -1.169786

6 -3.196774 0.074695 0.050627

9 -3.597234 0.184423 1.339236

9 -3.595207 1.201342 -0.576740

9 -3.892137 -0.952038 -0.485845

10-BH2-b3-ts-02-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H5B1F3N5 10-BH2-b3-ts-02-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-436.4 te_zpe=-867.856360 te_gfe=-867.898671 te_ms_zpe=-866.614316 te_ms_gfe=0.085699

6 1.228999 -1.418691 -0.005497

6 -0.131934 -1.653368 -0.003167

6 -0.970078 -0.535430 -0.001853

6 -0.547751 0.795968 -0.003294

6 0.840701 0.990573 -0.005601

6 1.706422 -0.095840 -0.006590

1 1.925438 -2.247232 -0.008808

1 -0.539766 -2.656157 -0.002995

1 1.242178 1.995617 -0.007747

7 -2.387914 -0.673307 0.000301

7 -3.235785 -1.486835 0.002109

7 -4.794335 -0.273516 0.003876

7 -4.148166 0.722525 0.002230

7 -2.931124 0.925537 0.000119

5 -1.701612 1.920929 -0.002435

1 -1.712574 2.581604 -1.010318

1 -1.709700 2.583227 1.004399

6 3.200909 0.111159 0.000840

9 3.544750 1.409723 -0.068891

9 3.758413 -0.393872 1.124119

9 3.787965 -0.519045 -1.040988

10-BH2-b3-ts-04-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H5B1F3N5 10-BH2-b3-ts-04-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-236.0 te_zpe=-867.861314 te_gfe=-867.901944 te_ms_zpe=-866.614915 te_ms_gfe=0.087581

6 1.242425 -1.406530 -0.028641

6 -0.130135 -1.593537 -0.017751

6 -0.925517 -0.448010 -0.010608

6 -0.429125 0.871348 -0.016337

6 0.956479 1.022140 -0.027452

6 1.775555 -0.107359 -0.033472

1 1.909050 -2.258921 -0.042973

1 -0.570462 -2.582664 -0.017667

1 1.404913 2.007615 -0.037750

7 -2.328073 -0.472893 -0.001093

7 -4.227693 -1.405015 0.015814

7 -4.653842 -0.328692 0.016852

7 -4.160772 0.883557 0.010391

7 -2.797098 0.694448 -0.000015

5 -1.673356 1.865524 -0.010900

1 -1.857275 2.510984 -1.010813

1 -1.844900 2.518546 0.986162

6 3.274083 0.049478 0.004674

9 3.894061 -0.864335 -0.774887

9 3.674095 1.267890 -0.409560

9 3.755756 -0.120021 1.257938

10-BH2-b3-ts-05-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H5B1F3N5 10-BH2-b3-ts-05-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-238.4 te_zpe=-867.847339 te_gfe=-867.888468 te_ms_zpe=-866.600808 te_ms_gfe=0.086883

6 1.130245 -1.343249 -0.017442

6 -0.249420 -1.464612 -0.010980

6 -0.963190 -0.270281 -0.006119

6 -0.421569 1.018841 -0.008878

6 0.974804 1.098535 -0.015170

6 1.730367 -0.070709 -0.019286

1 1.752006 -2.229254 -0.027487

1 -0.743431 -2.426688 -0.011565

1 1.472488 2.059693 -0.020234

7 -2.383605 -0.127449 -0.000366

7 -3.220982 -1.311463 0.003698

7 -4.391119 -0.803098 0.008737

7 -4.914542 0.226253 0.010753

7 -2.843393 1.016880 0.001210

5 -1.645765 2.051928 -0.004938

1 -1.774028 2.735667 -0.994023

1 -1.766141 2.739662 0.982233

6 3.236758 -0.006493 0.002657

9 3.780883 -0.803485 -0.944538

9 3.704695 1.238972 -0.203872

9 3.729470 -0.426464 1.190504

##
#

10-CH3BH2-iso-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H7B1F3N5
10-CH3BH2-iso-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=11.6 te_zpe=-907.199008 te_gfe=-907.240556 te_ms_zpe=-905.898122 te_ms_gfe=0.118787

7 -4.311236 0.030420 0.150793

7 -3.105270 0.511107 0.181795

7 -2.274378 -0.500314 -0.059610

7 -2.967200 -1.610890 -0.238487

7 -4.218575 -1.273601 -0.102302

6 -0.848656 -0.380079 -0.065802

6 -0.086648 -1.538110 0.075127

6 1.294297 -1.425035 0.082519

6 1.878559 -0.162722 -0.041252

6 1.092816 0.977394 -0.183960

6 -0.303064 0.904467 -0.207117

1 -0.572358 -2.498912 0.178032

1 1.912414 -2.306720 0.184730

1 1.566057 1.945149 -0.290927

6 -1.200507 2.100356 -0.387715

1 -1.444164 2.185294 -1.456865

1 -0.648781 3.008232 -0.132824

5 -2.553774 2.005215 0.504176

1 -2.346888 1.962484 1.695964

1 -3.438203 2.752540 0.198701

6 3.379344 -0.033760 0.032867

9 3.799723 0.068724 1.312945

9 3.999915 -1.107200 -0.499804

9 3.827090 1.057779 -0.618808

10-CH3BH2-ts-01-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H7B1F3N5 10-CH3BH2-ts-01-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-508.0 te_zpe=-907.154889 te_gfe=-907.198564 te_ms_zpe=-905.847144 te_ms_gfe=0.110947

7 4.298822 0.327959 -0.074072

7 3.081513 0.457070 -0.191867

7 2.240516 -0.487937 -0.070337

7 3.440742 -1.868361 0.340657

7 4.445403 -1.301834 0.268277

6 0.842273 -0.339402 -0.057087

6 0.083595 -1.492239 -0.271195

6 -1.300680 -1.414237 -0.256958

6 -1.914296 -0.180508 -0.046133

6 -1.145725 0.964224 0.163057

6 0.247404 0.919009 0.175505

1 0.586440 -2.433922 -0.449956

1 -1.898592 -2.299558 -0.426991

1 -1.639390 1.915523 0.319905

6 1.107719 2.131409 0.408843

1 1.441990 2.147331 1.454960

1 0.503626 3.037552 0.278648

5 2.349354 2.249990 -0.587793

1 2.161547 2.045294 -1.751609

1 3.267165 2.945311 -0.284407

6 -3.414884 -0.086825 0.013626

9 -3.867075 1.097689 -0.450506

9 -4.012547 -1.057998 -0.708597

9 -3.870485 -0.206840 1.282643

10-CH3BH2-ts-02-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H7B1F3N5 10-CH3BH2-ts-02-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-538.1 te_zpe=-907.163590 te_gfe=-907.205792 te_ms_zpe=-905.855978 te_ms_gfe=0.113942

7 4.325270 0.188083 -0.482822

7 3.277673 0.680036 -0.320241

7 2.244903 -0.532443 0.342498

7 3.006456 -1.552088 0.311794

7 4.160129 -1.514230 -0.031333

6 0.840996 -0.460735 0.238241

6 0.058112 -1.591974 0.002653

6 -1.316204 -1.444189 -0.108868

6 -1.880965 -0.171650 -0.016809

6 -1.079113 0.947494 0.199537

6 0.304236 0.835605 0.345833

1 0.522073 -2.566344 -0.082816

1 -1.943116 -2.308129 -0.285017

1 -1.534248 1.928366 0.257234

6 1.217915 2.010813 0.559172

1 1.611935 1.973403 1.584248

1 0.641260 2.936673 0.489569

5 2.449028 2.095722 -0.495737

1 2.124795 2.021187 -1.656278

1 3.267145 2.943887 -0.272285

6 -3.375829 -0.012861 -0.094434

9 -3.948307 -0.099868 1.128932

9 -3.733318 1.182571 -0.607790

9 -3.946251 -0.968056 -0.859717

10-CH3BH2-ts-03-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H7B1F3N5 10-CH3BH2-ts-03-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-274.9 te_zpe=-907.099471 te_gfe=-907.143592 te_ms_zpe=-905.797313 te_ms_gfe=0.107860

7 -4.966386 -0.309880 0.212766

7 -2.912445 0.675641 0.520079

7 -2.362273 -0.317198 0.005505

7 -2.672373 -1.391699 -0.572505

7 -4.658918 -1.273558 -0.257090

6 -0.802000 -0.345885 -0.097323

6 -0.091944 -1.495287 0.222198

6 1.290187 -1.399302 0.253256

6 1.902204 -0.174186 -0.031035

6 1.147229 0.952411 -0.327399

6 -0.257379 0.907054 -0.373798

1 -0.602968 -2.421484 0.436885

1 1.885732 -2.270270 0.493511

1 1.638802 1.894747 -0.529569

6 -1.125960 2.103292 -0.535524

1 -1.671922 2.071433 -1.484871

1 -0.533863 3.019049 -0.512360

5 -2.222522 2.041585 0.710326

1 -1.763446 2.106878 1.829733

1 -3.072873 2.892541 0.549621

6 3.407004 -0.090067 0.028644

9 3.877500 1.065956 -0.476810

9 3.852257 -0.182514 1.300729

9 3.984006 -1.098125 -0.660583

10-CH3BH2-ts-04-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H7B1F3N5 10-CH3BH2-ts-04-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-231.9 te_zpe=-907.154789 te_gfe=-907.196860 te_ms_zpe=-905.840253 te_ms_gfe=0.114380

7 -4.341797 0.265149 0.147820

7 -2.951805 0.495234 0.124543

7 -2.199970 -0.473458 -0.058034

7 -3.826753 -1.950982 -0.203888

7 -4.469394 -1.013099 -0.027698

6 -0.803243 -0.325222 -0.065999

6 -0.056348 -1.503375 0.034655

6 1.326922 -1.435424 0.053213

6 1.946184 -0.187570 -0.043841

6 1.192791 0.979785 -0.168273

6 -0.201230 0.945998 -0.186660

1 -0.574537 -2.451115 0.109218

1 1.921485 -2.335274 0.134687

1 1.696723 1.933657 -0.263199

6 -1.072807 2.157435 -0.363347

1 -1.260523 2.288117 -1.439285

1 -0.533678 3.053065 -0.042421

5 -2.461673 2.025457 0.455704

1 -2.331369 1.960426 1.660313

1 -3.352877 2.750915 0.120689

6 3.448912 -0.096433 0.033415

9 4.046447 -1.207242 -0.446856

9 3.929649 0.953684 -0.663207

9 3.866582 0.053763 1.310429

10-CH3BH2-ts-05-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C8H7B1F3N5 10-CH3BH2-ts-05-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-188.7 te_zpe=-907.139624 te_gfe=-907.181950 te_ms_zpe=-905.824075 te_ms_gfe=0.113605

7 -4.904705 -0.532954 0.125205

7 -3.004221 0.721637 0.177691

7 -2.287711 -0.220099 -0.036461

7 -2.924066 -1.639889 -0.224992

7 -4.133197 -1.367553 -0.076093

6 -0.848027 -0.228836 -0.077644

6 -0.154808 -1.432093 0.033133

6 1.231416 -1.401263 0.049541

6 1.890102 -0.174374 -0.042127

6 1.174788 1.014852 -0.159789

6 -0.222054 1.026085 -0.185266

1 -0.695234 -2.363439 0.112144

1 1.795566 -2.320501 0.130697

1 1.705931 1.954379 -0.245079

6 -1.043312 2.275405 -0.352568

1 -1.212593 2.425623 -1.428557

1 -0.467559 3.141507 -0.015790

5 -2.464642 2.182248 0.432637

1 -2.382719 2.165457 1.651285

1 -3.313036 2.960063 0.086369

6 3.395700 -0.133611 0.038396

9 3.909946 0.923426 -0.621706

9 3.814654 -0.041539 1.319908

9 3.956213 -1.246256 -0.479730

##
#

10-iso-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H4F3N5
10-iso-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=11.1 te_zpe=-842.454331 te_gfe=-842.495405 te_ms_zpe=-841.281976
te_ms_gfe=0.078248

7 -4.521628 -0.675754 0.015229

7 -3.300992 -1.099040 0.005810

7 -2.549332 0.000001 -0.000216

7 -3.301009 1.099032 0.005415

7 -4.521635 0.675720 0.014971

6 -1.123664 0.000012 -0.010772

6 -0.443905 1.216554 -0.017914

6 0.944682 1.208896 -0.029702

6 1.639779 0.000031 -0.035528

6 0.944693 -1.208848 -0.029922

6 -0.443889 -1.216525 -0.018143

1 1.486977 2.145202 -0.043096

1 1.486996 -2.145148 -0.043497

1 -0.997448 -2.144960 -0.017224

1 -0.997474 2.144983 -0.016819

6 3.145459 0.000003 0.004321

9 3.664155 -1.087793 -0.601775

9 3.664186 1.088431 -0.600601

9 3.605459 -0.000698 1.275502

10-ts-01-gas-b3-2d-d-p-cbs-qb3 charge=0 spin=1 mol=C7H4F3N5 10-ts-01-gas-b3-2d-d-p-cbs-qb3 CBS-QB3

lf=-550.6 te_zpe=-842.429627 te_gfe=-842.472206 te_ms_zpe=-841.250309 te_ms_gfe=0.072722

7 -4.642520 0.786247 0.005706

7 -3.581224 1.281604 -0.003166

7 -2.508688 -0.054588 0.004065

7 -3.296727 -1.064919 0.014560

7 -4.502676 -0.914137 0.018479

6 -1.104611 -0.068807 -0.007913

6 -0.383808 -1.268440 -0.020654

6 1.003120 -1.227528 -0.033440

6 1.674480 -0.004841 -0.036476

6 0.948021 1.185667 -0.025400

6 -0.439238 1.161163 -0.011818

1 1.565456 -2.152347 -0.050501

1 1.467272 2.135248 -0.036061

1 -1.009161 2.080273 -0.007040

1 -0.909459 -2.213821 -0.022844

6 3.176681 0.028755 0.003463

9 3.643936 0.032136 1.274000

9 3.722504 -1.044507 -0.607844

9 3.673656 1.131858 -0.595894