Electronic Supplementary Information for Mechanistic insight into catalytic hydrogenation of unactivated aldehydes with a Hantzsch ester in the presence of a series of organoboranes: NMR and DFT studies

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Contents

1. General Information

All reactions with oxygen- or moisture-sensitive reagents were performed under a nitrogen atmosphere, nitrogen gas was dried by passage through P_2O_5. Silica gel was purchased from Kanto chemical (Silica gel 60N, spherical neutral, particle size 40-50μm) or Yamazen corporation (Hi-FlashTM Column Silica gel 40 mm 60 Å). NMR spectra were recorded on a JEOL JNM ECS-400 spectrometer (396 MHz for ^{1}H, 100 MHz for ^{13}C, 373 MHz for ^{19}F, 127 MHz for ^{11}B). ^{1}H, ^{13}C, ^{19}F, and ^{11}B NMR spectra were recorded in $CDCl_3$ or CD_2Cl_2. Chemical shifts are reported in δ (ppm) referenced to tetramethylsilane (δ 0) as an internal standard or a solvent peak (CD_2Cl_2: δ 5.32) for ^{1}H NMR. Chemical shifts of ^{13}C NMR are given related to a solvent peak as an internal standard ($CDCl_3$: δ 77.0 or CD_2Cl_2: δ 53.80). Chemical shifts of ^{19}F and ^{11}B NMR are obtained related to CF_3CO_2H (δ −76.0) and $BF_3{\cdot}OEt_2$ (δ 0.00) as external standards, respectively. GC and GC-MS analyses were performed with an Agilent 6850 series II GC and an Agilent 6890 GC/5973N MS Detector, respectively. Commercially available chemicals (purchased from Sigma-Aldrich, TCI, Kanto chemical, Wako Pure Chemical Industries, Nacalai tesque, and Merck) were used without further purification unless otherwise noted. 1,4-Dioxane was distilled over CaH_2 prior to use. Tris[3,5-bis(trifluoromethyl)phenyl]borane (**B-a**) was synthesized according to literature method.[1]

2. Typical Procedure for the Hydrogenation of Benzaldehyde

In a glovebox, benzaldehyde (**1**; 27 mg, 0.25 mmol) and the Hantzsch ester **2** (95 mg, 0.38 mmol) were added to a solution of tris[3,5-bis(trifluoromethyl)phenyl]borane (**B-a**, 8.1 mg, 0.013 mmol) in distilled 1,4-dioxane (1 mL). After the reaction mixture was stirred at 25 °C for 12 h, the mixture was diluted with AcOEt and mesitylene was added as an internal standard. After filtration on celite, the resulting solution was analyzed with GC.

Benzyl alcohol (**3**):[2] ^{1}H NMR (396 MHz, $CDCl_3$): δ 1.86 (bs, 1H, -O***H***), 4.68 (s, 2H, ArC***H***$_2$OH), 7.28-7.36 (m, 5H, Ar***H***). ^{13}C NMR (100 MHz, $CDCl_3$) δ 65.3, 127.0, 127.6, 128.5, 140.8. MS (EI) *m/z* 108 ($[M]^+$).

3. Stoichiometric Reaction of Tris[3,5-bis(trifluoromethyl)phenyl]borane, Benzaldehyde, and Hantzsch Ester

In a glove box, benzaldehyde (**1**; 3.2 mg, 0.030 mmol) was added to a solution of tris[3,5-bis(trifluoromethyl)phenyl]borane (**B-a**, 19.5 mg, 0.030 mmol) in 0.75 mL of CD_2Cl_2 in a J-Young NMR tube at 25 ºC. The resulting sample was analyzed by ^{1}H, ^{13}C, ^{19}F and ^{11}B NMR measurements. Then, the Hantzsch ester **2** (7.6 mg, 0.030 mmol) was added to the sample in the glove box. The resulting solution was immediately analyzed by ^{1}H NMR (< 10 min) to determine the formation of tris[3,5-bis(trifluoromethyl)phenyl]borane-benzyl alcohol adduct **Int-IIIa**. Mesitylene (3.5 mg) was added to the solution as an internal standard. The yield of **Int-IIIa** was confirmed by ^{1}H NMR to be 90%. GC-MS analysis of the reaction mixture showed the formation of benzyl alcohol [**3**, *m/z* = 108 ($[M]^+$)].

Int-Ia: ^{1}H NMR (396 MHz, CD_2Cl_2): δ 9.17 (s, 1H, C*H*O), 8.25 (d, *J* = 8.1 Hz, 2H), 8.08 (t, *J* = 7.5 Hz, 1H), 7.99 (br s, 3H), 7.86 (br s, 6H), 7.79 (virt t, *J* = 7.5 and 8.1 Hz, 2H). ^{13}C NMR (100 MHz, CD_2Cl_2) δ 200.2 (CHO), 147.0 (br), 142.5, 135.4, 135.3, 131.4 (q, $J_{C\text{-}F}$ = 32.6 Hz), 131.1, 123.9 (q, $J_{C\text{-}F}$ = 274 Hz), 123.84, 123.78. ^{19}F NMR (373 MHz, CD_2Cl_2): δ –65.0. ^{11}B NMR (127 MHz, CD_2Cl_2): δ 36.0 (br). ESI-MS: *m/z* 779 ($[M + Na]^+$).

4. Stoichiometric Reaction of Tris[3,5-bis(trifluoromethyl)phenyl]borane and Hantzsch Ester

In a glove box, the Hantzsch ester (**2**; 7.6 mg, 0.030 mmol) was added to a solution of tris[3,5-bis(trifluoromethyl)phenyl]borane (**B-a**, 19.5 mg, 0.030 mmol) in 0.75 mL of CD_2Cl_2 in a J-Young NMR tube at 25 ºC. The resulting sample was analyzed by ^{1}H and ^{11}B NMR measurements. In the ^{1}H NMR spectrum, the characteristic signals derived from N-H and B-H protons were not detected (Figure S1a). In addition, a sharp doublet peak derived from B-H was not observed in the ^{11}B NMR spectrum (Figure S1b). Thus, **IntIVa** was not formed in this reaction.

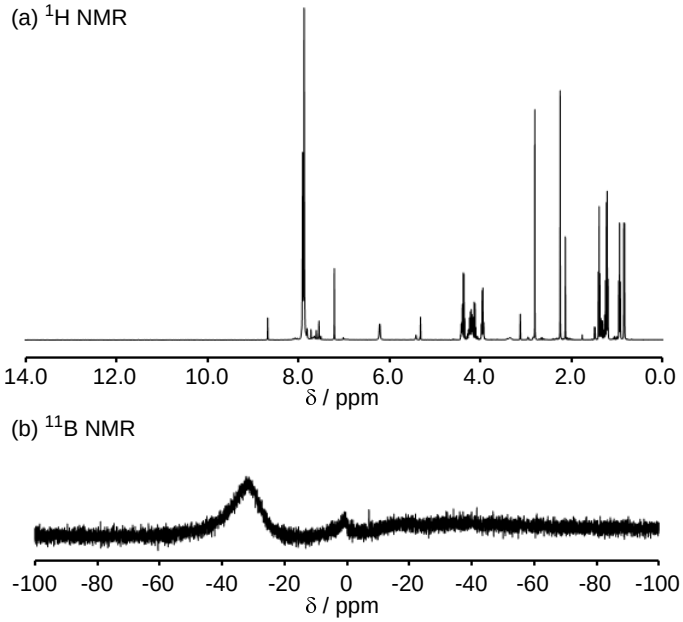


Figure S1. ^{1}H and ^{11}B NMR spectra in the reaction of **B-a** and **2**

5. Determination of Association Constants between Boron Reagents with Benzaldehyde or Benzyl Alcohol

5-1. Typical Procedure

In a glove box, benzaldehyde (**1**; 3.2 mg, 0.030 mmol) was added to a solution of tris[3,5-bis(trifluoromethyl)phenyl]borane (**B-a**; 19.5 mg, 0.030 mmol) in 0.75 mL of CD_2Cl_2 in a J-Young NMR tube at 25 ºC. The resulting sample was analyzed by ^{1}H NMR measurements at variable temperature. The obtained integration values of **Int-Ia** and benzaldehyde (**1**) were used to draw the van't Hoff plots and calculated the association constant and Gibbs free energy value at 25 °C.

5-2. The Reaction of Tris[3,5-bis(trifluoromethyl)phenyl]borane with Benzaldehyde

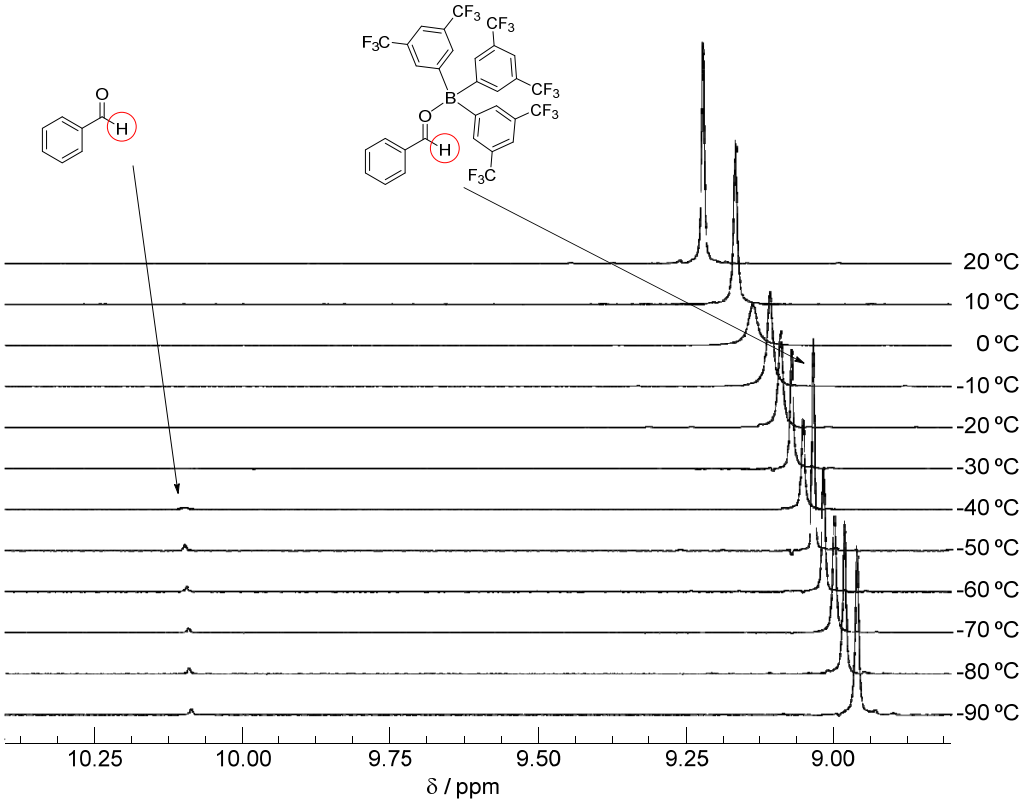


Figure S2. VT ^{1}H NMR spectra of a mixture of tris[3,5-bis(trifluoromethyl)phenyl]borane (**B-a**, 0.030 mmol) and benzaldehyde (**1**, 0.030 mmol) in CD_2Cl_2 (0.75 mL). Integration ratio of **Int-Ia**:benzaldehyde; 24.19:1.00 (–40 °C), 27.03:1.00 (–50 °C), 29.83:1 (–60 °C), 32.56:1.00 (–70 °C), 34.22:1.00 (–80 °C), 35.16:1.00 (–90 °C).

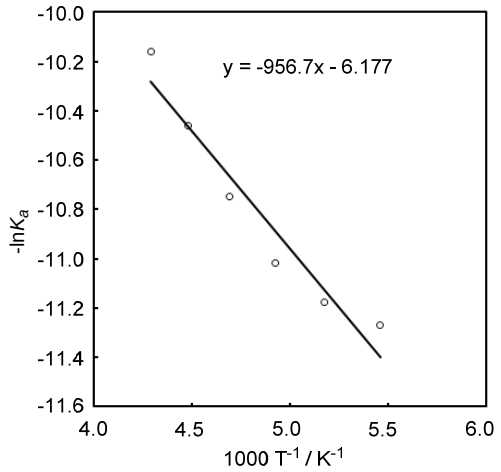


Figure S3. van't Hoff plot for a mixture of tris[3,5-bis(trifluoromethyl)phenyl]borane (**B-a**) and benzaldehyde (**1**) (–40 °C to –90 °C)

The association constant and Gibbs free energy at 25 °C were calculated to be 1.19×10^4 M^{-1} and –5.6 kcal·mol^{-1}, respectively.

5-3. The Reaction of Tris[3,5-bis(trifluoromethyl)phenyl]borane with Benzyl Alcohol

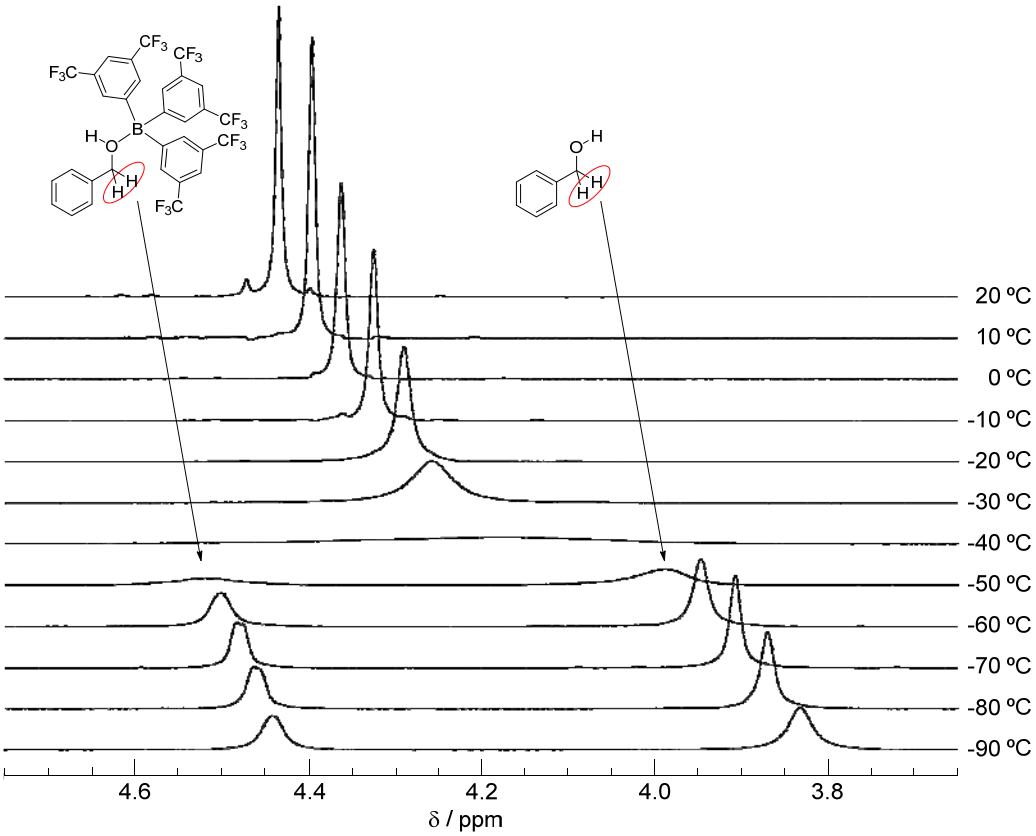


Figure S4. VT ^{1}H NMR spectra of a mixture of tris[3,5-bis(trifluoromethyl)phenyl]borane (**B-a**, 0.015 mmol) and benzyl alcohol (**3**, 0.030 mmol) in CD_2Cl_2 (0.75 mL). Integration ratio of **Int-IIIa**:benzyl alcohol; 2.00:3.17 (–60 °C), 2.00:3.11 (–70 °C), 2.00:3.55 (–80 °C), 2.00:2.97 (–90 °C).

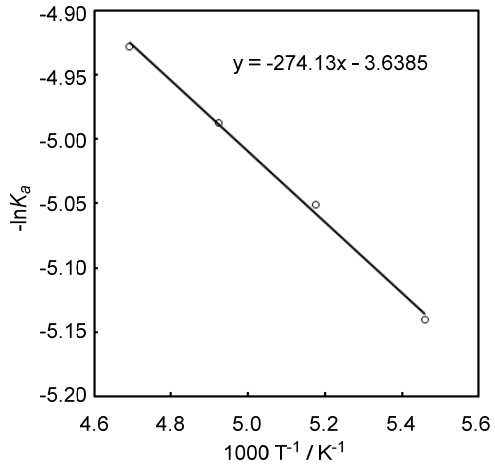


Figure S5. van't Hoff plot for a mixture of tris[3,5-bis(trifluoromethyl)phenyl]borane (**B-a**) and benzyl aocohol (**3**) (–60 °C to –90 °C)

The association constant and Gibbs free energy at 25 °C were calculated to be 95.4 M^{-1} and –2.7 kcal/·mol^{-1}, respectively.

5-4. The Reaction of Tris(pentafluorophenyl)borane with Benzaldehyde

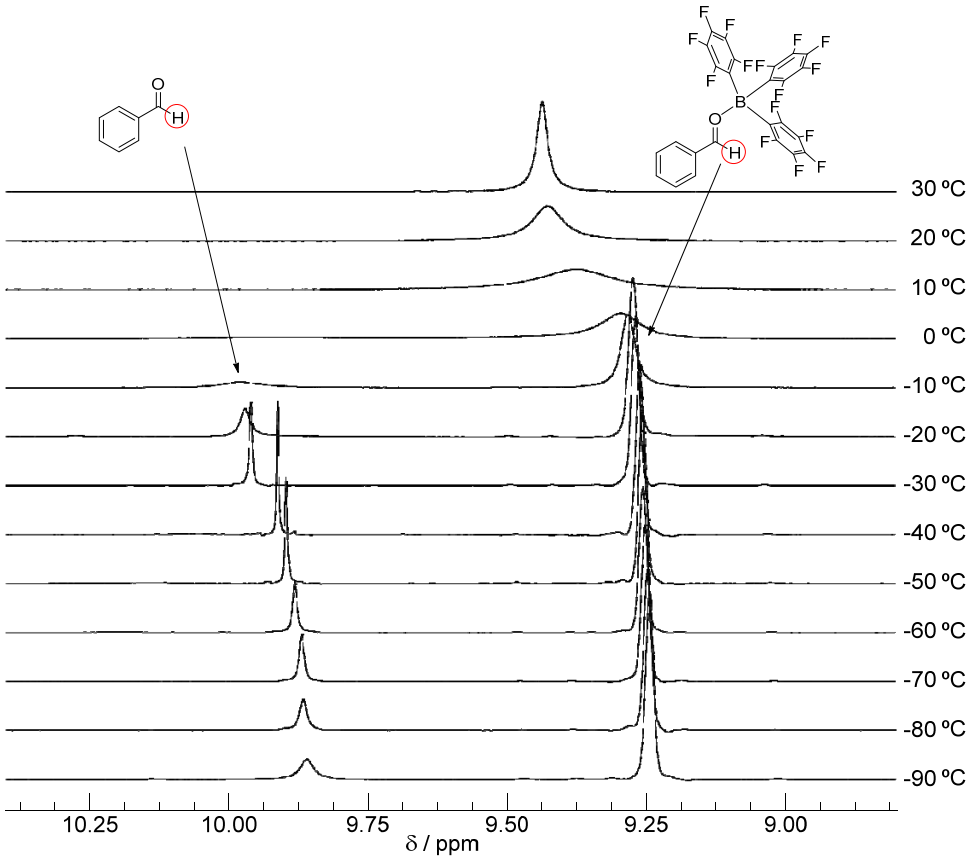


Figure S6. VT ^{1}H NMR spectra in a mixture of tris(pentafluorophenyl)borane (**B-b**, 0.031 mmol) and benzaldehyde (**1**, 0.030 mmol) in CD_2Cl_2 (0.75 mL). Integration ratio of **Int-Ib**:benzaldehyde; 4.05:1.00 (–50 °C), 4.24:1.00 (–60 °C), 4.16:1.00 (–70 °C), 4.30:1.00 (–80 °C), 4.48:1.00 (–90 °C).

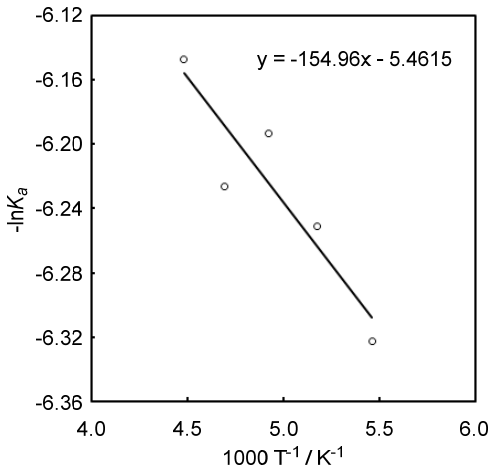


Figure S7. van't Hoff plot for a mixture of tris(pentafluorophenyl)borane (**B-b**) and benzaldehyde (**1**) (–50 °C to –90 °C)

The association constant and Gibbs free energy at 25 °C were calculated to be 396 and –3.5 kcal·mol^{-1}, respectively.

5-5. The Reaction of Tris(pentafluorophenyl)borane with Benzyl Alcohol

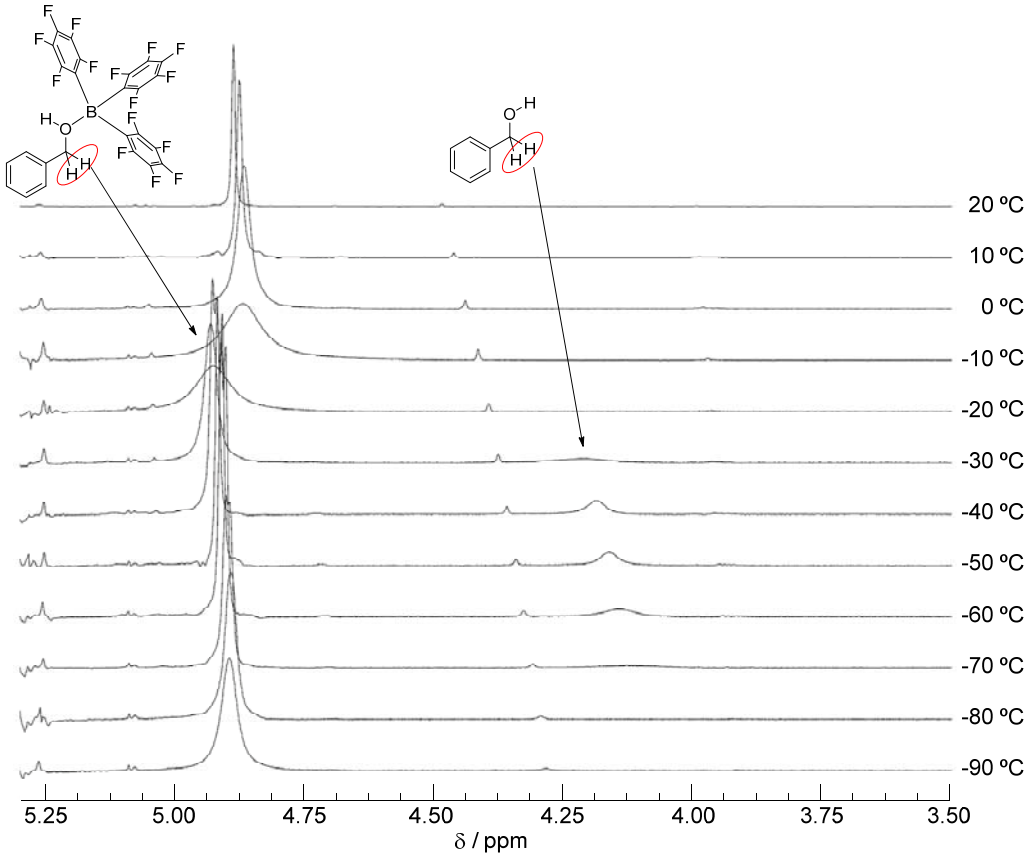


Figure S8. VT ^{1}H NMR spectra in a mixture of tris(pentafluorophenyl)borane (**B-b**, 0.030 mmol) and benzyl alcohol (**3**, 0.030 mmol) in CD_2Cl_2 (0.75 mL). Integration ratio of **Int-IIIb**:benzyl alcohol; 2.00:0.30 (–50 °C), 2.00:0.23 (–60 °C), 2.00:0.16 (–70 °C).

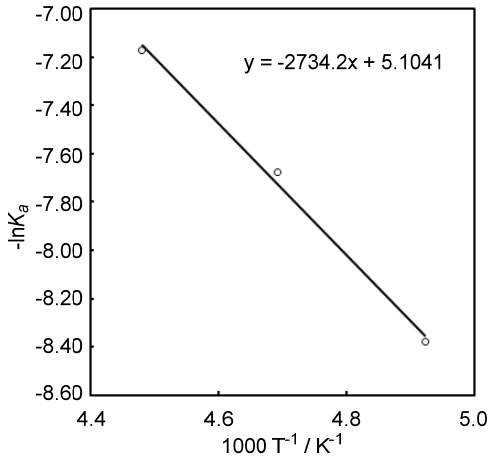


Figure S9. van't Hoff plot for a mixture of tris(pentafluorophenyl)borane (**B-b**) with benzyl alcohol (**3**) (–50 °C to –70 °C)

The association constant and Gibbs free energy at 25 °C were calculated to be 58.3 and –2.4 kcal·mol^{-1}, respectively.

5-6. The Raction of Trifluoroborane Etherate with Benzaldehyde

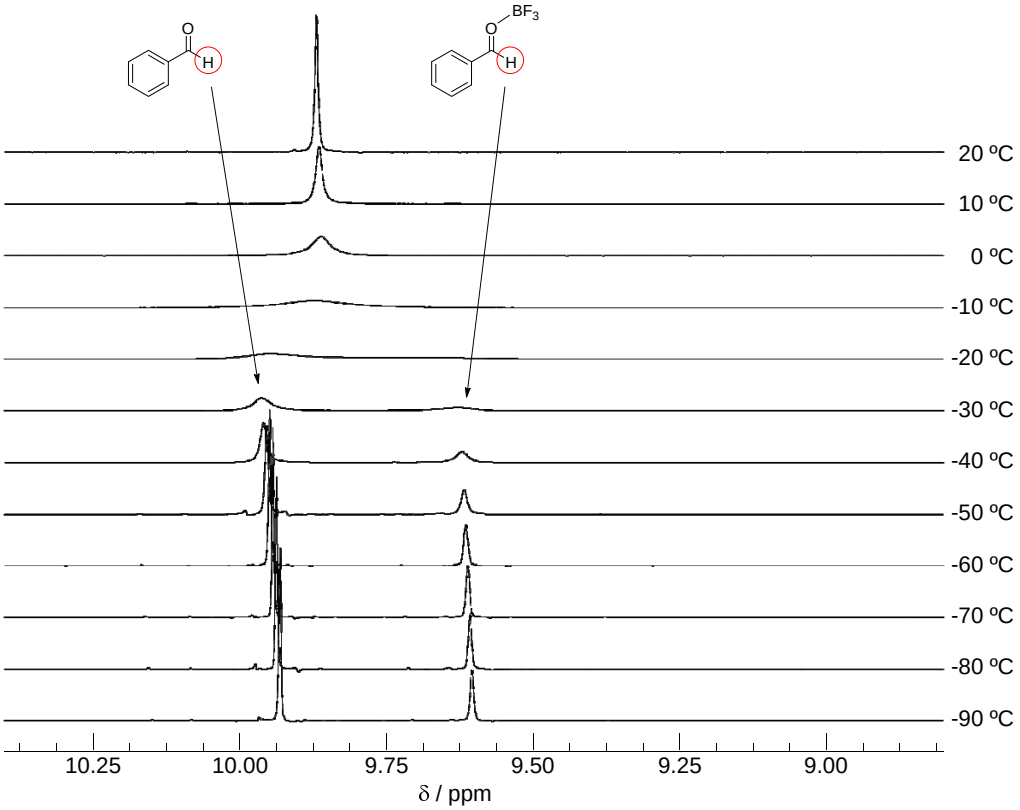


Figure S10. VT ^{1}H NMR spectra in a mixture of trifluoroborane etherate (**B-c**, 0.060 mmol) and benzaldehyde (**1**, 0.031 mmol) in CD_2Cl_2 (0.75 mL). Integration ratio of **Int-IIIc**:benzaldehyde: 0.43:1.00 (–40 °C), 0.45:1.00 (–50 °C), 0.46:1.00 (–60 °C), 0.48:1.00 (–70 °C), 0.49:1.00 (–80 °C), 0.51:1.00 (–90 °C).

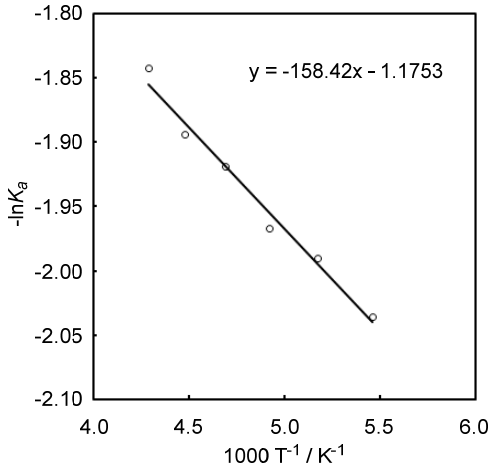


Figure S11. van't Hoff plot for a mixture of $BF_3{\cdot}OEt_2$ (**B-c**) and benzaldehyde (**1**) (–40 °C to –90 °C)

The association constant and Gibbs free energy at 25 °C were calculated to be 5.51 and –1.0 kcal·mol^{-1}, respectively.

5-7. The Reaction of Trifluoroborane Etherate with Benzyl Alcohol

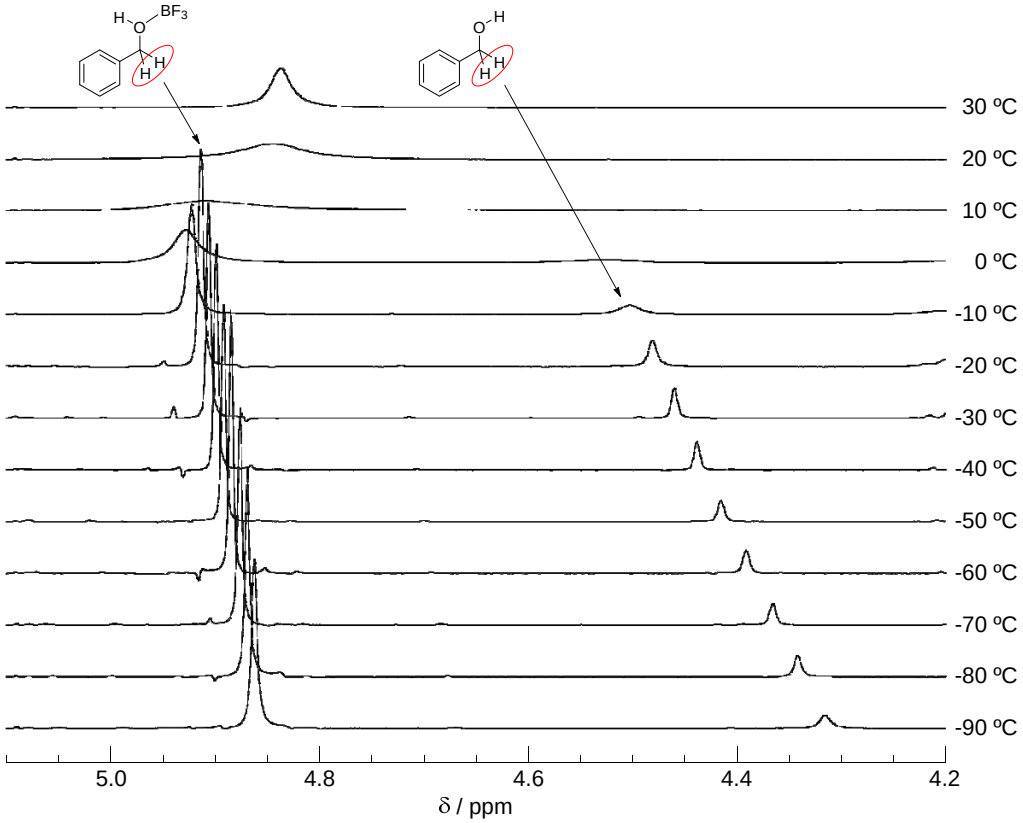


Figure S12. VT ^{1}H NMR spectra in a mixture of trifluoroborane etherate (**B-c**, 0.034 mmol) and benzyl alcohol (**3**, 0.032 mmol) in CD_2Cl_2 (0.75 mL). Integration ratio of **Int-IIIc**:benzyl alcohol: 1.82:0.43 (–10 °C), 1.78:0.37 (–20 °C), 1.75:0.33 (–30 °C), 1.68:0.29 (–40 °C), 1.71:0.26 (–50 °C), 1.66:0.23 (–60 °C).

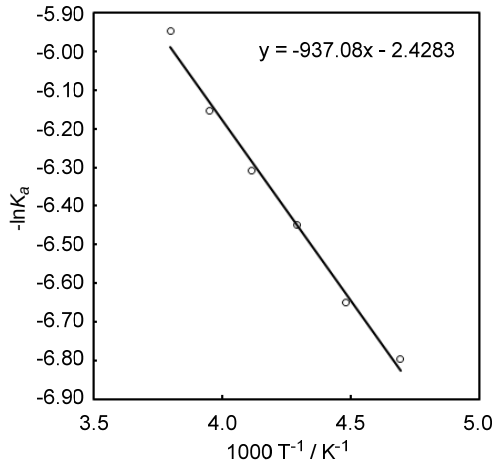


Figure S13. van't Hoff plot for a mixture of $BF_3{\cdot}OEt_2$ (**B-c**) and benzyl alcohol (**3**)

The association constant and Gibbs free energy at 25 °C were calculated to be 263 and –3.3 kcal·mol^{-1}, respectively.

5-8. The Reaction of Triphenylborane with Benzaldehyde

In the VT ^{1}H NMR measurements of the mixture of triphenylborane (**B-d**) and benzaldehyde (**1**), the peaks of aldehyde functionality derived from triphenylborane-benzaldehyde adduct (**Int-Id**) and benzaldehyde (**1**) were not observed independently (Figure S13). Only higher field shifts of the peak were observed below –70 °C. The observed chemical shifts of CHO may be used to calculate an association constant (K_a), by using following equation;[3]

$$K_a = \frac{\delta_{obs}}{(\delta_{adduct} - \delta_{obs})\left([BPh_3{}^0] - \frac{\Delta\delta_{obs} \times [PhCHO^0]}{\Delta\delta_{adduct}}\right)} \quad (1)$$

$$\Delta\delta_{obs} = \delta_{obs} - \delta_{PhCHO}$$

$$\Delta\delta_{adduct} = \delta_{adduct} - \delta_{PhCHO}$$

where δ_{obs} is observed chemical shift value of the 1:1 mixture of BPh_3 and PhCHO, δ_{PhCHO} is observed chemical shift value of PhCHO (Figure S14), δ_{adduct} is chemical shift value of BPh_3-PhCHO adduct, [$BPh_3{}^0$] is initial concentration of BPh_3, and [$PhCHO^0$] is initial concentration of PhCHO. The observed chemical shift value of the 50:1 mixture of BPh_3 and PhCHO (Figure S15) can be used as that of BPh_3-PhCHO adduct (**Int-Id**), because no change in this value was observed upon further addition of BPh_3. The obtained data are summarized in Table S1.

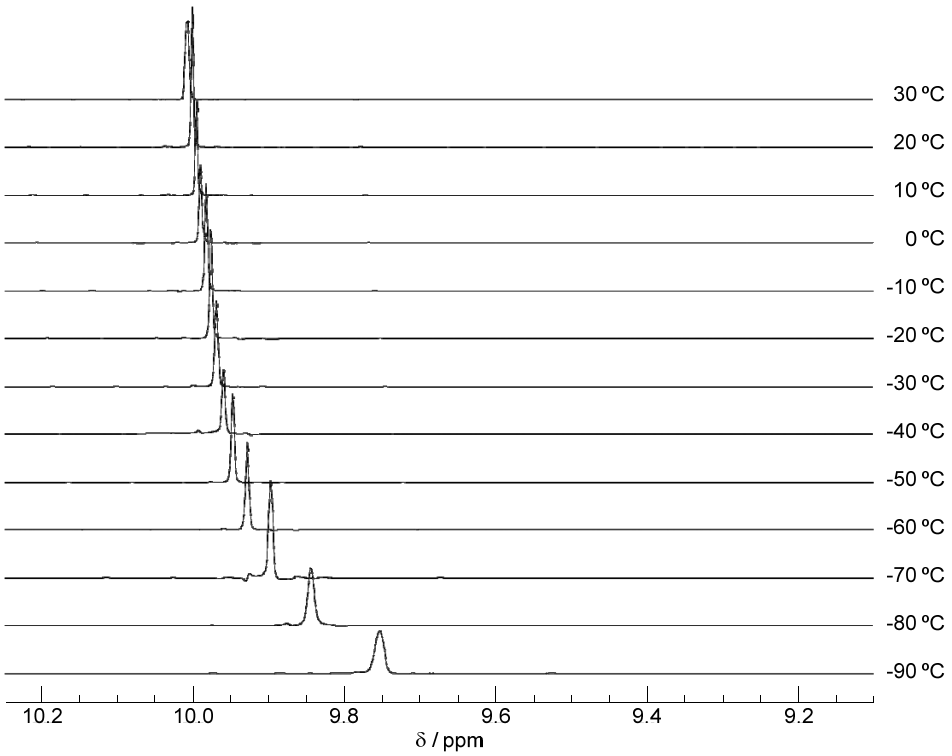


Figure S14. VT ^{1}H NMR spectra of a mixture of triphenylborane (**B-d**) and benzaldehyde (**1**) (1:1) in CD_2Cl_2 (0.75 mL).

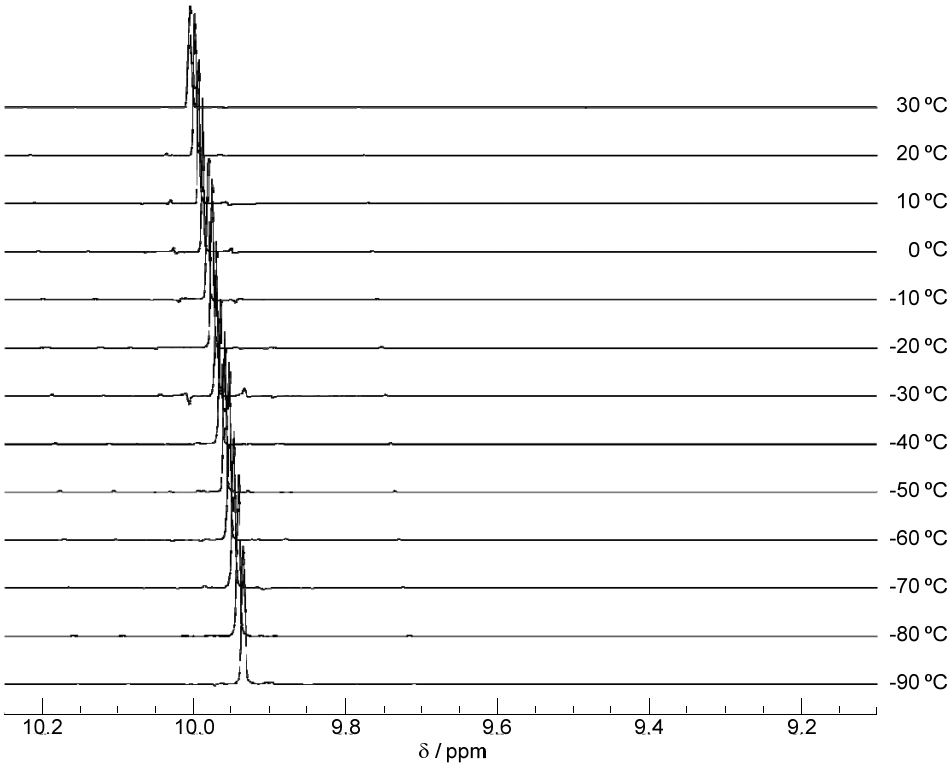


Figure S15. VT ^{1}H NMR spectra of benzaldehyde (**1**) in CD_2Cl_2.

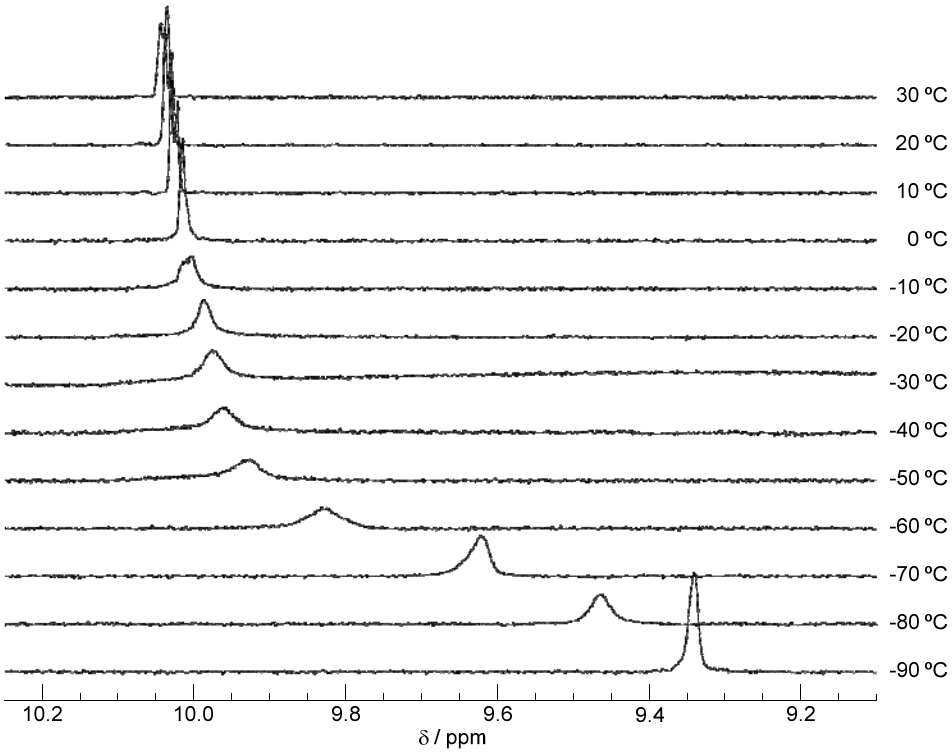


Figure S16. VT ^{1}H NMR spectra of a mixture of triphenylborane (**B-d**) and benzaldehyde (**1**) (50:1) in CD_2Cl_2 (0.75 mL).

Table S1. Summary of proton resonances at aldehyde functionality

	–70 °C	–80 °C	–90 °C
δ_{obs}	9.898	9.845	9.753
δ_{PhCHO}	9.947	9.941	9.935
δ_{adduct}	9.622	9.463	9.339
K_a	5.27	7.94	16.0

The association constant of BPh_3 and benzaldehyde at 25 °C was calculated by using van't Hoff plot (Figure S16) to be 0.195 (ΔG = 0.97 kcal·mol^{-1}).

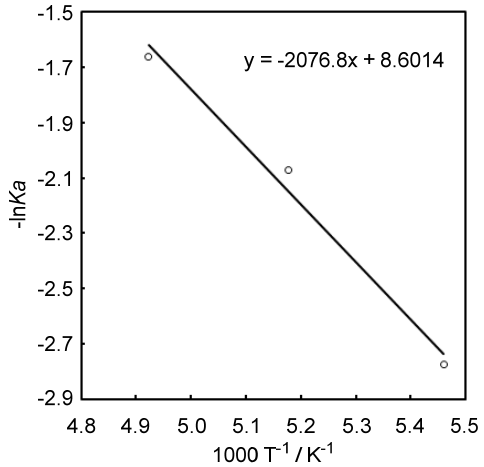


Figure S17. van't Hoff plot for a mixture of triphenylborane (**B-d**) with benzaldehyde (**1**) (–70 °C to –90 °C)

5-9. The Reaction of Triphenylborane with Benzyl Alcohol

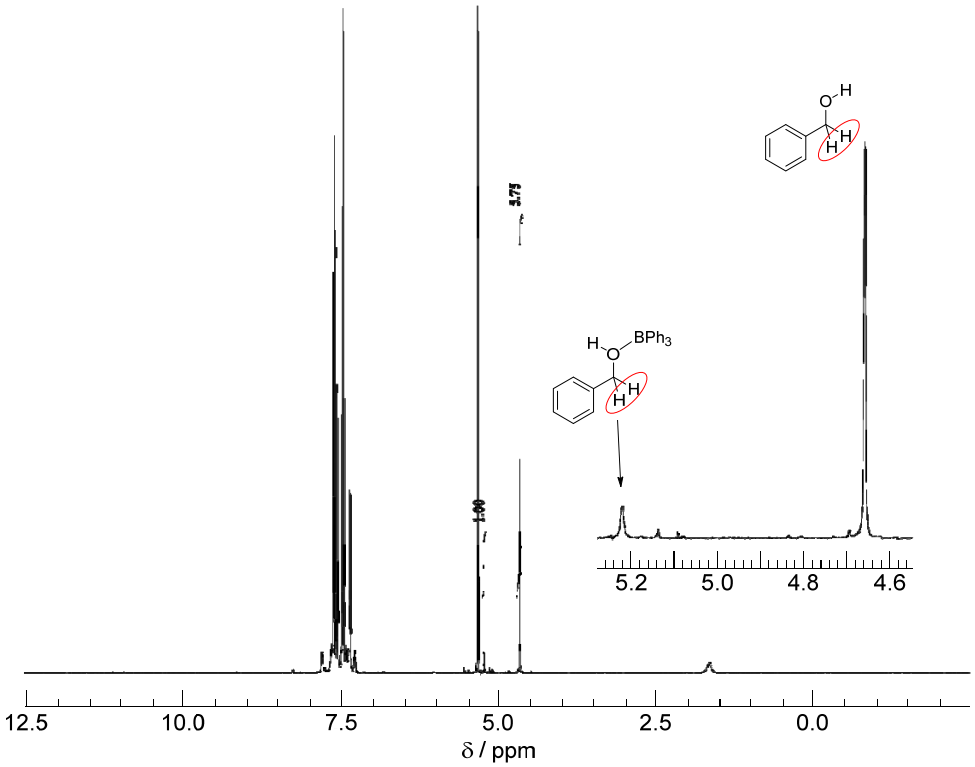


Figure S18. ^{1}H NMR spectrum at 25 ºC in a mixture of triphenylborane (**B-d**, 0.030 mmol) and benzyl alcohol (**3**, 0.030 mmol) in CD_2Cl_2 (0.75 mL): $K_a = 5.67 \times 10^{-3}$, $\Delta G = 3.1$ kcal·mol^{-1}.

Table S2. Summary of the association constants (K_a) and Gibbs free energy (ΔG) values for the reaction of borane reagents (**B-a** to **B-d**) with benzaldehyde (**1**) or benzyl alcohol (**3**), as estimated by ^{1}H NMR measurements

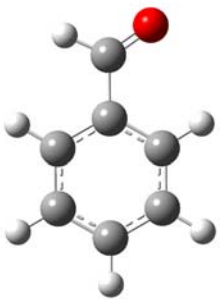
	Benzaldehyde (**1**)		Benzyl alcohol (**3**)	
	K_a, M^{-1}	ΔG, kcal·mol^{-1}	K_a, M^{-1}	ΔG, kcal·mol^{-1}
$B[3,5\text{-}(CF_3)_2C_6H_3]_3$	1.19×10^4	–5.6	95.4	–2.7
$B(C_6F_5)_3$	396	–3.5	58.3	–2.4
$BF_3 \cdot OEt_2$	5.51	–1.0	263	–3.3
BPh_3	0.195	1.0	5.67×10^{-3}	3.1

6. Computational Procedure

All calculations were carried out with the *Gaussian09* (Revision E.01) program.[4] Geometry optimizations and frequency calculations for all molecules were performed at the M06-2x[5] level of theory and with the basis sets 6-31G(d,p) for C and H and 6-31+G(d,p) for B, N, O, and F. Single -point energies were obtained by calculations at M06-2x/6-311++G(d,p) level of theory using the SMD[6] solvation model (1,4-dioxane). The computations were performed using Research Center for Computational Science, Okazaki, Japan.

Cartesian Coordinates

Benzaldehyde (**1**)

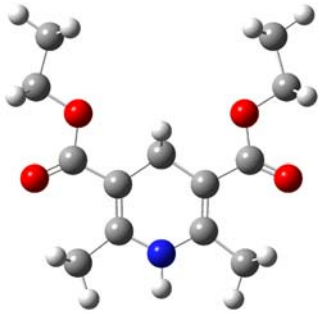


Zero-point correction = 0.111159 (Hartree/Particle)
Thermal correction to Energy = 0.117451
Thermal correction to Enthalpy = 0.118395
Thermal correction to Gibbs Free Energy = 0.080604
Sum of electronic and zero-point Energies = -345.317519
Sum of electronic and thermal Energies = -345.311227
Sum of electronic and thermal Enthalpies = -345.310283
Sum of electronic and thermal Free Energies = -345.348074

Single point energy = -345.5233977

C	1.72875700	1.06039200	0.00000000
C	2.20928300	−0.24688600	−0.00000100
C	1.32422900	−1.32718500	0.00000000
C	−0.04519100	−1.10149700	0.00000300
C	−0.52896800	0.21012500	0.00000300
C	0.35625900	1.28823300	0.00000200
C	−1.98721200	0.46883000	0.00001200
O	−2.83546900	−0.39522900	−0.00001400
H	2.42099300	1.89554400	0.00000000
H	3.27955200	−0.42743900	−0.00000300
H	1.70854900	−2.34175100	0.00000000
H	−0.75824900	−1.91987400	0.00000400
H	−0.03426700	2.30306100	0.00000400
H	−2.27576800	1.54021300	−0.00001000

Hantzsch ester (**2**)



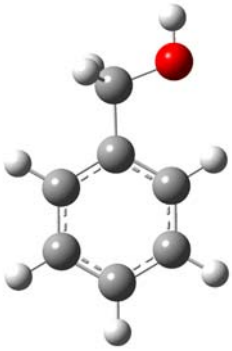
Zero-point correction = 0.313894 (Hartree/Particle)
Thermal correction to Energy = 0.333417
Thermal correction to Enthalpy = 0.334361
Thermal correction to Gibbs Free Energy = 0.264486
Sum of electronic and zero-point Energies = -861.849552
Sum of electronic and thermal Energies = -861.830029
Sum of electronic and thermal Enthalpies = -861.829085
Sum of electronic and thermal Free Energies = -861.898960

Single point energy = -862.3965672

C	−1.25607600	−0.72238300	0.00003900
C	−1.22194400	−2.07608700	−0.00011500
N	−0.00000500	−2.72533800	−0.00010100
C	1.22194400	−2.07611200	0.00003300
C	1.25614300	−0.72239900	0.00020300
C	0.00001600	0.12490700	0.00026500
C	−2.41059000	−2.99708800	−0.00031800
C	2.41055500	−2.99717200	−0.00002600
C	2.55367200	−0.03668900	0.00034600
O	2.39829400	1.30505500	0.00011500
O	3.65699800	−0.55425500	0.00003700
C	3.61090900	2.06876600	−0.00014400
C	3.22230600	3.53070500	−0.00042100
C	−2.55363400	−0.03672800	0.00000400
O	−2.39829500	1.30508400	0.00015900
O	−3.65692400	−0.55435500	−0.00022600
C	−3.61094000	2.06872200	0.00009000
C	−3.22238800	3.53067900	0.00028200
H	0.00002500	−3.73264500	−0.00015700
H	0.00000600	0.79709000	0.86767600
H	0.00011900	0.79738200	−0.86691800
H	−3.03955900	−2.81540200	0.87228200
H	−3.03936200	−2.81526300	−0.87303400
H	−2.08596700	−4.04115500	−0.00036600
H	3.03945000	−2.81536000	−0.87264700
H	3.03936100	−2.81558700	0.87270600
H	2.08588100	−4.04123900	−0.00018100
H	4.19808900	1.79845100	0.88233800
H	4.19795300	1.79807800	−0.88260200

H	4.11964700	4.15414500	−0.00061100
H	2.63132300	3.77266700	−0.88665200
H	2.63144500	3.77303200	0.88579200
H	−4.19794700	1.79829400	−0.88247400
H	−4.19815800	1.79811800	0.88245900
H	−4.11974700	4.15409000	0.00023500
H	−2.63157700	3.77276600	0.88659600
H	−2.63136000	3.77294200	−0.88584000

Benzyl alcohol (**3**)

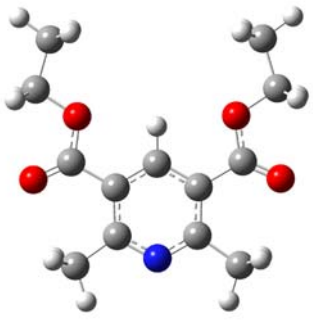


Zero-point correction = 0.134888 (Hartree/Particle)
Thermal correction to Energy = 0.141864
Thermal correction to Enthalpy = 0.142808
Thermal correction to Gibbs Free Energy = 0.103402
Sum of electronic and zero-point Energies = -346.494382
Sum of electronic and thermal Energies = -346.487405
Sum of electronic and thermal Enthalpies = -346.486461
Sum of electronic and thermal Free Energies = -346.525867

Single point energy = -346.7257841

C	1.87420200	−0.99966000	0.02638600
C	0.51637500	−1.29630600	0.01011100
C	−0.43311900	−0.27300200	−0.02273000
C	−0.00812000	1.05311200	−0.03407900
C	1.35383900	1.34984900	−0.01467800
C	2.29711400	0.32836800	0.01394300
H	2.60260800	−1.80407700	0.05320800
H	0.18800900	−2.33342500	0.02472300
H	−0.74887900	1.84432600	−0.05432700
H	1.67717000	2.38616300	−0.02178600
H	3.35672800	0.56254900	0.02905700
C	−1.89853500	−0.63031500	−0.06299600
H	−2.11469000	−1.35447200	0.73521500
H	−2.12274100	−1.11760000	−1.02312800
O	−2.67988200	0.53897700	0.09502200
H	−3.60968900	0.31244400	0.00111400

Hantzsch pyridine (**4**)

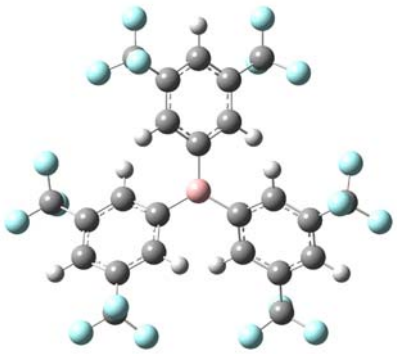


Zero-point correction = 0.290285 (Hartree/Particle)
Thermal correction to Energy = 0.309054
Thermal correction to Enthalpy = 0.309998
Thermal correction to Gibbs Free Energy = 0.241123
Sum of electronic and zero-point Energies = -860.688283
Sum of electronic and thermal Energies = -860.669514
Sum of electronic and thermal Enthalpies = -860.668569
Sum of electronic and thermal Free Energies = -860.737444

Single point energy = -861.2064701

O	−3.59613500	−0.53034200	−0.00051100
O	−2.31278000	1.30694900	0.00019900
O	3.59614000	−0.53031600	0.00001000
O	2.31276300	1.30696900	0.00014400
N	0.00001800	−2.83480200	0.00004500
C	−1.16594300	−2.17880900	0.00006200
C	−1.20620700	−0.76933200	0.00003800
C	0.00000300	−0.07711300	0.00007100
H	−0.00000200	1.00591600	0.00007500
C	1.20621800	−0.76932100	0.00007300
C	1.16597100	−2.17879700	0.00003200
C	−2.39260000	−3.04581600	0.00009300
H	−3.01638200	−2.83896600	−0.87266000
H	−3.01685200	−2.83836100	0.87234300
H	−2.07644500	−4.08803500	0.00048900
C	2.39264100	−3.04578700	−0.00003600
H	2.07650100	−4.08801000	−0.00004200
H	3.01670300	−2.83864000	0.87243000
H	3.01660600	−2.83861600	−0.87257600
C	−2.49558400	−0.02463800	−0.00011300
C	−3.51276800	2.09756000	−0.00006500
C	2.49558500	−0.02461600	0.00007000
C	3.51273700	2.09760000	0.00003000
H	4.10221700	1.83626900	−0.88316900
H	4.10211300	1.83669000	0.88343000
C	3.09372100	3.55038500	−0.00033100
H	2.49995400	3.78135500	−0.88758900
H	3.97913800	4.19029700	−0.00007200
H	2.49928100	3.78157500	0.88642100
C	−3.09376700	3.55035900	0.00028700
H	−2.49998400	3.78130700	0.88754800
H	−3.97919500	4.19025600	0.00009300
H	−2.49935800	3.78157000	−0.88646300
H	−4.10246600	1.83630700	0.88301100
H	−4.10190600	1.83656400	−0.88359500

B[3,5-$(CF_3)_2C_6H_3]_3$ (**B-a**)



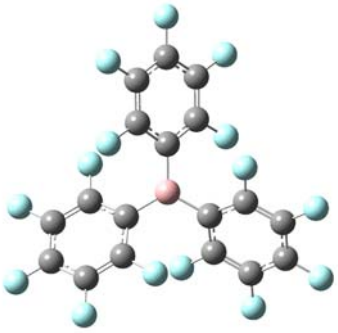
Zero-point correction = 0.309173 (Hartree/Particle)
Thermal correction to Energy = 0.346448
Thermal correction to Enthalpy = 0.347392
Thermal correction to Gibbs Free Energy = 0.227860
Sum of electronic and zero-point Energies = -2740.929771
Sum of electronic and thermal Energies = -2740.892496
Sum of electronic and thermal Enthalpies = -2740.891552

Sum of electronic and thermal Free Energies = -2741.011084

Single point energy = -2742.0007947

B	0.00000000	0.00000000	0.00000000
C	0.00000000	1.56612700	0.00000000
C	-1.02105100	2.29444700	0.63157300
C	1.02105100	2.29444700	-0.63157300
C	-1.01125400	3.68566000	0.63898000
H	-1.83106800	1.77096400	1.13347300
C	1.01125400	3.68566000	-0.63898000
H	1.83106800	1.77096400	-1.13347300
C	0.00000000	4.39556000	0.00000000
H	0.00000000	5.47981500	0.00000000
C	1.35630600	-0.78306300	0.00000000
C	1.47652400	-2.03148000	-0.63157300
C	2.49757500	-0.26296700	0.63157300
C	2.68624800	-2.71860200	-0.63898000
H	0.61816600	-2.47123300	-1.13347300
C	3.69750200	-0.96705800	0.63898000
H	2.44923400	0.70026900	1.13347300
C	3.80666700	-2.19778000	0.00000000
H	4.74565900	-2.73990700	0.00000000
C	-1.35630600	-0.78306300	0.00000000
C	-1.47652400	-2.03148000	0.63157300
C	-2.49757500	-0.26296700	-0.63157300
C	-2.68624800	-2.71860200	0.63898000
H	-0.61816600	-2.47123300	1.13347300
C	-3.69750200	-0.96705800	-0.63898000
H	-2.44923400	0.70026900	-1.13347300
C	-3.80666700	-2.19778000	0.00000000
H	-4.74565900	-2.73990700	0.00000000
C	2.10929300	4.40927200	-1.37150900
C	2.76389500	-4.03133800	-1.37150900
C	-4.87318900	-0.37793500	-1.37150900
C	-2.10929300	4.40927200	1.37150900
C	4.87318900	-0.37793500	1.37150900
C	-2.76389500	-4.03133800	1.37150900
F	-6.01534900	-1.02251000	-1.09596000
F	2.12215500	5.72070000	-1.09596000
F	3.89319400	-4.69819000	-1.09596000
F	-4.69528100	-0.42977700	-2.70360800
F	1.97544300	4.28112100	-2.70360800
F	2.71983800	-3.85134400	-2.70360800
F	1.73159300	-4.83055800	-1.05509000
F	3.31758900	3.91488300	-1.05509000
F	-5.04918200	0.91567500	-1.05509000
F	5.04918200	0.91567500	1.05509000
F	-3.31758900	3.91488300	1.05509000
F	-1.73159300	-4.83055800	1.05509000
F	4.69528100	-0.42977700	2.70360800
F	-1.97544300	4.28112100	2.70360800
F	-2.71983800	-3.85134400	2.70360800
F	6.01534900	-1.02251000	1.09596000
F	-2.12215500	5.72070000	1.09596000
F	-3.89319400	-4.69819000	1.09596000

$B(C_6F_5)_3$ (**B-b**)

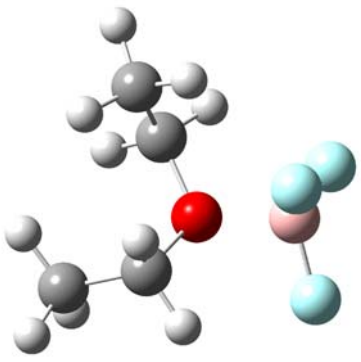


Zero-point correction = 0.158155 (Hartree/Particle)
Thermal correction to Energy = 0.186451
Thermal correction to Enthalpy = 0.187395
Thermal correction to Gibbs Free Energy = 0.099302
Sum of electronic and zero-point Energies = -2207.434484
Sum of electronic and thermal Energies = -2207.406187
Sum of electronic and thermal Enthalpies = -2207.405243
Sum of electronic and thermal Free Energies = -2207.493337

Single point energy = -2208.2126622

B	0.00000000	0.00000000	0.00215900
C	0.00043300	1.56718900	0.00173100
C	-0.98537900	2.31488500	0.65397200
C	0.98615900	2.31374200	-0.65190300
C	0.00000000	4.39484400	-0.00117800
C	1.35700900	-0.78397000	0.00173100
C	1.51068000	-2.01091000	-0.65190300
C	2.49743900	-0.30407900	0.65397200
C	3.80604700	-2.19742200	-0.00117800
C	-1.35744200	-0.78322000	0.00173100
C	-1.51206000	-2.01080600	0.65397200
C	-2.49683900	-0.30283200	-0.65190300
C	-3.80604700	-2.19742200	-0.00117800
C	0.99758600	3.69917800	-0.67212800
C	-0.99717600	3.70034500	0.67137600
C	3.70318100	-0.98659300	0.67137600
C	2.70478900	-2.71352400	-0.67212800
C	-2.70600500	-2.71375200	0.67137600
C	-3.70237500	-0.98565400	-0.67212800
F	-0.00028700	5.71916000	-0.00263300
F	1.94967100	4.36484700	-1.31875700
F	1.96929100	1.69697200	-1.31461500
F	-1.96844100	1.69922000	1.31769300
F	-1.94968300	4.36683800	1.31666500
F	2.45578800	0.85511000	1.31769300
F	4.75663400	-0.49494400	1.31666500
F	4.95308100	-2.85933100	-0.00263300
F	2.80523300	-3.87088800	-1.31875700
F	0.48497500	-2.55394200	-1.31461500
F	-0.48734700	-2.55433000	1.31769300
F	-2.80695100	-3.87189400	1.31666500
F	-4.95279400	-2.85982900	-0.00263300
F	-4.75490400	-0.49395900	-1.31875700
F	-2.45426600	0.85697000	-1.31461500

$BF_3{\cdot}OEt_2$ (**B-c**)

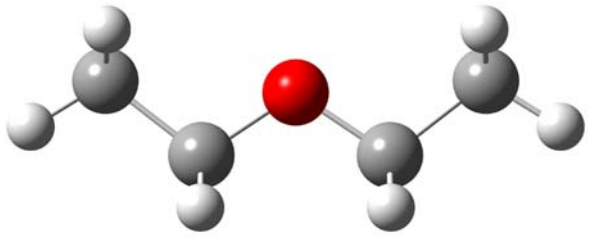


Zero-point correction = 0.154519 (Hartree/Particle)
Thermal correction to Energy = 0.164857
Thermal correction to Enthalpy = 0.165801
Thermal correction to Gibbs Free Energy = 0.118746
Sum of electronic and zero-point Energies = -557.896766
Sum of electronic and thermal Energies = -557.886428
Sum of electronic and thermal Enthalpies = -557.885484
Sum of electronic and thermal Free Energies = -557.932539

Single point energy = -558.2106606

O	−0.25779300	0.15749600	0.39457600
C	−0.83132100	−1.13539200	0.73434400
H	−0.04887300	−1.62470200	1.31156000
H	−1.67894100	−0.93181100	1.39230100
C	−1.07307800	1.02548400	−0.43867800
H	−0.47881900	1.93390300	−0.52763800
H	−1.16322400	0.56317200	−1.42552400
C	−2.41585400	1.30418700	0.20135200
H	−2.92293400	2.07864000	−0.37866800
H	−3.06371800	0.42427100	0.21575000
H	−2.28745700	1.67081700	1.22271000
C	−1.22593600	−1.94939500	−0.48241400
H	−0.38187500	−2.05164000	−1.16745700
H	−1.52895200	−2.94459500	−0.14808400
H	−2.07018600	−1.50792600	−1.01867000
B	1.32608500	0.17356500	−0.01113900
F	1.66577500	1.49079600	0.10108900
F	1.35434400	−0.30081400	−1.30026300
F	1.90588500	−0.65745200	0.90308300

Et_2O

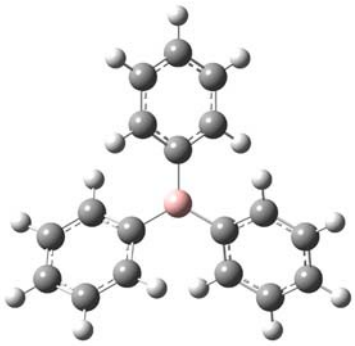


Zero-point correction = 0.138391 (Hartree/Particle)
Thermal correction to Energy = 0.145157
Thermal correction to Enthalpy = 0.146101
Thermal correction to Gibbs Free Energy = 0.108354
Sum of electronic and zero-point Energies = -233.412688
Sum of electronic and thermal Energies = -233.405922
Sum of electronic and thermal Enthalpies = -233.404978
Sum of electronic and thermal Free Energies = -233.442725

Single point energy = -233.6144183

O	0.00000000	0.26372200	−0.00000900
C	−1.17451000	−0.51852000	−0.00000700
H	−1.18773700	−1.17081700	0.88761700
H	−1.18774500	−1.17080800	−0.88763700
C	1.17451000	−0.51852000	0.00001800
H	1.18773900	−1.17078500	0.88766600
H	1.18774300	−1.17084000	−0.88758900
C	2.37068000	0.41036000	−0.00000800
H	3.30089200	−0.16304500	0.00002100
H	2.35295500	1.04933900	−0.88567600
H	2.35294100	1.04940300	0.88561400
C	−2.37068000	0.41036000	0.00000300
H	−2.35294500	1.04938300	−0.88563400
H	−3.30089200	−0.16304500	−0.00000900
H	−2.35295100	1.04935900	0.88565600

BPh_3 (**B-d**)

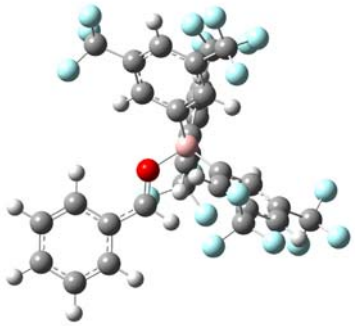


Zero-point correction = 0.280217 (Hartree/Particle)
Thermal correction to Energy = 0.295130
Thermal correction to Enthalpy = 0.296074
Thermal correction to Gibbs Free Energy = 0.237957
Sum of electronic and zero-point Energies = -719.241689
Sum of electronic and thermal Energies = -719.226775
Sum of electronic and thermal Enthalpies = -719.225831
Sum of electronic and thermal Free Energies = -719.283948

Single point energy = -719.7003129

B	0.00000000	0.00000000	0.00345500
C	0.00000000	1.56677800	0.00256800
C	−1.02205600	2.29855100	0.63402000
C	1.02194500	2.29651500	−0.63134800
H	−1.82674500	1.76240600	1.13056400
H	1.82654900	1.75880600	−1.12628500
C	−0.00039900	4.38592500	−0.00270000
H	−0.00066100	5.47166300	−0.00484100
C	1.35687000	−0.78338900	0.00256800
C	1.47786800	−2.03328800	−0.63134800
C	2.50163200	−0.26414900	0.63402000
H	0.60989600	−2.46124100	−1.12628500
H	2.43966100	0.70080500	1.13056400
C	3.79852200	−2.19261700	−0.00270000
H	4.73893000	−2.73525900	−0.00484100
C	−1.35687000	−0.78338900	0.00256800
C	−1.47957600	−2.03440200	0.63402000
C	−2.49981300	−0.26322700	−0.63134800
H	−0.61291600	−2.46321100	1.13056400
H	−2.43644500	0.70243500	−1.12628500
C	−3.79812300	−2.19330800	−0.00270000
H	−4.73826900	−2.73640400	−0.00484100
C	1.01744900	3.68756200	−0.64870400
H	1.80902000	4.22795900	−1.15825600
C	−1.01792600	3.68967600	0.64608000
H	−1.80968200	4.23178000	1.15356400
C	3.70431600	−0.96328800	0.64608000
H	4.56967000	−0.54865900	1.15356400
C	2.68479800	−2.72491800	−0.64870400
H	2.75701000	−3.68063700	−1.15825600
C	−2.68639000	−2.72638800	0.64608000
H	−2.75998800	−3.68312100	1.15356400
C	−3.70224700	−0.96264400	−0.64870400
H	−4.56603000	−0.54732200	−1.15825600

PhCHO-B[3,5-$(CF_3)_2C_6H_3]_3$ (**Int-Ia**)

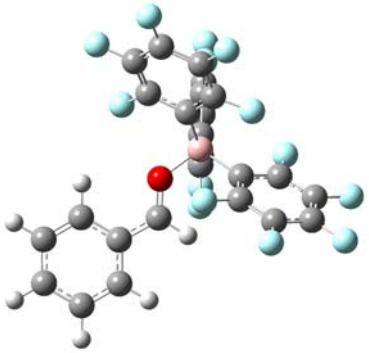


Zero-point correction = 0.422367 (Hartree/Particle)
Thermal correction to Energy = 0.467088
Thermal correction to Enthalpy = 0.468032
Thermal correction to Gibbs Free Energy = 0.329573
Sum of electronic and zero-point Energies = -3086.273857
Sum of electronic and thermal Energies = -3086.229136
Sum of electronic and thermal Enthalpies = -3086.228191
Sum of electronic and thermal Free Energies = -3086.366651

Single point energy = -3087.5512614

C	0.56498700	-0.45176700	5.96579900
C	1.65062500	0.19305200	6.56693000
C	2.55328400	0.93861600	5.80980600
C	2.37215400	1.04244600	4.43774500
C	1.28565300	0.39543000	3.83263300
C	0.37696600	-0.35464800	4.59770400
C	1.12512300	0.52215900	2.40377300
O	0.19333500	-0.02351100	1.79114700
H	-0.12761900	-1.02609900	6.57040400
H	1.79199700	0.11216900	7.63986500
H	3.38999800	1.43366300	6.28898100
H	3.06389800	1.62011100	3.83079800
H	-0.45794500	-0.84353600	4.10624600
H	1.84919300	1.12510400	1.83940200
B	-0.04280900	-0.00939700	0.18323900
C	-1.64835800	0.07045400	0.06798600
C	-2.29774500	0.84958800	-0.89429900
C	-2.45752400	-0.69912500	0.91489100
C	-3.68930300	0.86433400	-0.99730000
H	-1.71660200	1.46248300	-1.57984800
C	-3.84532000	-0.67144000	0.81856900
H	-1.99632200	-1.33536000	1.66731800
C	-4.48102600	0.11070500	-0.14070300
H	-5.56172000	0.13139800	-0.21716000
C	0.56602900	-1.42991300	-0.29254200
C	1.83999700	-1.84758300	0.10775800
C	-0.13793800	-2.28203100	-1.15194500
C	2.38431700	-3.05600000	-0.32046000
H	2.44264300	-1.22271300	0.76664000
C	0.40972100	-3.48849800	-1.58410700
H	-1.13514700	-2.00785200	-1.48670100
C	1.67521500	-3.89292400	-1.17347800
H	2.09484000	-4.83552600	-1.50545300
C	0.73101000	1.28557600	-0.39880000
C	1.79612900	1.20579900	-1.30225400
C	0.33860000	2.57126700	0.00704900
C	2.43639300	2.35326000	-1.77343700
H	2.13349400	0.23517000	-1.65777900
C	0.98873600	3.71247500	-0.45282600
H	-0.50092000	2.68757000	0.69195900
C	2.04715000	3.61787400	-1.35144900
H	2.54804200	4.50661700	-1.71744300
C	-4.64148800	-1.51676000	1.77179600
C	3.74594800	-3.44227200	0.18277800
C	0.53813700	5.04975000	0.06517800
C	-4.31452700	1.73238000	-2.05344100
C	-0.37608800	-4.34190400	-2.54161000
C	3.59364600	2.19105100	-2.72052300
F	1.15063500	6.07109000	-0.54981400
F	-5.96342600	-1.33629900	1.63965500
F	4.21538100	-4.55297500	-0.40089700
F	0.79595800	5.17022500	1.38541400
F	-4.32807700	-1.24168400	3.05517200
F	3.73525700	-3.66534800	1.51306600
F	4.64739100	-2.46440500	-0.02682000
F	-4.39758600	-2.82871800	1.59830900
F	-0.78503100	5.22234400	-0.08078200
F	-1.68196100	-4.36935500	-2.22851000
F	-3.99092400	3.02775900	-1.88230100
F	4.66708100	1.66966600	-2.09462200
F	-0.29010800	-3.87623200	-3.80175300
F	-3.89352700	1.39359000	-3.28562200
F	3.29671800	1.35852600	-3.73119100
F	0.05971900	-5.61200300	-2.56255700
F	-5.65405900	1.65396200	-2.05408500
F	3.97950700	3.35805400	-3.25820900

PhCHO-B$(C_6F_5)_3$ (**Int-Ib**)



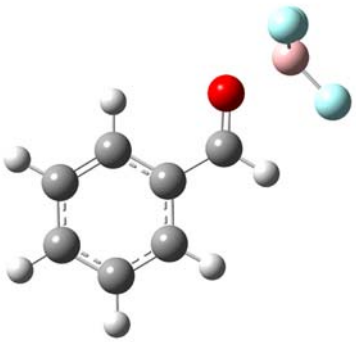
Zero-point correction = 0.271916 (Hartree/Particle)
Thermal correction to Energy = 0.307573
Thermal correction to Enthalpy = 0.308517
Thermal correction to Gibbs Free Energy = 0.201414
Sum of electronic and zero-point Energies = -2552.786616
Sum of electronic and thermal Energies = -2552.750958
Sum of electronic and thermal Enthalpies = -2552.750014
Sum of electronic and thermal Free Energies = -2552.857117

Single point energy = -2553.7718153

C	2.77842200	-1.52044000	4.64136300
C	3.96214900	-0.84986400	4.96453700
C	4.44449400	0.18527500	4.16433800
C	3.73847600	0.55705500	3.02868200
C	2.55156600	-0.11365500	2.70450000
C	2.06662000	-1.15713200	3.51065200
C	1.83310800	0.28774100	1.51955500
O	0.77205900	-0.26797500	1.19359800
H	2.41963800	-2.32339400	5.27522700
H	4.51467900	-1.14008700	5.85242700
H	5.36399000	0.69542800	4.42729100
H	4.09708700	1.36031800	2.39110900
H	1.14511600	-1.65862400	3.23072400
H	2.23394700	1.09380600	0.89428900
B	-0.12498600	-0.00554200	-0.09697900
C	-1.62522100	-0.09012000	0.51845800
C	-2.64876100	0.82214700	0.28285200
C	-1.97388700	-1.16219200	1.33975100
C	-3.92158100	0.69815000	0.82993200
C	-3.22666200	-1.32191300	1.90904100
C	-4.21154300	-0.37818800	1.65194900
C	0.27161900	-1.25166900	-1.06152300

C	1.60853500	-1.49071200	-1.36612900
C	-0.62715500	-2.13267900	-1.65512200
C	2.05182600	-2.52235600	-2.17650700
C	-0.23057900	-3.18015500	-2.47971800
C	1.11627100	-3.37922800	-2.73936600
C	0.25670300	1.45440900	-0.70332800
C	0.46996100	1.72507000	-2.05231900
C	0.28391200	2.57430500	0.12577900
C	0.69667700	3.00648400	-2.54438500
C	0.51517400	3.86640600	-0.31624700
C	0.72138300	4.08321000	-1.67206800
F	-3.49645700	-2.37003300	2.68856900
F	-5.42181800	-0.50931100	2.18758900
F	-1.07720100	-2.13441100	1.58810400
F	-2.46122400	1.88754400	-0.51316300
F	-4.86085900	1.60783600	0.57231600
F	0.07145500	2.41704100	1.44936600
F	0.53989200	4.89076100	0.53588100
F	0.94684400	5.31133400	-2.12669600
F	0.89404600	3.20642300	-3.84578800
F	0.44769700	0.74665200	-2.96730400
F	-1.94840800	-2.00357900	-1.47059900
F	-1.13469100	-3.99481600	-3.02089500
F	1.50965000	-4.37897200	-3.52274100
F	3.35071900	-2.69312100	-2.42400600
F	2.55868600	-0.66286300	-0.87319000

PhCHO-BF_3 (**Int-Ic**)

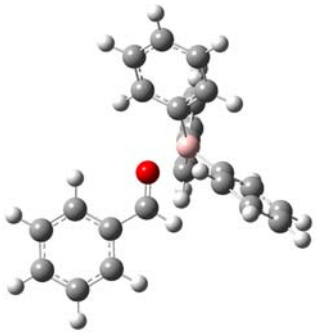


Zero-point correction = 0.126258 (Hartree/Particle)
Thermal correction to Energy = 0.136763
Thermal correction to Enthalpy = 0.137707
Thermal correction to Gibbs Free Energy = 0.087724
Sum of electronic and zero-point Energies = -669.797856
Sum of electronic and thermal Energies = -669.787351
Sum of electronic and thermal Enthalpies = -669.786407
Sum of electronic and thermal Free Energies = -669.836390

Single point energy = -670.1134181

C	-2.99087700	-1.36071500	0.00006000
C	-3.89019200	-0.29061700	0.00002600
C	-3.43600400	1.02723600	-0.00004100
C	-2.07054600	1.28001200	-0.00007300
C	-1.16838600	0.20928100	-0.00004300
C	-1.62713100	-1.11662400	0.00002900
C	0.25120200	0.50256900	-0.00009000
O	1.10733600	-0.39017800	0.00000000
B	2.71811400	-0.04111200	0.00002500
F	2.76165700	1.33461600	-0.00012200
F	3.15359800	-0.61636300	-1.15182900
F	3.15351400	-0.61611300	1.15203500
H	-3.36096000	-2.37981500	0.00011100
H	-4.95722800	-0.48888700	0.00005200
H	-4.14354800	1.84855800	-0.00006700
H	-1.69652200	2.30018500	-0.00012600
H	-0.90461200	-1.92623100	0.00005200
H	0.58627800	1.54705100	-0.00010800

PhCHO-BPh_3 (**Int-Id**)



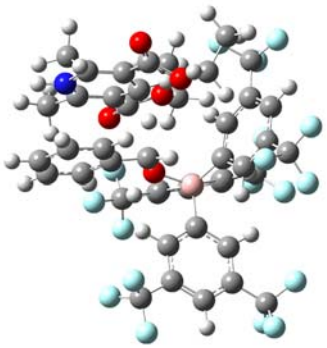
Zero-point correction = 0.392850 (Hartree/Particle)
Thermal correction to Energy = 0.415410
Thermal correction to Enthalpy = 0.416354
Thermal correction to Gibbs Free Energy = 0.337546
Sum of electronic and zero-point Energies = -1064.569353
Sum of electronic and thermal Energies = -1064.546793
Sum of electronic and thermal Enthalpies = -1064.545848
Sum of electronic and thermal Free Energies = -1064.624657

Single point energy = -1065.2353051

C	-4.57998600	-1.97631000	-0.65758800
C	-5.63967800	-1.07821000	-0.50553300
C	-5.40155900	0.26648000	-0.22792900
C	-4.09414200	0.71906300	-0.10069200
C	-3.03257800	-0.17906600	-0.25265700
C	-3.27329500	-1.53151100	-0.53200800
C	-1.67291600	0.32017200	-0.11322500
O	-0.69086300	-0.41440000	-0.24224800
H	-4.78080300	-3.01987500	-0.87320500
H	-6.66071400	-1.43247900	-0.60492200
H	-6.23102800	0.95499500	-0.11190100
H	-3.88841600	1.76405700	0.11488900
H	-2.42967200	-2.20485000	-0.64465700
H	-1.51694000	1.38478300	0.11043900
B	0.89764800	0.05917300	0.02119200
C	1.68585900	-0.78586900	-1.09608400
C	2.73336900	-0.23657900	-1.84652300
C	1.39450500	-2.14366300	-1.30618700
C	3.13449400	-2.33841300	-2.96400600
C	1.13735100	-0.45131500	1.53450300
C	0.26190500	-0.11109100	2.57709500
C	2.25751700	-1.22108000	1.87518500
C	1.60730300	-1.27560000	4.20032400
C	0.90230600	1.65962000	-0.18644200
C	1.17313100	2.56825100	0.84513300
C	0.60058200	2.20326800	-1.44926700
C	0.83118200	4.45585500	-0.62243000
C	2.09805500	-2.91150700	-2.22883500
C	3.45405700	-0.99909200	-2.76581200
C	2.49604900	-1.62501700	3.18818800
C	0.48263300	-0.51362500	3.89101700
C	1.14426500	3.94794200	0.63399200
C	0.55769600	3.57633600	-1.66964700
H	-0.61695900	0.49969700	2.36454900
H	-0.21788300	-0.23366100	4.67235800
H	1.78755400	-1.59372400	5.22257600
H	3.37544200	-2.21885500	3.41955600
H	2.95522000	-1.51054900	1.09351800
H	0.40700100	1.52578400	-2.28027800
H	0.32238700	3.96259000	-2.65714600
H	0.80646800	5.52851000	-0.78898600
H	1.36721600	4.62527600	1.45317800
H	1.41857900	2.18827500	1.83345600

H	2.99130200	0.81087300	-1.70927500
H	4.26351000	-0.54453900	-3.32959600
H	3.68999400	-2.93382500	-3.68224700
H	1.84529600	-3.95826500	-2.37152200
H	0.60249400	-2.60911900	-0.72219100

TSa

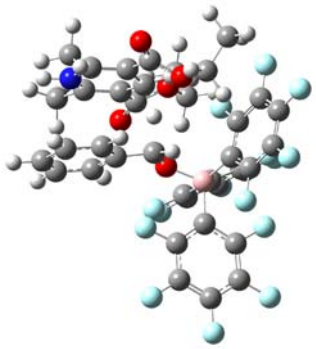


Zero-point correction = 0.735569 (Hartree/Particle)
Thermal correction to Energy = 0.799136
Thermal correction to Enthalpy = 0.800081
Thermal correction to Gibbs Free Energy = 0.628845
Sum of electronic and zero-point Energies = -3948.141966
Sum of electronic and thermal Energies = -3948.078399
Sum of electronic and thermal Enthalpies = -3948.077454
Sum of electronic and thermal Free Energies = -3948.248690

Single point energy = -3949.9608708

C	-2.15431100	-0.13728900	-4.74318800
C	-3.16066300	-1.09029000	-4.91934100
C	-3.45903100	-1.99692000	-3.90159200
C	-2.77329200	-1.93088300	-2.69332600
C	-1.77735600	-0.96329300	-2.50614400
C	-1.46354200	-0.06942400	-3.53888300
C	-1.12456700	-0.83465000	-1.19183100
O	-0.13008400	0.00728300	-1.10000600
H	-1.90189400	0.54219100	-5.55123800
H	-3.68871600	-1.14982200	-5.86623300
H	-4.21820600	-2.75723500	-4.05406300
H	-2.99304500	-2.63688700	-1.89474500
H	-0.67272800	0.65824400	-3.37999900
H	-1.10479900	-1.73338800	-0.56073400
B	0.97583400	-0.17051100	-0.03622800
C	1.59603000	1.31587300	0.14733800
C	2.19244900	1.76192300	1.32844300
C	1.60051000	2.20293100	-0.94235600
C	2.78159600	3.89227800	0.32992100
C	2.08803300	-1.16546000	-0.68019100
C	1.97301100	-1.68626700	-1.97018300
C	3.23393200	-1.52606500	0.04796300
C	4.06683000	-2.89019600	-1.77511700
C	0.30727800	-0.77342400	1.32757300
C	0.41220900	-2.11182500	1.72598900
C	-0.51140000	0.04632100	2.11607200
C	-1.07661600	-1.76875800	3.61517900
C	2.17834400	3.46235200	-0.85255800
C	2.77766700	3.02881700	1.41536000
C	4.19816000	-2.37242500	-0.48645200
C	2.94441300	-2.53510400	-2.50632000
C	-0.26356300	-2.59625600	2.84837200
C	-1.19385800	-0.43830300	3.22797800
C	-4.29961900	-0.09141400	-0.58342500
C	-4.93592700	0.15009900	-1.77016600
N	-4.45334500	1.14961500	-2.57177500
C	-3.41513800	1.98405600	-2.25168800
C	-2.77269300	1.79943400	-1.05248800
C	-3.08331800	0.63012300	-0.24554000
C	-6.13957300	-0.57198500	-2.29359500
C	-3.13671500	3.06527000	-3.25214200
C	-1.78163000	2.80915800	-0.59224400
O	-1.55537100	2.70596200	0.72075000
O	-1.28615400	3.65797600	-1.30222400
C	-0.72623200	3.72553200	1.32614700
C	-1.55888000	4.94498300	1.66424700
C	-4.71602300	-1.23407100	0.26256600
O	-3.69985300	-1.63693500	1.03850900
O	-5.80037200	-1.77577600	0.22614000
C	-3.95378300	-2.76831100	1.90145600
C	-4.67140600	-2.33671600	3.16356500
H	-4.89120200	1.27655000	-3.47418900
H	-2.14934200	-0.24920800	-0.52097900
H	-2.83581100	0.69359900	0.81418900
H	-7.02988400	-0.27930100	-1.73193800
H	-6.28860300	-0.34604100	-3.35262800
H	-6.02808700	-1.64861300	-2.16495200
H	-2.09841800	3.01806200	-3.58314800
H	-3.80258400	2.97037100	-4.11348100
H	-3.26870500	4.04975900	-2.79868000
H	-0.32004800	3.25240900	2.22307300
H	0.08758500	3.96565600	0.64080900
H	-0.93459800	5.67919000	2.17934500
H	-1.95082800	5.40605200	0.75461000
H	-2.38908700	4.67364800	2.32079400
H	-4.53207000	-3.50713400	1.34196300
H	-2.96011000	-3.16531000	2.11310300
H	-4.77678300	-3.19358500	3.83414900
H	-4.10586800	-1.55870300	3.68168600
H	-5.66774800	-1.95501100	2.93127000
H	-0.62829000	1.09155600	1.84721700
H	-1.59610800	-2.14950700	4.48795900
H	1.03358500	-2.79816400	1.15330000
H	1.13253200	1.90379900	-1.87499800
H	2.20142000	1.12272300	2.20982900
H	3.23097900	4.87739600	0.40225600
H	1.11497200	-1.42566500	-2.58567200
H	4.81751400	-3.55484600	-2.18771600
H	3.37341400	-1.14437600	1.05767500
C	2.72816400	-3.06699100	-3.89293900
C	5.43043500	-2.70314100	0.30741500
C	-0.13293200	-4.05346300	3.18984700
C	-2.08933000	0.51091400	3.96868400
C	3.33302300	3.47259500	2.73743800
C	2.14317000	4.41278200	-2.01515600
F	5.88347100	-3.94106100	0.03880000
F	5.21406300	-2.63460000	1.63125600
F	6.44218400	-1.85604200	0.03422700
F	1.62485900	-3.84155200	-3.96168200
F	3.75625600	-3.80877400	-4.33197700
F	2.54292900	-2.07420900	-4.78570500
F	2.34142500	3.74261400	3.61556700
F	4.07640700	4.58584200	2.63811100
F	4.09782500	2.52758100	3.30930200
F	1.51969600	5.56382600	-1.69622500
F	3.38403300	4.75635100	-2.41534100
F	1.51235200	3.90215400	-3.08383800
F	-1.46219200	1.65546900	4.28778300
F	-3.15622200	0.86667600	3.21337100
F	-2.57783000	-0.01272000	5.10397000
F	1.14668500	-4.43036700	3.32847100
F	-0.65902900	-4.83136800	2.21810700
F	-0.77276200	-4.37052500	4.32827400

TSb

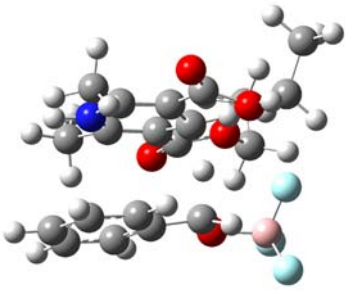


Zero-point correction = 0.584194 (Hartree/Particle)
Thermal correction to Energy = 0.639234
Thermal correction to Enthalpy = 0.640179
Thermal correction to Gibbs Free Energy = 0.493559
Sum of electronic and zero-point Energies = -3414.643335
Sum of electronic and thermal Energies = -3414.588294
Sum of electronic and thermal Enthalpies = -3414.587350
Sum of electronic and thermal Free Energies = -3414.733970

Single point energy = -3416.1732808

C	−2.23723100	−2.29176600	3.63761000
C	−3.28348800	−1.58488400	4.23599500
C	−3.55511900	−0.27001000	3.85518500
C	−2.79776700	0.32919800	2.85419400
C	−1.76001600	−0.38539500	2.24095600
C	−1.47666100	−1.69990800	2.63644700
C	−1.00966400	0.21950300	1.13033200
O	0.04879300	−0.41722000	0.70192400
H	−2.00711700	−3.30061000	3.96602400
H	−3.86363400	−2.04772400	5.02879100
H	−4.34562100	0.28787300	4.34735100
H	−2.98922600	1.35970100	2.56101200
H	−0.64653300	−2.21908700	2.16386000
H	−1.01295400	1.31672200	1.07374600
B	1.26977600	0.28019700	0.13543400
C	2.00844700	−0.88719100	−0.74943300
C	2.53396300	−0.76350100	−2.03069800
C	2.21952500	−2.12940200	−0.14826600
C	3.36088800	−3.01620600	−2.05753900
C	2.31423600	0.66473300	1.33983100
C	2.09836900	0.52939800	2.70378000
C	3.57803800	1.13755000	0.99430700
C	4.30209000	1.29231100	3.26681800
C	0.78013000	1.60606600	−0.71276000
C	0.99218300	2.93669500	−0.35954500
C	0.03990300	1.44016900	−1.88025600
C	−0.16494400	3.78463600	−2.28710500
C	2.87437400	−3.18548500	−0.76896800
C	3.19202400	−1.79503800	−2.69152100
C	4.56624400	1.45148800	1.91276900
C	3.05877600	0.83030500	3.66376800
C	0.54455100	4.01489500	−1.11982900
C	−0.42410300	2.47730100	−2.67260600
F	3.98424600	−4.01759200	−2.67864100
F	3.05023100	−4.34915600	−0.14047800
F	1.81698600	−2.34474600	1.11462900
F	2.43070200	0.38995700	−2.70995600
F	3.65547400	−1.62360800	−3.93237200
F	3.86925200	1.33418000	−0.30463500
F	5.75668400	1.90657900	1.51725600
F	5.23361300	1.58526800	4.17353700
F	2.79004400	0.67870400	4.96369700
F	0.91240700	0.10542600	3.18254500
F	1.63935800	3.26618100	0.76847100
F	0.77055700	5.26819000	−0.72124500
F	−0.62371600	4.80460400	−3.01159300
F	−1.11711200	2.23266200	−3.78916600
F	−0.26021400	0.19941800	−2.29834600
C	−4.09002000	0.02821800	−0.06883000
C	−4.88977800	−0.68467900	0.78377000
N	−4.56724200	−1.98833500	1.04447700
C	−3.50945700	−2.65747400	0.48751800
C	−2.68975400	−1.98339100	−0.37719200
C	−2.86038400	−0.55393100	−0.58472200
C	−6.12198800	−0.17668100	1.46890100
C	−3.39760700	−4.10474300	0.85942600
C	−1.58969400	−2.72090600	−1.05885000
O	−1.30806300	−2.17769800	−2.23958500
O	−1.04640600	−3.70587800	−0.60490300
C	−0.20017100	−2.74027400	−2.97132500
C	−0.64431500	−3.93616100	−3.78903300
C	−4.35721500	1.46758500	−0.29357500
O	−3.23236700	2.10522700	−0.65413900
O	−5.42451900	2.01825000	−0.12653400
C	−3.34217200	3.52882200	−0.88450700
C	−3.80202900	3.80901400	−2.30031500
H	−5.13578000	−2.48742300	1.71489700
H	−1.94228200	0.02909300	0.15573900
H	−2.46941700	−0.15820600	−1.52276000
H	−6.92651100	−0.03027400	0.74502100
H	−6.44897300	−0.88192200	2.23717200
H	−5.93333600	0.79438800	1.92816000
H	−2.51786100	−4.25839400	1.48757700
H	−4.29135500	−4.43451100	1.39483300
H	−3.25987500	−4.72266000	−0.02881200
H	0.14926300	−1.91905400	−3.59930300
H	0.57846600	−3.01220100	−2.25543400
H	0.19697900	−4.30403100	−4.38220600
H	−0.98372700	−4.74303900	−3.13604800
H	−1.45215100	−3.65804900	−4.47010600
H	−4.02996900	3.94620500	−0.14661600
H	−2.33510800	3.90702500	−0.69931600
H	−3.80456300	4.88749500	−2.47661500
H	−3.12939100	3.34489500	−3.02552100
H	−4.81460600	3.42992500	−2.45579200

TSc



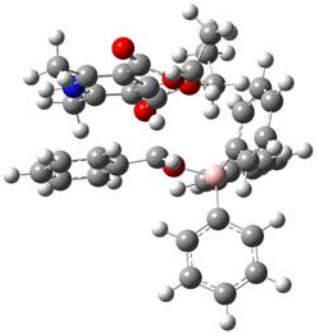
Zero-point correction = 0.438462 (Hartree/Particle)
Thermal correction to Energy = 0.468361
Thermal correction to Enthalpy = 0.469305
Thermal correction to Gibbs Free Energy = 0.376789
Sum of electronic and zero-point Energies = -1531.649324
Sum of electronic and thermal Energies = -1531.619426
Sum of electronic and thermal Enthalpies = -1531.618482
Sum of electronic and thermal Free Energies = -1531.710997

Single point energy = -1532.5107207

C	−1.06096900	−3.63431100	1.16915500
C	−2.43619100	−3.42606700	1.29016000
C	−2.92865900	−2.16503700	1.63080500

C	−2.04738900	−1.10621400	1.82193900
C	−0.66855500	−1.30748100	1.67906100
C	−0.17607000	−2.57756500	1.35705500
C	0.25808700	−0.15941400	1.74973200
O	1.53871200	−0.42242400	1.65315800
H	−0.68040500	−4.62380700	0.93418600
H	−3.12465100	−4.25444200	1.15203400
H	−3.99643700	−2.01193000	1.75341100
H	−2.42146400	−0.11954000	2.08861100
H	0.89911400	−2.70786700	1.27033500
H	−0.03510300	0.67915100	2.39649600
B	2.44373300	0.75431700	2.00175200
C	−1.61088300	0.63580100	−0.90787200
C	−2.32558700	−0.47583600	−1.27046000
N	−1.63560300	−1.61313300	−1.58343400
C	−0.26942600	−1.72324000	−1.61585000
C	0.48227700	−0.63510500	−1.25466000
C	−0.17495000	0.54178200	−0.71719100
C	−3.81650800	−0.57671300	−1.38060300
C	0.24994300	−3.04343500	−2.09932600
C	1.96876300	−0.68831100	−1.35456700
O	2.50015600	0.51635100	−1.20704800
O	2.59683300	−1.70442100	−1.57628300
C	3.94081000	0.60871500	−1.19710900
C	4.47556200	0.67998300	−2.61386600
C	−2.31407500	1.88661000	−0.54047000
O	−1.48559600	2.72612200	0.08879700
O	−3.48768600	2.11987400	−0.75025500
C	−2.02176300	4.00478100	0.48264200
C	−2.06859700	4.95630600	−0.69667500
H	−2.17347300	−2.44351800	−1.79152600
H	−0.06716200	0.42124900	0.61482700
H	0.40439000	1.46380600	−0.71947600
H	−4.17686200	0.00756400	−2.23024100
H	−4.11787300	−1.62039000	−1.50185500
H	−4.29319000	−0.16259100	−0.49191500
H	0.87380200	−3.50551400	−1.33332100
H	−0.57772200	−3.71063900	−2.35370800
H	0.88833500	−2.90468300	−2.97361700
H	4.13792300	1.51566500	−0.62625400
H	4.33519200	−0.24580400	−0.64643900
H	5.55942700	0.81954900	−2.58892300
H	4.26058200	−0.24400500	−3.15539900
H	4.03308400	1.52235700	−3.15191400
H	−3.01377000	3.84903100	0.91287200
H	−1.33442200	4.35021400	1.25521900
H	−2.41705800	5.93673600	−0.36254100
H	−1.07320000	5.07312000	−1.13101300
H	−2.75617000	4.58826800	−1.46073500
F	3.73133100	0.35851200	1.71236100
F	2.02894300	1.83428700	1.20556100
F	2.24677000	1.05085200	3.34405700

TSd



Zero-point correction = 0.704859 (Hartree/Particle)
Thermal correction to Energy = 0.746458
Thermal correction to Enthalpy = 0.747402
Thermal correction to Gibbs Free Energy = 0.630068

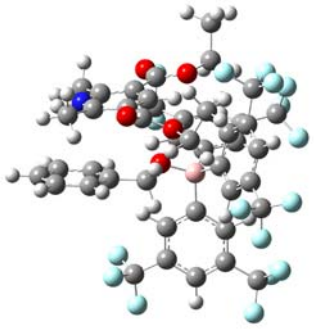
Sum of electronic and zero-point Energies = -1926.422955
Sum of electronic and thermal Energies = -1926.381357
Sum of electronic and thermal Enthalpies = -1926.380412
Sum of electronic and thermal Free Energies = -1926.497746

Single point energy = -1927.6285235

C	−1.94484800	−2.42508500	3.17727600
C	−3.10022800	−1.77596100	3.61705600
C	−3.30759500	−0.43009200	3.30949900
C	−2.37679500	0.25462300	2.53449600
C	−1.22932100	−0.40026400	2.07079700
C	−1.01141000	−1.74190700	2.40394500
C	−0.29784500	0.29434900	1.14634900
O	0.78634400	−0.36370600	0.80538600
H	−1.76958500	−3.46266600	3.44606600
H	−3.82155500	−2.30826500	4.23000900
H	−4.19001200	0.08334600	3.67932200
H	−2.52845700	1.30471100	2.29121600
H	−0.10130500	−2.21754500	2.04686200
H	−0.20614100	1.38099100	1.29235800
B	2.06009000	0.44695500	0.41342700
C	2.97861600	−0.60462300	−0.40939800
C	3.84679800	−0.22336100	−1.44195000
C	3.00389000	−1.95774900	−0.03181000
C	4.69235900	−2.47437900	−1.67836300
C	2.80313700	0.85281600	1.80303600
C	2.32730000	0.49355700	3.06996900
C	4.00285400	1.58364100	1.76666600
C	4.18051700	1.57876000	4.17302300
C	1.61162100	1.76285900	−0.45763200
C	1.60009100	3.06253400	0.07282800
C	1.17698200	1.63507100	−1.78819900
C	0.78286900	4.00728800	−1.99691200
C	3.84328000	−2.88203200	−0.64943900
C	4.69177700	−1.13853800	−2.07158100
C	4.68301900	1.94510800	2.92433600
C	2.99958400	0.84889800	4.24100600
C	1.19926000	4.16950000	−0.67782200
C	0.76488900	2.72771900	−2.54988400
C	−3.10384700	0.20439700	−0.63359500
C	−3.96827200	−0.64790600	0.00210000
N	−3.56874500	−1.94017000	0.19593000
C	−2.38457300	−2.47168300	−0.23369200
C	−1.49428400	−1.64907400	−0.88374900
C	−1.76661600	−0.23352100	−0.95621100
C	−5.33750900	−0.31031300	0.50753000
C	−2.21954800	−3.94006100	0.01654400
C	−0.26975100	−2.24020100	−1.49724100
O	0.24279500	−1.43977200	−2.42910200
O	0.15403800	−3.34450600	−1.23012000
C	1.39562300	−1.93653600	−3.14976400
C	0.96079500	−2.86325600	−4.26745400
C	−3.46130900	1.63446700	−0.80652000
O	−2.35996000	2.37434600	−0.94564800
O	−4.59160700	2.07692800	−0.78479900
C	−2.54016600	3.79447100	−1.13261300
C	−2.79096700	4.10324200	−2.59409800
H	−4.18089100	−2.54233800	0.73055100
H	−1.03532200	0.33591600	0.10147000
H	−1.19605200	0.35019000	−1.67788000
H	−6.03574900	−0.20299500	−0.32576100
H	−5.69505700	−1.09147700	1.18347000
H	−5.32633600	0.64425900	1.03379600
H	−1.33575900	−4.11957800	0.62974400
H	−3.10343700	−4.34423600	0.51657700
H	−2.05801700	−4.47165100	−0.92302200
H	1.88149800	−1.03659500	−3.52998900
H	2.06498000	−2.42666200	−2.44226900
H	1.83815800	−3.17250100	−4.84126900
H	0.48495900	−3.75869900	−3.86153500
H	0.26490400	−2.36061000	−4.94427600
H	−3.36754900	4.12466900	−0.50066000
H	−1.60054400	4.22388200	−0.78557400
H	−2.87067900	5.18465100	−2.73323300

H	-1.95926300	3.73525500	-3.19960600
H	-3.72132100	3.64285000	-2.93478000
H	1.17933200	0.64756300	-2.24174200
H	0.44930400	2.58390700	-3.58082400
H	0.48223500	4.86771800	-2.58974600
H	1.22436600	5.16174300	-0.23448300
H	1.93510800	3.21637000	1.09639400
H	1.41401300	-0.09315200	3.15184700
H	2.60097200	0.54955800	5.20683200
H	4.70881200	1.85668000	5.08018000
H	5.60816900	2.51113400	2.85692300
H	4.41024500	1.87626900	0.79936900
H	2.34561600	-2.29132500	0.76761900
H	3.83216500	-3.92140800	-0.33298700
H	5.35044600	-3.18975800	-2.16286300
H	5.35255000	-0.80683800	-2.86816600
H	3.86082400	0.81619100	-1.76549000

Int-IIa

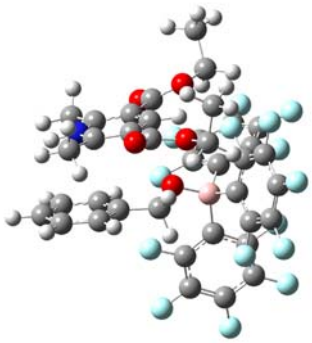


Zero-point correction = 0.740622 (Hartree/Particle)
Thermal correction to Energy = 0.804278
Thermal correction to Enthalpy = 0.805223
Thermal correction to Gibbs Free Energy = 0.635002
Sum of electronic and zero-point Energies = -3948.170411
Sum of electronic and thermal Energies = -3948.106754
Sum of electronic and thermal Enthalpies = -3948.105810
Sum of electronic and thermal Free Energies = -3948.276031

Single point energy = -3949.9967253

C	1.03779100	2.82368500	4.23918800
C	1.93534700	2.37589500	5.20820000
C	2.39507600	1.05828800	5.16019800
C	1.98131700	0.21073700	4.13583200
C	1.09819500	0.65739000	3.14737900
C	0.62292400	1.96974800	3.21631200
C	0.65631000	-0.27274800	2.03891800
O	0.12174500	0.45406000	0.97997800
H	0.64315100	3.83477800	4.28934400
H	2.24352200	3.03265300	6.01596700
H	3.07367000	0.69140300	5.92498700
H	2.34290100	-0.81634800	4.10137800
H	-0.07257700	2.31027400	2.45472300
H	-0.07905000	-0.98202700	2.45746600
B	-0.82650900	-0.26081400	0.06847500
C	-1.28660900	0.85690100	-1.02801200
C	-1.78168000	0.54995300	-2.29974600
C	-1.26974200	2.21363700	-0.67047700
C	-2.23749200	2.88428300	-2.78576000
C	-2.17506700	-0.70538700	0.88141500
C	-2.51226600	-0.07548200	2.08291300
C	-3.09042600	-1.64936100	0.39284000
C	-4.57519600	-1.32714700	2.28436600
C	-0.03958400	-1.52637300	-0.62199100
C	-0.12260100	-2.85975500	-0.19256500
C	0.89230200	-1.26141800	-1.62982800
C	1.59300900	-3.57288800	-1.76163800
C	-1.73007700	3.20614400	-1.52824700
C	-2.25025200	1.54615300	-3.15970500
C	-4.26215200	-1.95504900	1.08122100
C	-3.68405900	-0.38180600	2.77344300
C	0.66564600	-3.86027400	-0.76109600
C	1.70166200	-2.25366500	-2.18051000
C	3.94405700	0.44928600	1.21293800
C	4.21888100	1.33833700	2.24918500
N	3.61721900	2.54624200	2.18589600
C	2.82588400	3.00702200	1.18706300
C	2.63501300	2.16378300	0.09573700
C	3.14911100	0.86837400	0.14796600
C	5.14211200	1.10163500	3.40083300
C	2.25221800	4.37522500	1.36415400
C	1.90655300	2.66180000	-1.11796500
O	1.90836000	1.75685200	-2.08482300
O	1.43496300	3.77238300	-1.19685900
C	1.25129300	2.11574400	-3.32821100
C	2.22983200	2.81206800	-4.24906800
C	4.49136400	-0.94541200	1.26580200
O	3.74299400	-1.78054000	0.56176100
O	5.47593600	-1.24576300	1.90373800
C	4.14390300	-3.17530700	0.55822100
C	5.13846000	-3.43367900	-0.55305900
H	3.70263400	3.13910900	3.00891700
H	1.51525600	-0.88905500	1.71401700
H	2.94621000	0.17715400	-0.66504500
H	6.17272500	1.07459600	3.03740900
H	5.03050100	1.88861400	4.14944900
H	4.94425600	0.13427200	3.86137500
H	1.16951000	4.34766700	1.22083200
H	2.48408800	4.76126200	2.35921700
H	2.64282800	5.05112300	0.60001900
H	0.91011100	1.16344700	-3.73806600
H	0.38940200	2.73997400	-3.08908900
H	1.73754200	3.02822700	-5.20029800
H	2.56555400	3.75649900	-3.81394500
H	3.09453700	2.17323800	-4.44430900
H	4.55897600	-3.41304500	1.53956300
H	3.20972800	-3.71572000	0.41233100
H	5.38799000	-4.49746500	-0.57562900
H	4.71607700	-3.15519600	-1.52113400
H	6.05921100	-2.86840700	-0.39006300
H	0.99304200	-0.24189500	-1.99009000
H	2.20269800	-4.35646000	-2.20103300
H	-0.82494500	-3.13068100	0.59275100
H	-0.87798200	2.49071800	0.30355800
H	-1.80745500	-0.48554400	-2.63558800
H	-2.60150800	3.65496200	-3.45779400
H	-1.84007300	0.67475800	2.49631700
H	-5.48313800	-1.57350800	2.82319400
H	-2.88566200	-2.16549300	-0.54327500
C	-3.94345100	0.32342000	4.07166000
C	-5.23394800	-2.94179200	0.50052500
C	0.58648000	-5.27130300	-0.25366800
C	2.71929800	-1.84050000	-3.19968700
C	-2.68224600	1.16818200	-4.54636100
C	-1.67660000	4.65421000	-1.13531500
F	-5.91899400	-3.59907500	1.45477400
F	-4.62487000	-3.86726600	-0.26061500
F	-6.15108800	-2.34020800	-0.28318600
F	-2.98771300	0.05184200	4.98599000
F	-5.11981500	-0.01516900	4.62275000
F	-3.94614300	1.66333300	3.92380000
F	-1.61404300	1.01815100	-5.36463200
F	-3.46846500	2.09826900	-5.11284200
F	-3.34897200	0.00393100	-4.57606300
F	-0.97956400	5.38947300	-2.02210300
F	-2.90519200	5.20345500	-1.07472700
F	-1.10531200	4.84487400	0.07012200
F	2.18406100	-1.11145200	-4.19460200
F	3.67848800	-1.05633700	-2.64321000
F	3.35461300	-2.88145400	-3.76026200
F	-0.55916200	-5.53019600	0.38771600
F	1.58967300	-5.53287200	0.62180300
F	0.71280800	-6.17316100	-1.24269500

Int-IIb

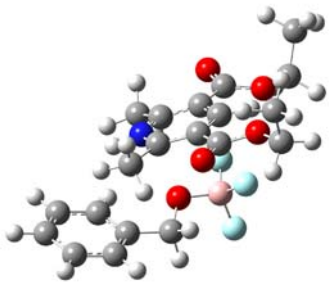


Zero-point correction = 0.589084 (Hartree/Particle)
Thermal correction to Energy = 0.644462
Thermal correction to Enthalpy = 0.645406
Thermal correction to Gibbs Free Energy = 0.498264
Sum of electronic and zero-point Energies = -3414.675208
Sum of electronic and thermal Energies = -3414.619829
Sum of electronic and thermal Enthalpies = -3414.618885
Sum of electronic and thermal Free Energies = -3414.766027

Single point energy = -3416.2139734

C	−1.65432100	−3.79731600	2.62739600
C	−2.74868200	−3.63621400	3.47885100
C	−3.21328700	−2.35124600	3.76249700
C	−2.59757200	−1.24380000	3.18197400
C	−1.50989100	−1.39973600	2.31785000
C	−1.04039000	−2.68804800	2.04649700
C	−0.82677000	−0.18786600	1.72579400
O	−0.09349500	−0.53481600	0.59078100
H	−1.26407300	−4.79220900	2.43028500
H	−3.21035300	−4.49983700	3.94826000
H	−4.04721900	−2.21193900	4.44470900
H	−2.95898800	−0.24128300	3.40878500
H	−0.18536900	−2.79049500	1.38366500
H	−0.17949300	0.25296300	2.50286000
B	1.06179300	0.31955700	0.26837000
C	1.76088300	−0.28440400	−1.09812300
C	2.29268000	0.45030100	−2.15479200
C	2.05433100	−1.64820300	−1.13891900
C	3.32008800	−1.47154500	−3.16397800
C	2.30736400	0.22457000	1.36366000
C	2.43321000	−0.68279400	2.40692400
C	3.42018100	1.04472200	1.18421000
C	4.62262700	0.08968600	3.01515100
C	0.49716100	1.87492200	0.13195500
C	0.62099200	2.86805100	1.09897400
C	−0.31462700	2.22953800	−0.94010700
C	−0.75432800	4.42409700	−0.09913100
C	2.80716600	−2.25191200	−2.13798000
C	3.05795800	−0.11038300	−3.17217100
C	4.55638800	1.00663400	1.97487900
C	3.55319400	−0.76128100	3.23041300
C	0.02755300	4.12352900	1.00273300
C	−0.92854800	3.46315800	−1.08408400
F	4.04239100	−2.02643000	−4.13893900
F	3.05242700	−3.56419400	−2.11438100
F	1.65133200	−2.45552400	−0.14287800
F	2.09551400	1.77481000	−2.24848800
F	3.52859600	0.64759400	−4.16736200
F	3.41325500	1.95023600	0.18818600
F	5.58062100	1.83438000	1.75216000
F	5.70384400	0.02882400	3.79429700
F	3.60531100	−1.65464700	4.22406700
F	1.44724900	−1.55478200	2.69396800
F	1.32244300	2.65645500	2.22599700
F	0.18183200	5.02933600	1.97158000
F	−1.36493000	5.60875000	−0.20057900
F	−1.71966200	3.72555300	−2.13424000
F	−0.55517300	1.33978700	−1.92546100
C	−3.86757300	−0.41274900	−0.00162800
C	−4.39026000	−1.52280600	0.66270400
N	−3.80811600	−2.71474300	0.40865800
C	−2.78220100	−2.94995900	−0.44462300
C	−2.28352400	−1.85790000	−1.14218600
C	−2.80779800	−0.59156900	−0.88898700
C	−5.55602300	−1.53416000	1.59949900
C	−2.30695800	−4.36095600	−0.56535100
C	−1.20035400	−2.04230000	−2.16279400
O	−1.16726200	−1.01015600	−2.98950000
O	−0.50209800	−3.02756000	−2.22755100
C	−0.16399000	−1.02142300	−4.02804700
C	−0.70977700	−1.69228800	−5.27187600
C	−4.46006100	0.94441000	0.23047700
O	−3.69026000	1.91111000	−0.25162600
O	−5.52111400	1.11349400	0.78980000
C	−4.21747300	3.26003400	−0.15461200
C	−5.13666500	3.54847300	−1.32222100
H	−4.11053300	−3.49986600	0.98135000
H	−1.58831200	0.58089000	1.49143100
H	−2.37862000	0.26267200	−1.40417400
H	−6.46594400	−1.26856900	1.05654600
H	−5.66810400	−2.51922000	2.05711800
H	−5.42458700	−0.78637400	2.38144200
H	−1.25158800	−4.41606500	−0.29096100
H	−2.89251800	−5.02262300	0.07652400
H	−2.37763000	−4.69295200	−1.60362800
H	0.06734000	0.03280600	−4.18814200
H	0.71596500	−1.53929500	−3.64595300
H	0.03652000	−1.64423700	−6.06853600
H	−0.93172900	−2.74372100	−5.07391300
H	−1.61726700	−1.19098100	−5.61635300
H	−4.72629500	3.35999600	0.80557700
H	−3.33403400	3.89566400	−0.16968300
H	−5.47646700	4.58543200	−1.26698000
H	−4.60429700	3.41077900	−2.26565000
H	−6.01441200	2.89837700	−1.29856400

Int-IIc



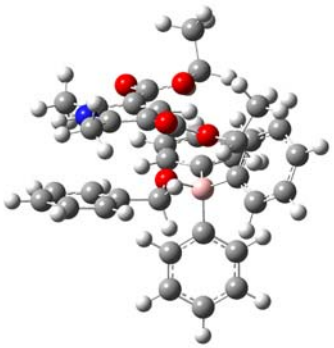
Zero-point correction = 0.442830 (Hartree/Particle)
Thermal correction to Energy = 0.473486
Thermal correction to Enthalpy = 0.474430
Thermal correction to Gibbs Free Energy = 0.378992
Sum of electronic and zero-point Energies = -1531.683571
Sum of electronic and thermal Energies = -1531.652915
Sum of electronic and thermal Enthalpies = -1531.651971
Sum of electronic and thermal Free Energies = -1531.747409

Single point energy = -1532.5498719

C	−4.43044800	−1.66984300	−1.09117200
C	−5.39650900	−0.67480900	−0.94518700
C	−5.27234300	0.25500500	0.08577900

C	−4.17382500	0.21072400	0.94096200
C	−3.18508100	−0.76343100	0.78635300
C	−3.33923200	−1.71952900	−0.22292000
C	−1.96347400	−0.78068300	1.67898100
O	−0.92452500	−1.47884300	1.05857800
H	−4.53716200	−2.41934700	−1.87032400
H	−6.24668900	−0.63468200	−1.61820500
H	−6.02712800	1.02424600	0.21620000
H	−4.07031800	0.95294100	1.72958700
H	−2.58877200	−2.50134800	−0.30151000
H	−2.21967000	−1.24288600	2.64452700
B	0.30970600	−1.57742000	1.83617000
C	0.27019300	1.56269500	−0.60603100
C	−0.90907400	1.03536400	−1.12207900
N	−0.87243500	−0.25178200	−1.53026900
C	0.18290600	−1.09132200	−1.46568600
C	1.38372600	−0.56234500	−0.99797800
C	1.40025600	0.74393200	−0.52987900
C	−2.21949100	1.74119700	−1.27256700
C	−0.05835200	−2.51614800	−1.82624700
C	2.59392400	−1.43741100	−0.88374800
O	3.49009700	−0.91272200	−0.05700800
O	2.73266800	−2.47182600	−1.49441100
C	4.60940000	−1.75547100	0.28316200
C	5.69748000	−1.67310600	−0.76952600
C	0.30986700	2.96729300	−0.09939400
O	1.51104100	3.28401300	0.38001900
O	−0.63579900	3.72403200	−0.12469100
C	1.65559800	4.60771600	0.93622100
C	1.88862600	5.63184400	−0.15684900
H	−1.77202700	−0.67092200	−1.76421100
H	−1.66868300	0.26131800	1.89497500
H	2.30565800	1.12943400	−0.07730400
H	−2.11410300	2.58307200	−1.96070600
H	−2.98977100	1.05308400	−1.63153000
H	−2.53361300	2.15532800	−0.31417400
H	0.14698600	−3.11005100	−0.92801900
H	−1.09329900	−2.66451300	−2.14138800
H	0.62800900	−2.84237400	−2.60688200
H	4.94384700	−1.37175700	1.24711200
H	4.23733700	−2.77434400	0.40821200
H	6.55728800	−2.26992000	−0.45452000
H	5.33872900	−2.06122500	−1.72446200
H	6.02702300	−0.63953900	−0.90185100
H	0.76145200	4.83650600	1.51939800
H	2.51364000	4.52078800	1.60267400
H	2.06193700	6.61281900	0.29242300
H	2.76573100	5.36536500	−0.75103800
H	1.01773500	5.70236100	−0.81114000
F	1.18434200	−2.40500300	1.09047600
F	0.89841500	−0.28897400	1.96074400
F	0.07964800	−2.10291900	3.10434800

Int-IId



Zero-point correction = 0.710175 (Hartree/Particle)
Thermal correction to Energy = 0.751802
Thermal correction to Enthalpy = 0.752746
Thermal correction to Gibbs Free Energy = 0.636117

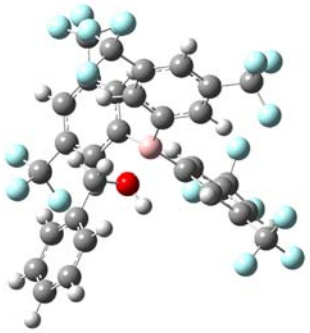
Sum of electronic and zero-point Energies = -1926.443464
Sum of electronic and thermal Energies = -1926.401837
Sum of electronic and thermal Enthalpies = -1926.400893
Sum of electronic and thermal Free Energies = -1926.517522

Single point energy = -1927.6564256

C	−2.01217800	−3.58916300	1.77735700
C	−3.22048100	−3.33433600	2.42715200
C	−3.50493000	−2.03733900	2.85927800
C	−2.59907000	−1.00669700	2.61863400
C	−1.39571700	−1.24789700	1.94772700
C	−1.10957400	−2.55304400	1.53706200
C	−0.41298100	−0.12689800	1.68876200
O	0.47093300	−0.48112500	0.68013000
H	−1.76656100	−4.60189700	1.46842600
H	−3.91702400	−4.14280200	2.62855800
H	−4.43184900	−1.83159600	3.38749100
H	−2.82415900	0.00441000	2.95612300
H	−0.16855400	−2.72684100	1.02244400
H	0.11700400	0.08718400	2.63319500
B	1.78722400	0.26865200	0.64632600
C	2.68349700	−0.44338900	−0.51459700
C	3.75256800	0.20015700	−1.15920200
C	2.52270700	−1.80963300	−0.79274700
C	4.43403800	−1.83721500	−2.26843200
C	2.61045300	0.00744500	2.04182000
C	2.36631200	−1.13913600	2.81303000
C	3.66532400	0.82828300	2.46871500
C	4.14389600	−0.60484000	4.35290700
C	1.49535800	1.86385500	0.36696800
C	1.37706200	2.80704400	1.40162500
C	1.29611800	2.35568400	−0.93430500
C	0.94837400	4.61198700	−0.14885600
C	3.37719600	−2.50319200	−1.64943600
C	4.61483700	−0.47699300	−2.02093100
C	4.42286500	0.53399300	3.60114300
C	3.10909200	−1.44504000	3.95106400
C	1.12128200	4.15697200	1.15764200
C	1.02267300	3.69841900	−1.19846900
C	−2.85663700	0.50287500	−0.54309400
C	−3.72962200	−0.54447300	−0.25433400
N	−3.34347800	−1.77912200	−0.63678700
C	−2.22109700	−2.09688700	−1.32748300
C	−1.37429600	−1.05191900	−1.67486400
C	−1.66498400	0.23511900	−1.21654400
C	−5.06311500	−0.43980600	0.41539300
C	−2.01952900	−3.54666400	−1.63206100
C	−0.18081300	−1.31317200	−2.54698000
O	0.38692100	−0.18219400	−2.92679800
O	0.14788900	−2.42339900	−2.89990500
C	1.56493000	−0.28881400	−3.76538000
C	1.16832500	−0.51177900	−5.21087300
C	−3.21540400	1.89476600	−0.11917500
O	−2.14948500	2.67035000	−0.04858500
O	−4.35470000	2.23280200	0.12507000
C	−2.36436200	4.05171400	0.33175500
C	−2.57858400	4.89360800	−0.90761200
H	−3.90932400	−2.55696900	−0.30640400
H	−0.97021700	0.79865000	1.44572200
H	−0.95041600	1.03737200	−1.39223500
H	−5.77807700	0.02788700	−0.26630400
H	−5.41832700	−1.42995900	0.70957100
H	−5.00290000	0.19821700	1.29610900
H	−1.05351900	−3.87382100	−1.24284400
H	−2.81746900	−4.14536100	−1.18635400
H	−1.98942800	−3.70772400	−2.71134800
H	2.07572800	0.66384300	−3.62104300
H	2.19380300	−1.08871000	−3.37167500
H	2.06688400	−0.51715800	−5.83287100
H	0.66443000	−1.47308500	−5.33112300
H	0.51085100	0.28720100	−5.56352900
H	−3.21961200	4.09277100	1.00849100
H	−1.44865700	4.32239000	0.85437500
H	−2.68944800	5.94308000	−0.62254300

H	−1.71565400	4.80320700	−1.57170500
H	−3.48272700	4.58477800	−1.43871500
H	1.38509600	1.66212200	−1.76776400
H	0.89337900	4.03765600	−2.22397200
H	0.76171800	5.66469700	−0.34667300
H	1.06746800	4.85779500	1.98750500
H	1.52795500	2.47846800	2.42840600
H	1.56913800	−1.81683500	2.50723200
H	2.88342300	−2.34127100	4.52325800
H	4.72881300	−0.83714100	5.23804000
H	5.23282900	1.19482700	3.89879400
H	3.90194000	1.72414800	1.89624500
H	1.70673500	−2.34350800	−0.30869400
H	3.21516700	−3.56125400	−1.83799700
H	5.10787200	−2.37107900	−2.93215800
H	5.43585500	0.05487200	−2.49493800
H	3.92240300	1.25897000	−0.96847200

$PhCH_2OH\text{-}B[3,5\text{-}(CF_3)_2C_6H_3]_3$ (**Int-IIIa**)

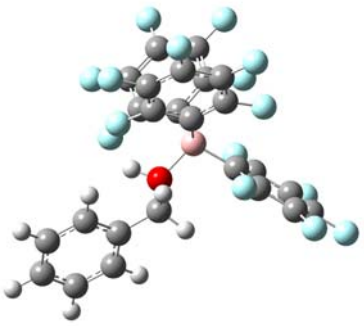


Zero-point correction = 0.446912 (Hartree/Particle)
Thermal correction to Energy = 0.491820
Thermal correction to Enthalpy = 0.492765
Thermal correction to Gibbs Free Energy = 0.357522
Sum of electronic and zero-point Energies = -3087.451454
Sum of electronic and thermal Energies = -3087.406546
Sum of electronic and thermal Enthalpies = -3087.405601
Sum of electronic and thermal Free Energies = -3087.540844

Single point energy = -3088.7545588

C	−0.39953300	−0.57274200	6.21722100
C	−0.03912900	0.07528300	5.03851300
C	−0.93821300	0.14125900	3.97295300
C	−2.20386100	−0.44105000	4.09265400
C	−2.56160100	−1.08777600	5.26953500
C	−1.65900300	−1.15448500	6.33033800
H	0.29948400	−0.61912900	7.04530100
H	0.93893000	0.54199700	4.94879300
H	−2.90883500	−0.37768700	3.26719300
H	−3.54544000	−1.53515600	5.36240500
H	−1.94158500	−1.65794800	7.24900900
C	−0.53130800	0.78892000	2.68570100
H	0.29811300	1.49043800	2.80980000
H	−1.36546100	1.28659800	2.18657600
O	−0.11990300	−0.24787300	1.74176100
H	0.46931700	−0.89704400	2.15714600
B	0.11546700	−0.00270400	0.11737900
C	−1.37849600	0.28389600	−0.41282700
C	0.70075700	−1.44312500	−0.31881400
C	1.13232300	1.24538600	−0.03525600
C	−1.64102000	1.16520700	−1.46724400
C	−2.47421600	−0.40028100	0.13021400
C	1.83974000	−1.98687900	0.29318000
C	0.08326800	−2.22403400	−1.30357600
C	2.45329000	1.10831800	−0.48079800
C	0.71025900	2.54709900	0.27580700
C	−2.93687100	1.35802700	−1.94575200
H	−0.82512000	1.71742000	−1.92885200
C	−3.76824600	−0.19229100	−0.33821900
H	−2.31457300	−1.11613500	0.93492100
C	2.32706200	−3.24641900	−0.04981500
H	2.38593100	−1.41629900	1.04620900
C	0.57773800	−3.47883700	−1.65136000
H	−0.80536200	−1.85274600	−1.80825900
C	3.30932400	2.20479900	−0.57753100
H	2.83165600	0.13212600	−0.77179000
C	1.56788700	3.63972900	0.18587700
H	−0.32026000	2.72601700	0.57824200
C	−4.01780500	0.69030900	−1.38377300
C	−3.13855100	2.31671000	−3.08693400
C	−4.89167100	−0.93143500	0.33127300
C	1.70247200	−4.00845500	−1.02921900
C	3.55151700	−3.75275400	0.65981500
C	−0.13160100	−4.25440700	−2.72807900
C	2.88222700	3.48253900	−0.23881500
C	4.70590800	1.98277700	−1.08962200
C	1.04366200	4.99233900	0.57831500
H	−5.02470700	0.85178500	−1.75068900
F	−2.65224500	3.53658900	−2.79630000
F	−2.49996600	1.90289300	−4.19596200
F	−4.43343100	2.46663900	−3.40448200
F	−6.07740400	−0.70150500	−0.24719800
F	−5.00583900	−0.57189800	1.62975900
F	−4.68942000	−2.26044100	0.32735100
H	2.07896000	−4.98828400	−1.29919500
F	3.89089500	−4.99092000	0.27748400
F	3.36582700	−3.78098100	1.99566600
F	4.61331800	−2.95719200	0.44191500
F	−1.45123200	−4.33980200	−2.48532400
F	0.00133200	−3.66540600	−3.92970900
F	0.33674700	−5.50655600	−2.84394300
H	3.55059300	4.33292400	−0.31100700
F	5.28770100	0.92551700	−0.49526700
F	4.71410500	1.73360000	−2.41179700
F	5.49745300	3.04611900	−0.88237000
F	1.91768000	5.97497100	0.32042800
F	0.76452400	5.04439000	1.89806600
F	−0.09978000	5.28752400	−0.06268800

$PhCh_2OH\text{-}B(C_6F_5)_3$ (**Int-IIIb**)



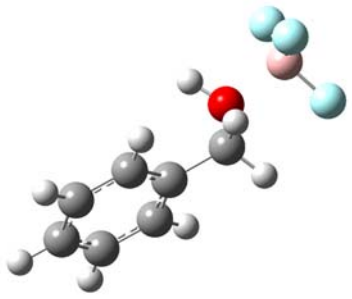
Zero-point correction = 0.295959 (Hartree/Particle)
Thermal correction to Energy = 0.331981
Thermal correction to Enthalpy = 0.332925
Thermal correction to Gibbs Free Energy = 0.225396
Sum of electronic and zero-point Energies = -2553.967130
Sum of electronic and thermal Energies = -2553.931108
Sum of electronic and thermal Enthalpies = -2553.930164
Sum of electronic and thermal Free Energies = -2554.037693

Single point energy = -2554.9772635

C	−5.27392200	−2.12543200	−1.34589500

C	−5.20302200	−2.76688600	−2.57956200
C	−3.97245900	−3.18431300	−3.08446600
C	−2.81146500	−2.96064800	−2.35352100
C	−2.87718800	−2.31685300	−1.11479200
C	−4.11205000	−1.89902700	−0.61340600
C	−1.62219300	−2.02700100	−0.35218400
O	−1.02238400	−0.80109300	−0.89342100
H	−6.23185600	−1.80265400	−0.95295200
H	−6.10894300	−2.94413300	−3.14964800
H	−3.91960100	−3.68605700	−4.04459400
H	−1.84869000	−3.28536300	−2.73917700
H	−4.16051500	−1.39843200	0.34990600
H	−1.80459400	−1.86638200	0.71299600
B	0.13801600	−0.03948700	−0.11558500
C	0.31792400	1.39367200	−0.87070000
C	1.40187500	2.18811000	−0.50099700
C	−0.53544300	1.97868400	−1.79495000
C	0.76872100	3.97864400	−1.95698600
C	1.39748800	−1.05978300	−0.22718100
C	1.53926200	−2.15144200	0.62877700
C	2.39055500	−0.95659300	−1.20027100
C	3.56329600	−2.89302100	−0.40675200
C	−0.38084300	0.29168000	1.39721300
C	0.42526300	0.30092300	2.53383800
C	−1.68520700	0.72870300	1.60859200
C	−1.35274400	1.08881300	3.94482800
C	−0.33513400	3.23840200	−2.34623900
C	1.64809800	3.44809200	−1.02103700
C	3.46224600	−1.83624000	−1.29770500
C	2.58860000	−3.05577400	0.56682300
C	−0.03517400	0.68448900	3.78834700
C	−2.19237900	1.11129100	2.84061300
F	0.98070100	5.18755200	−2.46725000
F	−1.19709400	3.73568100	−3.23171300
F	−1.65224000	1.32894500	−2.21663400
F	2.27283600	1.71428100	0.40184900
F	2.70899900	4.15259100	−0.63477800
F	2.35832900	0.02215800	−2.11593500
F	4.38286700	−1.68007200	−2.24763200
F	4.57520800	−3.74982800	−0.49264500
F	2.66107400	−4.07788900	1.41846400
F	0.61854200	−2.38138400	1.58404800
F	1.70800800	−0.07100500	2.46751700
F	0.77759800	0.66672300	4.84203800
F	−1.80670400	1.45409800	5.13931900
F	−3.46056400	1.50165200	2.96873300
F	−2.54304700	0.79563100	0.56098900
H	−0.85926700	−2.79479000	−0.48404200
H	−1.72277000	−0.19914400	−1.20883200

$PhCH_2OH\text{-}BF_3$ (**Int-IIIc**)

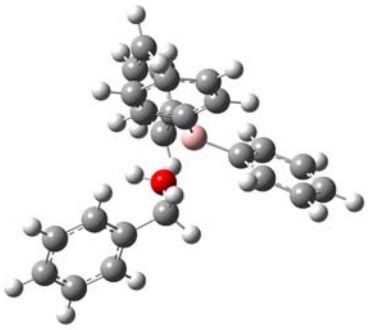


Zero-point correction = 0.150332 (Hartree/Particle)
Thermal correction to Energy = 0.161378
Thermal correction to Enthalpy = 0.162322
Thermal correction to Gibbs Free Energy = 0.111012
Sum of electronic and zero-point Energies = -670.978800
Sum of electronic and thermal Energies = -670.967755
Sum of electronic and thermal Enthalpies = -670.966810
Sum of electronic and thermal Free Energies = -671.018120

Single point energy = -671.3194863

C	3.09314400	−1.29674200	0.09583300
C	3.87495900	−0.17173900	0.35717400
C	3.32417400	1.10160900	0.25336200
C	1.98828700	1.25239900	−0.11154700
C	1.20367300	0.13090400	−0.37973100
C	1.76234800	−1.14666100	−0.27411600
C	−0.23972500	0.28825800	−0.75243500
O	−1.08148400	−0.21113100	0.33015100
B	−2.70603100	−0.03484500	0.12529900
F	−2.96461700	−0.85665100	−0.92795500
F	−2.86252400	1.29884700	−0.14830800
F	−3.18362800	−0.42629200	1.33936700
H	3.52415600	−2.28905500	0.17654000
H	4.91539200	−0.29038300	0.64164900
H	3.93138600	1.97709700	0.45764900
H	1.55407700	2.24511700	−0.19725200
H	1.14712700	−2.01760400	−0.48442100
H	−0.51068200	1.32969200	−0.94082400
H	−0.79435900	0.14194600	1.18679300
H	−0.52931400	−0.32482900	−1.60699700

$PhCH_2OH\text{-}BPh_3$ (**Int-IIId**)



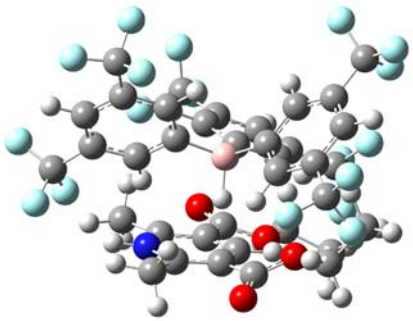
Zero-point correction = 0.417332 (Hartree/Particle)
Thermal correction to Energy = 0.440208
Thermal correction to Enthalpy = 0.441152
Thermal correction to Gibbs Free Energy = 0.362186
Sum of electronic and zero-point Energies = -1065.751122
Sum of electronic and thermal Energies = -1065.728247
Sum of electronic and thermal Enthalpies = -1065.727303
Sum of electronic and thermal Free Energies = -1065.806269

Single point energy = -1066.4413868

C	−4.93775700	0.19756900	0.09462000
C	−5.45739200	0.04915000	−1.18889100
C	−4.68462700	−0.52940300	−2.19409500
C	−3.39223200	−0.96121900	−1.91476700
C	−2.86544700	−0.81539900	−0.62882600
C	−3.64374700	−0.23253600	0.37471900
C	−1.45394200	−1.22739200	−0.33178900
O	−0.54299500	−0.16529100	−0.72719000
H	−5.54068400	0.64499400	0.87774700
H	−6.46676900	0.38265900	−1.40657900
H	−5.09106400	−0.64757900	−3.19301000
H	−2.78501600	−1.41757900	−2.69201900
H	−3.22726900	−0.12083500	1.37327700
H	−1.30869900	−1.40561600	0.73711500
B	0.95092000	0.06960500	0.08772000
C	1.36975800	1.48840800	−0.54660200
C	1.85415400	2.53687200	0.24888900

C	1.27771500	1.72700800	-1.92951200
C	2.12384700	3.97018900	-1.67510500
C	1.81136400	-1.21077600	-0.37332900
C	1.51588200	-2.50253500	0.09824800
C	2.87841900	-1.10259300	-1.27746200
C	3.27336400	-3.48393300	-1.22749000
C	0.54060200	0.13939800	1.64630400
C	1.23905900	-0.54832500	2.64715200
C	-0.52916400	0.94825800	2.06906500
C	-0.19828900	0.33637600	4.37576500
C	1.64102500	2.94923000	-2.49014900
C	2.23429000	3.75859600	-0.30337700
C	3.60265800	-2.21679700	-1.69865600
C	2.22444100	-3.62488500	-0.32215700
C	0.88266400	-0.45050300	3.99325500
C	-0.90766800	1.04229700	3.40472700
H	-1.13945900	-2.10352200	-0.90107300
H	-1.01208500	0.68249000	-0.77882200
H	1.55500200	3.10299900	-3.56179300
H	2.41285400	4.92356800	-2.10668100
H	2.61088100	4.54924000	0.33883700
H	1.93394000	2.39102700	1.32337400
H	0.92543300	0.92868000	-2.58090900
H	-1.08054900	1.53732800	1.33464500
H	-1.74300200	1.67476700	3.69149300
H	-0.48218000	0.40841400	5.42106800
H	1.44955900	-0.99465000	4.74283400
H	2.08235400	-1.17433000	2.36748800
H	0.72188800	-2.63364600	0.83150300
H	3.15388400	-0.12195400	-1.65544800
H	4.42636700	-2.09379700	-2.39565300
H	3.83449300	-4.35388800	-1.55482900
H	1.96562300	-4.60680500	0.06314500

Hantzsch ester–B[3,5-$(CF_3)_2C_6H_3]_3$ (C-H cleavage) **Int-IVa**



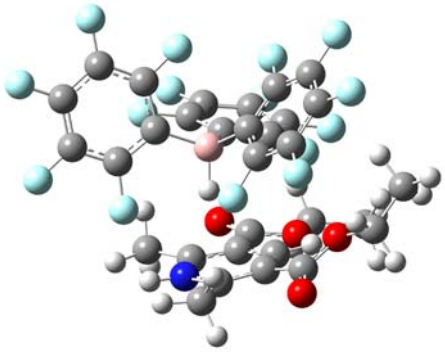
Zero-point correction = 0.624022 (Hartree/Particle)
Thermal correction to Energy = 0.680839
Thermal correction to Enthalpy = 0.681783
Thermal correction to Gibbs Free Energy = 0.526852
Sum of electronic and zero-point Energies = -3602.793011
Sum of electronic and thermal Energies = -3602.736194
Sum of electronic and thermal Enthalpies = -3602.735250
Sum of electronic and thermal Free Energies = -3602.890181

Single point energy = -3604.4144293

B	0.93968300	0.22778800	0.10830800
C	2.05034400	-0.93023900	-0.11673400
C	2.18855800	-1.65649400	-1.30614400
C	2.91155100	-1.28535100	0.93354200
C	3.95060400	-3.03994400	-0.37648400
C	1.47563200	1.74137100	-0.12291900
C	0.66941800	2.79312800	0.33777300
C	2.70050200	2.11459600	-0.68117600
C	2.28159200	4.47939200	-0.28133900
C	-0.44811900	-0.08866500	-0.68981500
C	-1.18542000	0.84014000	-1.43818200
C	-1.00518100	-1.37700700	-0.60167900
C	-2.94642100	-0.76578800	-1.92123500
C	3.83837600	-2.31689900	0.80843000
C	3.12005200	-2.68902100	-1.43289000
C	3.08855600	3.45754500	-0.76172800
C	1.05288000	4.12380500	0.27543300
C	-2.40761400	0.51121500	-2.03202800
C	-2.21996800	-1.70669300	-1.19632700
C	-2.65137300	-0.51288700	1.88964300
C	-3.56423400	0.38789900	1.33227400
C	-1.54485200	-0.07027300	2.61031400
C	-3.33723100	1.75497400	1.46856400
C	-4.76531000	-0.09602300	0.57868400
C	-1.34668000	1.29857600	2.77501200
C	-0.52409200	-1.02864900	3.15301200
N	-2.24807000	2.11987200	2.18729500
C	-4.17038900	2.86437400	0.91417700
O	-4.96896500	-1.39504500	0.76755800
O	-5.46658300	0.62268300	-0.09499000
C	-0.20970600	1.94887600	3.49179600
O	-0.50260000	-2.15673900	2.45806300
O	0.17904900	-0.77247300	4.10229900
H	-2.05960100	3.12019300	2.24938200
H	-4.16319800	2.82275600	-0.17668500
H	-5.21011600	2.74931200	1.22546800
H	-3.78901600	3.83302400	1.24408900
C	-6.12426400	-1.95739700	0.10000300
H	-0.22699800	1.67892200	4.54905500
H	0.73220500	1.57585100	3.07779700
H	-0.24789200	3.03521300	3.37941100
C	0.51291000	-3.12463700	2.82862800
C	-6.27939100	-3.37679500	0.59223600
H	-6.98913100	-1.33332300	0.33802300
H	-5.94682600	-1.90431900	-0.97753000
C	0.69455900	-4.06645700	1.66105000
H	1.43037400	-2.58230000	3.06663200
H	0.16672600	-3.63556300	3.73168000
H	1.39909600	-4.85306100	1.94152400
H	-0.25370300	-4.53010600	1.37652900
H	1.10925700	-3.53676900	0.79760100
H	0.65843300	0.17793000	1.30549300
H	-2.80901400	-1.57846500	1.74948800
C	4.40999000	3.78015600	-1.40169500
C	0.18173700	5.17833900	0.88281500
C	4.66099200	-2.72079300	1.99609900
C	3.17225600	-3.45546900	-2.72345100
C	-3.10828400	1.55075000	-2.85932900
C	-2.71863700	-3.11321100	-1.04364200
H	2.84181000	-0.74783400	1.87797100
H	4.66911200	-3.84597900	-0.47377500
H	1.54699700	-1.42659800	-2.15504600
H	-0.30199100	2.54635200	0.75201800
H	2.59824300	5.51532000	-0.33633400
H	3.37825400	1.34933900	-1.05464800
H	-0.80047800	1.84824000	-1.57798700
H	-0.47467900	-2.14292100	-0.04074800
H	-3.89001600	-1.01662800	-2.39354600
F	-2.44361300	1.81943500	-3.99554500
F	-3.20960700	2.72847000	-2.19750100
F	-4.35204300	1.18635800	-3.20183900
F	-1.89731300	-4.00906400	-1.61011000
F	-2.82241000	-3.46835900	0.25932700
F	-3.93756200	-3.29116600	-1.58838300
H	-7.13646000	-3.83969400	0.09788100
H	-5.38835200	-3.96370100	0.36497200
H	-6.45109200	-3.39410800	1.67085900
F	5.81964200	-3.30232100	1.64709000
F	4.95528100	-1.68226900	2.79468800
F	3.99997700	-3.61816600	2.76696000
F	4.24787900	-4.25654800	-2.80272700
F	2.08723400	-4.24169300	-2.87565600
F	3.20259500	-2.63913200	-3.79203800
F	4.40185800	3.50507700	-2.71928200
F	5.41205900	3.06110300	-0.86651400

F	4.73871400	5.07724400	-1.27305100
F	0.04706200	6.26390700	0.11547300
F	-1.08294400	4.71682200	1.13026300
F	0.64417500	5.59861300	2.07753500

Hantzsch ester–$B(C_6F_5)_3$ (C-H cleavage) **Int-IVb**

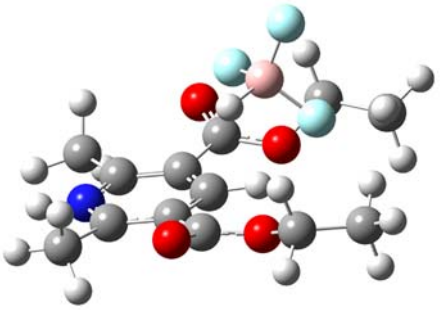


Zero-point correction = 0.473349 (Hartree/Particle)
Thermal correction to Energy = 0.521837
Thermal correction to Enthalpy = 0.522782
Thermal correction to Gibbs Free Energy = 0.391223
Sum of electronic and zero-point Energies = -3069.309745
Sum of electronic and thermal Energies = -3069.261257
Sum of electronic and thermal Enthalpies = -3069.260313
Sum of electronic and thermal Free Energies = -3069.391872

Single point energy = -3070.6430648

B	-0.82174700	-0.18289800	-0.10730700
C	-0.84923400	1.26842600	-0.86688200
C	-0.63477800	1.49051100	-2.22509400
C	-1.08439700	2.42477000	-0.13217600
C	-0.88867500	3.86969300	-2.02725300
C	-2.34714500	-0.74483200	0.03443700
C	-2.95263700	-1.02490700	1.24990700
C	-3.16098900	-0.96146400	-1.07393000
C	-5.02045200	-1.68839600	0.24814000
C	0.22744800	-1.23513200	-0.79376600
C	0.01884200	-2.60096000	-0.96280300
C	1.48439300	-0.80072600	-1.21440900
C	2.16822500	-2.96964700	-1.96166500
C	-1.10760400	3.70510600	-0.66829900
C	-0.64790300	2.75116700	-2.81119800
C	-4.46738500	-1.42161400	-0.99737700
C	-4.25462600	-1.48834700	1.38459400
C	0.94906000	-3.46633500	-1.53193100
C	2.43626300	-1.61801000	-1.80297500
F	-0.89298800	5.08902700	-2.56834800
F	-1.33155600	4.77400000	0.10754300
F	-1.29741600	2.34409400	1.20307900
F	-0.35888100	0.46827000	-3.04755500
F	-0.42008200	2.89932600	-4.11793200
F	-2.66759900	-0.73389200	-2.30033900
F	-5.19591800	-1.61338500	-2.09795600
F	-6.27473900	-2.12835500	0.35110300
F	-4.77048000	-1.73990100	2.59362700
F	-2.27351100	-0.86502900	2.42036300
F	-1.12831100	-3.17622200	-0.55266600
F	0.68225200	-4.76696000	-1.65485000
F	3.08712800	-3.77802300	-2.49412700
F	3.62013400	-1.12415700	-2.18872800
F	1.84088500	0.49105600	-1.04879800
C	2.19666900	0.47798300	1.88330400
C	1.99981600	-0.89334800	2.03861100
C	1.36094000	1.40474200	2.50227800
C	0.90552900	-1.33289900	2.78244700
C	2.89617100	-1.88509700	1.36118000
C	0.34357100	0.95240300	3.33773600
C	1.48196700	2.86868300	2.20941500
N	0.18935500	-0.38608400	3.42812700
C	0.41795300	-2.73853900	2.90716800
O	4.00029100	-1.30910800	0.89555800
O	2.65077100	-3.06652400	1.28066100
C	-0.60696400	1.79873300	4.11856800
O	2.04057400	3.05719400	1.02135500
O	1.09262400	3.74134700	2.94875700
H	-0.63410700	-0.71127400	3.92842500
H	0.08268300	-3.08144900	1.92262900
H	1.22039800	-3.40815700	3.21718000
H	-0.41799600	-2.79645600	3.60685700
C	4.97298200	-2.19886000	0.29622700
H	-0.06560400	2.34884900	4.89148000
H	-1.06767000	2.54005300	3.46441900
H	-1.38458100	1.18301200	4.57508200
C	2.10200500	4.42093700	0.54385100
C	6.11619000	-1.34430500	-0.19617700
H	5.28349500	-2.91633700	1.06121000
H	4.48699400	-2.75186300	-0.51080100
C	2.56453300	4.35702300	-0.89316900
H	1.10591500	4.86001700	0.64686600
H	2.78966700	4.97802700	1.18667900
H	6.87236300	-1.98349400	-0.65734500
H	5.76403400	-0.63034200	-0.94269400
H	6.57936300	-0.80064400	0.63051200
H	2.56694800	5.36068800	-1.32437200
H	3.57338900	3.94415600	-0.96236100
H	1.89189200	3.72599100	-1.48025300
H	-0.41988800	0.02659100	1.00883900
H	2.99297300	0.82723800	1.23436200

Hantzsch ester-BF_3 (C-H cleavage) **Int-IVc**



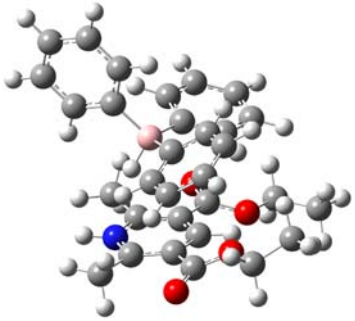
Zero-point correction = 0.326301 (Hartree/Particle)
Thermal correction to Energy = 0.350396
Thermal correction to Enthalpy = 0.351340
Thermal correction to Gibbs Free Energy = 0.271189
Sum of electronic and zero-point Energies = -1186.269039
Sum of electronic and thermal Energies = -1186.244944
Sum of electronic and thermal Enthalpies = -1186.244000
Sum of electronic and thermal Free Energies = -1186.324151

Single point energy = -1186.9368226

O	3.47459800	0.89873400	0.00891900
O	2.27511600	-0.74638600	-0.95713800
O	-3.57990300	0.78948300	0.14551800
O	-2.35600900	-0.82542900	-0.83921100
N	-0.08712600	3.15550700	0.00819000
C	1.13261100	2.57404500	-0.12772900
C	1.15100400	1.22104200	-0.42577600
C	-0.05578200	0.53255500	-0.54809000
H	-0.03898900	-0.54182300	-0.72112500

C	−1.27735800	1.17815500	−0.35895800
C	−1.29008300	2.53410400	−0.06269000
C	2.32536100	3.44678300	0.09690300
H	3.05935200	3.30489200	−0.69658000
H	2.81810700	3.15070700	1.02640100
H	2.03639100	4.49959800	0.14824700
C	−2.49925100	3.36842600	0.21651500
H	−2.23819500	4.42809500	0.27309200
H	−2.95165300	3.04766100	1.15792400
H	−3.25581700	3.21749500	−0.55397600
C	2.44018500	0.45199800	−0.43429400
C	3.29112100	−1.72564400	−0.64050600
C	−2.54368200	0.37306900	−0.32438700
C	−3.36221600	−1.82051200	−0.54288900
H	−4.30491100	−1.50331100	−0.99767400
H	−3.48187300	−1.84221400	0.54408700
C	−2.85020100	−3.13432800	−1.08440100
H	−2.72430700	−3.08281200	−2.16879200
H	−3.56800100	−3.92589500	−0.85625400
H	−1.89061600	−3.37034600	−0.61996200
C	2.77728300	−3.05970800	−1.12818200
H	1.82996300	−3.28610600	−0.63435900
H	3.50481800	−3.83923000	−0.88919100
H	2.62784600	−3.04596900	−2.21082600
H	3.42208400	−1.70844300	0.44465300
H	4.22523300	−1.42106700	−1.12111900
H	−0.09721400	4.14495000	0.23558400
B	−0.08322100	−1.53772700	1.64897600
F	1.06943100	−0.67754700	1.62251900
F	−0.05507100	−2.28680000	0.42407200
F	0.00974200	−2.40759000	2.72838300
H	−1.10750500	−0.84979400	1.68508500

Hantzsch ester-BPh_3 (C-H cleavage) **Int-IVd**



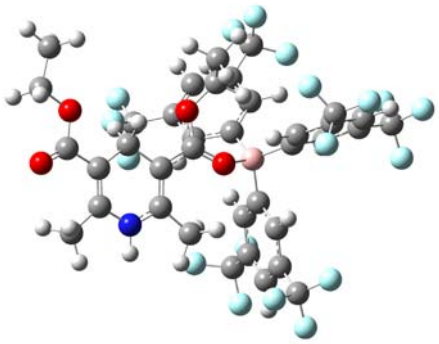
Zero-point correction = 0.592457 (Hartree/Particle)
Thermal correction to Energy = 0.627926
Thermal correction to Enthalpy = 0.628870
Thermal correction to Gibbs Free Energy = 0.523630
Sum of electronic and zero-point Energies = -1581.061457
Sum of electronic and thermal Energies = -1581.025988
Sum of electronic and thermal Enthalpies = -1581.025044
Sum of electronic and thermal Free Energies = -1581.130284

Single point energy = -1582.0703963

B	1.58584700	−0.01829600	−0.21455700
C	1.08536400	−1.43103500	−0.85502300
C	0.78830200	−1.63681700	−2.21246000
C	1.01368000	−2.57492100	−0.04048100
C	0.33490200	−3.98965000	−1.87085500
C	3.21103700	0.04623300	−0.15620800
C	3.88821800	0.51195300	0.98031700
C	4.01474100	−0.31053800	−1.25119900
C	6.04248000	0.27067600	−0.07411700
C	0.97428900	1.32004600	−0.93135400
C	1.62645300	2.56227200	−0.80741000
C	−0.22920400	1.33849000	−1.66048200
C	−0.05543000	3.70869800	−2.10828100
C	0.64589600	−3.83049900	−0.51984300
C	0.41922100	−2.88580100	−2.71604700
C	5.40258500	−0.20338000	−1.21831100
C	5.27701000	0.62985800	1.03099000
C	1.12642700	3.73469500	−1.37054500
C	−0.73031000	2.49912600	−2.25293600
C	−1.87510600	0.02484200	0.99805600
C	−1.36019700	1.24631600	1.42170800
C	−1.49669400	−1.17454000	1.59744700
C	−0.38116700	1.24800500	2.41190100
C	−1.81995300	2.53448300	0.81067500
C	−0.62248400	−1.14212800	2.67882600
C	−2.00385000	−2.48653500	1.08265300
N	−0.13174300	0.06745200	3.02436300
C	0.45451800	2.41326000	2.81898900
O	−2.90711700	2.35285200	0.06188600
O	−1.31237800	3.60662300	1.03522000
C	−0.15896500	−2.31523700	3.48003500
O	−2.48626100	−2.36689500	−0.14475300
O	−1.98309600	−3.51063000	1.72798600
H	0.60289300	0.07386600	3.72570800
H	1.01335400	2.74052400	1.93363400
H	−0.16113000	3.25477600	3.13734800
H	1.15432300	2.13164900	3.60912700
C	−3.44009700	3.54121100	−0.55688500
H	−0.99463400	−2.74399500	4.03742000
H	0.20587000	−3.09907900	2.81428600
H	0.63524400	−2.02198000	4.17028400
C	−2.95249400	−3.58591400	−0.76358700
C	−4.53932200	3.09729600	−1.49374000
H	−3.80816800	4.20065300	0.23498700
H	−2.62273100	4.04687000	−1.07542300
C	−3.27089000	−3.25768100	−2.20268600
H	−2.15505700	−4.32752200	−0.67707500
H	−3.82511400	−3.93747800	−0.20453400
H	−3.62715700	−4.15663700	−2.71158800
H	−4.04791300	−2.49215700	−2.26796700
H	−2.37104800	−2.90020100	−2.70863800
H	1.21574100	−0.00586000	0.96336900
H	−2.57242800	0.00540400	0.16770500
H	1.29645100	−2.46918900	1.00740700
H	0.04921100	−4.96304400	−2.26070900
H	0.85211900	−0.79496200	−2.89915400
H	3.30053700	0.79999000	1.85404900
H	7.12481200	0.35553100	−0.04450200
H	3.53526600	−0.69017400	−2.15239800
H	2.57253900	2.59971100	−0.26904900
H	−0.78148700	0.40823700	−1.79203600
H	−0.43814800	4.61514500	−2.56927500
H	−4.98009000	3.96798400	−1.98445100
H	−4.14014000	2.43071000	−2.26199500
H	−5.32697500	2.57058600	−0.94984100
H	1.66716400	4.66925800	−1.24825000
H	−1.64932000	2.45495700	−2.83498100
H	0.60921400	−4.68493500	0.15245100
H	0.20486300	−2.99960500	−3.77615700
H	5.98986000	−0.49077500	−2.08654100
H	5.76212400	0.99874600	1.93143300

Hantzsch ester–B[3,5-$(CF_3)_2C_6H_3]_3$ (B-O)

Int-Va

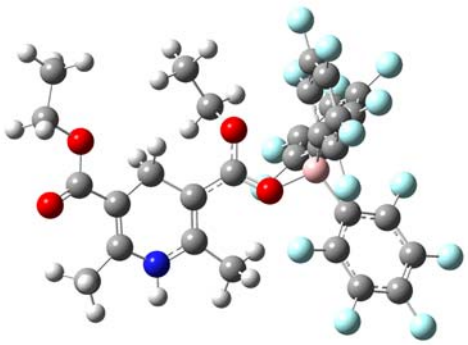


Zero-point correction = 0.625981 (Hartree/Particle)
Thermal correction to Energy = 0.683236
Thermal correction to Enthalpy = 0.684180
Thermal correction to Gibbs Free Energy = 0.522934
Sum of electronic and zero-point Energies = -3602.807927
Sum of electronic and thermal Energies = -3602.750672
Sum of electronic and thermal Enthalpies = -3602.749728
Sum of electronic and thermal Free Energies = -3602.910974

Single point energy = -3604.4264144

C	2.82496600	0.62313200	0.88029400
C	2.74032800	1.99475300	0.93454200
N	3.87849300	2.71554700	1.11390800
C	5.15007700	2.17228600	1.32991300
C	5.30079300	0.83483700	1.27244300
C	4.15871800	-0.09865400	0.94606800
C	1.49558900	2.82335800	0.81985800
C	6.21412200	3.19396700	1.61423200
C	6.63226300	0.24356000	1.51416200
O	6.59907700	-1.09449200	1.38896700
O	7.64751300	0.85109100	1.79129600
C	7.84830800	-1.77342400	1.60101900
C	7.59379900	-3.25141200	1.40910000
C	1.65626000	-0.19352300	0.74281600
O	1.94932400	-1.46517700	0.59242100
O	0.47044200	0.26210400	0.78952500
C	1.01678900	-2.56042300	0.75289300
C	1.46790400	-3.38657700	1.93812800
H	3.79394700	3.72048300	1.15115000
H	4.35750300	-0.61683100	-0.00158700
H	4.11184900	-0.89552800	1.69659800
H	0.96034800	2.59752400	-0.10397000
H	0.81023600	2.60881800	1.64223100
H	1.73877600	3.88804000	0.83361000
H	6.64315000	3.03878900	2.60543700
H	7.03677100	3.10270800	0.90413300
H	5.80155200	4.20470400	1.55753100
H	8.58123400	-1.38316100	0.88955900
H	8.20435100	-1.54133300	2.60880600
H	8.52178300	-3.80842100	1.55726700
H	6.85468200	-3.61316500	2.12757400
H	7.22612200	-3.45159300	0.40021600
H	0.00909800	-2.17701900	0.88984500
H	1.06068600	-3.11720300	-0.18572500
H	0.80821000	-4.25107900	2.04623900
H	2.49149800	-3.74100800	1.79849100
H	1.41711500	-2.80188700	2.86050700
B	-0.88513600	-0.00659500	-0.03755700
C	-1.93542800	-0.66755600	0.99875000
C	-0.49244900	-0.90059000	-1.33042300
C	-1.37825800	1.49455700	-0.41963200
C	-3.26044800	-0.90054200	0.60201400
C	-1.61695800	-0.97279600	2.32571400
C	0.62817900	-0.56044300	-2.10019900
C	-1.20468200	-2.03707500	-1.73147500
C	-1.39025600	2.01338300	-1.71692600
C	-1.77669700	2.35904500	0.61139700
C	-4.19790900	-1.44834200	1.47319300
H	-3.57526800	-0.64437500	-0.40890400
C	-2.56004400	-1.51344100	3.19967700
H	-0.61158200	-0.78323000	2.69729600
C	1.03094400	-1.32569500	-3.19243900
H	1.21763800	0.32066200	-1.84286800
C	-0.81206900	-2.79189900	-2.83537800
H	-2.07651600	-2.36159200	-1.16827900
C	-1.75456700	3.33925500	-1.96651500
H	-1.11078100	1.38555600	-2.55972800
C	-2.12281200	3.68200900	0.36256100
H	-1.80640900	1.99177900	1.63636800
C	-3.86042700	-1.76598300	2.78573600
C	-5.59342500	-1.68145700	0.96446900
C	-2.12420000	-1.82421800	4.60243100
C	0.31505600	-2.45343000	-3.57632100
C	2.26844400	-0.90590900	-3.93333800
C	-1.59214300	-4.03164900	-3.17359300
C	-2.11348700	4.19303800	-0.93332000
C	-1.71729000	3.83231900	-3.38560400
C	-2.45385300	4.56892400	1.52853300
H	-4.59104000	-2.19202400	3.46321400
F	-6.19898300	-0.52767100	0.63062900
F	-5.59186300	-2.44768300	-0.14228900
F	-6.37169800	-2.29177800	1.87143400
F	-3.10376800	-2.36062800	5.34253000
F	-1.69267700	-0.72283000	5.24566000
F	-1.09194900	-2.69484700	4.61536300
H	0.62327500	-3.04723000	-4.42916700
F	2.55526400	-1.71919600	-4.95952300
F	3.34525600	-0.89523100	-3.11943700
F	2.15586100	0.34070900	-4.42545700
F	-1.31735600	-5.03171700	-2.30984400
F	-2.91635600	-3.82295900	-3.10935100
F	-1.31278200	-4.48963100	-4.40326200
H	-2.38959000	5.22258300	-1.13002400
F	-0.46238300	3.81534400	-3.87860000
F	-2.45665100	3.06201200	-4.20196300
F	-2.16943700	5.09070700	-3.50337400
F	-2.99360300	5.73739700	1.15197800
F	-1.34305600	4.86280600	2.24300600
F	-3.30871400	3.98416200	2.38230700

Hantzsch ester-$B(C_6F_5)_3$ (B-O) **IntVb**

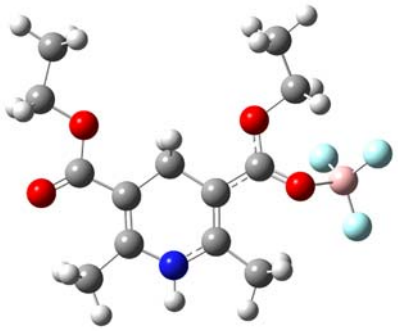


Zero-point correction = 0.474199 (Hartree/Particle)
Thermal correction to Energy = 0.522747
Thermal correction to Enthalpy = 0.523691
Thermal correction to Gibbs Free Energy = 0.389392
Sum of electronic and zero-point Energies = -3069.310682
Sum of electronic and thermal Energies = -3069.262133
Sum of electronic and thermal Enthalpies = -3069.261189
Sum of electronic and thermal Free Energies = -3069.395488

Single point energy = -3070.6387796

C	2.31770100	0.96219100	−0.85390400
C	2.17804800	2.29164500	−1.17769800
N	3.30382300	3.04669100	−1.31592300
C	4.57268600	2.65316200	−0.87536000
C	4.76794900	1.35717400	−0.56107500
C	3.69189400	0.32201600	−0.79441700
C	0.90000900	3.04651800	−1.39180800
C	5.57288800	3.76920200	−0.78451200
C	6.07989700	0.90807900	−0.05790100
O	6.11491300	−0.43043000	0.08112400
O	7.02936800	1.61917500	0.20237800
C	7.35050600	−0.97596400	0.57499500
C	7.17117100	−2.47444500	0.66999700
C	1.17332900	0.18688700	−0.47880000
O	1.22215500	−1.12527200	−0.40959900
O	0.09949200	0.73267600	−0.09592900
C	1.75599400	−1.94545200	−1.47895000
C	2.68870400	−2.98609900	−0.90376900
H	3.18129800	4.02076100	−1.55357400
H	3.93247000	−0.23867500	−1.70959600
H	3.71526900	−0.40991600	0.01723700
H	0.12267900	2.41078500	−1.81040000
H	0.54093100	3.42959900	−0.43250500
H	1.07881600	3.88836400	−2.06600300
H	5.80980500	3.98426600	0.25983800
H	6.51047200	3.49149500	−1.26494100
H	5.18033000	4.67545200	−1.25289300
H	8.15354600	−0.69677900	−0.11260700
H	7.56772000	−0.52182700	1.54556200
H	8.08905500	−2.93459800	1.04238600
H	6.35771400	−2.72384500	1.35528900
H	6.94499400	−2.89971800	−0.31060900
H	0.87466200	−2.41345900	−1.92757200
H	2.22641700	−1.30218800	−2.22621800
H	2.97705300	−3.68431200	−1.69311800
H	3.59480500	−2.53697900	−0.49043400
H	2.17640100	−3.54645100	−0.11855100
B	−1.27004400	0.02927600	0.16896000
C	−2.27242800	1.32668600	0.32385400
C	−1.09470500	−0.88207300	1.52811300
C	−1.67781700	−0.85918800	−1.15397600
C	−3.60216000	1.33819200	−0.09500300
C	−1.83812100	2.54843800	0.84939100
C	−0.70494700	−2.22600600	1.51577800
C	−1.27447500	−0.36605800	2.81285100
C	−2.61466200	−1.89114700	−1.07197000
C	−1.18687200	−0.64988000	−2.43614800
C	−4.42854000	2.45651600	−0.03795800
F	−4.18351900	0.23458700	−0.58922300
C	−2.62479500	3.68889600	0.91567600
F	−0.60399700	2.68527600	1.36562700
C	−0.49559900	−2.98646200	2.65722200
F	−0.52067300	−2.89614400	0.36378300
C	−1.08224600	−1.09471700	3.98223500
F	−1.65717700	0.90437900	3.00393900
C	−3.02014000	−2.66068100	−2.15018500
F	−3.18040900	−2.18363600	0.10543700
C	−1.55734900	−1.39652900	−3.55045300
F	−0.26084400	0.31009100	−2.68194600
C	−3.93528800	3.64680500	0.46516300
F	−5.68823600	2.38797800	−0.47024000
F	−2.13164300	4.82398300	1.41906300
C	−0.68340800	−2.41714500	3.90645500
F	−0.11379900	−4.26269500	2.55945800
F	−1.27312100	−0.52501000	5.17301200
C	−2.48472000	−2.41234000	−3.40742100
F	−3.91882200	−3.63205500	−1.99630400
F	−1.01882400	−1.14008900	−4.74613200
F	−4.70451600	4.73147800	0.52209300
F	−0.48559400	−3.13141800	5.01157300
F	−2.85809400	−3.14047100	−4.45691000

Hantzsch ester-BF_3 (B-O) **Int-Vc**

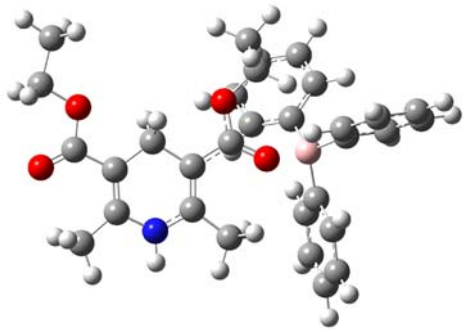


Zero-point correction = 0.328821 (Hartree/Particle)
Thermal correction to Energy = 0.352331
Thermal correction to Enthalpy = 0.353275
Thermal correction to Gibbs Free Energy = 0.274328
Sum of electronic and zero-point Energies = -1186.333760
Sum of electronic and thermal Energies = -1186.310250
Sum of electronic and thermal Enthalpies = -1186.309306
Sum of electronic and thermal Free Energies = -1186.388253

Single point energy = -1186.9902829

C	−0.32406300	−0.58333800	−0.16632900
C	−0.40841900	−1.95255600	−0.20143600
N	0.74288400	−2.67998300	−0.12465100
C	2.02807500	−2.13854600	−0.05580300
C	2.17186700	−0.79840600	−0.00229800
C	0.99193600	0.14651700	0.01066400
C	−1.65719300	−2.77852200	−0.32035800
C	3.12615600	−3.16409200	−0.05190000
C	3.52576100	−0.21763900	0.06305600
O	3.47642100	1.12670800	0.10548600
O	4.57505500	−0.83217800	0.08023200
C	4.74569900	1.79518100	0.17079300
C	4.46889800	3.28162800	0.20004500
C	−1.51081700	0.21004600	−0.25789900
O	−1.31253700	1.49405400	−0.08732400
O	−2.65102000	−0.27006000	−0.53405300
C	−2.39770300	2.43931300	−0.28826000
C	−1.75840700	3.79326200	−0.48974800
H	0.66304500	−3.68530400	−0.14585600
H	0.98391700	0.72192800	0.94556300
H	1.11214800	0.89869300	−0.77780100
H	−2.38223100	−2.52063900	0.45303300
H	−2.15374800	−2.59124900	−1.27441700
H	−1.41470600	−3.84121300	−0.24523800
H	3.81076400	−3.00100700	−0.88518400
H	3.72409300	−3.08614900	0.85735500
H	2.70975000	−4.17246200	−0.12163000
H	5.27442500	1.45463800	1.06574600
H	5.34038800	1.50207700	−0.69898500
H	5.41080300	3.83297200	0.24769000
H	3.93071700	3.59127500	−0.69871700
H	3.86783300	3.54570200	1.07294700
H	−2.98104900	2.11336100	−1.15167500
H	−3.03555900	2.40254700	0.59549800
H	−2.54062600	4.54254000	−0.63034600
H	−1.16274200	4.07444000	0.38129600
H	−1.11429200	3.79415400	−1.37197300
B	−3.99487500	−0.12000800	0.29953300
F	−4.47605600	−1.40277100	0.37615400
F	−4.81453700	0.73339100	−0.39419300
F	−3.59638900	0.38475000	1.52689200

Hantzsch ester-BPh_3 (B-O) **Int-Vd**

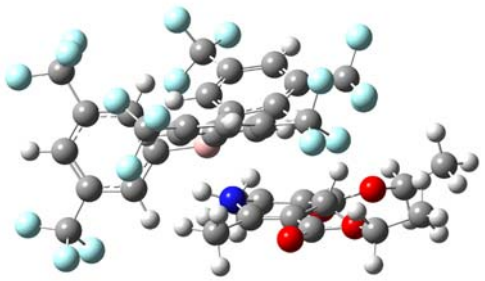


Zero-point correction = 0.595625 (Hartree/Particle)
Thermal correction to Energy = 0.631083
Thermal correction to Enthalpy = 0.632027
Thermal correction to Gibbs Free Energy = 0.526014
Sum of electronic and zero-point Energies = -1581.101345
Sum of electronic and thermal Energies = -1581.065887
Sum of electronic and thermal Enthalpies = -1581.064943
Sum of electronic and thermal Free Energies = -1581.170957

Single point energy = -1582.10 60345

C	−1. 47645200	0. 60309500	−0. 35541000
C	−1. 37606500	1. 96434200	−0. 42184500
N	−2. 52344200	2. 71466500	−0. 40797300
C	−3. 81370500	2. 19544900	−0. 36321400
C	−3. 97918500	0. 85789300	−0. 28650400
C	−2. 81345300	−0. 10313900	−0. 23120000
C	−0. 11657100	2. 77377300	−0. 50994900
C	−4. 89808200	3. 23468800	−0. 40989000
C	−5. 34043900	0. 29885500	−0. 24243200
O	−5. 31291600	−1. 04702100	−0. 17861300
O	−6. 38335400	0. 92595300	−0. 25715700
C	−6. 59233000	−1. 69438900	−0. 12967200
C	−6. 33864200	−3. 18457700	−0. 07763200
C	−0. 29630000	−0. 23418800	−0. 37279700
O	−0. 60045600	−1. 50308300	−0. 20448500
O	0. 86555600	0. 20398600	−0. 55890600
C	0. 34276000	−2. 59150200	−0. 33595600
C	−0. 25555200	−3. 59032800	−1. 30327300
H	−2. 42458000	3. 71683100	−0. 45770500
H	−2. 84819700	−0. 68061700	0. 70175400
H	−2. 91569500	−0. 85452200	−1. 02341600
H	0. 53553800	2. 58659900	0. 34631400
H	0. 46222800	2. 50289900	−1. 39397000
H	−0. 34860200	3. 84092400	−0. 54843000
H	−5. 56248000	3. 06215900	−1. 25756800
H	−5. 52116600	3. 18348600	0. 48421000
H	−4. 46640300	4. 23590700	−0. 48982600
H	−7. 13328500	−1. 33618400	0. 75114100
H	−7. 16739200	−1. 40365200	−1. 01342700
H	−7. 28902300	−3. 72209900	−0. 03993800
H	−5. 78906700	−3. 51253800	−0. 96298700
H	−5. 75620600	−3. 44642000	0. 80853500
H	1. 30028200	−2. 21306700	−0. 68749500
H	0. 46888600	−3. 00294300	0. 66787900
H	0. 40146800	−4. 46039600	−1. 37602300
H	−1. 23952300	−3. 92213200	−0. 96375800
H	−0. 35648900	−3. 15014000	−2. 29875800
B	2. 37552700	−0. 03063700	0. 13787400
C	3. 27817400	−0. 71858000	−1. 00438400
C	2. 09118700	−0. 89215700	1. 47650300
C	2. 84081100	1. 49724500	0. 40323400
C	4. 64482600	−0. 92315700	−0. 74838700
C	2. 81935500	−1. 06844500	−2. 28119800
C	1. 02153400	−0. 55099700	2. 32109000
C	2. 84617300	−2. 01493900	1. 84352000
C	2. 87746200	2. 09080800	1. 67161300
C	3. 16854000	2. 31506700	−0. 69158400
H	5. 05130000	−0. 62519300	0. 21696700
C	5. 49735600	−1. 47695500	−1. 69796700
H	1. 77468200	−0. 89656100	−2. 53604600
C	3. 66542100	−1. 61766300	−3. 24568000
H	0. 41228000	0. 32300200	2. 08478100
C	0. 69818600	−1. 29877000	3. 45056600
H	3. 67558700	−2. 32686800	1. 21382000
C	2. 54376500	−2. 76481900	2. 97983200
H	2. 65533300	1. 48852300	2. 54886900
C	3. 18749200	3. 44205400	1. 83985700
H	3. 17591200	1. 87669900	−1. 68851200
C	3. 46766700	3. 66477000	−0. 53872900
C	5. 00806100	−1. 83110400	−2. 95430600
H	6. 54754600	−1. 62475900	−1. 46330400
H	3. 27462300	−1. 87328700	−4. 22666300
C	1. 46172000	−2. 41545000	3. 78349000
H	−0. 14630400	−1. 01106700	4. 06995100
H	3. 14800400	−3. 63161600	3. 23185400
C	3. 47046700	4. 23635500	0. 73374800
H	3. 20809800	3. 87244400	2. 83719200
H	3. 70783800	4. 27150800	−1. 40740900
H	5. 67118700	−2. 25839300	−3. 70016400
H	1. 21656500	−3. 00450800	4. 66183600
H	3. 70778600	5. 28841100	0. 86134400

Hantzsch ester-$B[3,5\text{-}(CF_3)_2C_6H_3]_3$ (B-N) **Int-VIa**



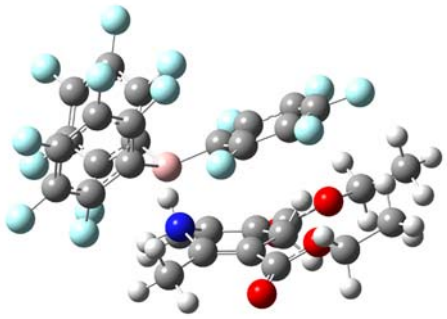
Zero-point correction = 0.629616 (Hartree/Particle)
Thermal correction to Energy = 0.685878
Thermal correction to Enthalpy = 0.686823
Thermal correction to Gibbs Free Energy = 0.533670
Sum of electronic and zero-point Energies = -3602.662161
Sum of electronic and thermal Energies = -3602.605899
Sum of electronic and thermal Enthalpies = -3602.604954
Sum of electronic and thermal Free Energies = -3602.758107

Single point energy = -3604.408933

C	−2. 29557800	−1. 20990000	−1. 83704900
C	−0. 96486200	−1. 19372700	−1. 97079500
N	−0. 24444300	0. 04476100	−1. 70793900
C	−0. 98508700	1. 28345200	−1. 90193100
C	−2. 31518800	1. 27428100	−1. 74806700
C	−3. 08885500	0. 01505500	−1. 47852000
C	−0. 06990700	−2. 34565300	−2. 32251400
C	−0. 11196500	2. 46307900	−2. 21811000
C	−3. 05695800	2. 56544200	−1. 73334600
O	−4. 36016100	2. 36543400	−1. 50947900
O	−2. 56205500	3. 66363500	−1. 85848100
C	−5. 14227200	3. 55162400	−1. 29085600
C	−6. 46802700	3. 10447200	−0. 71813100
C	−3. 02980400	−2. 49758100	−1. 98561700
O	−4. 24779900	−2. 40431200	−1. 43911900

O	−2.60317800	−3.49958900	−2.51238900
C	−5.06842600	−3.58229700	−1.52636300
C	−6.26666600	−3.35135400	−0.63446700
H	−3.42437100	−0.02481000	−0.43048300
H	−4.01804300	0.03037400	−2.05404200
H	−0.35401200	−3.23653000	−1.76097800
H	−0.16963900	−2.59463800	−3.38250200
H	0.97307500	−2.10764400	−2.10074200
H	−0.39963800	2.90159800	−3.17621600
H	−0.23518600	3.24373400	−1.46508000
H	0.94105700	2.16823000	−2.25119500
H	−4.59649500	4.20382000	−0.60485400
H	−5.25211200	4.07765000	−2.24414100
H	−7.10838700	3.97098100	−0.53860000
H	−6.98172700	2.42802300	−1.40494600
H	−6.30742800	2.58678700	0.23011700
H	−5.34836800	−3.72896200	−2.57459000
H	−4.47764300	−4.44450600	−1.21230500
H	−6.92409700	−4.22327300	−0.66082600
H	−5.93832800	−3.18980500	0.39388100
H	−6.83375000	−2.47732400	−0.96258700
H	0.54042800	0.07260400	−2.35740400
B	0.70461200	0.00694400	−0.09922500
C	2.27207300	−0.06294500	−0.51490100
C	0.21042700	−1.35541500	0.63737500
C	0.33773600	1.41961600	0.62003200
C	3.17617200	−0.07324200	0.56482000
C	2.85102200	−0.11871600	−1.78481800
C	−1.12984300	−1.57178500	1.00333100
C	1.08092800	−2.42507200	0.87124600
C	−0.96801900	1.75219400	1.01841300
C	1.29092500	2.43483100	0.76829100
C	4.55101000	−0.13617700	0.38324700
H	2.79034500	−0.02713300	1.58225400
C	4.23382100	−0.18195100	−1.97256100
H	2.25941900	−0.13419900	−2.69956500
C	−1.57350400	−2.77802600	1.52218300
H	−1.87581700	−0.80613000	0.84271700
C	0.64670900	−3.62809700	1.43428100
H	2.12864800	−2.35062900	0.59496700
C	−1.30988400	3.02410600	1.45718000
H	−1.77366200	1.03454400	0.93173300
C	0.96086900	3.70057000	1.25461800
H	2.32226600	2.26404300	0.47464900
C	5.10159700	−0.19141700	−0.89380500
C	5.43241700	−0.16776200	1.60169300
C	4.75767100	−0.21010100	−3.38045600
C	−0.68496900	−3.82606900	1.75439600
C	−3.03335000	−3.00495200	1.78625700
C	1.66185700	−4.70964800	1.67506200
C	−0.34590700	4.02068800	1.58410700
C	−2.73704600	3.32803700	1.80914400
C	2.04414300	4.73891400	1.32472300
H	6.17387900	−0.24305000	−1.03906600
F	5.13788400	0.83759700	2.43663300
F	5.26662600	−1.30688900	2.28754000
F	6.72863500	−0.06979500	1.28268300
F	6.05672600	−0.51931400	−3.42847100
F	4.60086800	0.97811200	−3.98334800
F	4.09177600	−1.10843700	−4.12454700
H	−1.02696200	−4.77227300	2.15985900
F	−3.25831700	−3.40224200	3.04423300
F	−3.51947600	−3.97376300	0.98504900
F	−3.77156300	−1.90770000	1.56585400
F	2.40429400	−4.93045000	0.57969100
F	2.50901200	−4.37399900	2.65714400
F	1.08597900	−5.86924500	2.01719200
H	−0.61056400	5.01829100	1.91629100
F	−3.58921000	2.51179200	1.15547000
F	−2.98098000	3.17970500	3.11685200
F	−3.06922000	4.58594700	1.48591100
F	1.63861600	5.84608500	1.95873100
F	2.44439900	5.10252300	0.09559900
F	3.12630200	4.27384900	1.96251200

Hantzsch ester-B(C_6F_5)$_3$ (B-N) **Int-VIb**



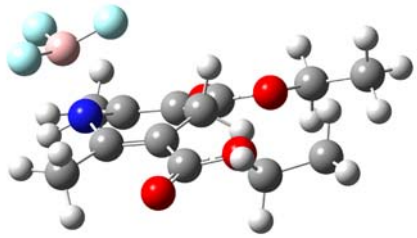
Zero-point correction = 0.476782 (Hartree/Particle)
Thermal correction to Energy = 0.524219
Thermal correction to Enthalpy = 0.525163
Thermal correction to Gibbs Free Energy = 0.396909
Sum of electronic and zero-point Energies = -3069.299851
Sum of electronic and thermal Energies = -3069.252415
Sum of electronic and thermal Enthalpies = -3069.251470
Sum of electronic and thermal Free Energies = -3069.379724

Single point energy = -3070.6297629

C	−1.91083300	−1.23908600	−1.75218000
C	−0.60729400	−1.23979700	−2.05735700
N	0.16680700	0.00003500	−1.80732300
C	−0.60724800	1.23992900	−2.05726900
C	−1.91077100	1.23925200	−1.75208200
C	−2.67218700	0.00009000	−1.39267900
C	0.16644200	−2.39863100	−2.60879100
C	0.16653800	2.39877100	−2.60863000
C	−2.68962500	2.51849700	−1.69302400
O	−3.69135000	2.37799000	−0.81374400
O	−2.47312400	3.54634300	−2.29162400
C	−4.48577300	3.55404500	−0.56244600
C	−5.59754700	3.14723000	0.37750400
C	−2.68980600	−2.51825300	−1.69325100
O	−3.69160100	−2.37771500	−0.81404400
O	−2.47340000	−3.54607900	−2.29192600
C	−4.48608000	−3.55375700	−0.56288000
C	−5.59765500	−3.14711800	0.37737600
H	−2.98423900	0.00005000	−0.34616300
H	−3.61472200	0.00014200	−1.95447700
H	0.68964000	−2.94165800	−1.81631200
H	−0.51501100	−3.08840600	−3.09677300
H	0.90545800	−2.05368000	−3.33426300
H	−0.51485800	3.08859600	−3.09660500
H	0.68976400	2.94174000	−1.81612300
H	0.90555000	2.05381900	−3.33410700
H	−3.83269000	4.31638500	−0.12792700
H	−4.86084800	3.92990700	−1.51782300
H	−6.21605500	4.01629600	0.61314100
H	−6.23208800	2.38523600	−0.08099500
H	−5.18715400	2.75126700	1.30893600
H	−4.86141600	−3.92931300	−1.51828200
H	−3.83297500	−4.31630400	−0.12876100
H	−6.21597700	−4.01628500	0.61311800
H	−5.18710700	−2.75116100	1.30874100
H	−6.23242300	−2.38518600	−0.08091200
H	0.97559500	0.00004000	−2.43725200
B	0.86425400	−0.00000100	−0.19777800
C	−0.45556300	0.00000200	0.75268200
C	1.87290800	1.28335400	0.00709500
C	1.87280700	−1.28340600	0.00716700
C	−1.09385400	−1.17171000	1.15756800
C	−1.09385200	1.17170100	1.15759400

C	2.76561500	1.74953800	-0.95532600
C	2.06785700	1.85085100	1.26949900
C	2.06771500	-1.85087700	1.26958200
C	2.76547900	-1.74966900	-0.95523900
C	-2.24983400	-1.19657700	1.92566000
F	-0.61928600	-2.37271400	0.78631700
C	-2.24985200	1.19655800	1.92566700
F	-0.61930300	2.37269300	0.78626300
C	3.72312800	2.72957200	-0.73528600
F	2.72790400	1.25474700	-2.21065400
C	3.01516600	2.83023900	1.54104900
F	1.33484300	1.45535800	2.31844600
C	3.01488400	-2.83039700	1.54113000
F	1.33474100	-1.45526000	2.31851200
C	3.72287500	-2.72981600	-0.73520600
F	2.72784900	-1.25476600	-2.21052300
C	-2.83549700	-0.00001300	2.31291200
F	-2.81484700	-2.35590900	2.26502600
F	-2.81493300	2.35586700	2.26500700
C	3.85019100	3.27978200	0.53015000
F	4.51789200	3.13391800	-1.72545800
F	3.13195800	3.33178200	2.76874200
C	3.84985600	-3.28004400	0.53023000
F	3.13162900	-3.33195200	2.76882600
F	4.51762000	-3.13422500	-1.72536700
F	-3.95532800	-0.00002200	3.03071800
F	4.76314400	4.21444700	0.77126700
F	4.76270500	-4.21480700	0.77136400

Hantzsch ester-BF_3 (B-N) **Int-VIc**



Zero-point correction = 0.328453 (Hartree/Particle)
Thermal correction to Energy = 0.352326
Thermal correction to Enthalpy = 0.353271
Thermal correction to Gibbs Free Energy = 0.272664
Sum of electronic and zero-point Energies = -1186.322738
Sum of electronic and thermal Energies = -1186.298865
Sum of electronic and thermal Enthalpies = -1186.297921
Sum of electronic and thermal Free Energies = -1186.378527

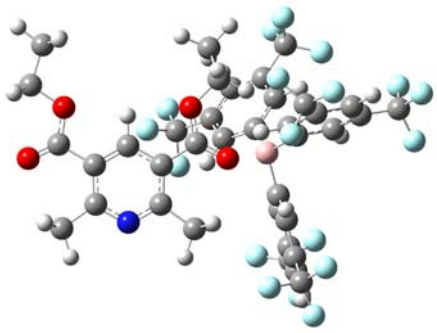
Single point energy = -1186.9794622

C	0.05978800	-1.24347300	-0.33468300
C	1.35521800	-1.24332500	-0.67341400
N	2.09316300	-0.00007900	-0.49631100
C	1.35532000	1.24323100	-0.67339700
C	0.05989000	1.24348000	-0.33466000
C	-0.63847400	0.00002800	0.15122700
C	2.18836200	-2.38793300	-1.17196700
C	2.18856100	2.38777800	-1.17192600
C	-0.70890100	2.51257500	-0.41957800
O	-1.95406400	2.36668500	0.05854000
O	-0.28999500	3.56531700	-0.85215100
C	-2.76875100	3.55127500	0.04465500
C	-4.11008300	3.17995700	0.63564400
C	-0.70910800	-2.51250000	-0.41963500
O	-1.95422200	-2.36654800	0.05859200
O	-0.29031800	-3.56524200	-0.85232300
C	-2.76900400	-3.55107300	0.04468200
C	-4.11026400	-3.17968900	0.63579200
H	-0.68627900	0.00002000	1.24750300
H	-1.67140100	0.00007300	-0.19945600
H	2.21085700	-3.19002400	-0.43212600
H	1.75928000	-2.80603000	-2.08380700
H	3.21586500	-2.06775600	-1.35439500
H	1.75941900	2.80604900	-2.08365600
H	2.21127600	3.18977200	-0.43198500
H	3.21599400	2.06747600	-1.35452900
H	-2.26120000	4.32802300	0.62316100
H	-2.85266200	3.90368300	-0.98717900
H	-4.76396700	4.05492600	0.64630800
H	-4.58928300	2.39627100	0.04466300
H	-3.99357900	2.82111600	1.66048700
H	-2.85301600	-3.90340300	-0.98717100
H	-2.26147400	-4.32790100	0.62309900
H	-4.76421600	-4.05460800	0.64644300
H	-3.99366000	-2.82092500	1.66065000
H	-4.58944500	-2.39592700	0.04489700
H	2.89181200	-0.00010700	-1.13298500
B	2.84609200	-0.00011500	1.08070600
F	1.79210700	-0.00007300	1.94568200
F	3.58658000	1.15010500	1.06844000
F	3.58648400	-1.15039600	1.06843700

Hantzsch ester-BPh_3 (B-N) **Int-VId**

Not converged.

Hantzsch pyridine-$B[3,5\text{-}(CF_3)_2C_6H_3]_3$ (B-O) **Int-VIIa**



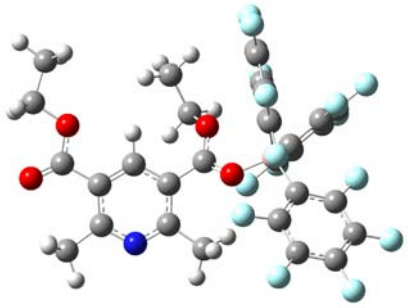
Zero-point correction = 0.601478 (Hartree/Particle)
Thermal correction to Energy = 0.658200
Thermal correction to Enthalpy = 0.659144
Thermal correction to Gibbs Free Energy = 0.499332
Sum of electronic and zero-point Energies = -3601.636239
Sum of electronic and thermal Energies = -3601.579518
Sum of electronic and thermal Enthalpies = -3601.578573
Sum of electronic and thermal Free Energies = -3601.738385

Single point energy = -3603.2251772

O	-7.50916100	0.87983000	-1.78022100
O	-6.37013700	-1.05272000	-1.76262800
O	-0.39983900	0.30709900	-0.97397100
O	-1.86684200	-1.41570700	-1.12072600
N	-3.76784300	2.88282900	-1.27903200
C	-4.97459900	2.32776100	-1.44263600
C	-5.12398300	0.92527600	-1.52016700
C	-3.98728800	0.14104200	-1.41919800

H	-4.07958900	-0.93623100	-1.47297200
C	-2.73165500	0.73066300	-1.24179300
C	-2.66110800	2.14252400	-1.17336500
C	-6.11898200	3.29105000	-1.53422500
H	-6.85329600	3.09581600	-0.74916300
H	-6.65143300	3.17109700	-2.48074600
H	-5.72657300	4.30262500	-1.44457900
C	-1.39577800	2.92361000	-0.97985400
H	-1.64378400	3.98368600	-0.99790600
H	-0.66450600	2.70166100	-1.76104800
H	-0.91998700	2.67599600	-0.02615700
C	-6.46013800	0.28331600	-1.69954600
C	-7.61769200	-1.75575400	-1.91742900
C	-1.55907300	-0.15035600	-1.10006600
C	-0.92190000	-2.51892100	-1.18724600
H	0.06257400	-2.18476000	-0.87461200
H	-0.88810400	-2.81153200	-2.24048400
C	-1.45940600	-3.61644900	-0.29932600
H	-1.54574200	-3.26145600	0.73108500
H	-0.77117400	-4.46491500	-0.31631800
H	-2.43994900	-3.95261300	-0.64318700
C	-7.29748100	-3.23237200	-1.96213500
H	-6.64526000	-3.46223700	-2.80770900
H	-8.22056300	-3.80586100	-2.07246500
H	-6.80258100	-3.54827000	-1.04091400
H	-8.10001000	-1.40659900	-2.83446000
H	-8.26569000	-1.49684800	-1.07579100
B	0.90319900	-0.01527000	-0.00122400
C	2.01587000	-0.72222100	-0.92517000
C	0.29179200	-0.87274300	1.22911100
C	1.39115100	1.46708700	0.42045000
C	3.26200600	-1.04977600	-0.37153600
C	1.85089100	-0.96756300	-2.29129700
C	-0.89146100	-0.43416200	1.84002400
C	0.86360400	-2.04351300	1.73921300
C	1.36430900	1.95195500	1.73016700
C	1.85821400	2.34013000	-0.57305900
C	4.26939500	-1.62846700	-1.13843700
H	3.46148000	-0.83979400	0.67852200
C	2.86418200	-1.54064300	-3.05849100
H	0.91498500	-0.70501900	-2.78039600
C	-1.48260300	-1.13402700	2.88765200
H	-1.37294800	0.48249500	1.49662400
C	0.28079400	-2.73328500	2.80322500
H	1.77304300	-2.44449000	1.29616000
C	1.76174500	3.25760200	2.02837000
H	1.02769100	1.31376200	2.54380900
C	2.23332600	3.64464200	-0.27631600
H	1.91700500	1.99788200	-1.60539000
C	4.08416500	-1.88607000	-2.49310600
C	5.57252200	-1.96256700	-0.46605000
C	2.58905000	-1.79269800	-4.51349700
C	-0.90085200	-2.29323700	3.38884100
C	-2.77478200	-0.60905200	3.44850400
C	0.92930500	-4.00974200	3.26379400
C	2.18815100	4.12291000	1.03118200
C	1.69839800	3.71110500	3.45999900
C	2.64996800	4.54334500	-1.40604400
H	4.86953900	-2.33642000	-3.08871400
F	6.17558000	-0.86295500	0.01825500
F	5.38597700	-2.78998700	0.57940400
F	6.43815000	-2.56072900	-1.29784900
F	3.64118600	-2.31758200	-5.15488000
F	2.24529500	-0.66320700	-5.15827300
F	1.55639900	-2.64860400	-4.67379900
H	-1.35727200	-2.83816100	4.20708200
F	-3.24704500	-1.36954300	4.44540400
F	-3.73010200	-0.55708500	2.49697700
F	-2.64042400	0.64148900	3.91998500
F	0.86088400	-4.95934800	2.30770100
F	2.23109300	-3.83800000	3.54048200
F	0.34440500	-4.51274100	4.36054600
H	2.48554600	5.13901500	1.26301300
F	0.44123800	3.65397500	3.94029400
F	2.44698600	2.93116300	4.26094700
F	2.12649800	4.97275000	3.61669200
F	3.15372400	5.70958600	-0.97607900
F	1.60366200	4.83505400	-2.20705000
F	3.57793800	3.96657800	-2.18840400

Hantzsch pyridine-B(C_6F_5)$_3$ (B-O) **Int-VIIb**



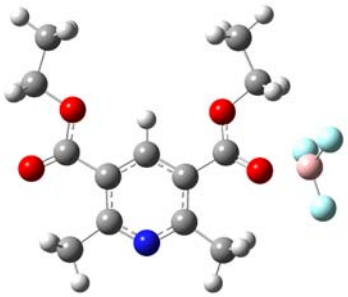
Zero-point correction = 0.450500 (Hartree/Particle)
Thermal correction to Energy = 0.498314
Thermal correction to Enthalpy = 0.499258
Thermal correction to Gibbs Free Energy = 0.366637
Sum of electronic and zero-point Energies = -3068.139268
Sum of electronic and thermal Energies = -3068.091455
Sum of electronic and thermal Enthalpies = -3068.090510
Sum of electronic and thermal Free Energies = -3068.223131

Single point energy = -3069.4379757

C	2.35370600	1.14721100	-0.56952200
C	2.23438200	2.50096100	-0.95627500
N	3.32251900	3.26789600	-1.06416800
C	4.54386000	2.79959200	-0.77954300
C	4.73413900	1.46214600	-0.36522200
C	3.61846600	0.64661000	-0.26891500
C	0.93012200	3.17488700	-1.26355200
C	5.66509400	3.78354200	-0.92770000
C	6.08042800	0.91709100	-0.02465700
O	6.03079700	-0.39842300	0.23962500
O	7.10196600	1.56195200	0.01375500
C	7.28176400	-1.00884600	0.61245700
C	7.01190700	-2.47902400	0.83787200
C	1.19257900	0.26786100	-0.38713100
O	1.26759600	-1.02406000	-0.52742300
O	0.10812300	0.75211000	-0.00497700
C	2.08369500	-1.70966700	-1.51682700
C	2.82831400	-2.83867300	-0.84234900
H	0.23947800	2.52096400	-1.79751500
H	0.44925300	3.46507300	-0.32376700
H	1.13621700	4.07184800	-1.84599300
H	6.16429000	3.94256500	0.03129200
H	6.43121000	3.40500600	-1.60823400
H	5.25549600	4.72132600	-1.29927300
H	8.00413300	-0.83666300	-0.18965000
H	7.65233600	-0.51148100	1.51300900
H	7.93522000	-2.98268700	1.13227800
H	6.27462100	-2.62123500	1.63157300
H	6.64030400	-2.94896800	-0.07601600
H	1.35933700	-2.08845000	-2.24328400
H	2.73944400	-0.98904600	-2.00970500
H	3.34353900	-3.42900800	-1.60371900
H	3.57450100	-2.47080300	-0.13285900
H	2.12669700	-3.48755100	-0.31422100
B	-1.28547700	0.01933400	0.15641700
C	-2.29247000	1.30129700	0.33908600
C	-1.12839300	-0.96081600	1.46392300
C	-1.61284500	-0.80629200	-1.22253800
C	-3.59584800	1.34162600	-0.15446800
C	-1.88924100	2.48458300	0.96760700
C	-0.70657800	-2.29240400	1.38226700

C	-1.37302100	-0.52871700	2.76928400
C	-2.56675500	-1.82460200	-1.22152100
C	-1.03463600	-0.57956300	-2.46426800
C	-4.42668000	2.45383900	-0.06708200
F	-4.14483500	0.27539100	-0.75647200
C	-2.68321100	3.61721900	1.07017200
F	-0.68257800	2.58399800	1.54979900
C	-0.52576900	-3.11883900	2.48189300
F	-0.46520200	-2.88357200	0.19772900
C	-1.21093600	-1.32618900	3.89681000
F	-1.79623600	0.71687800	3.01918200
C	-2.91654800	-2.56356800	-2.33991500
F	-3.20372900	-2.13413400	-0.08513700
C	-1.34354100	-1.29817500	-3.61485300
F	-0.07925100	0.37092100	-2.62964500
C	-3.96641900	3.60567600	0.54506200
F	-5.65825600	2.41665100	-0.57636400
F	-2.22351900	4.71291900	1.67727200
C	-0.77810600	-2.63323000	3.75458500
F	-0.11376100	-4.37877100	2.31954400
F	-1.46518700	-0.83947700	5.11114000
C	-2.29650600	-2.29907600	-3.55408400
F	-3.83803200	-3.52152900	-2.26229400
F	-0.72304300	-1.02804600	-4.76650500
F	-4.74191000	4.68271500	0.63296800
F	-0.61037600	-3.41161300	4.81943200
F	-2.61289100	-2.99666500	-4.64183300
H	3.73939400	-0.37520200	0.07241200

Hantzsch pyridine-BF_3 (B-O) **Int-VIIc**

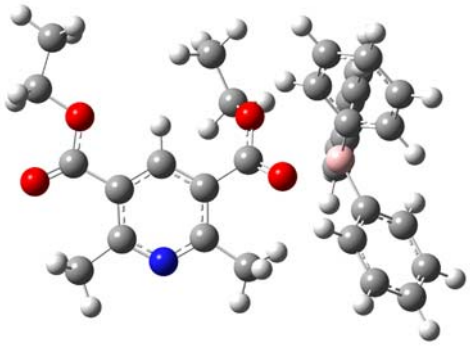


Zero-point correction = 0.304345 (Hartree/Particle)
Thermal correction to Energy = 0.327510
Thermal correction to Enthalpy = 0.328454
Thermal correction to Gibbs Free Energy = 0.249017
Sum of electronic and zero-point Energies = -1185.163358
Sum of electronic and thermal Energies = -1185.140194
Sum of electronic and thermal Enthalpies = -1185.139249
Sum of electronic and thermal Free Energies = -1185.218686

Single point energy = -1185.7890485

O	4.55855000	-0.78125400	0.09050300
O	3.41372500	1.14483900	-0.00334800
O	-2.54627000	-0.30272500	-0.46011500
O	-1.23771400	1.42896200	0.15621400
N	0.79997800	-2.81642400	-0.03646300
C	2.01170800	-2.24857300	-0.01667900
C	2.16036100	-0.84353600	-0.00657500
C	1.01268200	-0.06543000	-0.03788400
H	1.09382900	1.01504200	-0.03589600
C	-0.24229800	-0.67080400	-0.07866800
C	-0.31700600	-2.08288300	-0.06459700
C	3.16798200	-3.20420000	-0.00447300
H	3.77326900	-3.06809400	0.89491500
H	3.83650600	-3.01901600	-0.84825100
H	2.77585200	-4.21907400	-0.04517200
C	-1.60020800	-2.86241200	-0.06119700
H	-1.35664300	-3.91321600	0.08622900
H	-2.13660100	-2.73659200	-1.00524700
H	-2.28175600	-2.52102500	0.72152000
C	3.50214800	-0.19397200	0.03251300
C	4.66621600	1.85233000	0.03800900
C	-1.44460000	0.17492400	-0.12871900
C	-2.27169000	2.43423200	-0.06686300
H	-2.98513400	2.35872900	0.75336800
H	-2.78054800	2.19077500	-1.00106100
C	-1.56746300	3.76933900	-0.10983800
H	-1.04629700	3.96402900	0.82980000
H	-2.30784800	4.55738600	-0.26344800
H	-0.84687300	3.80710300	-0.92979300
C	4.34836700	3.32975100	-0.00590200
H	3.81280900	3.58310100	-0.92353500
H	5.27494500	3.90727600	0.02404700
H	3.73330000	3.61842100	0.84930100
H	5.27317100	1.53289700	-0.81343500
H	5.19459800	1.56860700	0.95216400
B	-4.07986200	-0.07055300	0.07994300
F	-3.89591500	0.40094600	1.35987300
F	-4.59678000	-1.32433100	0.01112600
F	-4.65070900	0.83340700	-0.76997500

Hantzsch pyridine-BPh_3 (B-O) **Int-VIId**



Zero-point correction = 0.571630 (Hartree/Particle)
Thermal correction to Energy = 0.606497
Thermal correction to Enthalpy = 0.607441
Thermal correction to Gibbs Free Energy = 0.502289
Sum of electronic and zero-point Energies = -1579.926797
Sum of electronic and thermal Energies = -1579.891930
Sum of electronic and thermal Enthalpies = -1579.890986
Sum of electronic and thermal Free Energies = -1579.996138

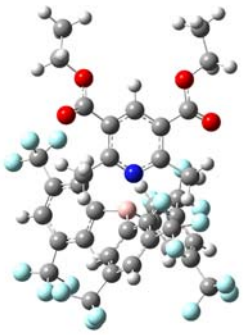
Single point energy = -1580.9039107

C	-1.44069100	0.90981000	-0.02101300
C	-1.35718400	2.31031500	0.12975300
N	-2.46003400	3.06492500	0.08116100
C	-3.66727300	2.52449100	-0.12537800
C	-3.82651000	1.12977200	-0.27800700
C	-2.69112400	0.33427300	-0.22354100
C	-0.06927000	3.04612000	0.35382400
C	-4.81052300	3.49449500	-0.17729200
C	-5.16121800	0.50196500	-0.49217100
C	-5.09015500	-0.83941100	-0.46146600
O	-6.19632800	1.10224100	-0.66870600
C	-6.33064000	-1.53704000	-0.67554100
C	-6.03839500	-3.01553800	-0.55578100
C	-0.24704800	0.04109000	-0.02892800
O	-0.35591200	-1.22513500	0.31150800
O	0.83454800	0.47413000	-0.43973300
C	-1.05894800	-1.67580600	1.49777700
C	-1.73973800	-2.98353500	1.16787000
H	0.60471900	2.51511700	1.02929300

H	0.47495200	3.15107700	−0.59002100
H	−0.29889300	4.03640100	0.74510000
H	−5.31512700	3.44407900	−1.14505400
H	−5.56780000	3.24804100	0.57093100
H	−4.42054600	4.49659000	−0.00570800
H	−7.05414000	−1.19475100	0.06926700
H	−6.71317800	−1.26813000	−1.66418500
H	−6.95528000	−3.58742100	−0.71540100
H	−5.30339100	−3.32735700	−1.30168300
H	−5.65159800	−3.25355500	0.43806600
H	−0.28385100	−1.80465100	2.25797200
H	−1.76273300	−0.90599800	1.82469700
H	−2.19578100	−3.39241400	2.07248000
H	−2.52126000	−2.85523400	0.41322500
H	−1.00465100	−3.70096900	0.79603500
B	2.39516200	−0.14020500	−0.11611200
C	3.22688400	1.23849400	−0.08760000
C	2.75561100	−1.09193500	−1.36131200
C	2.24463200	−0.87121800	1.31978000
C	4.16991600	1.52473000	0.90729300
C	3.08352800	2.18185000	−1.11908100
C	1.86715200	−2.04322700	−1.88948900
C	4.03431500	−1.03520300	−1.93460700
C	2.42220200	−2.25109700	1.48756700
C	1.89099400	−0.13542600	2.46363300
C	4.92603700	2.69758600	0.88666600
C	3.82061000	3.36148800	−1.14360000
C	2.23070900	−2.88601000	−2.93714100
C	4.41328900	−1.88177200	−2.97454700
C	2.25438100	−2.86834000	2.72813000
C	1.71763700	−0.73819600	3.70886600
C	4.74794000	3.62364500	−0.13513300
C	3.50931500	−2.80968300	−3.48336200
C	1.90045000	−2.11353000	3.84484900
H	−2.78269500	−0.73811000	−0.36008700
H	1.76916600	0.94433300	2.38061000
H	1.45000500	−0.13654600	4.57288000
H	1.77451400	−2.58965700	4.81258500
H	2.40465300	−3.93999700	2.82425700
H	2.69037200	−2.85446500	0.62377400
H	0.86965500	−2.13554400	−1.46677200
H	1.51646100	−3.60595000	−3.32706200
H	3.79716600	−3.46574900	−4.29929000
H	5.41273800	−1.80955000	−3.39368300
H	4.74790900	−0.30600800	−1.55864600
H	2.37711600	1.97839800	−1.92271000
H	4.32123400	0.81392400	1.71605300
H	5.65323300	2.88633600	1.67116300
H	5.33030800	4.53992400	−0.15195400
H	3.68170400	4.07437700	−1.95142300

Hantzsch pyridine–B[3,5-$(CF_3)_2C_6H_3]_3$ (B-N)

Int-VIIIa



Zero-point correction = 0.602696 (Hartree/Particle)
Thermal correction to Energy = 0.659173
Thermal correction to Enthalpy = 0.660117
Thermal correction to Gibbs Free Energy = 0.499658

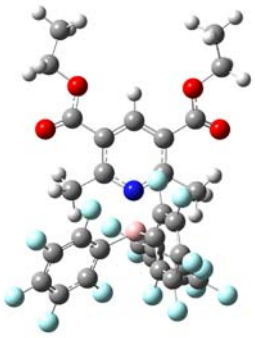
Sum of electronic and zero-point Energies = -3601.631170
Sum of electronic and thermal Energies = -3601.574693
Sum of electronic and thermal Enthalpies = -3601.573749
Sum of electronic and thermal Free Energies = -3601.734208

Single point energy = -3603.225321

O	−3.23228100	−1.03948400	3.69694100
O	−5.05391600	−1.39530400	2.43935800
O	−3.40054800	−2.14648500	−3.35175500
O	−5.13102100	−1.34150500	−2.17210100
N	−0.99414900	−0.94870200	0.04119900
C	−1.61057400	−1.12008900	1.25117100
C	−3.00915000	−1.20581900	1.30558100
C	−3.72838800	−1.29876000	0.12127200
H	−4.80965500	−1.35420500	0.14747200
C	−3.05761100	−1.40095500	−1.08791200
C	−1.66471200	−1.22111500	−1.11761700
C	−0.78814600	−1.36725200	2.48541500
H	−1.22242200	−2.22856000	2.99789500
H	−0.82826800	−0.53426700	3.18949200
H	0.24621500	−1.57941900	2.23538400
C	−0.91687200	−1.34747700	−2.41437400
H	0.11777400	−1.04132300	−2.34140400
H	−1.41478600	−0.78016500	−3.20205500
H	−0.95978800	−2.39879700	−2.71604500
C	−3.74231500	−1.20700800	2.61484100
C	−5.85588000	−1.34832500	3.63886400
C	−3.84753800	−1.67389400	−2.33386200
C	−5.98392600	−1.56681500	−3.31455400
H	−5.95644100	−2.63211200	−3.55897600
H	−5.57120900	−1.01325300	−4.16209700
C	−7.36925900	−1.09560100	−2.93737700
H	−7.74925500	−1.65518600	−2.07953600
H	−8.04988800	−1.24851900	−3.77771700
H	−7.36081400	−0.03256700	−2.68757200
C	−7.29311200	−1.56421800	3.22554700
H	−7.61991200	−0.78291400	2.53579600
H	−7.93552400	−1.53607300	4.10838300
H	−7.41549600	−2.53527900	2.74075800
H	−5.69965300	−0.37722900	4.11584500
H	−5.49707200	−2.12278300	4.32183300
B	0.51228000	−0.19272400	−0.07790400
C	0.33352700	1.08933900	−1.08935000
C	1.56651600	−1.35994300	−0.50819900
C	0.92416300	0.54627000	1.31771500
C	1.46595500	1.87399600	−1.36735200
C	−0.87770600	1.59437000	−1.57444200
C	1.40101100	−2.66772900	−0.02904000
C	2.67888600	−1.15033300	−1.33532900
C	2.11844800	0.28342200	1.99364100
C	0.11332200	1.56465700	1.83929100
C	1.40128000	3.02072500	−2.15224700
H	2.42767300	1.61150400	−0.93272200
C	−0.94678100	2.75125800	−2.35039600
H	−1.82122900	1.10327900	−1.35037100
C	2.29608900	−3.69045600	−0.33323800
H	0.54393500	−2.92048300	0.59039200
C	3.57439300	−2.17424800	−1.63953600
H	2.86039400	−0.17822900	−1.78277800
C	2.46586800	0.98128900	3.15215100
H	2.79154300	−0.48920600	1.62732400
C	0.44873700	2.24050400	3.00634500
H	−0.81109000	1.83581400	1.32942900
C	0.19212000	3.47531100	−2.66844500
C	2.67333800	3.78234400	−2.40452200
C	−2.30159400	3.18081000	−2.83395600
C	3.40162300	−3.45917000	−1.14110800
C	2.01582000	−5.06413400	0.20694300
C	4.73111500	−1.85741300	−2.54760400
C	1.63441300	1.95946700	3.68009500
C	3.77043300	0.64579500	3.81956000
C	−0.49224500	3.29519700	3.51659500
H	0.14258900	4.36731900	−3.28148100
F	3.15159300	4.33662400	−1.27609000

F	3.64374800	2.97954000	-2.87783500
F	2.50379100	4.77340000	-3.29341000
F	-2.25260000	4.26362600	-3.62028800
F	-3.13001300	3.46386700	-1.81011700
F	-2.90486500	2.19974600	-3.54111700
H	4.10166100	-4.25201500	-1.37715400
F	3.03457100	-5.91158800	0.00892800
F	0.92665800	-5.60951600	-0.37258600
F	1.76519100	-5.03678900	1.52974600
F	4.31027200	-1.52424900	-3.78229100
F	5.44748700	-0.81556600	-2.09230700
F	5.57168000	-2.89478400	-2.68128200
H	1.90086900	2.49219500	4.58536600
F	3.85197500	-0.66578100	4.11424900
F	4.81811700	0.92376500	3.02321400
F	3.94912300	1.32248600	4.96418900
F	-0.12804700	3.76822000	4.71757000
F	-1.74647300	2.81568500	3.63907400
F	-0.56752600	4.34522900	2.67909900

Hantzsch pyridine–B(C_6F_5)$_3$ (B-N) **Int-VIIIb**

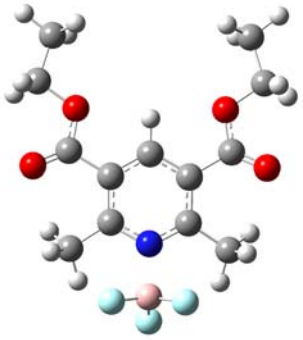


Zero-point correction = 0.453011 (Hartree/Particle)
Thermal correction to Energy = 0.500064
Thermal correction to Enthalpy = 0.501008
Thermal correction to Gibbs Free Energy = 0.371571
Sum of electronic and zero-point Energies = -3068.140164
Sum of electronic and thermal Energies = -3068.093111
Sum of electronic and thermal Enthalpies = -3068.092167
Sum of electronic and thermal Free Energies = -3068.221605

Single point energy = -3069.4449414

O	3.09251900	3.41494500	-1.46775300
O	4.91634700	2.11888600	-1.34242100
O	3.45632000	-3.42517400	0.43138800
O	4.97284500	-1.87697300	1.01344800
N	0.82718900	-0.07854800	-0.36821900
C	1.47538500	0.97749100	-0.95599600
C	2.86799200	1.10339700	-0.81554900
C	3.59969500	0.06345700	-0.26975100
H	4.67717300	0.13812600	-0.19007200
C	2.95110100	-1.09237400	0.12738500
C	1.55110500	-1.13211300	0.12988100
C	0.77988600	1.96456100	-1.85301200
H	1.42948500	2.13654100	-2.71253300
H	0.66497700	2.93186700	-1.36038000
H	-0.17267200	1.60328700	-2.20857000
C	0.88417900	-2.34620200	0.71278600
H	-0.11264900	-2.16286400	1.08656600
H	1.49132800	-2.73146100	1.53003700
H	0.84158200	-3.13350100	-0.04688900
C	3.59932800	2.34003600	-1.25283000
C	5.72000100	3.26781300	-1.68115000
C	3.78480300	-2.26779000	0.54182500
C	5.87915500	-2.93704300	1.38229300
H	6.07841400	-3.54363500	0.49445200
H	5.38228200	-3.57168800	2.12069100
C	7.12865800	-2.28723900	1.93028900
H	7.59671500	-1.64891400	1.17741100
H	7.84461100	-3.05857000	2.22270600
H	6.89473700	-1.68068900	2.80773200
C	7.15894900	2.80877800	-1.73156500
H	7.47427700	2.41319900	-0.76341100
H	7.80359000	3.65304000	-1.98575800
H	7.29159800	2.03235400	-2.48809100
H	5.55389100	4.03824600	-0.92347700
H	5.37347000	3.65833000	-2.64141000
B	-0.83801400	-0.12784300	-0.11749500
C	-1.35395300	-1.41569600	-0.99926200
C	-1.62036900	1.26954800	-0.48877800
C	-1.15815800	-0.19306300	1.50422500
C	-2.01314000	-2.54975100	-0.52661100
C	-1.13067200	-1.43384400	-2.37440600
C	-1.28439300	2.43745100	0.19881700
C	-2.75574200	1.38120700	-1.28658800
C	-2.49755700	-0.29731200	1.88821100
C	-0.28235900	0.02173800	2.56326400
C	-2.44676900	-3.58950200	-1.34130800
F	-2.22592000	-2.73548700	0.78699100
C	-1.53895300	-2.44539700	-3.22879600
F	-0.49701900	-0.39636100	-2.95518500
C	-1.97430200	3.63236200	0.09693500
F	-0.18818700	2.44021100	0.98385800
C	-3.48480300	2.56104800	-1.41581400
F	-3.22726100	0.34056400	-1.98688900
C	-2.93845600	-0.23881400	3.20058000
F	-3.44387900	-0.45220300	0.94862700
C	-0.67709400	0.09090900	3.89430400
F	1.03953400	0.18395400	2.35139500
C	-2.21310700	-3.53808900	-2.70543800
F	-3.05989500	-4.64800800	-0.81276600
F	-1.29447500	-2.37253700	-4.53707500
C	-3.09383100	3.69386600	-0.72352500
F	-1.57477800	4.71530700	0.76309100
F	-4.56254900	2.60205300	-2.19767300
C	-2.01572600	-0.04343400	4.21898600
F	-4.23297300	-0.35936200	3.49098800
F	0.22640600	0.29335400	4.85482500
F	-2.61467800	-4.52682100	-3.49809300
F	-3.77758200	4.82785100	-0.84146600
F	-2.41367900	0.02369800	5.48629400

Hantzsch pyridine–BF_3 (B-N) **Int-VIIIc**

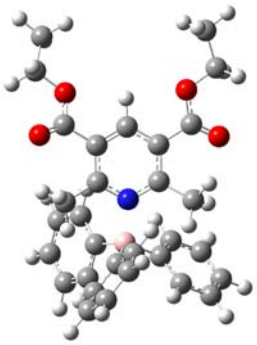


Zero-point correction = 0.306024 (Hartree/Particle)
Thermal correction to Energy = 0.328476
Thermal correction to Enthalpy = 0.329421
Thermal correction to Gibbs Free Energy = 0.252648
Sum of electronic and zero-point Energies = -1185.169194
Sum of electronic and thermal Energies = -1185.146742
Sum of electronic and thermal Enthalpies = -1185.145797
Sum of electronic and thermal Free Energies = -1185.222570

Single point energy = -1185.8007942

O	-0.40329100	-3.58090000	-0.25554800
O	-2.21402800	-2.28969800	0.03357500
O	-0.40334200	3.58082000	-0.25547900
O	-2.21411700	2.28963200	0.03357700
N	1.91551500	0.00004200	0.14171300
C	1.26119200	-1.18800400	0.17206900
C	-0.13250700	-1.20526100	0.00486500
C	-0.81310400	-0.00004200	-0.10793700
H	-1.88720200	-0.00006800	-0.24744400
C	-0.13257400	1.20520700	0.00489200
C	1.26111500	1.18804100	0.17207700
C	2.04364300	-2.42960800	0.48919300
H	2.26569400	-2.99557500	-0.41743900
H	1.43997800	-3.06843700	1.13273600
H	2.97812800	-2.17292700	0.98288500
C	2.04342900	2.42974200	0.48914100
H	2.97784900	2.17321200	0.98303600
H	1.43960800	3.06861000	1.13250700
H	2.26557600	2.99560400	-0.41753000
C	-0.89403900	-2.49019600	-0.08190800
C	-3.03431100	-3.46789200	-0.08562200
C	-0.89411900	2.49013100	-0.08182400
C	-3.03438500	3.46783900	-0.08558800
H	-2.85177800	3.91874900	-1.06490100
H	-2.72109600	4.18453400	0.67832400
C	-4.47147800	3.03311400	0.08896300
H	-4.75527400	2.31297700	-0.68186600
H	-5.13029900	3.90082600	0.01038600
H	-4.61972500	2.57357500	1.06861800
C	-4.47138500	-3.03317400	0.08910300
H	-4.61952600	-2.57373500	1.06882200
H	-5.13021900	-3.90087500	0.01051100
H	-4.75525000	-2.31296100	-0.68162800
H	-2.72096300	-4.18465500	0.67820600
H	-2.85178900	-3.91871500	-1.06499200
B	3.59604800	0.00004500	-0.15130100
F	3.83678800	-1.13079900	-0.89211900
F	4.19041300	-0.00016100	1.08842400
F	3.83688900	1.13108500	-0.89177700

Hantzschpyridine–BPh_3 (B-N) **Int-VIIId**



Zero-point correction = 0.573077 (Hartree/Particle)
Thermal correction to Energy = 0.607372
Thermal correction to Enthalpy = 0.608316
Thermal correction to Gibbs Free Energy = 0.504720
Sum of electronic and zero-point Energies = -1579.926131
Sum of electronic and thermal Energies = -1579.891836
Sum of electronic and thermal Enthalpies = -1579.890892
Sum of electronic and thermal Free Energies = -1579.994488

Single point energy = -1580.907157

O	-2.06537600	3.62187300	0.02881900
O	-3.90031600	2.36503100	0.31059300
O	-2.37512400	-3.44026200	0.97984000
O	-3.89324700	-2.24495500	-0.15790000
N	0.20838400	0.00326200	0.42014800
C	-0.44815900	1.19726300	0.49961300
C	-1.83888500	1.24056600	0.30551200
C	-2.54898900	0.05265000	0.21218200
H	-3.62142100	0.07078900	0.06370200
C	-1.89088400	-1.15478100	0.38240200
C	-0.48748800	-1.16788900	0.48243900
C	0.27843600	2.43608300	0.94396200
H	-0.36309100	2.95692600	1.65801300
H	0.47119100	3.12400900	0.11905500
H	1.22358700	2.18310600	1.41185600
C	0.22837000	-2.47288100	0.68414200
H	1.30115300	-2.38568200	0.58913600
H	-0.14381600	-3.21999600	-0.01788800
H	-0.01747900	-2.83130700	1.68856000
C	-2.57411800	2.54018700	0.20557600
C	-4.69641400	3.55611600	0.17045500
C	-2.70593600	-2.40887500	0.44458300
C	-4.77717000	-3.38067400	-0.11060900
H	-4.96427000	-3.63109200	0.93730400
H	-4.27157000	-4.23168700	-0.57471900
C	-6.04156500	-2.99563500	-0.84438200
H	-6.52315200	-2.14024400	-0.36508200
H	-6.74075800	-3.83484900	-0.83691000
H	-5.82179000	-2.73694200	-1.88244700
C	-6.14310000	3.15046800	0.33687600
H	-6.43310600	2.42636600	-0.42796200
H	-6.78523700	4.02906800	0.24218800
H	-6.30853500	2.70525600	1.32046000
H	-4.49749100	3.99268500	-0.81230000
H	-4.37701400	4.27644000	0.92848400
B	1.88602900	-0.09069400	0.02469300
C	2.60126100	-0.62312900	1.38875000
C	2.45564600	1.34987800	-0.47539900
C	1.98668200	-1.01572000	-1.32430400
C	3.67309100	-1.52927100	1.40662600
C	2.16798700	-0.16167900	2.64349500
C	1.95743300	1.94099400	-1.64848000
C	3.50131200	2.01632300	0.17519600
C	3.27868800	-1.27041700	-1.82137600
C	0.92922200	-1.44068300	-2.14131300
H	4.03199600	-1.95599200	0.47561400
C	4.28368700	-1.93409200	2.59216800
H	1.32174900	0.51989100	2.70333500
C	2.76841500	-0.55679600	3.83686800
H	1.17435900	1.42954100	-2.20768700
C	2.43123700	3.16171800	-2.11677100
H	3.92423200	1.58533100	1.08014600
C	4.00065800	3.23153600	-0.29627500
H	4.13709400	-0.87424800	-1.28453500
C	3.50205500	-1.96491100	-3.00495100
H	-0.10239900	-1.22473900	-1.86926500
C	1.13643300	-2.12570600	-3.33933000
C	3.83791400	-1.44605800	3.81670400
H	5.10823100	-2.64037500	2.55653200
H	2.39549700	-0.17336100	4.78237300
C	3.45805500	3.81580700	-1.43592600
H	2.01030300	3.59920100	-3.01737400
H	4.81202300	3.72397800	0.23210400
C	2.42600200	-2.40877100	-3.77044500
H	4.51959000	-2.14282600	-3.34067900
H	0.28238300	-2.43093100	-3.93739700
H	4.31083900	-1.76115800	4.74163100
H	3.83835800	4.76524500	-1.80019000
H	2.59297400	-2.94498400	-4.69928900

7. References

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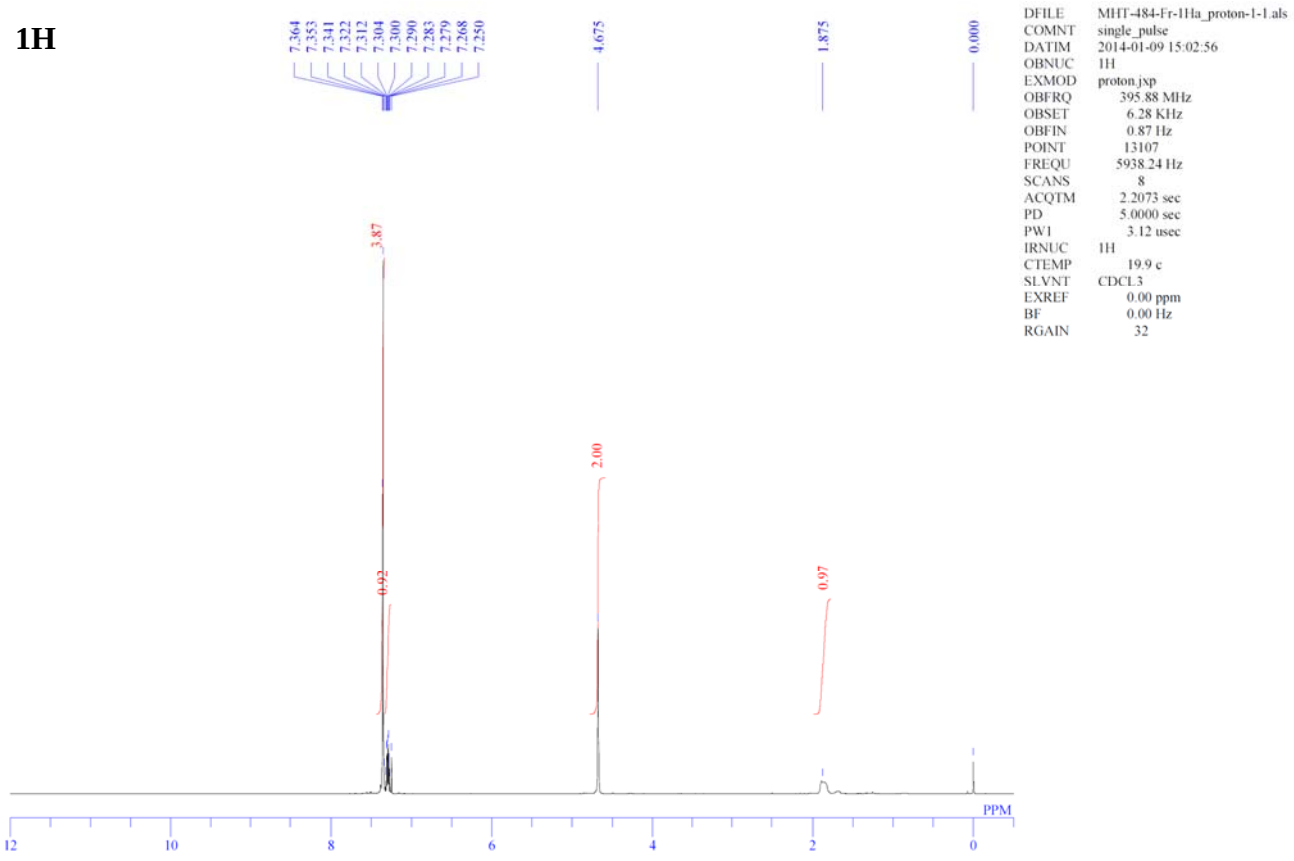
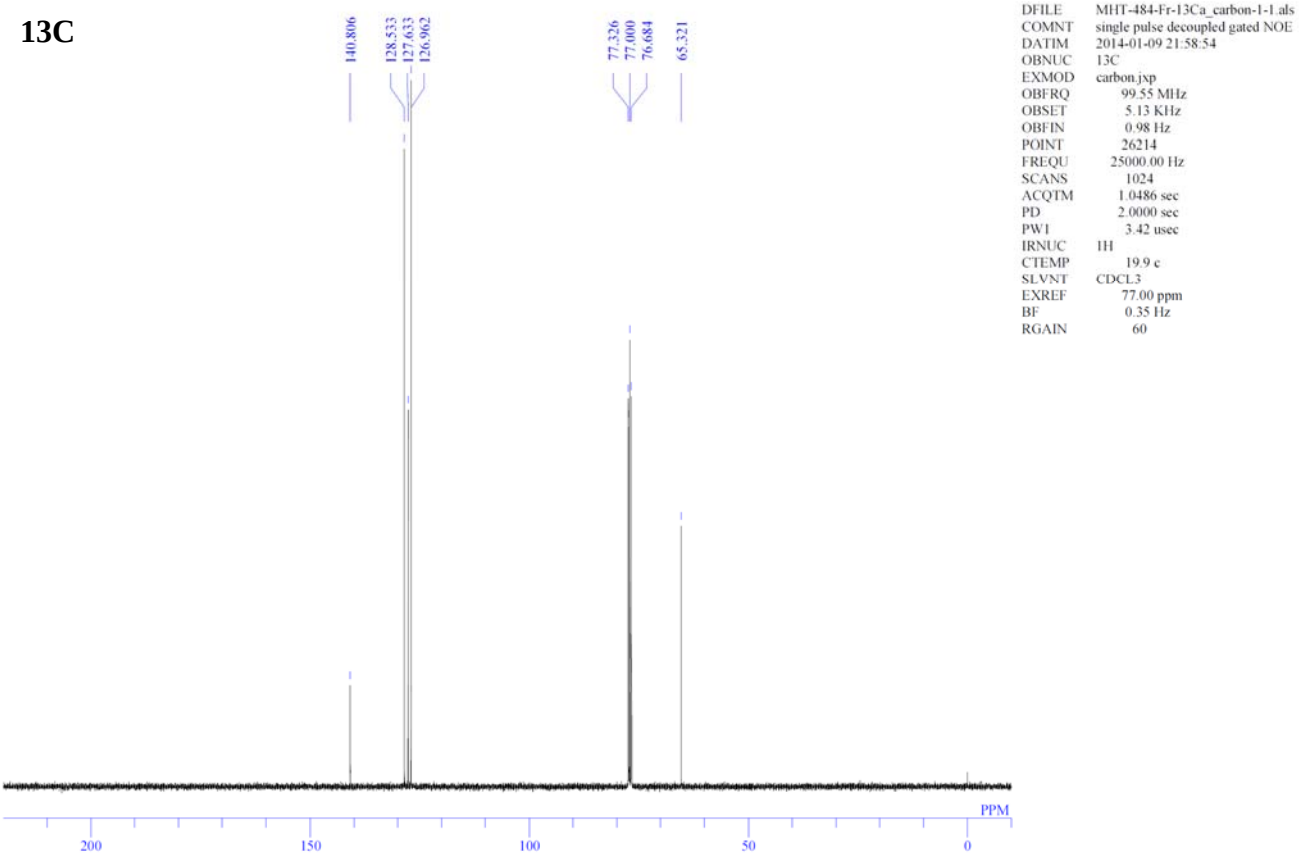
8. Copies of NMR spectra of benzyl alcohol and **Int-Ia**

Benzyl alcohol

1H

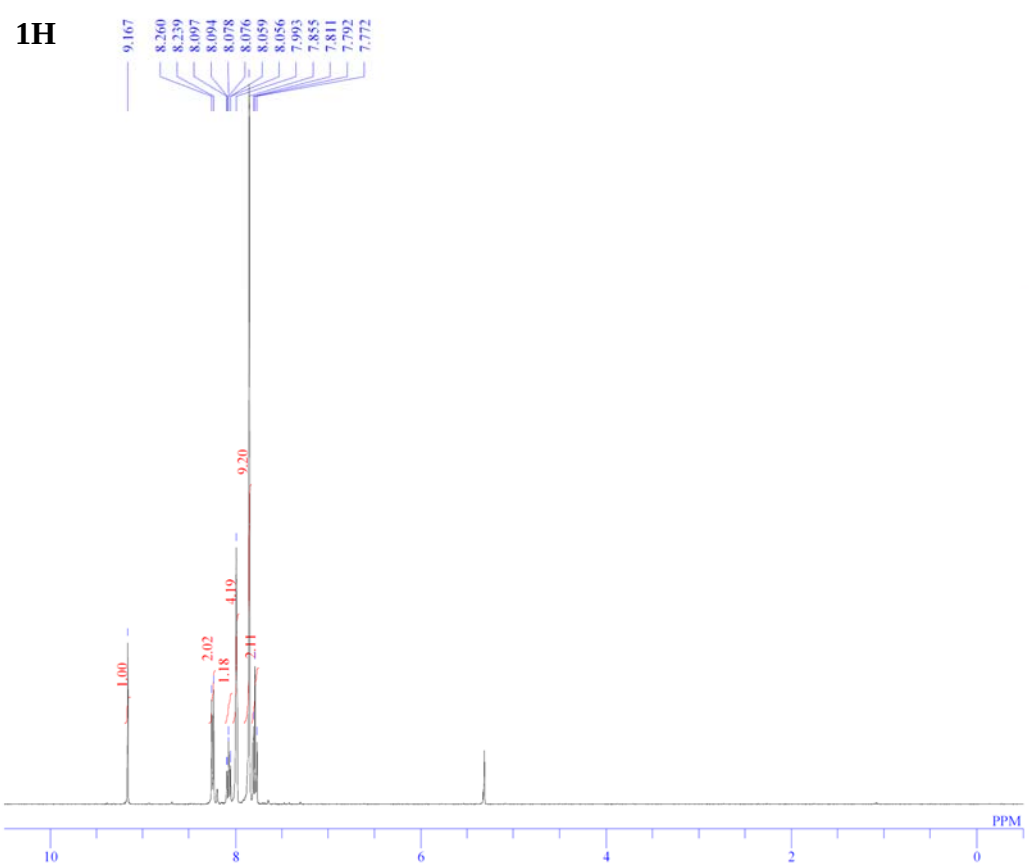


13C



Int-Ia

1H



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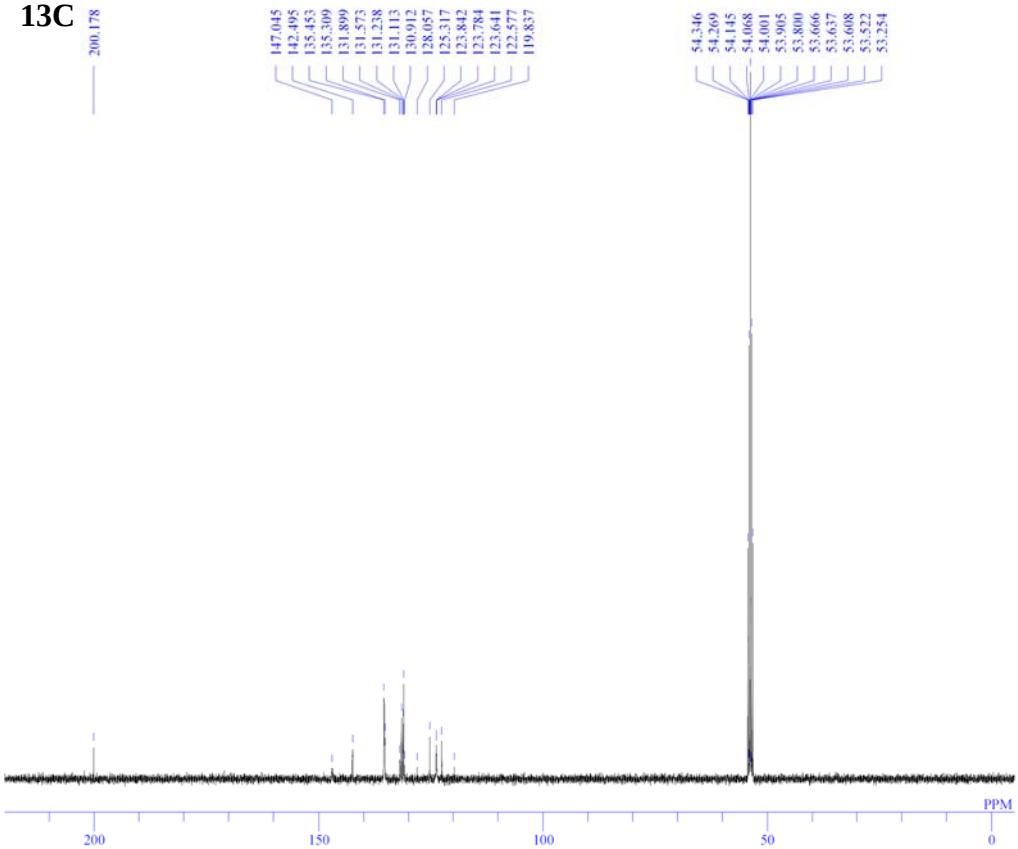
OBSET	6.28 KHz
OBFIN	0.87 Hz
POINT	16384
FREQU	7422.80 Hz
SCANS	8
ACQTM	2.2073 sec
PD	5.0000 sec
PW1	3.12 usec
IRNUC	1H
CTEMP	19.3 c
SLVNT	CD2CL2
EXREF	5.32 ppm
BF	0.00 Hz
RGAIN	44

13C



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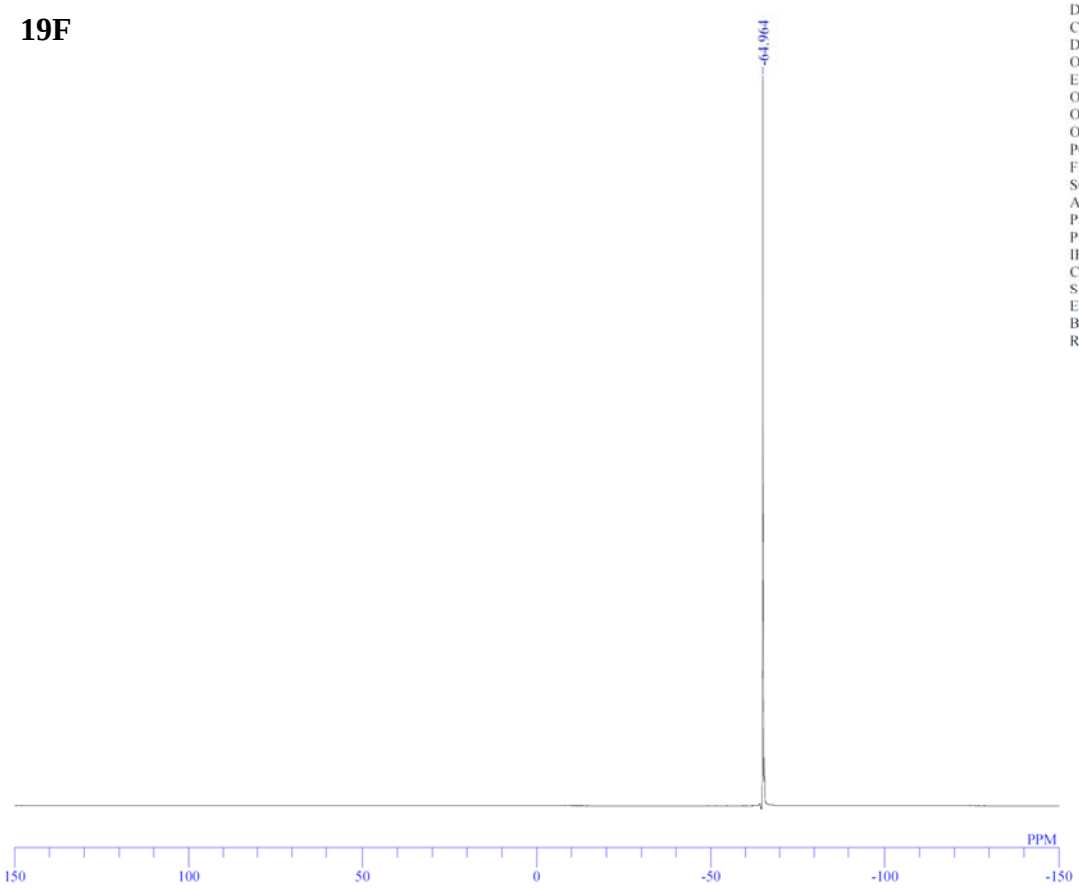
OBFRQ	99.55 MHz
OBSET	5.13 KHz
OBFIN	0.98 Hz
POINT	32767
FREQU	31250.00 Hz
SCANS	1024
ACQTM	1.0486 sec
PD	2.0000 sec
PW1	3.42 usec
IRNUC	1H
CTEMP	19.6 c
SLVNT	CD2CL2
EXREF	53.80 ppm
BF	1.00 Hz
RGAIN	60

19F



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OBSET	3.36 KHz
OBFIN	6.86 Hz
POINT	16384
FREQU	186567.17 Hz
SCANS	32
ACQTM	0.0878 sec
PD	5.0000 sec
PW1	3.67 usec
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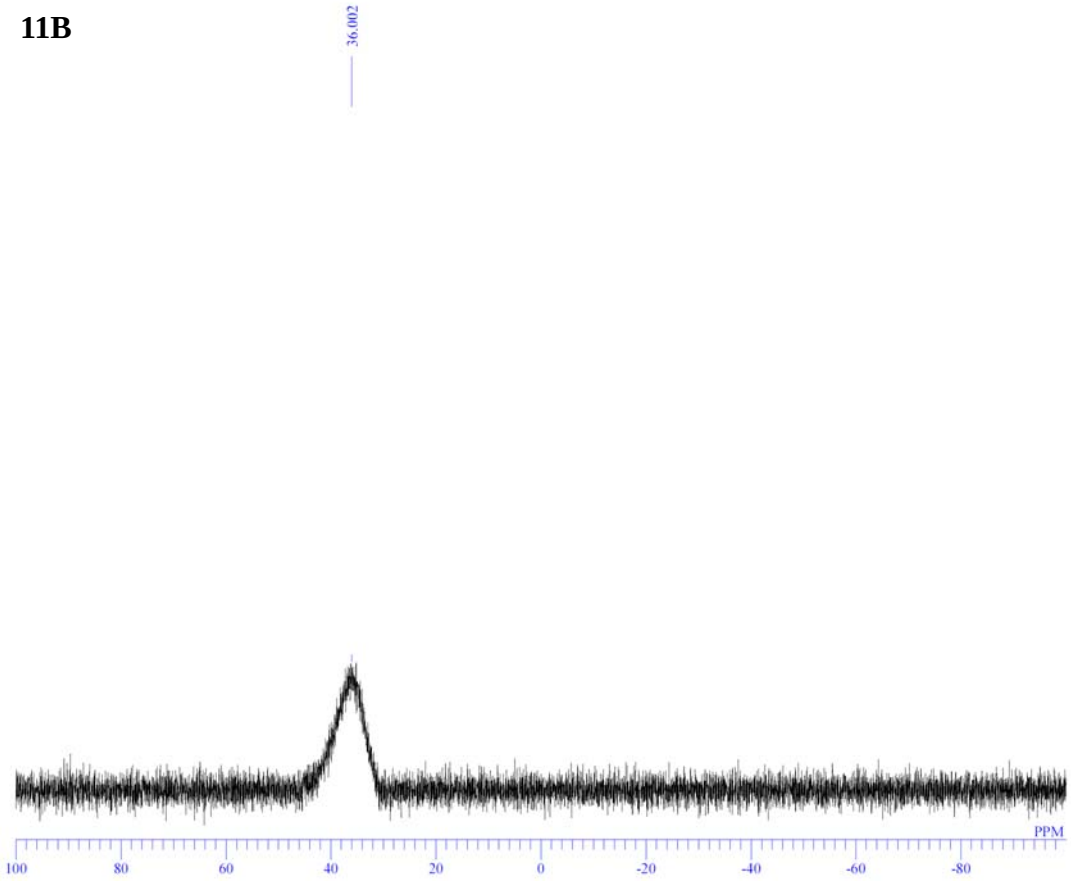
EXREF	-78.20 ppm
BF	30.00 Hz
RGAIN	50

11B



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OBSET	5.53 KHz
OBFIN	4.57 Hz
POINT	13107
FREQU	31847.13 Hz
SCANS	6000
ACQTM	0.4116 sec
PD	5.0000 sec
PW1	5.00 usec
IRNUC	11B
CTEMP	19.5 c
SLVNT	CD2CL2
EXREF	0.00 ppm
BF	0.40 Hz
RGAIN	42