

Electronic Supplementary Information

Scope and mechanism of nitrile dihydroboration mediated by a β -diketiminato manganese hydride catalyst

Thao T. Nguyen,^a Jun-Hyeong Kim,^{b,c} Suyeon Kim,^{b,c} Changjin Oh,^{b,c} Marco Flores,^a Thomas L. Groy,^a Mu-Hyun Baik^{*b,c} and Ryan J. Trovitch^{*a}

^aSchool of Molecular Sciences, Arizona State University, Tempe, Arizona, 85287, USA.

^bDepartment of Chemistry, Korea Advanced Institute of Science and Technology (KAIST), Daejeon 34141, Republic of Korea.

^cCenter for Catalytic Hydrocarbon Functionalizations, Institute for Basic Science (IBS), Daejeon 34141, Republic of Korea.

Email: mbaik2805@kaist.ac.kr, ryan.trovitch@asu.edu

EXPERIMENTAL PROCEDURES

General Considerations: All reactions were performed inside an MBraun glovebox under an atmosphere of purified nitrogen. Toluene, tetrahydrofuran, diethyl ether, and pentane were purchased from Sigma-Aldrich, purified using a Pure Process Technology solvent system, and stored in the glovebox over activated 4 Å molecular sieves and potassium before use. Benzene-*d*₆ was purchased from Oakwood Chemicals and dried over 4 Å molecular sieves and potassium. Celite, pinacolborane, phenylsilane, catecholborane, benzonitrile, *p*-tolunitrile, 4-methoxybenzonitrile, 4-(dimethylamino)benzonitrile, 4-fluorobenzonitrile, 4-chlorobenzonitrile, 2-bromobenzonitrile, 4-(trifluoromethyl)benzonitrile, 4-acetylbenzonitrile, acetonitrile, cyclohexanecarbonitrile, and 2-phenoxyacetonitrile were purchased from Oakwood Chemicals. 9-Borabicyclo[3.3.1]nonane and 3-(dimethylamino)propionitrile were purchased from Sigma Aldrich. All substrates were dried over 3 Å molecular sieves prior to catalyst screening. 3-(Diphenylphosphino)propanenitrile¹ and [(^{2,6-iPr₂Ph}BDI)Mn(μ-H)]₂ (**1**)² were synthesized according to literature procedures.

Solution nuclear magnetic resonance (NMR) spectra were recorded at room temperature on a Varian 400 MHz or a Bruker 400 MHz NMR spectrometer. All ¹H NMR and ¹³C NMR chemical shifts (ppm) are reported relative to Si(Me)₄ using ¹H (residual) and ¹³C chemical shifts of the solvent as secondary standards. ¹⁹F NMR chemical shifts (ppm) are reported relative to trichlorofluoromethane upon referencing an external trifluorotoluene standard at -63.72 ppm. ³¹P NMR chemical shifts (ppm) are reported relative to phosphoric acid upon referencing an external triphenylphosphate standard at -17.54 ppm. Elemental analyses were performed at Robertson Microlit Laboratories Inc. (Ledgewood, NJ). Solution state magnetic susceptibility was determined via Evans method on the Varian 400 MHz NMR spectrometer.^{3,4}

Synthesis of [(^{2,6-iPr₂Ph}BDI)Mn(μ-NCHPh)]₂ (2**):** A 20 mL vial was charged with **1** (0.0728 g, 0.077 mmol) dissolved in 10 mL toluene. Then, a solution of benzonitrile (15.9 μL, 0.154 mmol) in 5 mL of toluene was added to the vial. A color change from yellow to orange was observed. After stirring at room temperature for 1 h, the orange solution was filtered through Celite and the solvent was removed under vacuum to obtain a reddish-orange solid. The solid was washed with Et₂O and recrystallized in toluene layered with pentane upon cooling to -35 °C, affording orange crystals of **2** (0.0631 g, 0.055 mmol, 71%). Elemental analysis for C₇₂H₉₄N₆Mn₂: Calcd. C, 74.97; H, 8.21; N, 7.29. Found: C, 74.65; H, 8.02; N, 7.01. Magnetic susceptibility (Evans method, 25 °C): μ_{eff} = 6.54 μ_B (considering a dimeric structure in solution). ¹H NMR (benzene-*d*₆, 25 °C): 26.82 (peak width at half-height = 14,988 Hz), 14.92 (7,011 Hz), 3.90 (2,891 Hz), -12.36 (23,042 Hz).

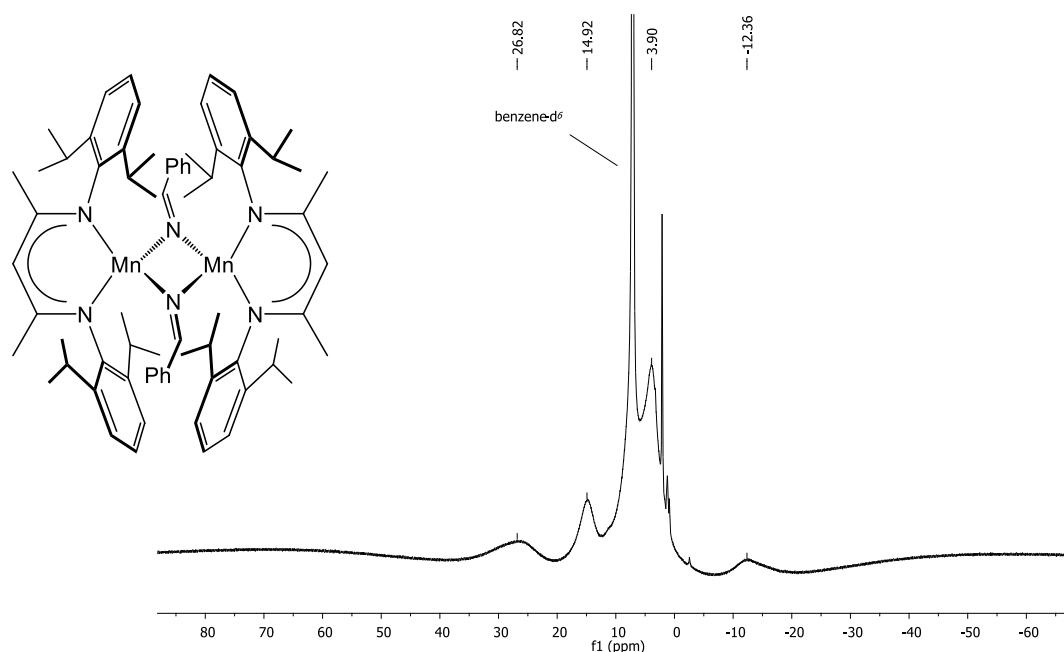


Figure S1. ¹H NMR spectrum of **2** in benzene-*d*₆ at 25 °C.

X-ray Crystallography: A single crystal of **2** was coated with polyisobutylene oil in the glovebox and transferred to a glass fiber, which was then mounted on the goniometer head of a Bruker APEX Diffractometer equipped with Mo K_α radiation (Arizona State University). A hemisphere routine was used for data collection and determination of the lattice constants. The space group was identified and the data was processed using the Bruker SAINT+ program and corrected for absorption using SADABS. The structures were solved using direct methods (SHELXS), completed by subsequent Fourier synthesis, and refined by full-matrix, least square procedures on [F²] (SHELXL). The crystallographic parameters for **2** are provided in Table S1.

EPR Spectroscopy:

Instrumentation. Studies were performed at the EPR Facility of Arizona State University. Continuous wave (CW) EPR spectra were recorded at 114 K using a Bruker ELEXSYS E580 CW X-band spectrometer (Bruker, Rheinstetten, Germany) equipped with a liquid nitrogen temperature control system (ER 4131VT). The magnetic field modulation frequency was 100 kHz with a field modulation amplitude of 0.5 mT peak-to-peak. The microwave power was 1 mW, the microwave frequency was 9.43 GHz and the sweep time was 168 seconds.

Spin Hamiltonian. The EPR spectra of a coupled dimer system can be described with the spin Hamiltonian:⁵

$$H = -2J_0h\mathbf{S}_1 \cdot \mathbf{S}_2 + h\mathbf{S}_1 \cdot \mathbf{J} \cdot \mathbf{S}_2 + H_1 + H_2 \quad (1)$$

where J_0 is the isotropic exchange coupling constant between the two Mn(II) ions of the dimer, $\mathbf{J}$ is the tensor describing the dipole-dipole interaction between the two Mn(II) spin centers, both in frequency units, h is Planck's constant, and H_i ($i = 1, 2$) are the spin Hamiltonians corresponding to each individual Mn(II) ion. The spin Hamiltonian of each Mn(II) spin center contains the electron Zeeman interaction with the applied magnetic field $\mathbf{B}_0$, the zero-field interaction, and the hyperfine coupling (hfc) interaction with the nucleus of ⁵⁵Mn:

$$H_i = \beta_e\mathbf{S}_i \cdot \mathbf{g}_i \cdot \mathbf{B}_0 + h\mathbf{S}_i \cdot \mathbf{d}_i \cdot \mathbf{S}_i + h\mathbf{S}_i \cdot \mathbf{a}_i \cdot \mathbf{I}_i \quad (2)$$

where $\mathbf{S}_i$ and $\mathbf{I}_i$ are the electron and nuclear spin operators, respectively, $\mathbf{d}_i$ and $\mathbf{a}_i$ are the zero-field splitting and hfc tensors, respectively, all in frequency units, $\mathbf{g}_i$ is the electronic g -tensor, and β_e is the electron magneton. For Mn(II) dimers, the electron and nuclear spins of each Mn(II) ion are $S_i = 5/2$ and $I_i = 5/2$, respectively. Mn(II) ions have a singlet orbital ground state (⁶A), with the first excited orbital state (⁴T) more than 10,000 cm⁻¹ above the ground state. Consequently, the zero-field energies of Mn(II) ions are generally small, $|D_i| < 0.1$ cm⁻¹.^{6,7} For dimeric manganese complexes, the bridging atoms typically give a Mn–Mn exchange interaction that is significantly larger than 0.1 cm⁻¹. In this strong exchange regimen, the isotropic exchange coupling energy is much larger than the electronic Zeeman energy ($|J_0| \gg g_i\beta_e B_0/h$) and the zero-field splitting ($|J_0| \gg |D_i|$). The dimer system may then be regarded as a ladder of isolated spin manifolds. These spin manifolds have total spin quantum numbers of $S = 0, 1, 2, 3, 4$, and 5 , each with a degeneracy of $(2S+1)$. The energy separation between the spin manifolds is much larger than the microwave energy ($h\nu$) at the X-band (9.40 GHz) frequency and no transitions are observable between spin manifolds. The individual spin manifolds can be considered independently and their corresponding spectra can be simulated using a spin Hamiltonian for each individual spin manifold given by:⁸

$$H_S = \beta_e\mathbf{S} \cdot \mathbf{G}_S \cdot \mathbf{B}_0 + h\mathbf{S} \cdot \mathbf{D}_S \cdot \mathbf{S} + h\mathbf{S} \cdot \mathbf{A}_1 \cdot \mathbf{I}_1 + h\mathbf{S} \cdot \mathbf{A}_2 \cdot \mathbf{I}_2 \quad (3)$$

where $\mathbf{G}_S$, $\mathbf{D}_S$, and $\mathbf{A}_i$ ($i = 1, 2$) are the electronic Zeeman, zero-field splitting, and hfc tensors, respectively, of the spin manifolds of the coupled system, and $\mathbf{S}$ is the spin operator of the coupled spin manifolds. The parameters of the coupled spin system can be expressed as linear combinations of the parameters of the individual spin centers:

$$\mathbf{G}_S = c_1\mathbf{g}_1 + c_2\mathbf{g}_2 \quad (4)$$

$$\mathbf{D}_S = d_1\mathbf{d}_1 + d_2\mathbf{d}_2 + d_{12}\mathbf{J} \quad (5)$$

$$\mathbf{A}_i = c_i\mathbf{a}_i \quad (6)$$

where the coefficients c_1 , c_2 , d_1 , d_2 , and d_{12} are specific to the particular spin manifold and have been tabulated elsewhere.⁸ For Mn(II) ions, the contributions from spin-orbit coupling to the $\mathbf{g}_i$ tensor and hfc tensor are small, thus we will assume that both tensors $\mathbf{g}_i$ and $\mathbf{a}_i$ are isotropic. In the complex studied here, the two manganese centers of the dimer have identical ligation. The

coordination geometry of one manganese ion is related to the other by a mirror plane, thus, we assume $g_1 = g_2 = g_{\text{iso}}$, $a_1 = a_2 = a$, and $\mathbf{d}_1 = \mathbf{d}_2$. In this study, hfc's due to Mn(II) were not explicitly included in the spin Hamiltonian (Eq. 3).

Fitting of EPR spectra. To quantitatively compare experimental and simulated spectra, we divided the spectra into N intervals (*i.e.*, we treated the spectrum as an N -dimensional vector $\mathbf{R}$). Each component R_j has the amplitude of the EPR signal at a magnetic field B_j , with j varying from 1 to N . The amplitudes of the experimental and simulated spectra were normalized so that the span between the maximum and minimum values of R_j is 1. We compared the calculated amplitudes R_j^{calc} of the signal with the observed values R_j defining a root-mean-square deviation σ by:

$$\sigma(p_1, p_2, \dots, p_n) = [\sum_j (R_j^{\text{calc}}(p_1, p_2, \dots, p_n) - R_j^{\text{exp}})^2 / N]^{1/2} \quad (7)$$

where the sums are over the N values of j , and p 's are the fitting parameters that produced the calculated spectrum. For our simulations, N was set equal to 2048. The EPR spectrum was simulated using EasySpin (v 5.2.25), a computational package developed by Stoll and Schweiger⁹ and based on Matlab (The MathWorks, Natick, MA, USA). EasySpin calculates EPR resonance fields using the energies of the states of the spin system obtained by direct diagonalization of the spin Hamiltonian (see Eq. 3). The EPR fitting procedure used a Monte Carlo type iteration to minimize the root-mean-square deviation, σ (see Eq. 7) between measured and simulated spectra. We searched for the optimum values of the following parameters: the isotropic g -value (g_{iso}), the zero-field splitting parameters (D and E), the principal components of the $\mathbf{J}$ tensor (J_x , J_y , and J_z) and the isotropic peak-to-peak linewidth (ΔB).

Computational Details

All calculations were carried out using DFT¹⁰ as implemented in the Jaguar 9.1 suite¹¹ of ab initio quantum chemistry programs. Geometry optimizations were performed with B3LYP¹²⁻¹⁶ functional including Grimme's D3 dispersion correction¹⁷ and the 6-31G** basis set for main group atoms. Mn was represented using the Los Alamos LACVP basis.¹⁸⁻²⁰ The energies of the optimized structures were reevaluated by additional single-point calculations on each optimized geometry using Dunning's correlation consistent triple- ζ basis set cc-pVTZ(-f),²¹ which includes a double set of polarization functions. For Mn, we used a modified version of LACVP, designated as LACV3P, in which the exponents were decontracted to match the effective core potential with triple- ζ quality. For boron, 6-311G** containing the decontracted exponent with triple- ζ quality was used. Solvation energies were evaluated by a self-consistent reaction field (SCRF) approach based on accurate numerical solutions of the Poisson–Boltzmann equation. In the results reported, solvation calculations were carried out with the 6-31G**/LACVP basis at the optimized gas-phase geometry employing the dielectric constant of $\epsilon = 2.284$ for benzene. As is the case for all continuum models, the solvation energies are subject to empirical parametrization of the atomic radii that are used to generate the solute surface. We employed the standard set of optimized radii in Jaguar for H (1.150 Å), B (2.042 Å), C (1.900 Å), N (1.600 Å), O (1.600 Å), and Mn (1.480 Å).²² Analytical vibrational frequencies within the harmonic approximation were computed with the 6-31G**/LACVP basis to confirm proper convergence to well-defined minima or saddle points on the potential energy surface. The energy components have been computed with the following protocol. The free energy in solution-phase, $G(\text{sol})$, has been calculated as follows:

$$G(\text{sol}) = G(\text{gas}) + G_{\text{solv}} \quad (8)$$

$$G(\text{gas}) = H(\text{gas}) - TS(\text{gas}) \quad (9)$$

$$H(\text{gas}) = E(\text{SCF}) + \text{ZPE} \quad (10)$$

$$\Delta E(\text{SCF}) = \sum E(\text{SCF}) \text{ for products} - \sum E(\text{SCF}) \text{ for reactants} \quad (11)$$

$$\Delta G(\text{sol}) = \sum G(\text{sol}) \text{ for products} - \sum G(\text{sol}) \text{ for reactants} \quad (12)$$

CRYSTALLOGRAPHIC DATA

Table S1. Crystallographic data for **2**.

	2
chemical formula	C ₇₂ H ₉₄ Mn ₂ N ₆
formula weight	1153.41
crystal dimensions	0.264 x 0.212 x 0.171
crystal system	monoclinic
space group	P 1 2 ₁ /n 1
<i>a</i> (Å)	12.3092(5)
<i>b</i> (Å)	12.7350(5)
<i>c</i> (Å)	20.5570(9)
α (deg)	90
β (deg)	92.9550(10)
γ (deg)	90
<i>V</i> (Å ³)	3218.2(2)
<i>Z</i>	2
<i>T</i> (°C)	123.00(10)
ρ_{calcd} (g cm ⁻³)	1.190
μ (mm ⁻¹)	0.438
reflections collected	26289
data/restraints/parameters	5849/0/371
<i>R</i> ₁ [<i>I</i> > 2 σ (<i>I</i>)]	0.0486
<i>wR</i> ₂ (all data)	0.1269
Goodness-of-fit	1.065
Largest peak, hole (eÅ ⁻³)	0.890, -0.205

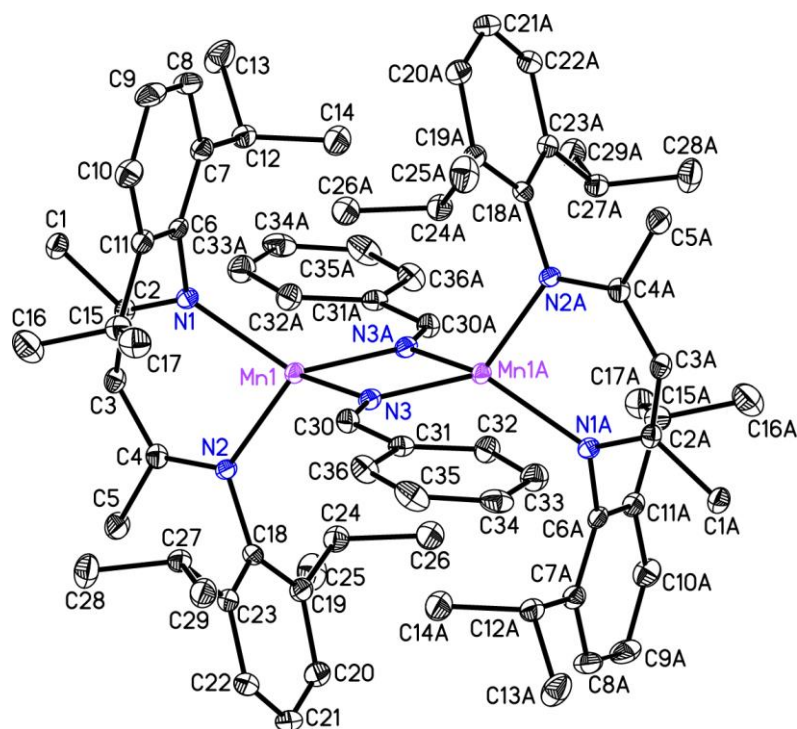


Figure S2. The molecular structure of **2** shown at 30% probability ellipsoids. Hydrogen atoms omitted for clarity.

Table S2. Bond length (Å) and angles (°) for **2**.

Mn1–N3	2.1086(18)	C6–C11	1.409(3)	C21–C22	1.375(4)
Mn1–N2	2.1099(18)	C7–C8	1.391(3)	C22–C23	1.391(3)
Mn1–N1	2.1211(18)	C7–C12	1.521(3)	C23–C27	1.516(3)
Mn1–N3A	2.1230(19)	C8–C9	1.381(4)	C24–C26	1.523(3)
Mn1–Mn1A	3.0819(6)	C9–C10	1.381(4)	C24–C25	1.536(3)
N1–C2	1.336(3)	C10–C11	1.390(3)	C27–C29	1.526(4)
N1–C6	1.438(3)	C11–C15	1.523(3)	C27–C28	1.532(3)
N2–C4	1.330(3)	C12–C14	1.520(3)	C30–C31	1.493(3)
N2–C18	1.449(3)	C12–C13	1.525(3)	C31–C36	1.389(3)
N3–C30	1.267(3)	C15–C16	1.525(4)	C31–C32	1.391(3)
N3–Mn1A	2.1231(19)	C15–C17	1.531(3)	C32–C33	1.377(3)
C1–C2	1.519(3)	C18–C23	1.398(3)	C33–C34	1.388(4)
C2–C3	1.393(3)	C18–C19	1.405(3)	C34–C35	1.377(4)
C3–C4	1.406(3)	C19–C20	1.393(3)	C35–C36	1.385(4)
C4–C5	1.518(3)	C19–C24	1.523(4)		
C6–C7	1.406(3)	C20–C21	1.380(4)		
N3–Mn1–N2	119.08(7)	N2–C4–C5	120.4(2)	C20–C19–C24	120.1(2)
N3–Mn1–N1	124.95(7)	C3–C4–C5	115.4(2)	C18–C19–C24	122.5(2)
N2–Mn1–N1	89.91(7)	C7–C6–C11	120.6(2)	C21–C20–C19	121.3(2)
N3–Mn1–N3A	86.52(8)	C7–C6–N1	120.6(2)	C22–C21–C20	120.3(2)
N2–Mn1–N3A	112.79(7)	C11–C6–N1	118.8(2)	C21–C22–C23	120.8(3)
N1–Mn1–N3A	126.38(7)	C8–C7–C6	118.5(2)	C22–C23–C18	118.2(2)
N3–Mn1–Mn1A	43.44(5)	C8–C7–C12	121.2(2)	C22–C23–C27	120.4(2)
N2–Mn1–Mn1A	126.83(5)	C6–C7–C12	120.3(2)	C18–C23–C27	121.3(2)
N1–Mn1–Mn1A	143.19(5)	C9–C8–C7	121.5(2)	C26–C24–C19	109.9(2)
N3A–Mn1–Mn1A	43.07(5)	C10–C9–C8	119.3(2)	C26–C24–C25	109.4(2)
C2–N1–C6	115.51(18)	C9–C10–C11	121.8(2)	C19–C24–C25	113.4(2)
C2–N1–Mn1	121.54(14)	C10–C11–C6	118.2(2)	C23–C27–C29	113.5(2)
C6–N1–Mn1	122.87(14)	C10–C11–C15	120.5(2)	C23–C27–C28	110.9(2)
C4–N2–C18	116.03(18)	C6–C11–C15	121.2(2)	C29–C27–C28	110.1(2)
C4–N2–Mn1	122.75(15)	C14–C12–C7	109.8(2)	N3–C30–C31	128.1(2)
C18–N2–Mn1	121.21(13)	C14–C12–C13	110.1(2)	C36–C31–C32	117.5(2)
C30–N3–Mn1	128.33(16)	C7–C12–C13	114.3(2)	C36–C31–C30	119.3(2)
C30–N3–Mn1A	138.18(16)	C11–C15–C16	111.3(2)	C32–C31–C30	123.1(2)
Mn1–N3–Mn1A	93.48(8)	C11–C15–C17	113.4(2)	C33–C32–C31	121.6(2)
N1–C2–C3	124.9(2)	C16–C15–C17	109.6(2)	C32–C33–C34	120.0(3)
N1–C2–C1	120.1(2)	C23–C18–C19	121.7(2)	C35–C34–C33	119.3(2)
C3–C2–C1	115.0(2)	C23–C18–N2	118.1(2)	C34–C35–C36	120.3(2)
C2–C3–C4	129.7(2)	C19–C18–N2	120.3(2)	C35–C36–C31	121.3(2)
N2–C4–C3	124.1(2)	C20–C19–C18	117.5(2)		

PROCEDURES AND SPECTROSCOPIC DATA FOR CATALYTIC TRIALS

Hydroboration of benzonitrile catalyzed by 0.5 mol% of **1 (1 mol% based on Mn):** In the glove box, HBPin (337.25 μ L, 2.32 mmol) and benzonitrile (110 μ L, 1.06 mmol) were added to a vial containing a benzene- d_6 solution of **1** (0.005 g, 0.00528 mmol). The vial was sealed under N_2 atmosphere and stirred at 80 $^{\circ}$ C. After 24 h of heating, I_2 was added to the solution to deactivate the catalyst. Greater than 99% conversion was observed by 1H NMR spectroscopy. The solvent and remaining borane were removed under vacuum, resulting in a white solid. Recrystallization from pentane at -35 $^{\circ}$ C yielded 0.316 g (83%) of *N*-benzyl-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine. 1H NMR (benzene- d_6 , 400 MHz): 7.60 (d, $J = 7.6$ Hz, 2H, *phenyl*), 7.26 (pseudo t, $J = 7.6$ Hz, 2H, *phenyl*), 7.12 (m, 1H, *phenyl*), 4.63 (s, 2H, CH_2), 1.04 (s, 24H, CCH_3). ^{13}C NMR (benzene- d_6 , 100 MHz): 144.61 – 143.76 (m, *phenyl*), 128.71 (s, *phenyl*), 128.41 (s, *phenyl*), 127.00 (s, *phenyl*), 82.94 (s, CCH_3), 48.32 (s, CH_2), 25.15 (s, CH_3).

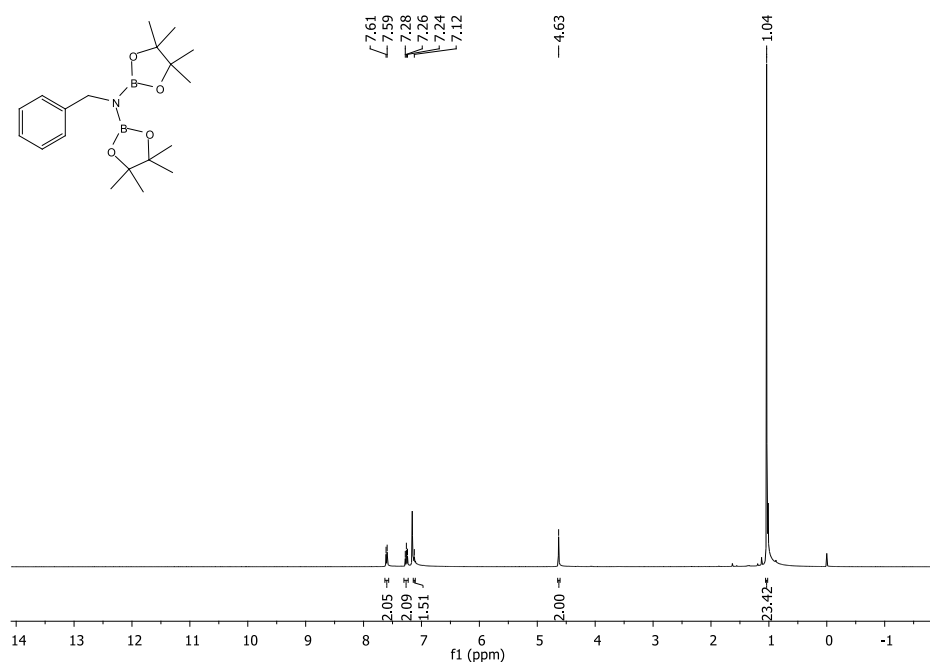


Figure S3. 1H NMR spectrum of *N*-benzyl-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine in benzene- d_6 .

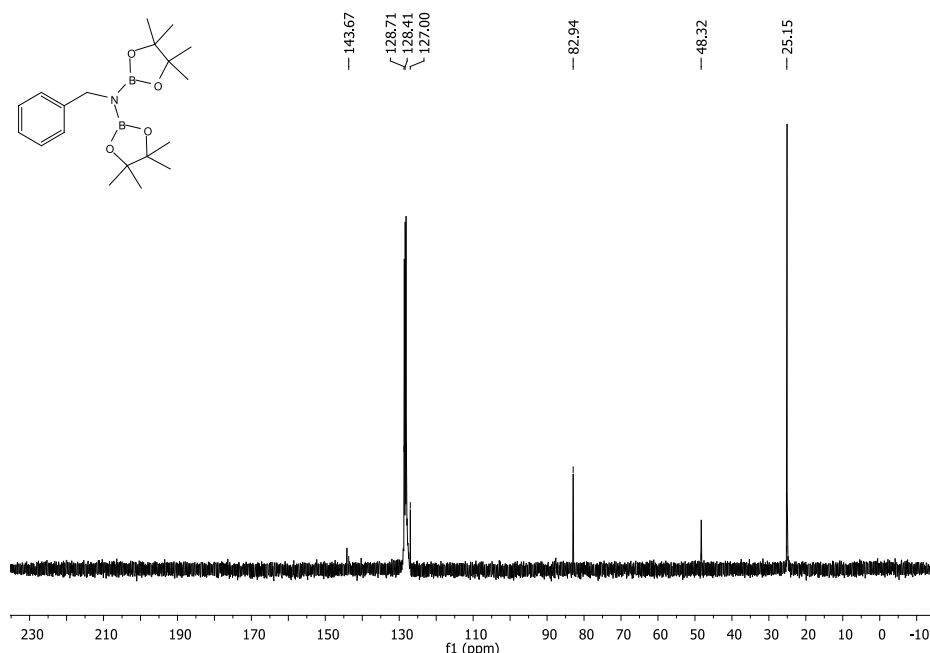


Figure S4. ¹³C NMR spectrum of *N*-benzyl-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine in benzene-*d*₆.

Hydroboration of *p*-tolunitrile catalyzed by 0.5 mol% of **1 (1 mol% based on Mn):** In the glove box, HBPIn (278 μL, 1.92 mmol) and *p*-tolunitrile (0.102 g, 0.871 mmol) were added to a vial containing a benzene-*d*₆ solution of **1** (0.0042 g, 0.00435 mmol). The vial was sealed under N₂ atmosphere and stirred at 80 °C. After 24 h of heating, I₂ was added to the solution to deactivate the catalyst. Greater than 99% conversion was observed by ¹H NMR spectroscopy. The solvent and remaining borane were removed under vacuum, resulting in a white solid. Recrystallization from pentane at −35 °C yielded 0.2665 g (82%) of 4,4,5,5-tetramethyl-*N*-(4-methylbenzyl)-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine. ¹H NMR (benzene-*d*₆, 400 MHz): 7.55 (d, *J* = 7.6 Hz, 2H, *phenyl*), 7.09 (d, *J* = 7.6 Hz, 2H, *phenyl*), 4.63 (s, 2H, CH₂), 2.16 (s, 3H, CH₃), 1.05 (s, 24H, CCH₃). ¹³C NMR (benzene-*d*₆, 100 MHz): 141.26 (s, *phenyl*), 136.12 (s, *phenyl*), 129.43 (s, *phenyl*), 128.47 (s, *phenyl*), 82.91 (s, CCH₃), 47.99 (s, CH₂), 25.10 (s, CCH₃), 21.50 (s, CH₃).

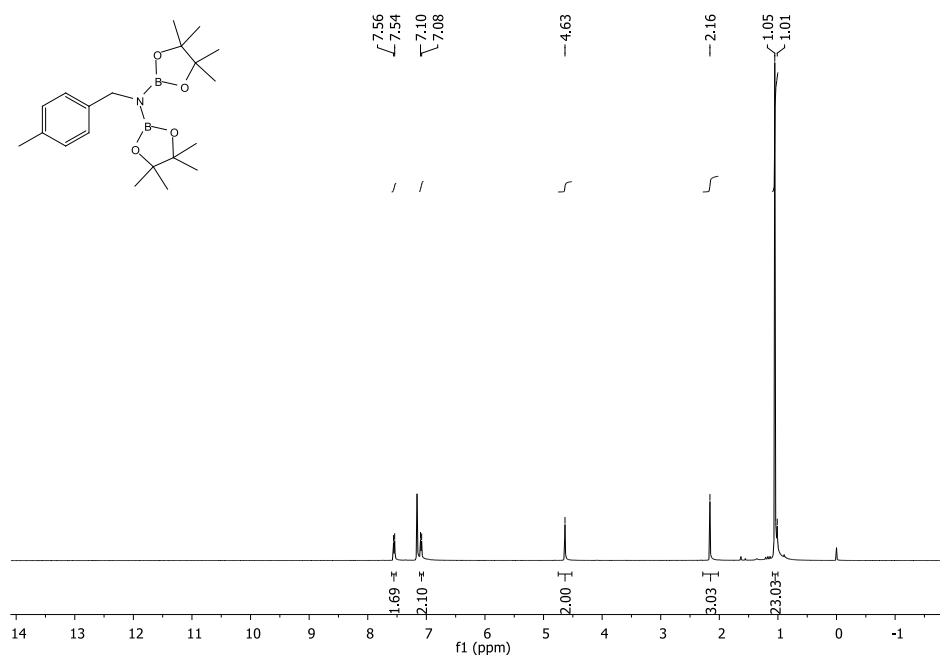


Figure S5. ¹H NMR spectrum of 4,4,5,5-tetramethyl-*N*-(4-methylbenzyl)-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine in benzene-*d*₆.

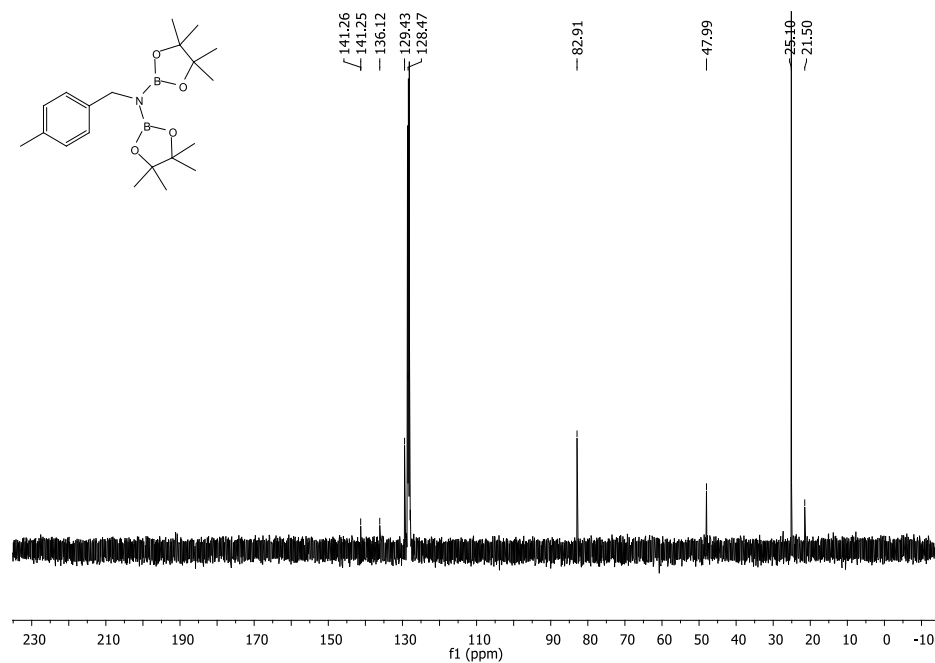


Figure S6. ^{13}C NMR spectrum of 4,4,5,5-tetramethyl-*N*-(4-methylbenzyl)-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine in benzene- d_6 .

Hydroboration of 4-methoxybenzonitrile catalyzed by 0.5 mol% of **1 (1 mol% based on Mn):** In the glove box, HBPin (404.7 μ L, 2.79 mmol) and 4-methoxybenzonitrile (0.169 g, 1.27 mmol) were added to a vial containing a benzene- d_6 solution of **1** (0.006 g, 0.00634 mmol). The vial was sealed under N_2 atmosphere and stirred at 80 $^{\circ}$ C. After 24 h of heating, I_2 was added to the solution to deactivate the catalyst. Greater than 99% conversion was observed by 1H NMR spectroscopy. The solvent and remaining borane were removed under vacuum, resulting in a white solid. Recrystallization from pentane at -35 $^{\circ}$ C yielded 0.3509 g (71%) of *N*-(4-methoxybenzyl)-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine. 1H NMR (benzene- d_6 , 400 MHz): 7.58 (d, J = 8.1 Hz, 2H, *phenyl*), 6.89 (d, J = 8.1 Hz, 2H, *phenyl*), 4.61 (s, 2H, CH_2), 3.35 (s, 3H, $-OCH_3$), 1.06 (s, 24H, CCH_3). ^{13}C NMR (benzene- d_6 , 100 MHz): 159.36 (s, *phenyl*), 136.43 (s, *phenyl*), 129.83 (s, *phenyl*), 114.22 (s, *phenyl*), 82.90 (s, CCH_3), 55.10 (s, CH_2), 47.68 (s, CH_3), 25.12 (s, CCH_3).

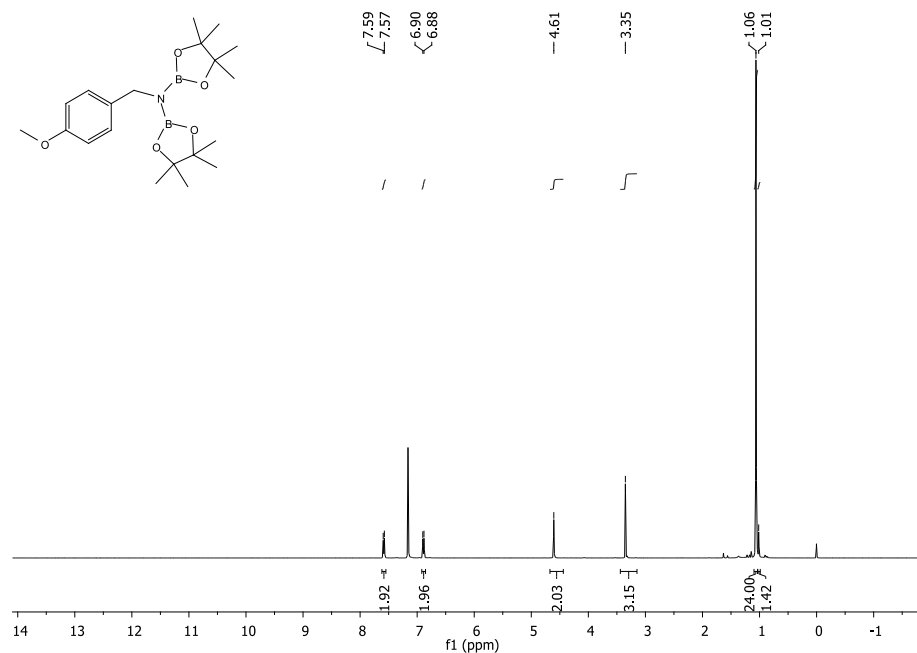


Figure S7. 1H NMR spectrum of *N*-(4-methoxybenzyl)-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine in benzene- d_6 .

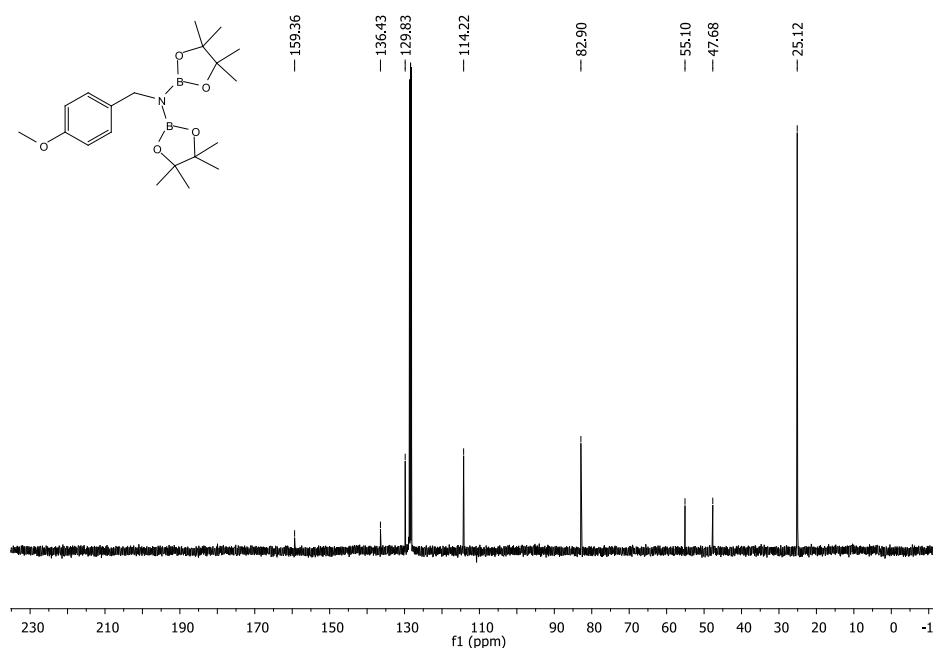


Figure S8. ^{13}C NMR of *N*-(4-methoxybenzyl)-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine in benzene- d_6 .

Hydroboration of 4-(dimethylamino)benzonitrile catalyzed by 0.5 mol% of **1 (1 mol% based on Mn):** In the glove box, HBPin (346.9 μ L, 2.5147 mmol) and 4-(dimethylamino)benzonitrile (167.1 mg, 1.143 mmol) were added to vial containing a benzene- d_6 solution of **1** (0.0054 g, 0.0057 mmol). The vial was sealed under N_2 atmosphere and stirred at 80 $^{\circ}$ C. After 24 h of heating, I_2 was added to the solution to deactivate the catalyst. 1H NMR spectroscopy revealed 84% conversion. The solvent and remaining borane were removed under vacuum and the resulting solid was washed with Et_2O . Recrystallization from pentane at -35 $^{\circ}$ C yielded 0.2026 g (44%) of *N*-(4-(dimethylamino)benzyl)-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine. 1H NMR (benzene- d_6 , 400 MHz): 7.55 (d, J = 8.6 Hz, 2H, *phenyl*), 6.67 (d, J = 8.6 Hz, 2H, *phenyl*), 4.55 (s, 2H, CH_2), 2.57 (s, 6H, NCH_3), 1.05 (s, 24H, CCH_3). ^{13}C NMR (benzene- d_6 , 100 MHz): 150.22 (s, *phenyl*), 132.61 (s, *phenyl*), 129.56 (s, *phenyl*), 113.30 (s, *phenyl*), 82.75 (s, CCH_3), 47.65 (s, CH_2), 40.95 (s, NCH_3), 25.15 (s, CCH_3).

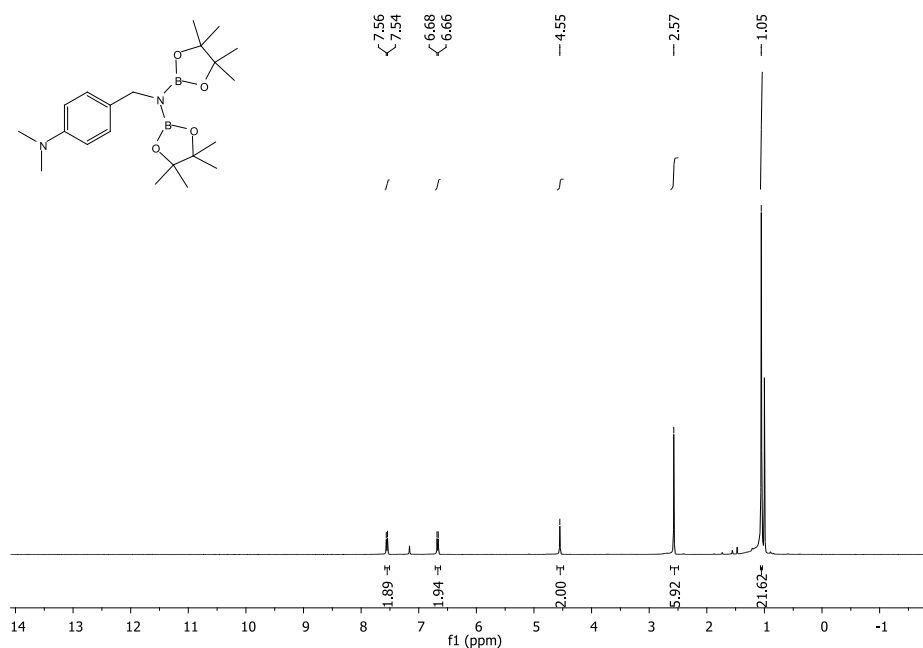


Figure S9. 1H NMR spectrum of *N*-(4-(dimethylamino)benzyl)-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine in benzene- d_6 .

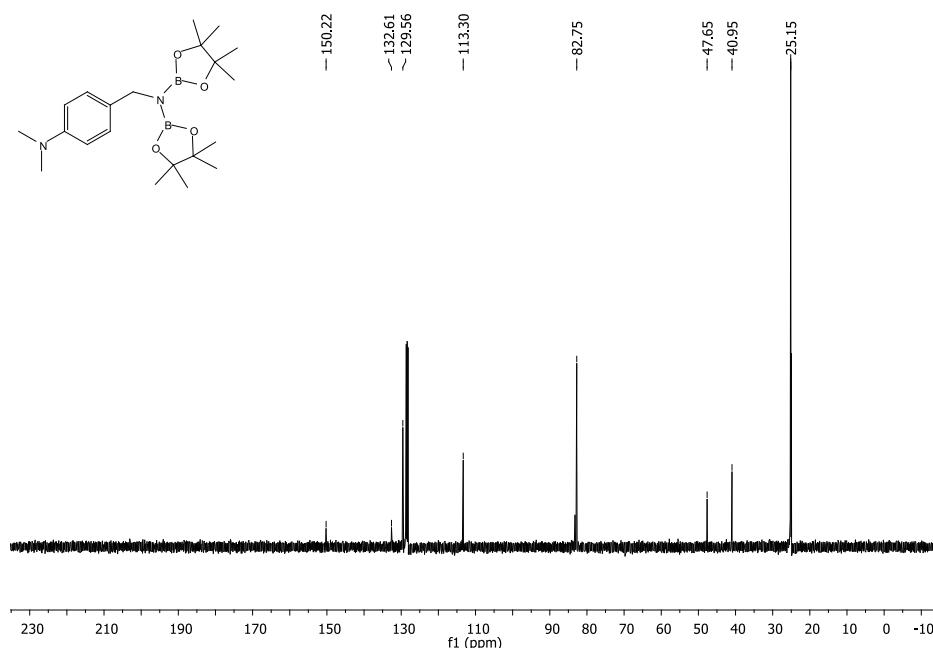


Figure S10. ^{13}C NMR of *N*-(4-(dimethylamino)benzyl)-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine in benzene- d_6 .

Hydroboration of 4-fluorobenzonitrile catalyzed by 0.5 mol% of **1 (1 mol% based on Mn):** In the glove box, HBPIn (344.2 μ L, 2.372 mmol) and 4-fluorobenzonitrile (0.131 g, 1.08 mmol) were added to a vial containing a benzene- d_6 solution of **1** (0.0052 g, 0.0054 mmol). The vial was sealed under N_2 atmosphere and stirred at 80 $^{\circ}$ C. After 24 h of heating, I_2 was added to the solution to deactivate the catalyst. Greater than 99% conversion was observed by 1H NMR spectroscopy. The solvent and remaining borane were removed under vacuum, resulting in a white solid. Recrystallization from pentane at -35 $^{\circ}$ C yielded 0.3584 g (88%) of *N*-(4-fluorobenzyl)-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine. 1H NMR (benzene- d_6 , 400 MHz): 7.45-7.41 (dd, J = 8.5, 5.7 Hz, 2H, *phenyl*), 6.92-6.88 (t, J = 8.8 Hz, 2H, *phenyl*), 4.49 (s, 2H, CH_2), 1.03 (s, 24H, CCH_3). ^{13}C NMR (benzene- d_6 , 100 MHz): 130.15 (d, J = 7.8 Hz, *phenyl*), 128.87 (d, J = 11.4 Hz, *phenyl*), 115.36 (d, J = 21.0 Hz, *phenyl*), 83.00 (s, CCH_3), 47.50 (s, CH_2), 25.06 (s, CCH_3). ^{19}F NMR (benzene- d_6 , 407.6 MHz): -118.41.

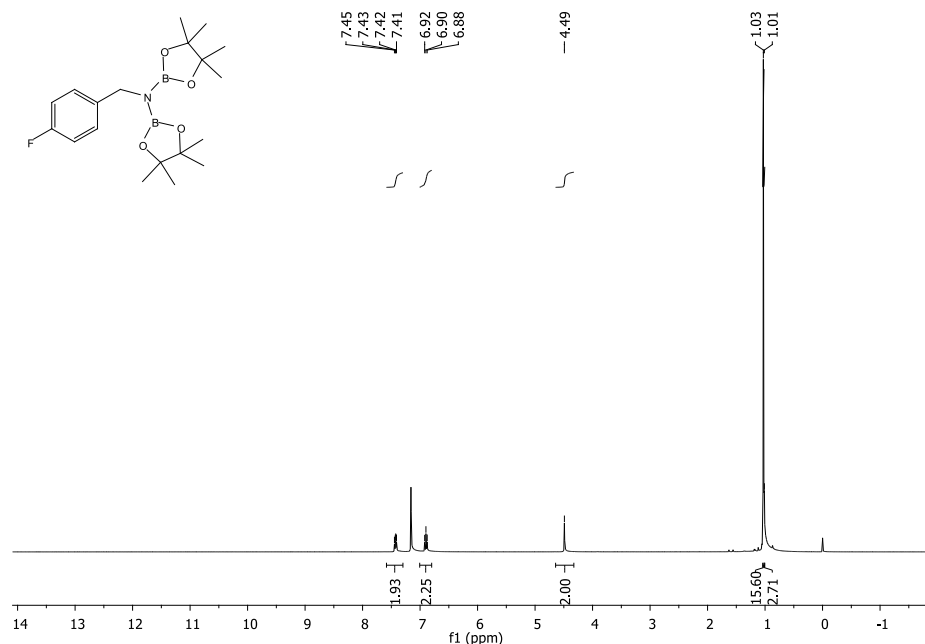


Figure S11. 1H NMR spectrum of *N*-(4-fluorobenzyl)-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine in benzene- d_6 .

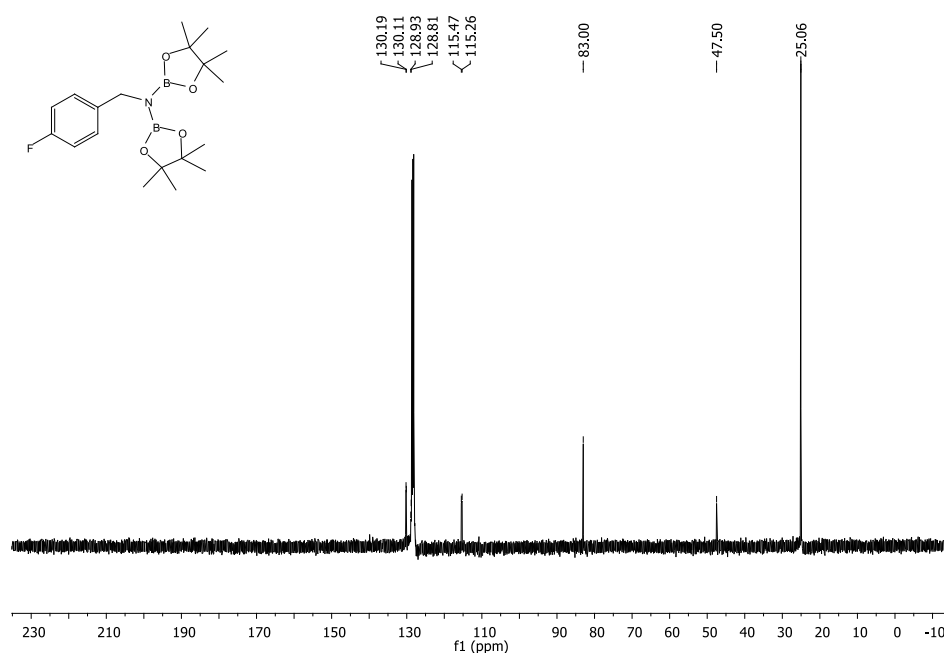


Figure S12. ^{13}C NMR spectrum of *N*-(4-fluorobenzyl)-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine in benzene- d_6 .

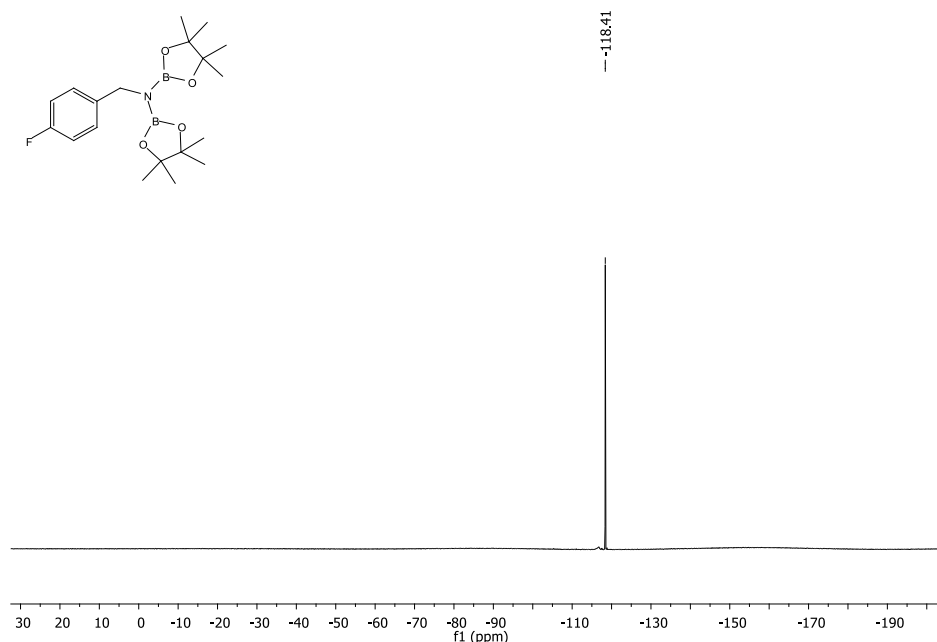


Figure S13. ^{19}F NMR spectrum of *N*-(4-fluorobenzyl)-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine in benzene- d_6 .

Hydroboration of 4-chlorobenzonitrile catalyzed by 0.5 mol% of **1 (1 mol% based on Mn):** In the glove box, HBPin (472.2 μL , 3.254 mmol) and 4-chlorobenzonitrile (0.203 g, 1.48 mmol) were added to vial containing a benzene- d_6 solution of **1** (0.007 g, 0.0074 mmol). The vial was sealed under N_2 atmosphere and stirred at 80 $^\circ\text{C}$. After 24 h of heating, I_2 was added to the solution to deactivate the catalyst. Greater than 99% conversion was observed by ^1H NMR spectroscopy. The solvent and remaining borane were removed under vacuum, resulting in a white solid. Recrystallization from pentane at -35 $^\circ\text{C}$ yielded 0.5355 g (92%) of *N*-(4-chlorobenzyl)-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine. ^1H NMR (benzene- d_6 , 400 MHz): 7.35 (d, $J = 7.7$ Hz, 2H, *phenyl*), 7.18 (d, $J = 13.7$ Hz, 2H, *phenyl*), 4.44 (s, 2H, CH_2), 1.02 (s, 24H, CCH_3). ^{13}C NMR (benzene- d_6 , 100 MHz): 142.59 (s, *phenyl*), 132.80 (s, *phenyl*), 129.89 (s, *phenyl*), 128.83 (s, *phenyl*), 83.03 (s, CCH_3), 47.53 (s, CH_2), 25.05 (s, CCH_3).

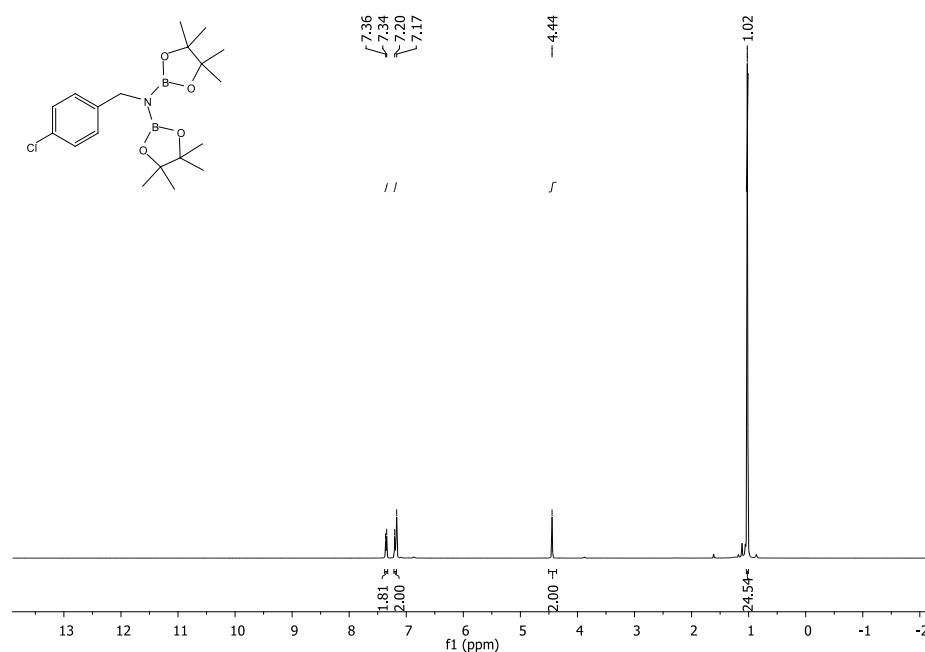


Figure S14. ^1H NMR spectrum of *N*-(4-chlorobenzyl)-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine in benzene- d_6 .

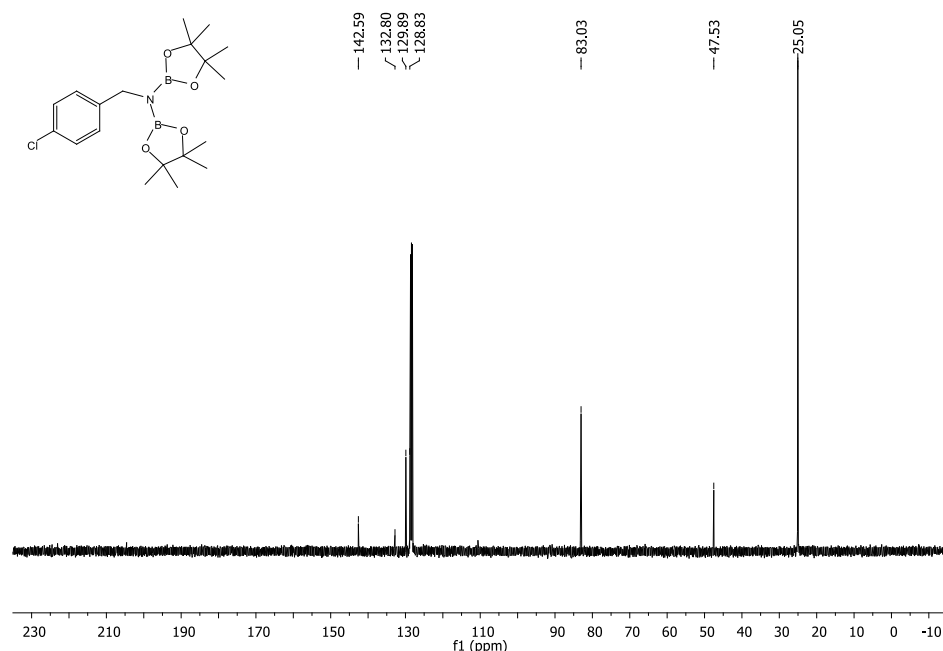


Figure S15. ¹³C NMR spectrum of *N*-(4-chlorobenzyl)-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine in benzene-*d*₆.

Hydroboration of 2-bromobenzonitrile catalyzed by 0.5 mol% of **1 (1 mol% based on Mn):** In the glove box, HBPIn (263 μL, 1.813 mmol) and 2-bromobenzonitrile (0.150 g, 0.824 mmol) were added to a vial containing a benzene-*d*₆ solution of **1** (0.0039 g, 0.00412 mmol). The vial was sealed under N₂ atmosphere and stirred at 80 °C. After 24 h of heating, I₂ was added to the solution to deactivate the catalyst. Greater than 99% conversion was observed by ¹H NMR spectroscopy. The solvent and remaining borane were removed under vacuum, resulting in a white solid. Recrystallization from pentane at –35 °C yielded 0.310 g (86%) of *N*-(2-bromobenzyl)-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine. ¹H NMR (benzene-*d*₆, 400 MHz): 7.57 (d, *J* = 7.7 Hz, 1H, *phenyl*), 7.35 (d, *J* = 7.9 Hz, 1H, *phenyl*), 7.10 (d, *J* = 7.5 Hz, 1H, *phenyl*), 6.72 (t, *J* = 7.6 Hz, 1H, *phenyl*), 4.85 (s, 2H, CH₂), 1.01 (s, 24H, CCH₃). ¹³C NMR (benzene-*d*₆, 100 MHz): 142.53 (s, *phenyl*), 133.14 (s, *phenyl*), 128.81 (s, *phenyl*), 128.10 (s, *phenyl*), 127.55 (s, *phenyl*), 127.34 (s, *phenyl*), 83.10 (s, CCH₃), 48.88 (s, CH₂), 24.94 (s, CCH₃).

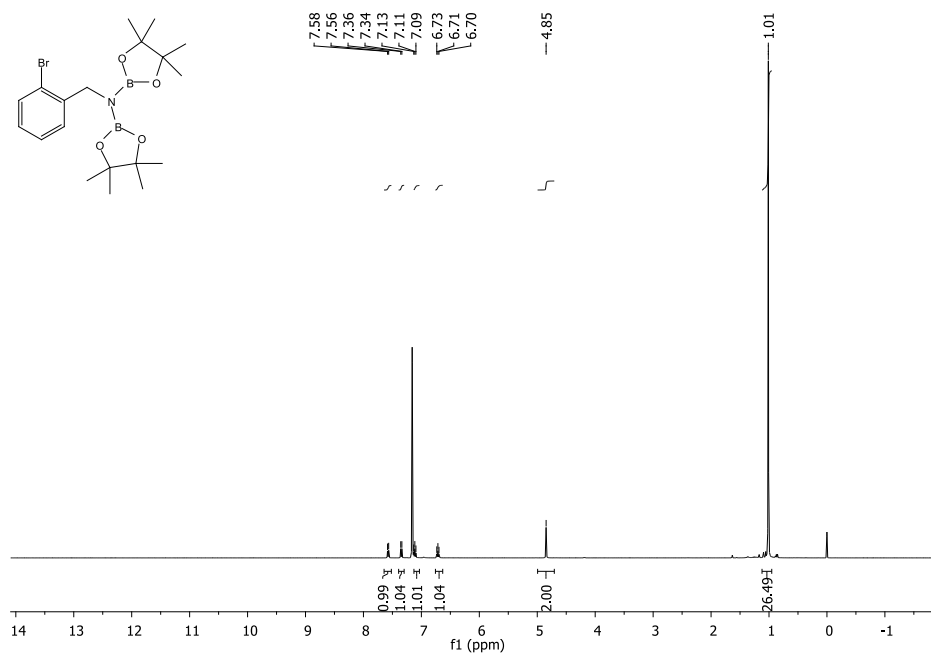


Figure S16. ¹H NMR spectrum of *N*-(2-bromobenzyl)-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine in benzene-*d*₆.

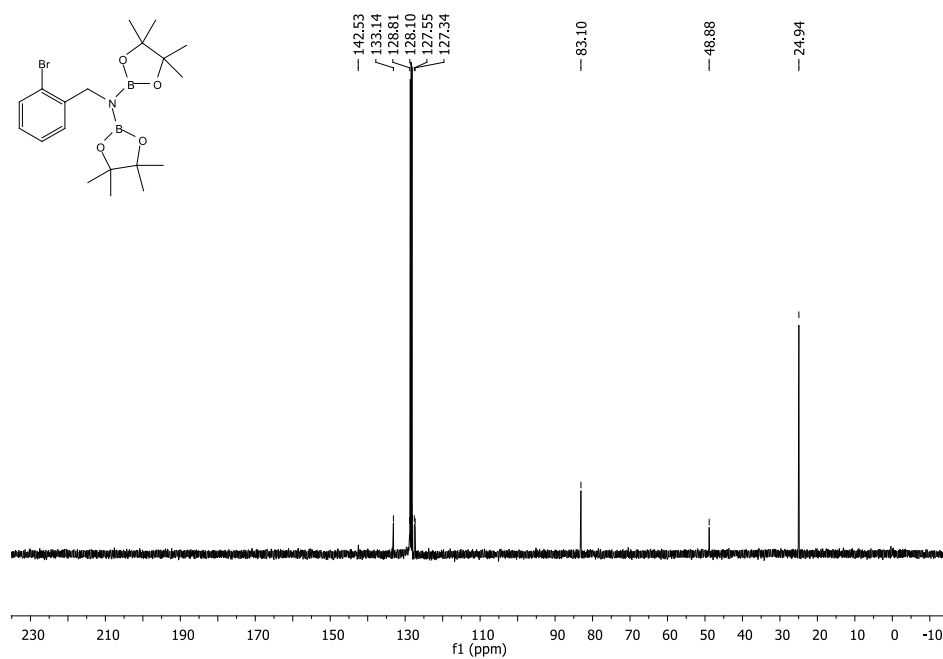


Figure S17. ¹³C NMR spectrum of *N*-(2-bromobenzyl)-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine in benzene-*d*₆.

Hydroboration of 4-(trifluoromethyl)benzonitrile catalyzed by 0.5 mol% of **1 (1 mol% based on Mn):** In the glove box, HBPin (371 μ L, 2.555 mmol) and 4-(trifluoromethyl)benzonitrile (0.199 mg, 1.16 mmol) were added to a vial containing a benzene- d_6 solution of **1** (0.0056 g, 0.0058 mmol). The vial was sealed under N_2 atmosphere and stirred at 80 $^{\circ}C$. After 24 h of heating, I_2 was added to the solution to deactivate the catalyst. Greater than 99% conversion was observed by 1H NMR spectroscopy. The solvent and remaining borane were removed under vacuum, resulting in a white solid. Recrystallization from pentane at -35 $^{\circ}C$ yielded 0.4061 g (82%) of 4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-*N*-(4-trifluoromethyl)benzyl)-1,3,2-dioxaborolan-2-amine. 1H NMR (benzene- d_6 , 400 MHz): 7.41 (s, 4H, *phenyl*), 4.47 (s, 2H, CH_2), 1.01 (s, 24H, CCH_3). ^{13}C NMR (benzene- d_6 , 100 MHz): 148.06 (s, *phenyl*), 128.51 (s, *phenyl*), 128.26 (s, *phenyl*), 125.62 (q, $J = 3.7$ Hz, CF_3), 83.13 (s, CCH_3), 47.81 (s, CH_2), 25.02 (s, CCH_3) one resonance not located. ^{19}F NMR (benzene- d_6 , 470.6 MHz): -63.57.

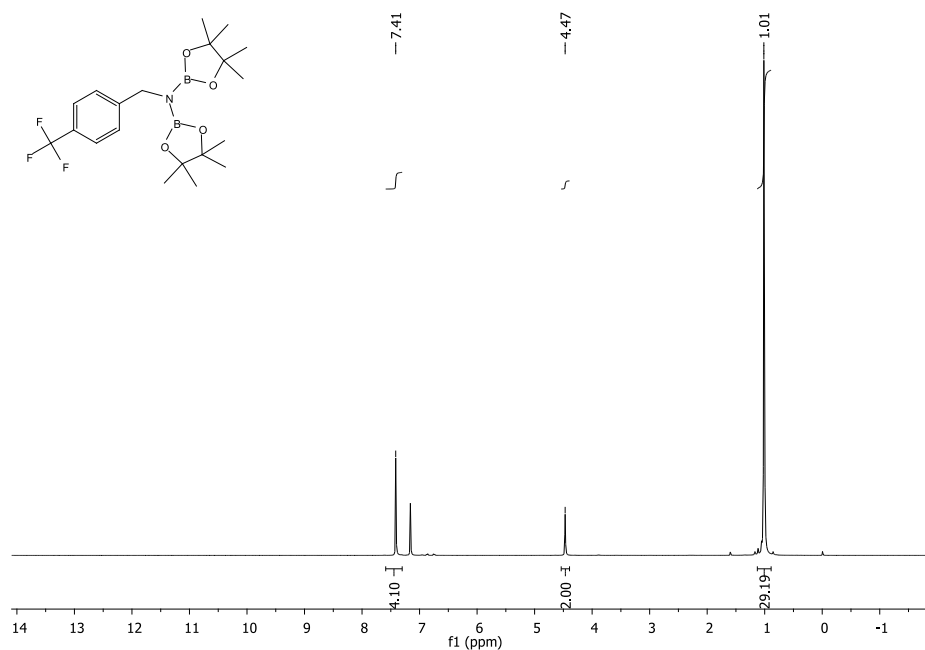


Figure S18. 1H NMR spectrum of 4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-*N*-(4-trifluoromethyl)benzyl)-1,3,2-dioxaborolan-2-amine in benzene- d_6 .

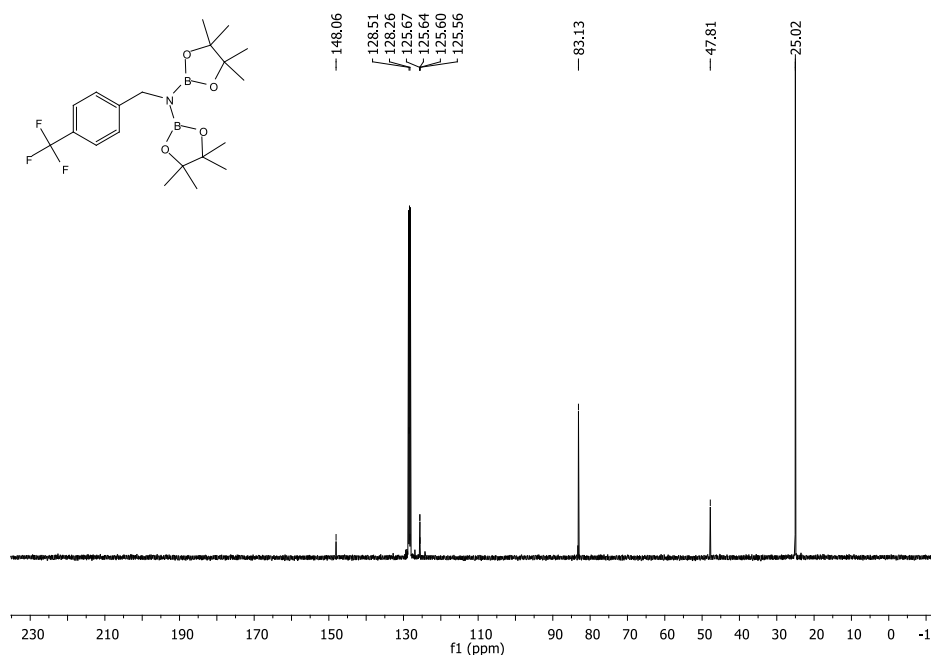


Figure S19. ^{13}C NMR spectrum of 4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-*N*-(4-trifluoromethyl)benzyl)-1,3,2-dioxaborolan-2-amine in benzene- d_6 .

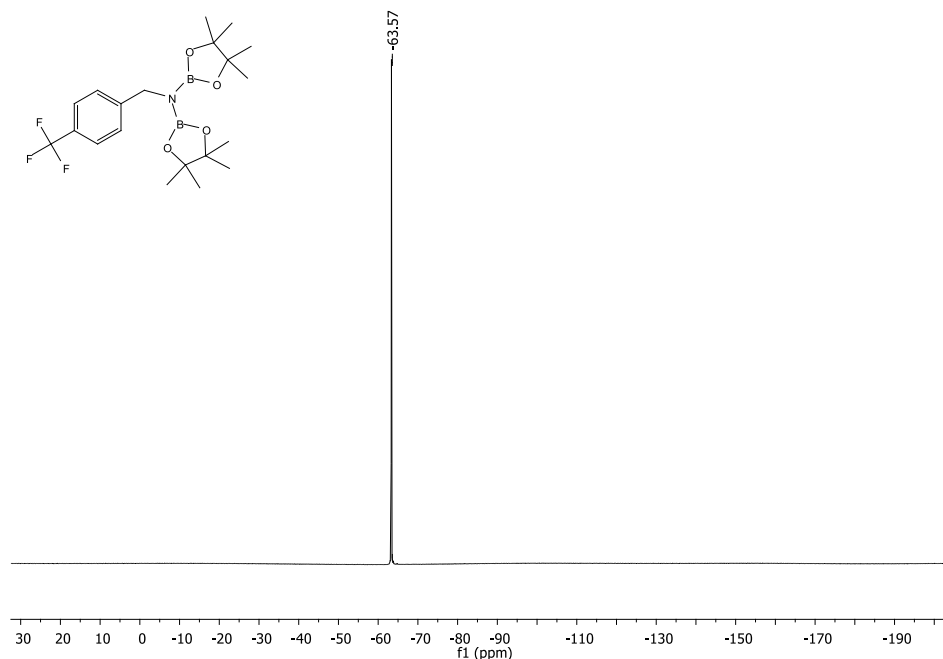


Figure S20. ^{19}F NMR spectrum of 4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-*N*-(4-(trifluoromethyl)benzyl)-1,3,2-dioxaborolan-2-amine in benzene- d_6 .

Hydroboration of 4-acetylbenzonitrile catalyzed by 0.5 mol% of **1 (1 mol% based on Mn):** In the glove box, HBPin (635.44 μL , 4.379 mmol) and 4-acetylbenzonitrile (0.193 mg, 1.327 mmol) were added to a vial containing a benzene- d_6 solution of **1** (0.0064 g, 0.0066 mmol). The vial was sealed under N_2 atmosphere and stirred at 80 $^\circ\text{C}$. After 24 h of heating, I_2 was added to the solution to deactivate the catalyst. Greater than 99% conversion was observed by ^1H NMR spectroscopy. The solvent and remaining borane were removed under vacuum, resulting in a white solid. Recrystallization from pentane at -35 $^\circ\text{C}$ yielded 0.463 g (87%) of 4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-*N*-(4-(1-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)oxy)ethyl)benzyl)-1,3,2-dioxaborolan-2-amine. ^1H NMR (benzene- d_6 , 400 MHz): 7.56 (d, $J = 11.3$ Hz, 2H, *phenyl*), 7.43 (d, $J = 7.8$ Hz, 2H, *phenyl*), 5.46 (q, $J = 11.2, 5.1$ Hz, 1H, CH), 4.59 (s, 2H, CH_2), 1.49 (d, $J = 10.2$ Hz, 3H, CH_3), 1.04 (s, 12H, CCH_3), 1.03 (s, 12H, CCH_3), 1.01 (s, 12H, CCH_3). ^{13}C NMR (benzene- d_6 , 100 MHz): 143.73 (s, *phenyl*), 142.96 (s, *phenyl*), 125.87 (s, *phenyl*), 82.92 (s, CCH_3), 82.79 (s, CCH_3), 73.31 (s, CH), 47.99 (s, CH_2), 26.05 (s, CH_3), 25.08 (s, CH_3), one resonance not located.

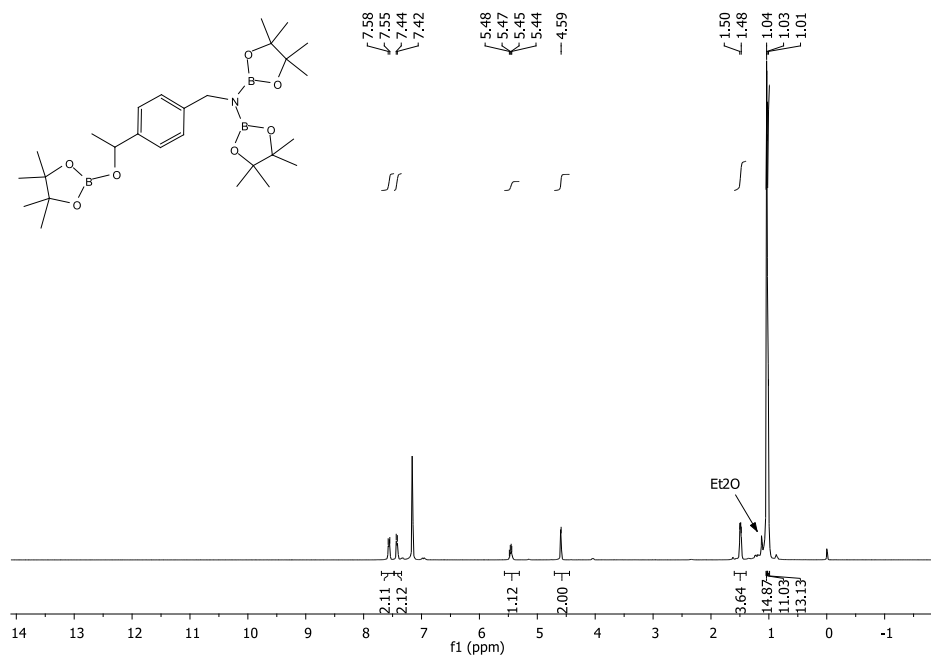


Figure S21. ^1H NMR spectrum of 4,4,5,5-tetramethyl-N-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-N-(4-(1-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)oxy)ethyl)benzyl)-1,3,2-dioxaborolan-2-amine in benzene- d_6 .

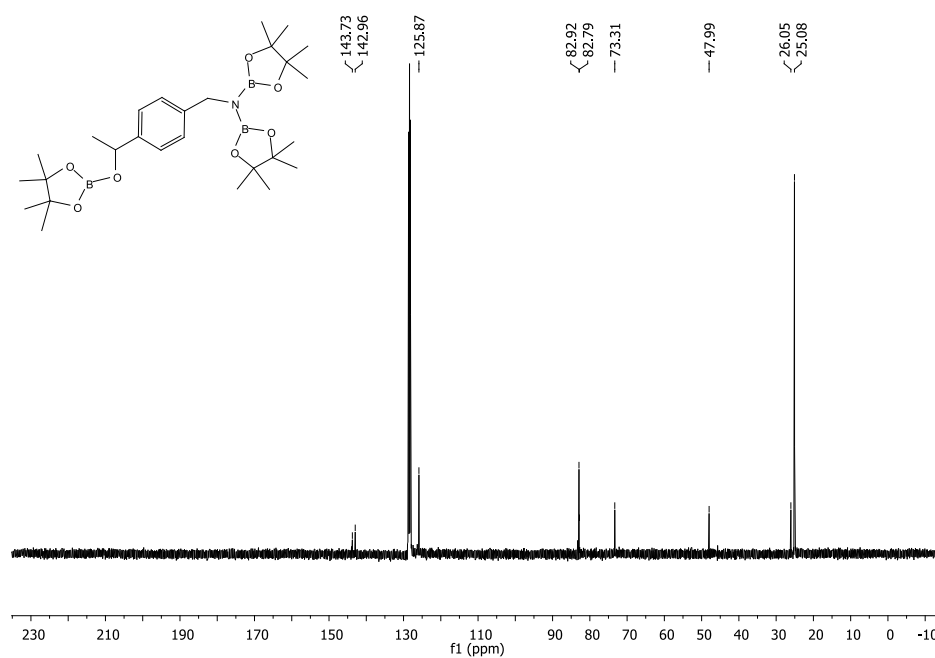


Figure S22. ^{13}C NMR spectrum of 4,4,5,5-tetramethyl-N-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-N-(4-(1-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)oxy)ethyl)benzyl)-1,3,2-dioxaborolan-2-amine in benzene- d_6 .

Hydroboration of acetonitrile catalyzed by 0.5 mol% of **1 (1 mol% based on Mn):** In the glove box, HBPIn (230 μ L, 1.58 mmol) and acetonitrile (37.52 μ L, 0.7184 mmol) were added to a vial containing a benzene- d_6 solution of **1** (0.0034 g, 0.0036 mmol). The vial was sealed under N_2 atmosphere and stirred at 80 $^{\circ}C$. After 24 h of heating, I_2 was added to the solution to deactivate the catalyst. Greater than 99% conversion was observed by 1H NMR spectroscopy. The solvent and remaining borane were removed under vacuum, resulting in a white solid. Recrystallization from pentane at -35 $^{\circ}C$ yielded 0.1259 g (59%) of *N*-ethyl-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine. 1H NMR (benzene- d_6 , 400 MHz): 3.44 (q, $J = 6.2$ Hz, 2H, CH_2), 1.29 (t, 3H, CH_3), 1.06 (s, 24H, CH_3). ^{13}C NMR (benzene- d_6 , 100 MHz): 82.53 (s, CCH₃), 39.44 (s, CH_2), 25.15 (s, CCH₃), 19.54 (s, CH_3).

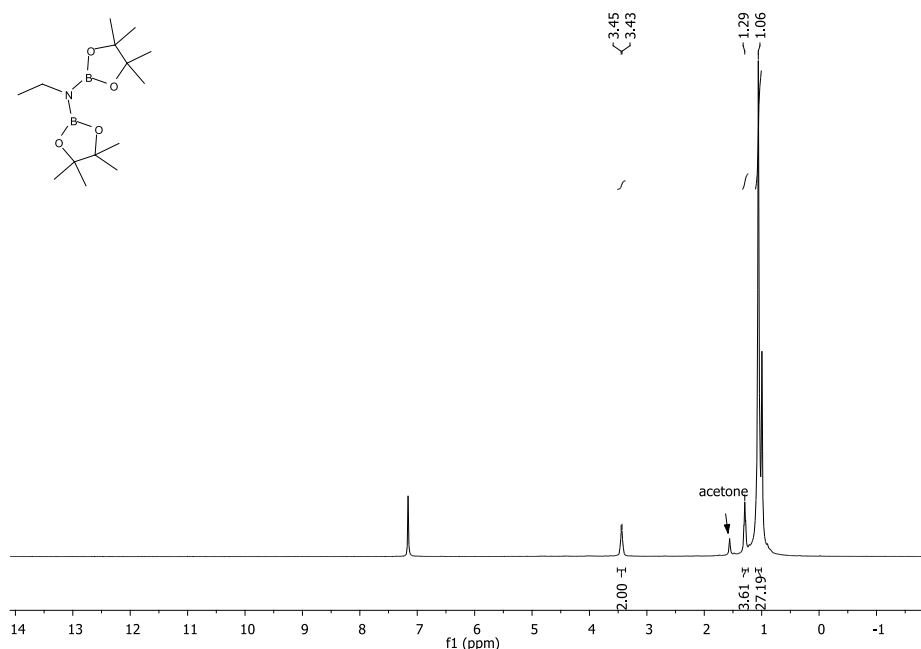


Figure S23. 1H NMR spectrum of *N*-ethyl-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine in benzene- d_6 .

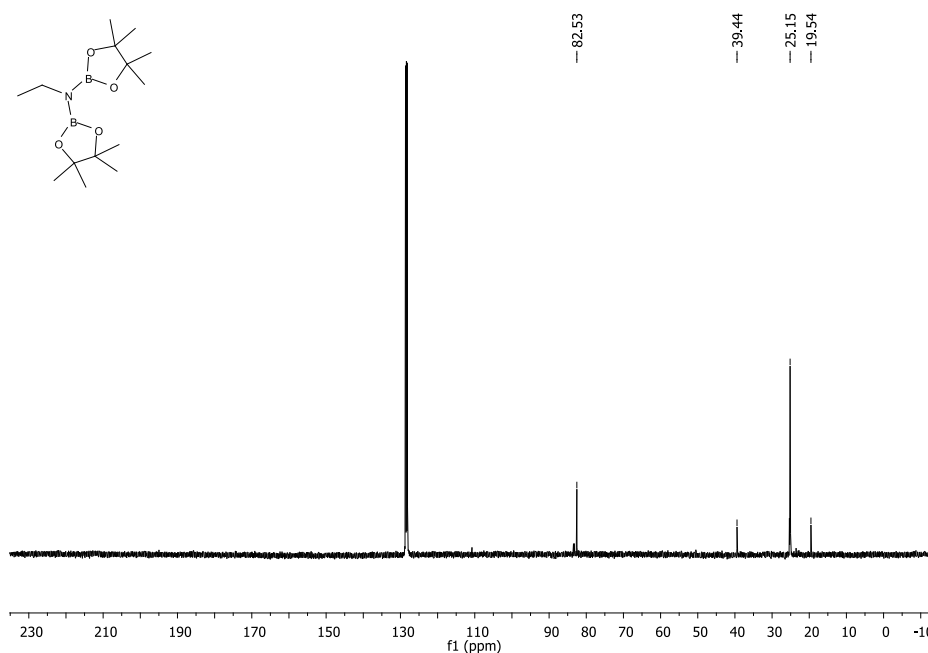


Figure S24. ^{13}C NMR spectrum of *N*-ethyl-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine in benzene- d_6 .

Hydroboration of cyclohexanecarbonitrile catalyzed by 0.5 mol% of **1 (1 mol% based on Mn):** In the glove box, HBPIn (271 μ L, 1.87 mmol) and cyclohexanecarbonitrile (101 μ L, 0.85 mmol) were added to a vial containing a benzene- d_6 solution of **1** (0.0041 g, 0.00425 mmol). The vial was sealed under N₂ atmosphere and stirred at 80 °C. After 24 h of heating, I₂ was added to the solution to deactivate the catalyst. Greater than 99% conversion was observed by ¹H NMR spectroscopy. The solvent and remaining borane were removed under vacuum, resulting in a white solid. Recrystallization from pentane at -35 °C yielded 0.4079 g (89%) of *N*-(cyclohexylmethyl)-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine. ¹H NMR (benzene- d_6 , 400 MHz): 3.30 (d, J = 7.0 Hz, 2H, CH₂), 2.76 (pseudo t, J = 7.1 Hz, 1H, CH), 1.89 (d, J = 12.4 Hz, 2H, CH₂), 1.72 (d, J = 12.3 Hz, 4H, CH₂), 1.65 – 1.53 (m, 4H, CH₂), 1.07 (s, 24H, CCH₃). ¹³C NMR (benzene- d_6 , 100 MHz): 82.48 (s, CCH₃), 50.71 (s, CH₂), 41.13 (s, CH), 31.47 (s, CH₂), 27.64 (s, CH₂), 26.96 (s, CH₂), 25.16 (s, CCH₃).

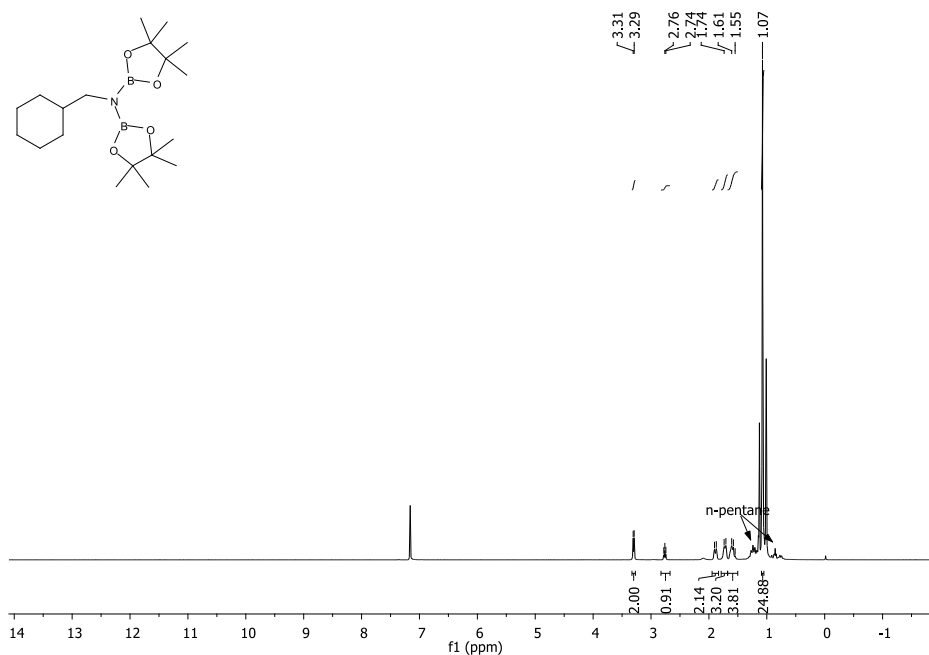


Figure S25. ¹H NMR spectrum of *N*-(cyclohexylmethyl)-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine in benzene- d_6 .

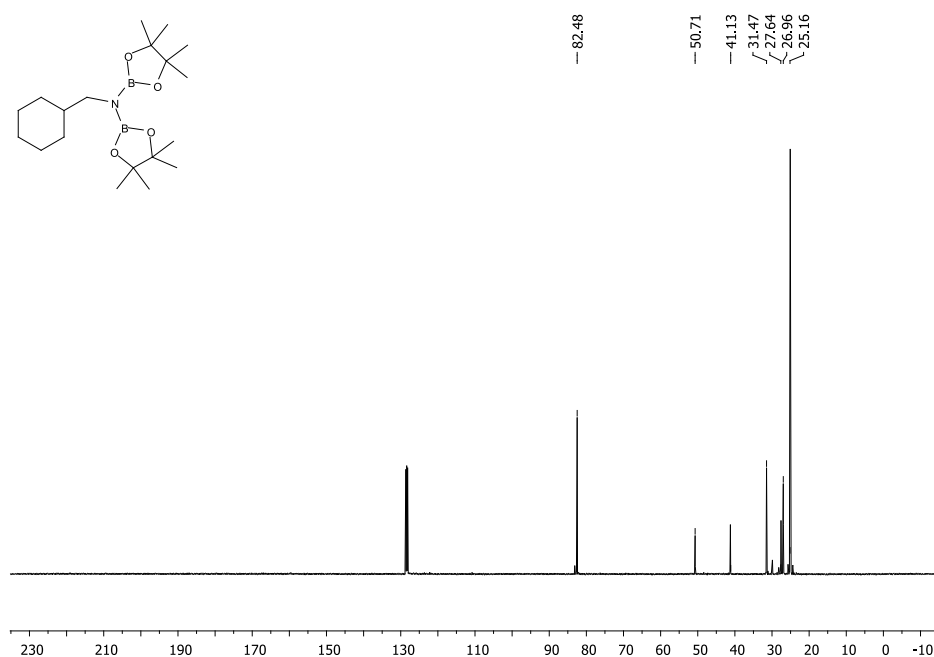


Figure S26. ¹³C NMR spectrum of *N*-(cyclohexylmethyl)-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine in benzene- d_6 .

Hydroboration of 3-(dimethylamino)propionitrile catalyzed by 0.5 mol% of **1 (1 mol% based on Mn):** In the glove box, HBPin (472 μ L, 3.25 mmol) and 3-(dimethylamino)propionitrile (157 μ L, 1.4 mmol) were added to a vial containing a benzene- d_6 solution of **1** (0.0066 g, 0.007 mmol). The vial was sealed under N_2 atmosphere and stirred at 80 $^{\circ}$ C. After 24 h of heating, I_2 was added to the solution to deactivate the catalyst. Greater than 99% conversion was observed by 1H NMR spectroscopy. The solvent and remaining borane were removed under vacuum, resulting in a white solid. Recrystallization from pentane at -35 $^{\circ}$ C yielded 0.322 g (65%) of *N1,N1*-dimethyl-*N3,N3*-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propane-1,3-diamine. 1H NMR (benzene- d_6 , 400 MHz): 3.35 (t, $J = 7.2$ Hz, 2H, CH_2), 2.23 (t, $J = 7.2$ Hz, 2H, CH_2), 2.08 (s, 6H, CH_3), 1.85 – 1.73 (m, 2H, CH_2), 1.02 (s, 24H, CCH_3). ^{13}C NMR (benzene- d_6 , 100 MHz): 81.69 (s, CCH_3), 57.31 (s, CH_2), 45.12 (s, CH_3), 42.15 (s, CH_2), 31.62 (s, CH_2), 24.30 (s, CCH_3).

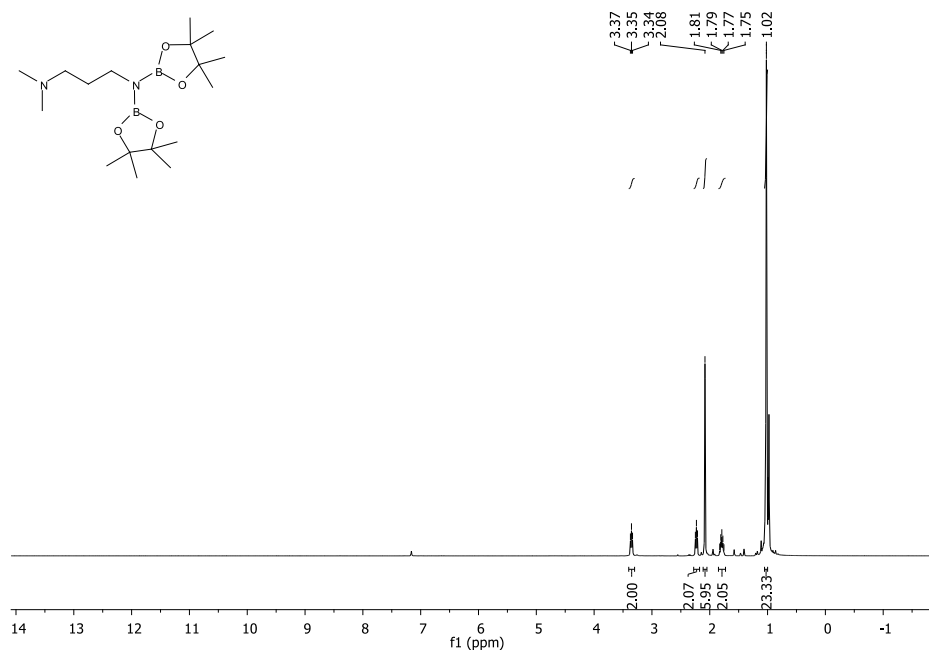


Figure S27. 1H NMR spectrum of *N1,N1*-dimethyl-*N3,N3*-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propane-1,3-diamine in benzene- d_6 .

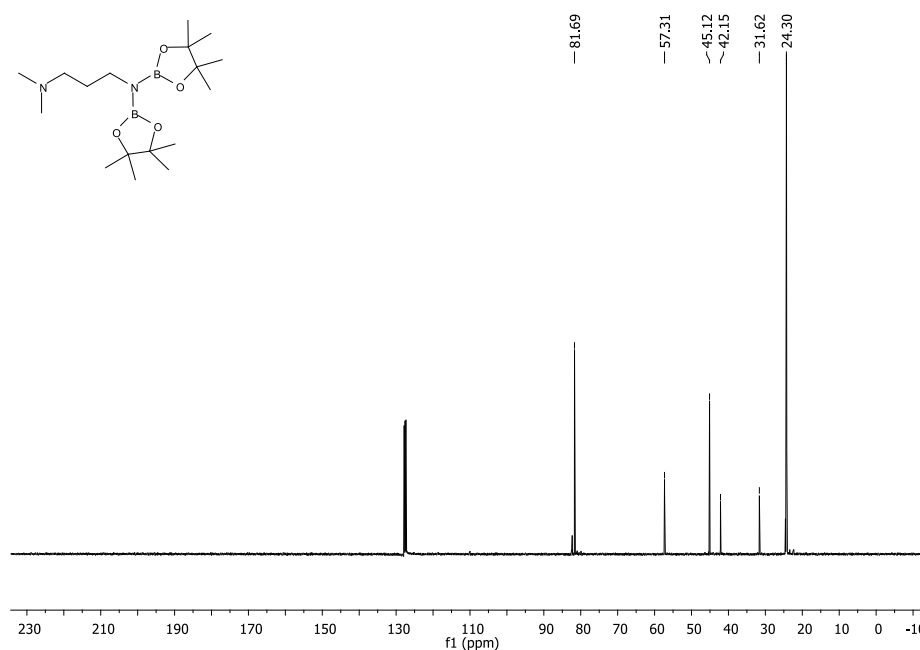


Figure S28. ^{13}C NMR spectrum of *N1,N1*-dimethyl-*N3,N3*-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propane-1,3-diamine in benzene- d_6 .

Hydroboration of 2-phenoxyacetonitrile catalyzed by 0.5 mol% of **1 (1 mol% based on Mn):** In the glove box, HBPIn (209 μ L, 1.441 mmol) and 2-phenoxyacetonitrile (80 μ L, 0.655 mmol) were added to a vial containing a benzene- d_6 solution of **1** (0.0031 g, 0.0033 mmol). The vial was sealed under N_2 atmosphere and stirred at 80 $^{\circ}C$. After 24 h of heating, I_2 was added to the solution to deactivate the catalyst. Greater than 99% conversion was observed by 1H NMR spectroscopy. The solvent and remaining borane were removed under vacuum, resulting in a white solid. Recrystallization from pentane at -35 $^{\circ}C$ yielded 0.2064 g (81%) of 4,4,5,5-tetramethyl-*N*-(2-phenoxyethyl)-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine. 1H NMR (benzene- d_6 , 400 MHz): 7.17 (m, 2H, *phenyl*), 7.03 (d, $J = 8.4$ Hz, 2H, *phenyl*), 6.85 (t, $J = 7.3$ Hz, 1H, *phenyl*), 4.12 (t, $J = 6.5$ Hz, 2H, CH_2), 3.81 (t, $J = 6.5$ Hz, 2H, CH_2), 1.06 (s, 24H, CCH_3). ^{13}C NMR (benzene- d_6 , 100 MHz): 160.22 (s, *phenyl*), 130.03 (s, *phenyl*), 121.00 (s, *phenyl*), 115.28 (s, *phenyl*), 82.92 (s, CCH_3), 69.55 (s, CH_2), 43.69 (s, CH_2), 25.08 (s, CCH_3).

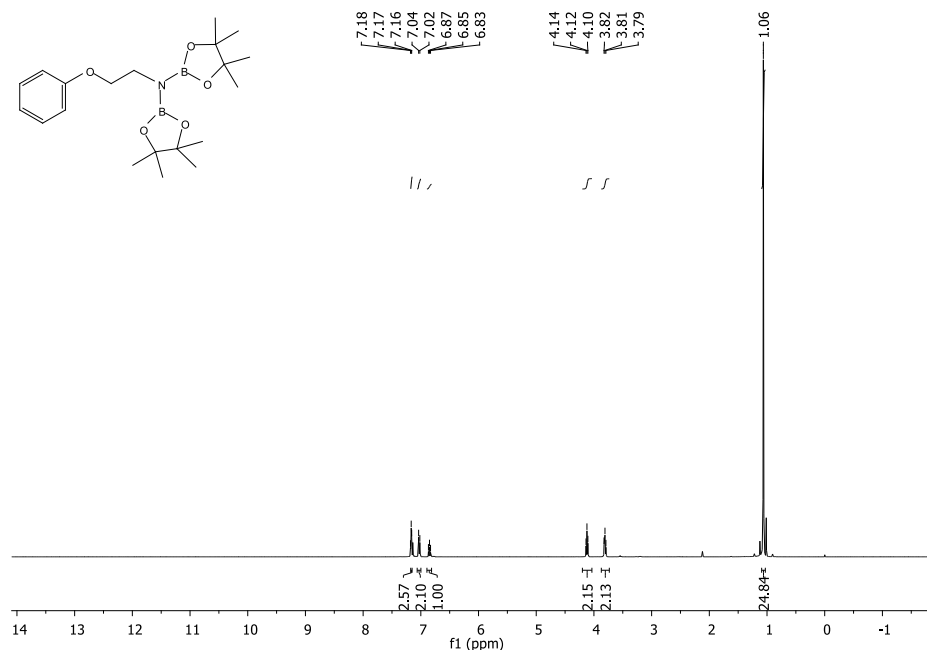


Figure S29. 1H NMR spectrum of 4,4,5,5-tetramethyl-*N*-(2-phenoxyethyl)-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine in benzene- d_6 .

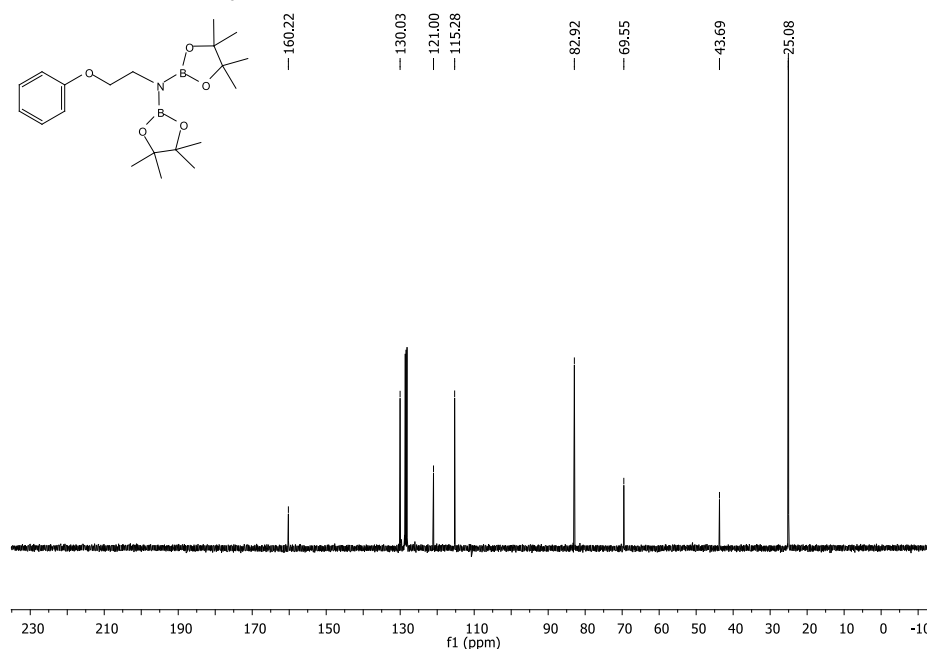


Figure S30. ^{13}C NMR spectrum of 4,4,5,5-tetramethyl-*N*-(2-phenoxyethyl)-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine in benzene- d_6 .

Hydroboration of 3-(diphenylphosphino)propanenitrile catalyzed by 0.5 mol% of **1 (1 mol% based on Mn):** In the glove box, HBPIn (73.2 μ L, 0.5045 mmol) and 3-(diphenylphosphino)propanenitrile (0.054 g, 0.23 mmol) were added to a vial containing a benzene- d_6 solution of **1** (0.0011 g, 0.0012 mmol). The vial was sealed under N_2 atmosphere and stirred at 80 $^{\circ}$ C. After 24 h of heating, I_2 was added to the solution to deactivate the catalyst. Greater than 99% conversion was observed by 1H NMR spectroscopy. The solvent and remaining borane were removed under vacuum, resulting in a white solid. Recrystallization from pentane at -35 $^{\circ}$ C yielded 0.0736 g (65%) of *N*-(3-(diphenylphosphino)propyl)-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine. 1H NMR (benzene- d_6 , 400 MHz): 7.47 (t, J = 7.1 Hz, 4H, *phenyl*), 7.08 (dt, J = 21.5, 7.2 Hz, 6H, *phenyl*), 3.51 (t, J = 6.9 Hz, 2H, CH_2), 2.15 – 2.05 (m, 2H, CH_2), 1.94 – 1.84 (m, 2H, CH_2), 1.05 (s, 24H, CCH_3). ^{13}C NMR (benzene- d_6 , 100 MHz): 139.54 (s, *phenyl*), 132.79 (d, J = 18.5 Hz, *phenyl*), 128.30 (s, *phenyl*), 128.22 (d, J = 6.5 Hz, *phenyl*), 81.65 (s, CCH_3), 42.37 (s, CH_2), 30.10 (s, CH_2), 25.21 (s, CH_2), 24.46 (s, CCH_3). ^{31}P NMR (benzene- d_6 , 162 MHz): -16.04.

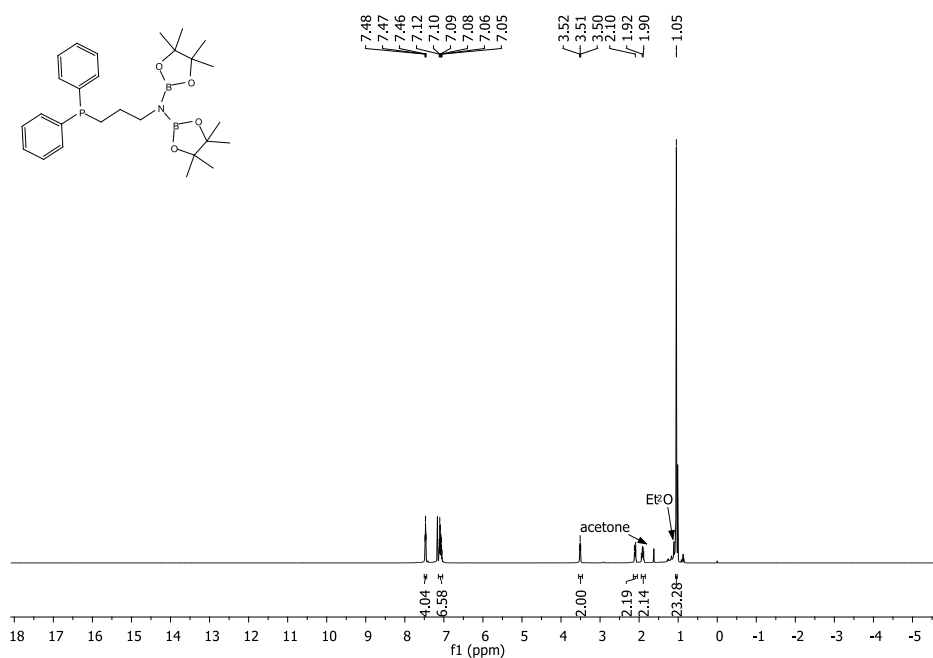


Figure S31. 1H NMR spectrum of *N*-(3-(diphenylphosphino)propyl)-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine in benzene- d_6 .

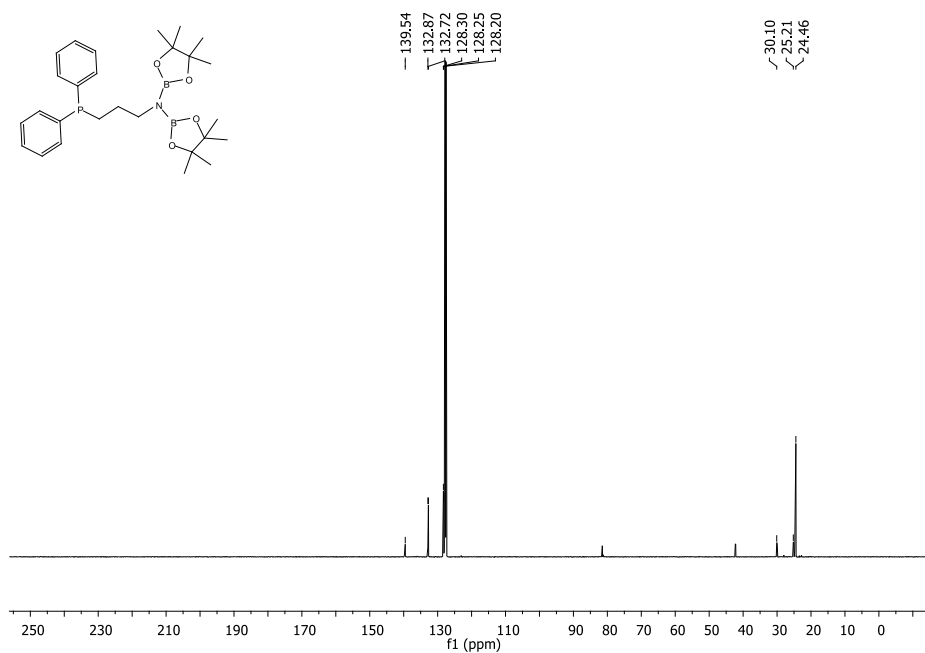


Figure S32. ¹³C NMR spectrum of *N*-(3-(diphenylphosphino)propyl)-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine in benzene-*d*₆.

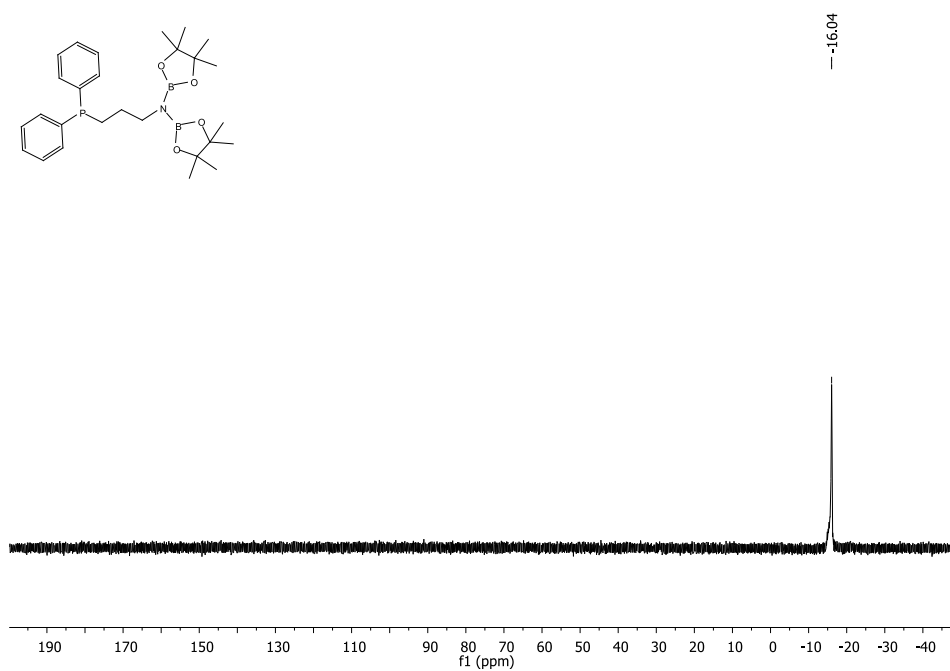


Figure S33. ³¹P NMR spectrum of *N*-(3-(diphenylphosphino)propyl)-4,4,5,5-tetramethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,2-dioxaborolan-2-amine in benzene-*d*₆.

Determination of maximum benzonitrile dihydroboration turnover frequency using 0.1 mol% of **1 under neat conditions:**

In the glove box, HBPin (1.653 mL, 11.39 mmol) and benzonitrile (0.534 mL, 5.18 mmol) were added to a vial containing 0.0049 g of **1** (0.00528 mmol). The vial was sealed under N₂ atmosphere and stirred at 80 °C. After 2 h of heating, the resulting solid was dissolved in benzene and I₂ was added to the solution to deactivate the catalyst. ¹H NMR spectroscopy revealed 52% conversion. Repeating this trial without **1** afforded 6% conversion, which when subtracted, equates to a maximum TOF of 230 h⁻¹ at 80 °C for **1** (115 h⁻¹ relative to Mn).

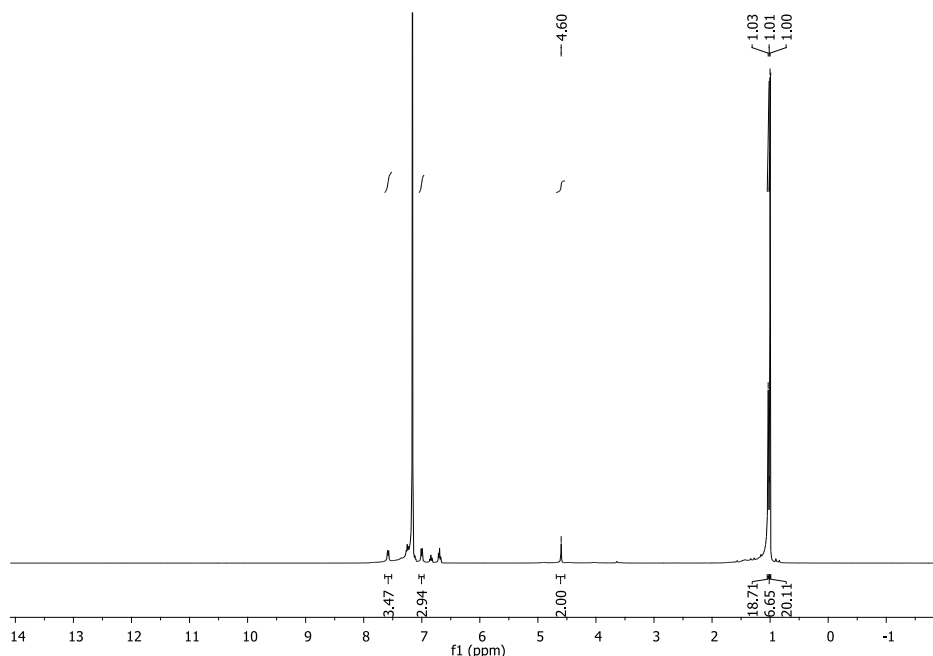


Figure S34. ¹H NMR spectrum showing 52% conversion of benzonitrile to diborylamine after 2 h in benzene-*d*₆.

Figure S35. Two different conformations after addition of HBPin to ⁶C.

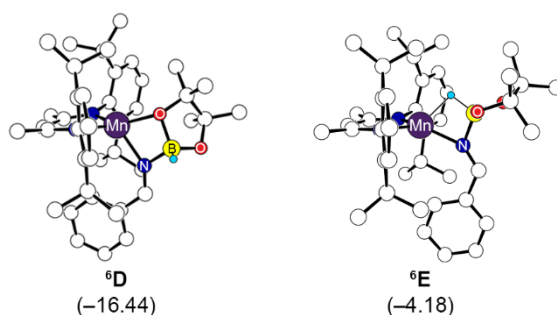


Figure S36. Two different conformations after addition of HBPin to ⁶H.

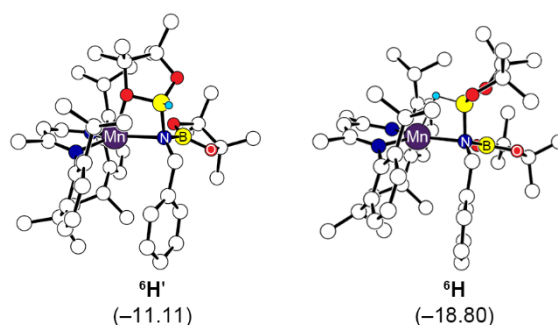


Table S3. Computed energy components for DFT-optimized structures.

	E(SCF)/(eV) cc-pVTZ(-f)/LACV3P**	ZPE/(kcal mol⁻¹) 6-31G**/LACVP**	S(gas)/(cal mol⁻¹ K⁻¹) 6-31G**/LACVP**	G(solv)/(kcal mol⁻¹) 6-31G**/LACVP**
1	-73166.750	811.47	372.94	-5.54
Benzonitrile	-8832.844	62.35	78.55	-3.66
HBPIn	-11211.936	120.07	91.03	-2.24
⁶A	-36582.516	403.59	225.32	-5.18
⁶B	-45415.895	467.08	264.00	-8.16
⁶B-TS	-45415.387	466.55	259.36	-3.89
⁶C	-45416.727	470.22	262.05	-3.49
2	-90836.516	944.95	440.47	-4.25
⁶D	-56630.262	593.51	290.02	-5.20
⁶E	-56629.547	592.24	299.81	-4.70
⁶E-TS	-56629.520	590.45	294.61	-5.08
⁶F	-56629.594	590.96	299.22	-5.55
⁶F-TS	-56629.008	590.51	290.61	-5.00
⁶G	-56630.902	594.65	298.02	-3.73
⁶H	-67843.383	716.78	331.21	-3.27
⁶H-TS	-67842.805	714.27	331.97	-4.69
⁶I	-67842.938	714.64	341.43	-4.77
Borylimine	-20045.932	185.18	130.43	-3.91
Diborylamine	-31260.059	309.21	175.70	-3.93

Table S4. Cartesian coordinates of the optimized geometries.

=====

1							
=====							
Mn	2.723260000	0.824722500	12.543915000	H	1.763609900	5.538744000	16.162831000
N	3.887879300	0.666488700	10.799892000	C	2.444401200	4.238729000	14.586423000
N	3.460014700	2.772720200	12.880367000	C	1.244848200	4.478616600	13.675974000
C	5.064144000	1.534524500	8.808557000	H	1.592563800	4.406781000	12.640220000
H	5.911763700	0.850557300	8.911773000	C	0.187305460	3.383984300	13.881718000
H	5.429589000	2.483291400	8.412201000	H	0.590559200	2.384060300	13.698792000
H	4.389216000	1.084841900	8.074536000	H	-0.657394400	3.530301500	13.198659000
C	4.365243400	1.730086900	10.144470000	H	-0.192136100	3.408232400	14.905031000
C	4.293539000	3.053894300	10.611360000	C	0.617593950	5.872742500	13.842416000
H	4.670341000	3.803340500	9.927321000	H	-0.123525100	6.045802400	13.054263000
C	3.985392000	3.521960500	11.901403000	H	1.371374600	6.666098000	13.779226000
C	4.345006000	4.978389400	12.168677000	H	0.100025460	5.975197500	14.803178000
H	3.459957000	5.568307500	12.425726000	C	5.651125600	2.078735900	14.631503000
H	4.819913000	5.428941000	11.295403000	H	5.161210400	1.330195800	13.997261000
H	5.030352500	5.057543000	13.016942000	C	6.766755000	2.727599300	13.786391000
C	4.234164300	-0.623694600	10.276488000	H	7.230672000	3.558458800	14.332784000
C	5.392912000	-1.267320600	10.766880000	H	6.384165300	3.111719600	12.836612000
C	5.752461500	-2.502396000	10.216548000	H	7.548455700	1.994514700	13.555451000
H	6.651829600	-3.001324500	10.569527500	C	6.270657000	1.338413400	15.829652000
C	4.970459600	-3.105708200	9.234244000	H	6.931971000	0.541727670	15.474370000
H	5.256266000	-4.071871700	8.826092000	H	5.504181300	0.885029530	16.463343000
C	3.812052700	-2.472949500	8.784881000	H	6.879261000	2.004920700	16.453490000
H	3.198408300	-2.956530200	8.030086000	H	2.666523200	-0.398741840	13.908931000
C	3.433378100	-1.219584700	9.279064000	Mn	0.792243500	-0.839476900	13.865618000
C	2.197012300	-0.508449360	8.744484000	N	-0.352500130	-0.713256140	15.618695000
H	2.264858500	0.545280100	9.030406000	N	0.018167495	-2.764876600	13.475523000
C	2.087917200	-0.569703200	7.210132600	C	-1.417024900	-1.634999600	17.647844000
H	2.994597000	-0.197626110	6.719680700	H	-2.237399200	-0.911937100	17.634937000
H	1.245449900	0.043066510	6.869757700	H	-1.796644600	-2.586537000	18.024570000
H	1.910429200	-1.590525400	6.854077700	H	-0.674797000	-1.250488200	18.353822000
C	0.933463700	-1.077190300	9.404288000	C	-0.808314300	-1.794061100	16.263944000
H	0.843040440	-2.149357800	9.214535000	C	-0.789680200	-3.099305500	15.746175000
H	0.038474957	-0.585174130	9.006938000	H	-1.166612300	-3.863494900	16.413693000
H	0.947939700	-0.926411450	10.487932000	C	-0.531620600	-3.526739500	14.429782000
C	6.275851000	-0.619523750	11.828929000	C	-0.965319360	-4.952763600	14.112009000
H	5.791349400	0.312518400	12.132933000	H	-0.112021354	-5.577094000	13.829085500
C	7.665275500	-0.259779760	11.268526000	H	-1.459100400	-5.409837300	14.971342000
H	8.211827000	-1.157352200	10.954486000	H	-1.656705500	-4.967281400	13.264946000
H	8.269366000	0.244941550	12.031515000	C	-0.666819440	0.565637040	16.186496000
H	7.590364600	0.407842080	10.403627000	C	-1.850969300	1.216812900	15.770269000
C	6.386680000	-1.498150100	13.088532000	C	-2.174356100	2.446364000	16.354121000
H	5.399063600	-1.669793100	13.529096000	H	-3.092500500	2.950199400	16.061648000
H	7.018249800	-1.013940450	13.841498000	C	-1.331068400	3.041102400	17.290906000
H	6.831005600	-2.474926400	12.863500000	H	-1.587972600	4.005691400	17.721417000
C	3.477206600	3.360208000	14.191029000	C	-0.152305640	2.399810000	17.667505000
C	4.580195000	3.091203700	15.036627000	H	0.506763870	2.873837700	18.389680000
C	4.660137000	3.775711200	16.254352000	C	0.189200630	1.147271700	17.145106000
H	5.506322500	3.603894300	16.912418000	C	1.442826300	0.422856530	17.616078000
C	3.655318000	4.654827000	16.652698000	H	1.372075500	-0.618020000	17.286919000
H	3.729692400	5.168574000	17.608024000	C	1.588037800	0.422477570	19.148715000
C	2.547202000	4.863219600	15.834166000	H	0.696820300	0.022324594	19.644824000
				H	2.444503800	-0.193679830	19.445463000
				H	1.761980400	1.430787900	19.540189000
				C	2.687404400	1.023831900	16.951825000
				H	2.800291700	2.078541000	17.213314000

H	3.587827000	0.491607630	17.278891000
H	2.632238300	0.948400150	15.862202500
C	-2.796150300	0.574331500	14.758543000
H	-2.301861500	-0.323811440	14.376115000
C	-4.117366600	0.133612980	15.420475000
H	-4.667430000	0.997019400	15.816075000
H	-4.764117000	-0.367468780	14.690443000
H	-3.943960800	-0.563121800	16.247521000
C	-3.058948000	1.491202200	13.549946000
H	-2.125327200	1.722031300	13.025933000
H	-3.738167000	1.003698800	12.841667000
H	-3.521736600	2.439509500	13.849022000
C	-0.035238741	-3.295195600	12.141820000
C	-1.130793300	-2.934744600	11.323457500
C	-1.277495800	-3.582622000	10.091492000
H	-2.128217800	-3.346311000	9.458934000
C	-0.339580480	-4.514632000	9.654277000
H	-0.465950530	-5.003281000	8.691364000
C	0.774359540	-4.803474500	10.441667000
H	1.509082500	-5.515166200	10.079121000
C	0.941680670	-4.216554000	11.700363000
C	2.141942000	-4.546646300	12.581286000
H	1.797381400	-4.556852000	13.620864000
C	3.214173800	-3.453293200	12.461477000
H	2.829015800	-2.465684800	12.727757000
H	4.061096000	-3.667037900	13.123561000
H	3.586320200	-3.399039100	11.437405000
C	2.754142700	-5.928001000	12.299306000
H	3.500982900	-6.167338000	13.064216000
H	1.994938700	-6.718652700	12.308190000
H	3.262361000	-5.957069600	11.328470000
C	-2.138832000	-1.881517500	11.782866000
H	-1.635170600	-1.249294800	12.524551000
C	-3.345923100	-2.530765100	12.493032500
H	-3.848127600	-3.247921000	11.829577000
H	-3.036736700	-3.062604000	13.399840000
H	-4.076170300	-1.767771600	12.788366000
C	-2.612570200	-0.960233600	10.643783000
H	-3.279227400	-0.188231000	11.043438000
H	-1.766740700	-0.459230100	10.159400000
H	-3.174955000	-1.507267700	9.873670000
H	0.854536900	0.375603370	12.488962000

Benzonitrile

C	0.407542527	-0.007355646	-1.877812266
C	-0.748744249	-0.361969620	-1.187595844
C	1.562913895	0.347055376	-1.177343607
H	-1.651228189	-0.638785839	-1.722021937
H	2.462058067	0.622852206	-1.720320582
C	-0.746395171	-0.361251235	0.217235535
C	1.565107822	0.347817242	0.219503209
H	2.463770390	0.623555660	0.762669563
C	0.415533543	-0.004803194	0.921809196
H	0.406731635	-0.007487478	2.006540537

H	0.407233179	-0.007515664	-2.963475227
C	-1.933968425	-0.725680530	0.934474528
N	-2.896923304	-1.021240354	1.516104341

HBPIn

B	0.079749167	0.032325376	-1.580637574
O	0.758988261	0.049014367	-2.767875195
O	0.573222101	0.901538312	-0.646648586
C	1.682018995	1.176437855	-2.717876911
C	1.831683874	1.422901154	-1.167622209
C	0.992628515	2.331853390	-3.452431917
H	0.744557083	2.007316351	-4.466374874
H	0.063145824	2.616367102	-2.951688290
H	1.640449286	3.210902452	-3.515866995
C	2.967957258	0.785368979	-3.440027952
H	3.713019371	1.583873034	-3.359540939
H	3.393745184	-0.133604258	-3.034947157
H	2.756977797	0.620498657	-4.500261784
C	1.962662578	2.885550499	-0.751611233
H	2.863070250	3.330921888	-1.187667847
H	1.096498013	3.471645594	-1.061677456
H	2.042081833	2.951524973	0.336978465
C	2.944247484	0.586524010	-0.524782181
H	3.935646057	0.946756780	-0.814169288
H	2.852542162	0.653243542	0.562409163
H	2.857374430	-0.466238499	-0.807324052
H	-0.853790224	-0.675308049	-1.378973603

⁶A

Mn	3.618494511	0.834519207	12.652955055
N	4.319438457	0.825560808	10.717077255
N	4.015269279	2.845215797	12.796641350
C	5.277987480	1.651808262	8.615464211
H	6.079537868	0.906135082	8.592133522
H	5.643075466	2.576797724	8.166120529
H	4.465606213	1.253901124	7.997738361
C	4.799791813	1.869397163	10.037082672
C	4.887305260	3.173231602	10.562168121
H	5.286138535	3.924147129	9.891655922
C	4.519807339	3.630832434	11.841627121
C	4.715789318	5.103048801	12.143250465
H	3.759593964	5.566958904	12.406698227
H	5.146847248	5.636393070	11.294350624
H	5.370753288	5.230725288	13.011700630
C	4.282513142	-0.477875471	10.126828194
C	5.375004292	-1.354314208	10.317078590
C	5.268054008	-2.660809040	9.829323769
H	6.092131138	-3.353871584	9.973752022
C	4.118788719	-3.090855122	9.170319557
H	4.052559376	-4.111052990	8.802258492
C	3.050646067	-2.214523077	8.991312981

H	2.153781176	-2.561952353	8.486325264
C	3.109927893	-0.899274945	9.461696625
C	1.913141847	0.035953149	9.326107025
H	2.261136770	1.051943779	9.536516190
C	1.312582612	0.042540386	7.910933971
H	2.073079348	0.273290575	7.157403469
H	0.520912886	0.796251595	7.838405132
H	0.867100835	-0.923659086	7.651005745
C	0.842362940	-0.308874995	10.381706238
H	0.441612244	-1.314690351	10.211356163
H	0.009699505	0.403161615	10.342453957
H	1.257497787	-0.295689166	11.396815300
C	6.614411354	-0.908868551	11.086834908
H	6.578781128	0.181094989	11.174221992
C	7.924500942	-1.266242027	10.365781784
H	8.072555542	-2.349596739	10.301218987
H	8.781585693	-0.850751519	10.907074928
H	7.939190388	-0.866232157	9.346366882
C	6.594484329	-1.480550170	12.518590927
H	5.672514439	-1.208405018	13.045850754
H	7.444996357	-1.107185602	13.100625992
H	6.646041870	-2.575160980	12.500902176
C	3.660625696	3.384805918	14.074349403
C	4.610351086	3.357756138	15.120782852
C	4.209899426	3.783847570	16.390792847
H	4.921998978	3.762314796	17.211000443
C	2.909501314	4.226472378	16.623609543
H	2.615293503	4.550543308	17.618156433
C	1.984863997	4.245867729	15.582148552
H	0.969910383	4.581885338	15.774832726
C	2.338609934	3.830335140	14.294494629
C	1.305991173	3.798917532	13.172909737
H	1.844396949	3.665116549	12.229577065
C	0.367660880	2.586269617	13.340308189
H	0.928592563	1.645480037	13.398915291
H	-0.333225012	2.514857292	12.500671387
H	-0.213453397	2.671757936	14.265678406
C	0.504079401	5.105981827	13.061121941
H	-0.159804195	5.070947170	12.190443993
H	1.166429639	5.971103191	12.949937820
H	-0.122850291	5.276904583	13.942890167
C	6.017227650	2.818405628	14.886252403
H	6.180504799	2.773401260	13.805393219
C	7.111053467	3.722035170	15.477768898
H	7.062179565	3.762567043	16.571361542
H	7.026082993	4.747052193	15.101505280
H	8.102855682	3.341829538	15.209577560
C	6.135474682	1.378496885	15.425088882
H	7.119405270	0.954482675	15.193903923
H	5.369998932	0.722876012	14.993210793
H	6.001390934	1.359068513	16.512653351
H	3.015208006	-0.356271297	13.678769112

=====

⁶B

Mn	2.704378605	0.603332043	12.851152420
N	3.591908932	0.575033367	10.958418846
N	3.326441765	2.582747936	13.144082069
C	4.213088036	1.567139983	8.798160553
H	5.206617355	1.115352869	8.718837738
H	4.233633041	2.539914131	8.303494453
H	3.528609514	0.905297339	8.258818626
C	3.803405046	1.687906027	10.255059242
C	3.703545332	2.991738558	10.780852318
H	3.865502596	3.789948702	10.066932678
C	3.573239326	3.405011654	12.124619484
C	3.742470503	4.890989304	12.393193245
H	2.791929960	5.330824375	12.710294724
H	4.091085434	5.421161652	11.505237579
H	4.451689243	5.059640408	13.207738876
C	3.956692696	-0.692170084	10.406125069
C	5.280777931	-1.158428788	10.579401970
C	5.612428665	-2.424898148	10.088376045
H	6.625555992	-2.796712875	10.217959404
C	4.666935444	-3.220879555	9.446083069
H	4.943016529	-4.203440189	9.073025703
C	3.363966465	-2.755209684	9.292625427
H	2.625100374	-3.384027719	8.802567482
C	2.986476421	-1.492991567	9.762862206
C	1.546562314	-1.018230081	9.616398811
H	1.513456225	0.027536258	9.932257652
C	1.045660019	-1.077161789	8.162643433
H	1.695806742	-0.504407763	7.492527962
H	0.033541702	-0.660853028	8.090330124
H	1.003511429	-2.105062246	7.785989761
C	0.623289824	-1.817007303	10.556762695
H	0.626560092	-2.880825758	10.293457985
H	-0.410672098	-1.456200719	10.490196228
H	0.952454031	-1.726028204	11.597425461
C	6.323985577	-0.333395332	11.325697899
H	5.883098602	0.639315426	11.558563232
C	7.586263180	-0.079274185	10.483016968
H	8.117009163	-1.011075020	10.257348061
H	8.280654907	0.573289394	11.024263382
H	7.343945503	0.403428137	9.530537605
C	6.682200909	-1.002011657	12.666088104
H	5.793982983	-1.117790461	13.295804977
H	7.415969372	-0.398691684	13.211635590
H	7.115697384	-1.996375322	12.509160995
C	3.371680975	3.079623699	14.484281540
C	4.549407482	2.858918428	15.238783836
C	4.605835438	3.364965200	16.540859222
H	5.503627300	3.222309113	17.133096695
C	3.522244930	4.036917686	17.104578018
H	3.589536905	4.421578884	18.118663788
C	2.346681118	4.186175346	16.376260757
H	1.490255117	4.673892975	16.834259033
C	2.245673418	3.708677292	15.064069748
C	0.914504468	3.799991369	14.326891899

H	1.083908319	3.515087366	13.285243034
C	-0.078835733	2.782503843	14.923633575
H	0.330457240	1.767982841	14.881722450
H	-1.028261423	2.799232960	14.374312401
H	-0.291345835	3.017126083	15.972937584
C	0.310936838	5.214734554	14.339565277
H	-0.595439255	5.247950077	13.724237442
H	1.013285041	5.957511902	13.948163986
H	0.031255554	5.527504921	15.351741791
C	5.709003448	2.062713861	14.644688606
H	5.264388561	1.293377757	14.001461029
C	6.617731571	2.926255465	13.747908592
H	7.044836044	3.760064363	14.317771912
H	6.074132919	3.335072756	12.893577576
H	7.447330475	2.326199770	13.355163574
C	6.546814919	1.337066293	15.709136963
H	7.254100800	0.655482113	15.227262497
H	5.914959431	0.749585271	16.382390976
H	7.134366512	2.037153959	16.314472198
H	2.529859543	-0.638689876	14.000431061
C	-3.997006178	1.000819802	10.490493774
C	-2.611454487	1.105148792	10.584294319
C	-4.761895657	0.745825648	11.633908272
H	-4.481269360	1.116806746	9.524957657
H	-2.003198862	1.297977328	9.705283165
C	-1.997297049	0.950333595	11.839023590
H	-5.842653751	0.665015101	11.552757263
C	-4.146182060	0.591639102	12.880349159
C	-2.761946678	0.691369832	12.991527557
C	-0.578112245	1.038489580	11.961345673
H	-4.744242668	0.390967011	13.765083313
H	-2.265669107	0.572554171	13.949951172
N	0.573383212	1.085632205	12.101522446

=====

⁶B-TS

=====

Mn	3.530660152	0.076341122	12.828281403
N	3.881945610	0.441078156	10.864637375
N	3.523485899	2.112803459	13.270283699
C	4.644552708	1.689475060	8.897222519
H	5.379354954	0.919807255	8.638991356
H	5.045800686	2.668229342	8.628892899
H	3.759706974	1.494478583	8.282612801
C	4.292665005	1.614753842	10.370480537
C	4.398499489	2.798384666	11.120945930
H	4.782895565	3.657034397	10.584035873
C	3.990995884	3.049768448	12.451877594
C	4.135443211	4.475067616	12.952718735
H	3.305606127	4.755434990	13.604888916
H	4.197211266	5.184941292	12.125662804
H	5.052175999	4.562703609	13.547021866
C	3.571030855	-0.650273144	9.992613792
C	4.520652771	-1.672625065	9.775562286
C	4.144996166	-2.774121284	8.998677254

H	4.860599041	-3.573795080	8.826799393
C	2.869700909	-2.864239454	8.446440697
H	2.596003056	-3.727752686	7.846129417
C	1.943327785	-1.848098993	8.670319557
H	0.946287036	-1.929106474	8.245448112
C	2.269393206	-0.728744626	9.441886902
C	1.224100471	0.351001084	9.708535194
H	1.711236000	1.166799426	10.249734879
C	0.650218129	0.939308822	8.406942368
H	1.441383719	1.327638745	7.756817341
H	-0.036185179	1.763055801	8.632868767
H	0.089727573	0.190289393	7.836606026
C	0.099388428	-0.185464501	10.615063667
H	-0.425576270	-1.020619154	10.136878014
H	-0.636182487	0.602057099	10.816400528
H	0.493059307	-0.534150243	11.573911667
C	5.908844471	-1.603009105	10.399632454
H	6.022780418	-0.606573701	10.838609695
C	7.028225899	-1.783110023	9.359413147
H	7.014702797	-2.786052465	8.918427467
H	8.009236336	-1.642393351	9.826597214
H	6.933426857	-1.060115814	8.542101860
C	6.041660309	-2.627109051	11.543579102
H	5.295179844	-2.441248178	12.324161530
H	7.034075737	-2.566377640	12.005355835
H	5.899879456	-3.648599863	11.171805382
C	3.021131992	2.429551840	14.570141792
C	3.898774624	2.504189491	15.673873901
C	3.352973938	2.737564802	16.941740036
H	4.012880802	2.790443182	17.803459167
C	1.982072353	2.896399498	17.117313385
H	1.577470183	3.086175203	18.108123779
C	1.125742078	2.796490908	16.021314621
H	0.056279279	2.905787230	16.171768188
C	1.618666887	2.545500755	14.737136841
C	0.676578283	2.400540590	13.545187950
H	1.175597906	1.753730297	12.816855431
C	-0.652010560	1.721332312	13.907287598
H	-0.473265499	0.764105380	14.404167175
H	-1.228485346	1.525637984	12.997424126
H	-1.274601102	2.348082066	14.556227684
C	0.427783698	3.755391598	12.855060577
H	-0.249204814	3.632260084	12.001700401
H	1.357410669	4.194118023	12.482920647
H	-0.029938642	4.468714237	13.550643921
C	5.400773525	2.293551683	15.519096375
H	5.624845505	2.248635769	14.449163437
C	6.217691898	3.451763153	16.121007919
H	6.110464573	3.496772528	17.210575104
H	5.901771545	4.420029640	15.718876839
H	7.283352375	3.321668148	15.901854515
C	5.825704098	0.943949997	16.129501343
H	6.904525757	0.789079607	16.009838104
H	5.304724216	0.115404502	15.642024040
H	5.593871593	0.907060325	17.199998856

H	4.202299118	-1.072109103	14.054814339
C	2.092792749	-1.261267185	18.323398590
C	1.905200481	-0.951019168	16.979423523
C	3.145372868	-2.094944715	18.709634781
H	1.421934128	-0.846189320	19.070074081
H	1.107904792	-0.288302660	16.659984589
C	2.788841724	-1.472530603	16.022130966
H	3.288269281	-2.335527182	19.759576797
C	4.023060322	-2.609865189	17.751457214
C	3.855937243	-2.288647890	16.406698227
C	2.546552420	-1.105152369	14.633600235
H	4.845197201	-3.251365185	18.055017471
H	4.545979023	-2.645657063	15.648571014
N	1.738312483	-0.750331640	13.822659492

=====

⁶C

=====

Mn	6.626139641	5.346853256	11.863155365
N	5.624547005	4.548085690	13.445819855
N	7.310999393	3.512523651	11.273583412
N	6.893334866	7.054590225	11.142162323
C	4.854654312	2.843521595	15.030834198
H	5.218005657	3.381119728	15.913445473
H	4.931976318	1.770582080	15.214201927
H	3.798049688	3.109192610	14.918085098
C	5.637170792	3.261090755	13.801690102
C	6.342195034	2.258430719	13.106396675
H	6.268232346	1.261705041	13.523408890
C	7.107599258	2.367854834	11.927397728
C	7.726511955	1.100540280	11.372287750
H	7.345893860	0.902588487	10.364778519
H	7.518085480	0.236009240	12.004748344
H	8.811507225	1.218775749	11.276914597
C	4.884700775	5.516078472	14.199591637
C	3.564931870	5.835046768	13.808825493
C	2.893425703	6.851152420	14.498211861
H	1.880982518	7.116118908	14.205428123
C	3.508848429	7.538671970	15.542258263
H	2.973189592	8.327130318	16.063999176
C	4.817622662	7.225753784	15.906446457
H	5.297539711	7.780651569	16.707984924
C	5.527694702	6.216393948	15.247405052
C	2.919602871	5.151563644	12.608359337
H	3.541917801	4.291101933	12.343195915
C	1.506756902	4.624057770	12.905266762
H	1.509181261	3.941169500	13.761945724
H	1.113759518	4.080981255	12.038403511
H	0.806939900	5.436964512	13.128487587
C	2.921589375	6.107332230	11.396893501
H	2.292300701	6.983798981	11.589996338
H	2.542832851	5.604951382	10.499045372
H	3.933803082	6.471124172	11.185391426
C	6.984792709	5.932938099	15.596550941
H	7.260112286	4.983540535	15.129264832

C	7.225852966	5.787864685	17.108161926
H	8.265802383	5.502325535	17.300863266
H	6.575705051	5.021306038	17.543605804
H	7.040985584	6.725649834	17.643228531
C	7.897202492	7.017199516	14.986309052
H	7.759682178	7.092728615	13.900728226
H	8.952716827	6.795213699	15.183658600
H	7.668266296	7.999442577	15.416226387
C	8.024376869	3.536601305	10.031696320
C	7.302947521	3.369513512	8.826676369
C	7.989726067	3.505375385	7.616961479
H	7.450507164	3.391350031	6.680594921
C	9.351961136	3.798395395	7.591534615
H	9.867869377	3.904568911	6.640923023
C	10.047484398	3.967100859	8.785924911
H	11.106276512	4.210174084	8.757752419
C	9.403690338	3.839209795	10.021828651
C	5.795776367	3.133744240	8.842452049
H	5.515430927	2.825999022	9.854582787
C	5.349234581	2.018708944	7.882489204
H	4.276733398	1.825125098	7.998173237
H	5.887259007	1.084911346	8.080122948
H	5.520461559	2.287108898	6.833919525
C	5.053950787	4.453505993	8.543655396
H	5.364960670	5.248005390	9.231186867
H	3.968935966	4.324675083	8.636308670
H	5.273033142	4.802256584	7.527659893
C	10.159987450	4.085780621	11.320565224
H	9.525192261	3.742684126	12.143004417
C	11.480451584	3.300590992	11.397834778
H	11.315405846	2.228019714	11.246215820
H	11.949511528	3.438736916	12.378302574
H	12.198409081	3.636953831	10.641558647
C	10.390537262	5.596498966	11.522255898
H	11.029020309	5.997284412	10.726283073
H	10.881205559	5.790106773	12.483157158
H	9.443124771	6.148082733	11.498913765
C	7.242045403	8.193681717	10.724433899
H	8.146455765	8.706832886	11.118712425
C	6.536008835	8.985177040	9.679313660
C	5.364743233	8.504334450	9.069379807
H	4.978420734	7.538464546	9.380675316
C	4.722911835	9.252600670	8.087788582
H	3.816499233	8.871507645	7.620820045
C	5.242482662	10.494166374	7.698071957
H	4.740456104	11.077534676	6.930434227
C	6.406607628	10.981060982	8.298181534
H	6.813944340	11.944057465	7.997512341
C	7.047355175	10.229772568	9.283880234
H	7.956608772	10.605717659	9.752214432

=====

2

=====

Mn	6.019448757	5.193267345	11.246610641
----	-------------	-------------	--------------

N	5.502881050	4.623636723	13.216644287	C	6.427616596	1.001312733	7.817183971
N	7.203913212	3.454492092	11.049800873	H	5.387177467	0.678874254	7.695860386
N	6.752255917	7.093950272	10.736754417	H	6.935038567	0.275140345	8.460669518
C	4.899048805	2.969163895	14.949459076	H	6.902610779	0.955510080	6.830406666
H	5.068684101	3.714118719	15.728224754	C	5.811505318	3.411846638	7.425497055
H	5.256875515	1.999955297	15.301548958	H	5.826567650	4.431880951	7.813978672
H	3.816339731	2.902803183	14.801739693	H	4.766412258	3.131278276	7.252234459
C	5.566729069	3.361170530	13.641724586	H	6.327687263	3.416529179	6.462421894
C	6.206148624	2.315580368	12.948276520	C	9.791104317	4.496815205	11.684869766
H	6.137901783	1.342682958	13.419305801	H	8.842490196	4.898382187	12.057908058
C	7.027927399	2.369114399	11.805159569	C	10.260584831	3.440579653	12.704416275
C	7.727873325	1.072122812	11.432912827	H	9.496242523	2.679270983	12.876799583
H	7.257717609	0.640973866	10.544272423	H	10.484565735	3.909985781	13.669901848
H	7.670406818	0.342750400	12.242886543	H	11.170197487	2.940493822	12.350721359
H	8.776622772	1.241722584	11.181916237	C	10.794962883	5.659415722	11.622236252
C	5.003190517	5.617450714	14.119331360	H	11.807758331	5.315412998	11.382502556
C	3.619135380	5.872317314	14.213523865	H	10.846664429	6.159092426	12.596966743
C	3.186314106	6.838509083	15.129255295	H	10.504175186	6.401803493	10.874557495
H	2.124636650	7.057992458	15.206823349	C	7.772935867	7.652570248	11.253074646
C	4.089752197	7.511446953	15.947426796	H	8.354467392	7.139635563	12.038133621
H	3.730211973	8.242748260	16.667104721	C	8.333613396	8.988844872	10.941100121
C	5.457810402	7.264437199	15.829314232	C	7.785696507	9.848693848	9.976634979
H	6.155667782	7.813101292	16.454521179	H	6.914078712	9.547520638	9.408785820
C	5.940130234	6.335950851	14.902306557	C	8.349842072	11.097413063	9.739379883
C	2.616792440	5.129534245	13.340291023	H	7.906918526	11.747637749	8.989850044
H	3.155721664	4.339651108	12.813897133	C	9.473967552	11.509949684	10.462532043
C	1.486590624	4.469150066	14.151276588	H	9.912881851	12.486920357	10.277891159
H	1.872352123	3.831002951	14.952939034	C	10.030272484	10.663692474	11.423255920
H	0.864894867	3.851046085	13.493436813	H	10.903364182	10.978923798	11.988643646
H	0.832712591	5.218283176	14.612607002	C	9.462842941	9.412151337	11.658214569
C	2.025976419	6.067547798	12.278014183	H	9.890867233	8.749675751	12.407518387
H	1.427420139	6.856800556	12.739648819	Mn	5.238417149	7.537220478	9.287350655
H	1.381218195	5.504708290	11.593688011	N	5.736313343	8.090353966	7.302154541
H	2.807334661	6.548440456	11.686445236	N	4.071702480	9.290361404	9.483432770
C	7.434115887	6.068274975	14.740881920	N	4.505492687	5.641571522	9.803850174
H	7.579545975	5.715353012	13.713759422	C	6.318826199	9.728385925	5.544838905
C	7.919754028	4.939295769	15.671856880	H	6.117493153	8.984092712	4.772794247
H	8.996500015	4.773912430	15.545973778	H	5.967876434	10.702153206	5.198615074
H	7.413991451	3.994959354	15.458828926	H	7.406016350	9.777037621	5.663877010
H	7.735592365	5.198294163	16.721307755	C	5.675127506	9.351002693	6.869496346
C	8.301960945	7.322015285	14.929377556	C	5.058509827	10.407333374	7.567028999
H	7.947468758	8.149248123	14.309822083	H	5.130702972	11.376880646	7.089907169
H	9.338986397	7.103077888	14.648012161	C	4.253947735	10.369825363	8.721967697
H	8.315041542	7.660056114	15.971948624	C	3.584543943	11.680788040	9.099575996
C	8.197325706	3.401479006	10.018671036	H	4.108889103	12.125913620	9.950333595
C	7.883009911	2.885418653	8.743755341	H	3.606842518	12.391080856	8.271168709
C	8.903462410	2.815768242	7.788320065	H	2.549518108	11.529766083	9.410109520
H	8.677287102	2.433432341	6.796572208	C	6.226027489	7.092283249	6.397798538
C	10.202111244	3.212723732	8.092204094	C	7.609701633	6.847139835	6.277822018
H	10.986358643	3.128749132	7.343963146	C	8.031392097	5.881524086	5.356422901
C	10.491541862	3.747902155	9.347717285	H	9.092699051	5.669749737	5.257683277
H	11.501114845	4.085280418	9.563459396	C	7.118023396	5.200535297	4.556065559
C	9.496311188	3.880073547	10.319693565	H	7.469357491	4.470386505	3.831270218
C	6.472305298	2.426059246	8.399727821	C	5.750550747	5.437352657	4.699441433
H	5.884637833	2.428173065	9.320430756	H	5.045217514	4.883195400	4.087461472

C	5.279127121	6.365147114	5.633836746
C	8.623326302	7.602529526	7.127202988
H	8.094687462	8.410167694	7.637000561
C	9.753016472	8.235434532	6.294164181
H	9.366446495	8.853379250	5.477052212
H	10.379362106	8.868694305	6.932812214
H	10.403147697	7.472351551	5.851183414
C	9.214227676	6.685896397	8.207751274
H	9.792536736	5.874528885	7.759038925
H	9.878428459	7.256872177	8.866797447
H	8.433783531	6.235205650	8.824444771
C	3.786582232	6.628281593	5.818631172
H	3.656807184	6.983553886	6.846998215
C	3.283617973	7.753696918	4.893195629
H	2.208781004	7.917071342	5.036304951
H	3.790777683	8.699611664	5.095777988
H	3.451048851	7.492583275	3.841403246
C	2.919211626	5.371979237	5.647459507
H	3.280833960	4.549932480	6.269974232
H	1.884836435	5.591588020	5.937739372
H	2.895823240	5.026348591	4.607490540
C	3.082255840	9.357030869	10.517696381
C	3.408356428	9.860675812	11.794610023
C	2.392381668	9.938253403	12.754632950
H	2.628129005	10.311226845	13.747861862
C	1.087917566	9.558993340	12.454075813
H	0.308318377	9.647552490	13.206647873
C	0.785241008	9.040678978	11.194832802
H	-0.230186611	8.720908165	10.980233192
C	1.774297476	8.903026581	10.217483521
C	4.823739529	10.306709290	12.134954453
H	5.414391994	10.275774002	11.216706276
C	4.882240772	11.744035721	12.686449051
H	5.925482273	12.057191849	12.808177948
H	4.387180805	12.462081909	12.024657249
H	4.400180340	11.815923691	13.668395042
C	5.468995094	9.336230278	13.134199142
H	5.437227249	8.306670189	12.773112297
H	6.518387318	9.605978012	13.297660828
H	4.955401421	9.364248276	14.098463058
C	1.464199662	8.307445526	8.846507072
H	2.405112743	7.896724224	8.463805199
C	1.005451679	9.383878708	7.843149662
H	1.778452277	10.137974739	7.678720474
H	0.772354186	8.930772781	6.872134209
H	0.103447095	9.890524864	8.206800461
C	0.442229956	7.160264492	8.898427963
H	-0.563787162	7.517091274	9.147451401
H	0.378281236	6.675089359	7.917089462
H	0.723943293	6.403420925	9.634939194
C	3.470721960	5.096849442	9.301181793
H	2.870090008	5.628904343	8.543394089
C	2.915292740	3.755081892	9.597186089
C	3.487696648	2.868978024	10.523663521
H	4.376592159	3.153419018	11.073712349

C	2.924154997	1.616837978	10.745873451
H	3.384771824	0.946108043	11.466109276
C	1.777098060	1.228057027	10.046023369
H	1.338552356	0.248916179	10.219182968
C	1.197638988	2.100369692	9.123044014
H	0.306791067	1.803529739	8.575911522
C	1.764461398	3.354263544	8.902067184
H	1.318508983	4.037124634	8.182177544

=====

⁶D

=====

Mn	6.693281651	5.209829330	11.295761108
N	6.840274334	3.702181101	12.731276512
N	7.883931637	4.157855511	9.967864990
N	7.182307720	7.088650227	12.154510498
C	7.684275627	1.602102876	13.718674660
H	8.675271988	1.155683517	13.833382607
H	6.994562626	0.807875633	13.406965256
H	7.339824677	1.968919277	14.685972214
C	7.699814796	2.691410303	12.660331726
C	8.616129875	2.508749008	11.598654747
H	9.304766655	1.681529284	11.725239754
C	8.666060448	3.138554811	10.341376305
C	9.697072983	2.592694759	9.367709160
H	9.344698906	2.639290571	8.335764885
H	9.958489418	1.560229897	9.607802391
H	10.609461784	3.195642233	9.426898003
C	5.852688789	3.739889383	13.768138885
C	4.635252953	3.051709414	13.569652557
C	3.658938169	3.123127699	14.567874908
H	2.713298559	2.605916500	14.429273605
C	3.877441406	3.853447199	15.733325005
H	3.111280441	3.893430471	16.503061295
C	5.073842049	4.545524120	15.904605865
H	5.229931355	5.127075672	16.808507919
C	6.074714661	4.516999245	14.928416252
C	4.355895519	2.319287777	12.261853218
H	5.298997402	2.230140209	11.715290070
C	3.811895370	0.897757411	12.467321396
H	4.486711502	0.302455962	13.091715813
H	3.701958656	0.389238209	11.502936363
H	2.828536272	0.901527107	12.950037956
C	3.409825087	3.168749094	11.392201424
H	2.425698280	3.263579607	11.865535736
H	3.271739483	2.718039036	10.402336121
H	3.809854269	4.179488659	11.264442444
C	7.370238781	5.294094086	15.114757538
H	7.801527023	5.417939663	14.122439384
C	8.393201828	4.516679764	15.963770866
H	9.316428185	5.097185135	16.073173523
H	8.655268669	3.558297157	15.506567955
H	7.995257378	4.315161228	16.965076447
C	7.147707939	6.702255726	15.689223289
H	6.388590813	7.243821144	15.118476868

H	8.084220886	7.270057201	15.641961098
H	6.837288380	6.674587250	16.740200043
C	7.884701729	4.616586685	8.611165047
C	6.847198486	4.164099216	7.751576900
C	6.804606438	4.667953491	6.447813988
H	6.024975300	4.338731289	5.769179344
C	7.739587784	5.601418495	6.001245022
H	7.680922031	5.984134197	4.985763550
C	8.741640091	6.043133736	6.857686996
H	9.463990211	6.775012493	6.506500244
C	8.839381218	5.560378075	8.169070244
C	5.798735619	3.164068460	8.246361732
H	5.531982899	3.459187031	9.270482063
C	6.343765736	1.722233415	8.321026802
H	5.550732613	1.035272598	8.639578819
H	7.164288044	1.626705170	9.032072067
H	6.698279858	1.394762397	7.336788654
C	4.503555298	3.165477514	7.418268681
H	4.103234768	4.171412468	7.271134377
H	3.738951683	2.569447756	7.927964687
H	4.658761024	2.714907169	6.431028843
C	9.959160805	6.063409805	9.072430611
H	9.899352074	5.521059990	10.018128395
C	11.350434303	5.797451019	8.464521408
H	11.473812103	4.751523495	8.166583061
H	12.132137299	6.042543411	9.192310333
H	11.522002220	6.414280891	7.574941635
C	9.800065994	7.560512543	9.396292686
H	9.828292847	8.166591644	8.483343124
H	10.609965324	7.894226074	10.053640366
H	8.853610039	7.758187771	9.902331352
C	8.147669792	7.762160778	12.638443947
H	7.982746124	8.799837112	12.964068413
C	9.526141167	7.266930580	12.816765785
C	9.883618355	5.921607971	12.618482590
H	9.135508537	5.190071583	12.338897705
C	11.200854301	5.507456303	12.783442497
H	11.453897476	4.462815762	12.624934196
C	12.187334061	6.429124355	13.148990631
H	13.217155457	6.105295181	13.273314476
C	11.843939781	7.765920162	13.360388756
H	12.604982376	8.485537529	13.649072647
C	10.521628380	8.178236961	13.201472282
H	10.253688812	9.219794273	13.364345551
O	5.541926861	8.802520752	11.224042892
B	5.715134144	7.634554863	12.054607391
O	5.043784142	6.489542007	11.249836922
H	5.256012917	7.746895790	13.174761772
C	5.020265579	8.434310913	9.950636864
C	4.200850010	7.130344391	10.261317253
C	6.182633877	8.163346291	8.978219032
C	4.166174889	9.588546753	9.422833443
C	4.017420769	6.201063633	9.069659233
C	2.854248047	7.418278694	10.936085701
H	6.854621410	9.025961876	8.987053871

H	6.765810013	7.290019035	9.281604767
H	5.843194962	7.996488094	7.950785160
H	3.642004490	9.305889130	8.502619743
H	3.432524681	9.902049065	10.167978287
H	4.807735443	10.446871758	9.200284958
H	3.497999191	6.719365120	8.256496429
H	4.979242802	5.853059769	8.689517021
H	3.419965744	5.329324722	9.348916054
H	2.132205486	7.834077358	10.226356506
H	2.451197624	6.482819080	11.335604668
H	2.981828451	8.119692802	11.763910294

=====

⁶E

=====

Mn	6.958727837	5.557921886	11.337343216
N	6.480830193	3.975168228	12.539214134
N	7.830972195	4.423272610	9.879817009
N	7.374023914	7.493199825	11.889616966
C	6.417922497	1.607501507	13.192323685
H	6.780296803	1.805409193	14.205671310
H	6.798439026	0.638946176	12.863629341
H	5.326713562	1.553835750	13.258740425
C	6.836941719	2.720082045	12.249625206
C	7.554126263	2.336082458	11.097410202
H	7.768410206	1.277125478	11.027577400
C	7.970678806	3.098439693	9.986315727
C	8.586279869	2.333348751	8.829311371
H	8.000547409	2.484826565	7.917051792
H	8.640650749	1.264013052	9.039623260
H	9.593008041	2.703387022	8.614151001
C	5.603235722	4.226073265	13.650328636
C	4.205909252	4.197645187	13.423629761
C	3.350597143	4.476624489	14.493224144
H	2.276483297	4.478061199	14.327760696
C	3.851290464	4.772287369	15.758558273
H	3.171919346	4.988567829	16.578866959
C	5.226501465	4.798614025	15.965277672
H	5.613678932	5.038170338	16.952402115
C	6.124824524	4.534803867	14.924591064
C	3.622597933	3.965273619	12.032687187
H	4.450326920	3.748913527	11.349329948
C	2.667478800	2.758249998	11.992196083
H	3.159301043	1.840744376	12.335400581
H	2.309804678	2.589556932	10.969774246
H	1.788685322	2.921268940	12.627596855
C	2.919827700	5.241909981	11.526758194
H	2.026764393	5.459352493	12.125965118
H	2.606715202	5.122077465	10.482735634
H	3.585061789	6.105658054	11.601708412
C	7.620606422	4.659765244	15.179662704
H	8.136371613	4.427571774	14.242667198
C	8.126720428	3.668055058	16.242977142
H	9.212326050	3.759660721	16.363754272
H	7.905251980	2.631454706	15.968111992

H	7.666114807	3.858998299	17.218566895
C	7.972549915	6.106360912	15.578628540
H	7.593163490	6.818841457	14.840517044
H	9.055644989	6.236739159	15.665246964
H	7.521961689	6.361155510	16.544609070
C	8.145410538	5.071374893	8.636941910
C	7.109356403	5.242178440	7.686604977
C	7.411223888	5.875610828	6.476952553
H	6.622251987	6.025017738	5.744602203
C	8.697567940	6.332558632	6.203883171
H	8.914122581	6.824941635	5.259588718
C	9.702618599	6.166183472	7.151662350
H	10.701769829	6.537638187	6.939508438
C	9.451995850	5.541576862	8.379144669
C	5.670855522	4.821549416	7.975556374
H	5.644995213	4.363227844	8.969673157
C	5.166944504	3.764589548	6.975886345
H	4.149437904	3.449395180	7.233776569
H	5.805966377	2.874614954	6.976320744
H	5.144679070	4.159509182	5.953691959
C	4.735361099	6.047200203	8.000653267
H	5.094078064	6.809002876	8.697362900
H	3.725782871	5.752357006	8.309096336
H	4.660873890	6.504518032	7.006960392
C	10.551178932	5.500702381	9.433789253
H	10.156147957	4.981974125	10.313656807
C	11.804310799	4.738222599	8.964035034
H	11.568701744	3.712487698	8.661434174
H	12.546055794	4.691827774	9.769570351
H	12.276652336	5.234027386	8.108370781
C	10.926147461	6.937256336	9.848707199
H	11.391857147	7.471421719	9.012907028
H	11.630905151	6.933603287	10.685305595
H	10.040168762	7.500953197	10.151997566
C	8.234210014	8.268928528	12.423281670
H	8.003763199	9.339327812	12.543584824
C	9.567379951	7.856672764	12.895467758
C	9.942473412	6.507154942	13.007876396
H	9.231408119	5.725996494	12.761186600
C	11.210894585	6.158938408	13.454358101
H	11.483195305	5.110073566	13.542790413
C	12.128786087	7.157279968	13.801729202
H	13.118493080	6.884619236	14.157952309
C	11.769344330	8.503055573	13.697924614
H	12.479145050	9.280998230	13.966007233
C	10.493338585	8.848435402	13.253499031
H	10.210508347	9.896283150	13.170289040
O	4.995064259	7.978998184	12.600789070
B	5.903081894	7.864208221	11.489392281
O	5.793247223	9.027796745	10.665716171
H	5.568205357	6.764292717	10.824486732
C	4.354012966	9.261414528	12.521950722
C	4.552868366	9.665856361	11.005094528
C	5.078326225	10.215129852	13.489391327
C	2.895905972	9.106134415	12.958177567

C	4.693686962	11.169399261	10.756030083
C	3.455186605	9.090867043	10.091993332
H	5.076075077	9.769319534	14.490036011
H	6.118521214	10.361922264	13.185159683
H	4.594147682	11.196948051	13.544822693
H	2.346935272	10.048303604	12.836505890
H	2.391975164	8.325627327	12.383377075
H	2.857316017	8.820911407	14.015862465
H	3.792224884	11.705937386	11.075136185
H	5.554403305	11.583085060	11.286023140
H	4.838184834	11.351970673	9.685065269
H	2.488529444	9.579970360	10.252858162
H	3.752847910	9.241518021	9.048741341
H	3.333561420	8.015673637	10.254107475

=====

⁶E-TS

=====

Mn	6.059555531	5.644661427	11.345999718
N	5.553912163	4.471654892	12.968777657
N	7.306348801	4.157547951	10.566412926
N	7.392708302	7.352250576	11.628293037
C	5.936078548	2.741767645	14.676463127
H	5.904477119	3.500313520	15.464597702
H	6.682728767	1.988722920	14.936090469
H	4.951542377	2.262667656	14.663352013
C	6.243785858	3.385821581	13.335452080
C	7.225354195	2.759884834	12.544759750
H	7.659375191	1.864289880	12.973240852
C	7.624865055	3.043180466	11.214968681
C	8.407734871	1.952440381	10.504912376
H	9.135161400	2.354802608	9.799142838
H	7.707895279	1.336516261	9.926641464
H	8.917459488	1.300420403	11.217823982
C	4.370799065	4.829919338	13.693958282
C	3.180979013	4.094495296	13.459365845
C	2.021215439	4.470291138	14.141107559
H	1.099782467	3.920458794	13.975657463
C	2.022864342	5.545187473	15.030141830
H	1.111223578	5.818339348	15.554980278
C	3.190830708	6.271171570	15.233000755
H	3.187669754	7.115004539	15.918311119
C	4.376978874	5.936086178	14.568992615
C	3.155609846	2.970994949	12.426144600
H	4.163177967	2.554105043	12.345685005
C	2.218848467	1.810651064	12.795123100
H	2.435794592	1.425484538	13.797446251
H	2.339725494	0.988826752	12.080933571
H	1.164630651	2.107448339	12.770719528
C	2.802348137	3.546582222	11.041246414
H	1.787532926	3.961120605	11.040614128
H	2.857578516	2.769933939	10.269341469
H	3.487958193	4.353031635	10.761485100
C	5.632327557	6.765389919	14.787434578
H	6.412210941	6.338491440	14.156469345

C	6.140871048	6.686985493	16.237131119
H	7.089732170	7.225904942	16.336151123
H	6.311228275	5.648941994	16.542089462
H	5.423656940	7.128432751	16.938835144
C	5.422550678	8.224106789	14.343867302
H	5.130715847	8.277769089	13.290424347
H	6.347911835	8.798027039	14.469502449
H	4.644702435	8.714658737	14.939868927
C	7.764144421	4.373740673	9.226115227
C	6.944399357	3.990687847	8.144761086
C	7.395707130	4.243566513	6.844304085
H	6.774306297	3.957811356	5.999535084
C	8.624769211	4.856321335	6.616633892
H	8.966228485	5.033903599	5.600034714
C	9.407827377	5.259672165	7.696576118
H	10.350841522	5.765991211	7.512158394
C	8.990468025	5.049085617	9.012871742
C	5.565429211	3.384778261	8.374694824
H	5.463995457	3.177536249	9.444761276
C	5.370639324	2.054011822	7.629633904
H	4.399520397	1.613062978	7.881954670
H	6.151618481	1.333336234	7.895217419
H	5.398418427	2.188669443	6.542606354
C	4.474982262	4.408025265	8.001411438
H	4.583329201	5.323684692	8.594030380
H	3.475081205	3.999300241	8.182424545
H	4.544518471	4.683001041	6.942589283
C	9.818513870	5.564972401	10.184563637
H	9.133061409	5.652335644	11.026698112
C	10.938234329	4.590995312	10.596057892
H	10.542366982	3.623468876	10.914899826
H	11.514374733	5.004757881	11.432125092
H	11.627655983	4.416644096	9.761709213
C	10.398998260	6.967777729	9.933006287
H	11.218362808	6.949656963	9.204714775
H	10.806491852	7.370968342	10.868010521
H	9.622685432	7.643467903	9.568170547
C	8.163688660	7.930211544	12.469999313
H	8.335768700	9.013785362	12.406537056
C	8.878843307	7.235563278	13.547581673
C	8.866418839	5.834318638	13.672793388
H	8.322010994	5.227616310	12.961008072
C	9.549445152	5.216417313	14.712871552
H	9.524424553	4.133653641	14.794192314
C	10.259038925	5.984417915	15.642366409
H	10.791230202	5.499271393	16.456079483
C	10.285573006	7.375549316	15.523779869
H	10.836709976	7.974214077	16.243341446
C	9.601712227	7.996450424	14.479791641
H	9.617892265	9.080042839	14.386276245
O	6.296834469	9.390875816	10.598441124
B	6.783572674	8.100841522	10.496820450
O	7.247859478	7.791666031	9.226499557
H	5.189773083	6.991102695	10.600857735
C	6.535210609	10.030761719	9.314451218

C	6.717871666	8.802647591	8.337933540
C	7.816251278	10.859631538	9.478281021
C	5.351264000	10.935670853	8.991437912
C	7.728858471	9.012473106	7.213826180
C	5.395745277	8.274209976	7.769977570
H	7.681001186	11.557020187	10.310403824
H	8.669753075	10.214438438	9.708713531
H	8.048221588	11.435658455	8.577021599
H	5.462059021	11.376518250	7.994676590
H	4.411173344	10.383171082	9.029605865
H	5.297486782	11.748785019	9.721571922
H	7.403102875	9.813165665	6.541109562
H	8.717939377	9.261029243	7.603423595
H	7.820353985	8.086651802	6.638690472
H	4.966571808	8.968662262	7.041135788
H	5.591197968	7.319141388	7.274689674
H	4.671433926	8.095050812	8.567802429

=====

⁶F

=====

Mn	6.341652870	6.034845352	10.650824547
N	6.190172195	4.834235191	12.384690285
N	7.810781002	4.758110046	9.874444962
N	7.077137470	8.026366234	11.551719666
C	6.601635456	2.849917650	13.807472229
H	5.998402596	3.343450069	14.569127083
H	7.511308193	2.454407215	14.267929077
H	6.026112080	1.995077252	13.431890488
C	6.936642170	3.766268253	12.641529083
C	8.038471222	3.362371445	11.848294258
H	8.608137131	2.530634642	12.247083664
C	8.411083221	3.779985189	10.555900574
C	9.556860924	3.024405003	9.904277802
H	9.184034348	2.339197636	9.135918617
H	10.115363121	2.441655397	10.639885902
H	10.238091469	3.718772173	9.404621124
C	5.083674431	5.179362774	13.225712776
C	3.791051388	4.717883587	12.896370888
C	2.719291449	5.101886749	13.710277557
H	1.718779445	4.750735283	13.471279144
C	2.912091494	5.923807144	14.816726685
H	2.068940878	6.203438282	15.443453789
C	4.189524651	6.396118164	15.112715721
H	4.331907749	7.052657127	15.966703415
C	5.289436340	6.050685883	14.323547363
C	3.541873217	3.848777533	11.668946266
H	4.507330894	3.660055876	11.189143181
C	2.941565275	2.483249903	12.047710419
H	3.576133251	1.956743479	12.768952370
H	2.836425781	1.850320101	11.159155846
H	1.947890997	2.592014551	12.497567177
C	2.662446022	4.591787815	10.645702362
H	1.682146192	4.837234020	11.070472717
H	2.500533581	3.973410130	9.756136894

H	3.150374889	5.520250797	10.330877304	O	5.752716064	9.990279198	10.711889267
C	6.672590256	6.610098839	14.633346558	H	5.151347160	6.736587048	9.631360054
H	7.251277447	6.524930477	13.713952065	C	3.793265820	9.570889473	11.985985756
C	7.407934189	5.802454472	15.719512939	C	4.323917866	10.318693161	10.698282242
H	8.397709846	6.233820438	15.910215378	C	3.905053139	10.406000137	13.266803741
H	7.550928116	4.760246277	15.426253319	C	2.401309013	8.962334633	11.859646797
H	6.845536709	5.814467430	16.660659790	C	4.183368683	11.836286545	10.733391762
C	6.644834042	8.099034309	15.016212463	C	3.761995316	9.748023987	9.393532753
H	6.059432983	8.674776077	14.297283173	H	3.716855049	9.756847382	14.126402855
H	7.667363167	8.493817329	15.037856102	H	4.908660412	10.828722954	13.374778748
H	6.216580391	8.259808540	16.012351990	H	3.178613424	11.223998070	13.279359818
C	8.056449890	4.887917995	8.469424248	H	1.649945021	9.742338181	11.697060585
C	7.441260338	3.971600533	7.578200817	H	2.357956886	8.247442245	11.036685944
C	7.653261662	4.130494595	6.205950260	H	2.158483744	8.426416397	12.781796455
H	7.188155651	3.439757109	5.508956432	H	3.128536224	12.121237755	10.806656837
C	8.445374489	5.167824268	5.713664055	H	4.722698212	12.273243904	11.575927734
H	8.604465485	5.271032810	4.643352032	H	4.588696957	12.263339996	9.811869621
C	9.018650055	6.076707840	6.596474171	H	2.698411465	9.981449127	9.286418915
H	9.624612808	6.892763615	6.210394859	H	4.301936626	10.193167686	8.552891731
C	8.827430725	5.962981701	7.978514194	H	3.905720234	8.664531708	9.348827362
C	6.498463631	2.890768528	8.100476265	=====			
H	6.747965336	2.691710949	9.145595551	⁶ F-TS			
C	6.618016243	1.556333899	7.347675800	=====			
H	6.007524490	0.790869951	7.839337349	Mn	6.481675625	6.014771938	11.161996841
H	7.654358387	1.201395273	7.323748589	N	6.006129265	4.322256088	12.260279655
H	6.267645359	1.633802891	6.312591076	N	7.090009212	4.815066338	9.551836967
C	5.048676014	3.413045883	8.084728241	N	7.760445118	7.606781960	12.024449348
H	4.960376263	4.352876663	8.639806747	C	4.685824871	2.248025179	12.424598694
H	4.368636608	2.679832697	8.534760475	H	5.200822353	1.885641932	13.316985130
H	4.717700481	3.603832722	7.057114601	H	4.392966270	1.391402602	11.814682961
C	9.432802200	6.990015030	8.922505379	H	3.780507088	2.756145477	12.774413109
H	9.106822014	6.725049973	9.927600861	C	5.535306454	3.232144833	11.636788368
C	10.970430374	6.948414326	8.926571846	C	5.782559395	2.919292450	10.290663719
H	11.337987900	5.949728489	9.185990334	H	5.362594604	1.982614994	9.945041656
H	11.370461464	7.653794765	9.663951874	C	6.628433704	3.581093550	9.371112823
H	11.380684853	7.212545872	7.944849014	C	7.021236420	2.805202484	8.125457764
C	8.906851768	8.406152725	8.629310608	H	6.601368427	3.261502504	7.223448753
H	9.198491096	8.744965553	7.628748894	H	6.681613445	1.769492149	8.181336403
H	9.312598228	9.122353554	9.353786469	H	8.108654022	2.812954903	8.001667976
H	7.814638138	8.438990593	8.696055412	C	6.083511829	4.290978432	13.686302185
C	8.148202896	8.592735291	11.975915909	C	5.107228279	4.932084560	14.478411674
H	8.164610863	9.679634094	12.140815735	C	5.200279713	4.814044952	15.870464325
C	9.402082443	7.910032272	12.304630280	H	4.452346325	5.294734001	16.495681763
C	9.499413490	6.510578156	12.382207870	C	6.228417873	4.087179184	16.465637207
H	8.631074905	5.893435001	12.204750061	H	6.274221420	3.993032217	17.547492981
C	10.710630417	5.907367706	12.695476532	C	7.210536003	3.497459412	15.670063019
H	10.761486053	4.824061871	12.747800827	H	8.024365425	2.951995611	16.140733719
C	11.842256546	6.691775799	12.940178871	C	7.173038483	3.603655577	14.277441978
H	12.789755821	6.218893528	13.183795929	C	3.989498615	5.753178120	13.847349167
C	11.756422043	8.084741592	12.877133369	H	4.059569836	5.634098530	12.761895180
H	12.633882523	8.695339203	13.069720268	C	2.590268373	5.283276081	14.281180382
C	10.540764809	8.690402985	12.566788673	H	2.438675642	4.220577717	14.064728737
H	10.469771385	9.774715424	12.516463280	H	1.817326665	5.850888252	13.751044273
O	4.742599010	8.478302002	12.123142242	H	2.428145409	5.429455280	15.355315208
B	5.860536575	8.830842018	11.423764229				

H	2.900167704	4.991597176	13.953185081	C	6.355792522	10.822092056	8.397069931
H	2.491581202	6.500603199	13.114394188	H	6.140342236	11.174962044	7.391134262
H	3.033567905	6.541865826	14.795684814	C	7.328356743	9.840368271	8.593419075
C	5.033331394	7.652615547	13.154332161	H	7.852616310	9.421413422	7.738177299
H	4.998783588	8.189457893	14.109706879	O	9.633710861	9.082124710	12.657520294
H	4.367931843	8.162258148	12.449408531	B	9.065953255	7.831321716	12.420245171
H	6.053917885	7.730917931	12.766316414	O	9.039778709	7.048863888	13.580477715
C	8.561909676	2.975409746	13.964686394	H	9.665225983	8.803116798	10.099215508
H	8.208054543	2.650367498	12.982767105	C	9.714990616	9.236024857	14.092034340
C	8.786179543	1.711519957	14.810055733	C	9.836008072	7.745219707	14.572241783
H	9.466294289	1.026536822	14.292022705	C	8.408047676	9.897205353	14.556645393
H	7.846597672	1.180545807	14.997098923	C	10.905961037	10.128885269	14.426657677
H	9.237063408	1.942854166	15.781357765	C	9.264242172	7.465704441	15.956687927
C	9.885724068	3.729298353	13.736311913	C	11.273517609	7.218942165	14.467616081
H	9.730724335	4.641040802	13.151495934	H	8.263270378	10.824390411	13.994835854
H	10.614518166	3.092238426	13.221628189	H	7.551185131	9.243945122	14.365767479
H	10.318386078	4.034761906	14.696089745	H	8.431014061	10.134464264	15.624785423
C	7.334311485	5.400974751	8.243469238	H	11.056962967	10.186739922	15.510214806
C	6.310114384	6.213329315	7.697276115	H	11.822447777	9.759920120	13.962586403
C	6.626683712	7.031785011	6.608946800	H	10.722341537	11.140635490	14.052430153
H	5.863056183	7.676939487	6.185254097	H	9.772925377	8.073939323	16.712850571
C	7.912115574	7.041539669	6.067259789	H	8.193218231	7.669314384	15.993525505
H	8.139773369	7.684682846	5.221215248	H	9.402137756	6.411180496	16.207843781
C	8.905703545	6.232181072	6.613912582	H	11.921606064	7.666485310	15.227403641
H	9.906044006	6.250916481	6.189429283	H	11.270594597	6.136238575	14.610224724
C	8.639200211	5.399767876	7.707275867	H	11.693268776	7.433336735	13.480419159
C	4.911557198	6.226362705	8.310414314	=====			
H	4.797879219	5.315762043	8.903218269	6H			
C	3.794932365	6.215776443	7.253954887	=====			
H	2.819060326	6.102737904	7.738775253	Mn	7.713521957	5.566616058	11.068408012
H	3.922672987	5.388639927	6.547125340	N	6.588004112	4.326596737	12.268135071
H	3.764766932	7.147050381	6.678135395	N	7.034594059	4.690253258	9.318717003
C	4.743056297	7.407287598	9.285613060	N	8.916191101	7.293002605	11.276574135
H	5.503896236	7.393312931	10.073019981	C	5.295154095	2.256834984	12.752477646
H	3.759051800	7.370292187	9.767786980	H	5.346394539	2.565397024	13.796456337
H	4.844425201	8.369259834	8.774310112	H	5.691877842	1.238224506	12.664365768
C	9.735894203	4.533725262	8.316361427	H	4.239631653	2.218776226	12.454574585
H	9.265121460	3.895218611	9.070993423	C	6.057238579	3.187963247	11.819772720
C	10.386985779	3.610095739	7.272300720	C	6.112999916	2.760037184	10.477713585
H	9.637733459	2.989449263	6.769142151	H	5.684823036	1.780119061	10.295112610
H	11.114491463	2.945216656	7.751175880	C	6.470876694	3.475692987	9.321634293
H	10.918481827	4.181116581	6.502852917	C	6.104022980	2.803799152	8.006731987
C	10.789359093	5.395903587	9.039465904	H	5.042981625	2.965073347	7.787125587
H	11.273144722	6.090018272	8.342532158	H	6.263312340	1.724347353	8.081422806
H	11.568574905	4.762055874	9.478896141	H	6.680374622	3.191990614	7.166997910
H	10.334746361	5.986594677	9.842057228	C	6.401896477	4.712235451	13.634171486
C	8.693793297	8.288890839	10.042559624	C	5.339104176	5.586557388	13.950848579
H	8.719416618	7.698761940	9.120884895	C	5.114519596	5.898902893	15.294087410
C	7.619783878	9.356908798	9.875669479	H	4.286077976	6.549569607	15.560733795
C	6.921040535	9.895375252	10.960287094	C	5.942855835	5.395477772	16.295570374
H	7.147484303	9.548032761	11.959746361	H	5.750354290	5.641512394	17.336744308
C	5.938631058	10.868944168	10.769334793	C	7.031102657	4.594546795	15.956938744
H	5.400758266	11.263888359	11.628039360	H	7.687084675	4.223627090	16.740087509
C	5.646837234	11.336412430	9.486054420	C	7.287805557	4.242757320	14.626642227
H	4.879713058	12.091536522	9.336083412				

C	4.460387707	6.180239677	12.855410576	H	4.920895100	10.241640091	11.150662422
H	4.971580982	6.015250206	11.899959564	C	5.518773556	10.534850121	9.098767281
C	3.099048615	5.464817047	12.764190674	H	4.670614243	11.167527199	8.850963593
H	3.225571632	4.394519806	12.568676949	C	6.465308189	10.211280823	8.122416496
H	2.491593122	5.888105392	11.955676079	H	6.349153042	10.580829620	7.106842041
H	2.538972139	5.572185516	13.701812744	C	7.555815697	9.406474113	8.442567825
C	4.277284145	7.699003696	13.023601532	H	8.279100418	9.145608902	7.674221992
H	3.644344091	7.941154003	13.885946274	O	9.545147896	9.248814583	12.697950363
H	3.801918507	8.123894691	12.133275032	B	8.884048462	8.060550690	12.518916130
H	5.245343208	8.188164711	13.168568611	O	8.108868599	7.692000389	13.591870308
C	8.476387978	3.351685524	14.284827232	H	9.814346313	8.837970734	10.130497932
H	8.526959419	3.266407490	13.194542885	C	9.130031586	9.796154976	13.977746010
C	8.303631783	1.934094310	14.864333153	C	8.496483803	8.543875694	14.709720612
H	9.143421173	1.295220971	14.568305016	C	8.120858192	10.910011292	13.673875809
H	7.379967690	1.460846305	14.518187523	C	10.357995033	10.378642082	14.672180176
H	8.274830818	1.960537195	15.960068703	C	7.258118153	8.861647606	15.540507317
C	9.802254677	3.975543976	14.753652573	C	9.500090599	7.737982273	15.539943695
H	9.977405548	4.940350056	14.272617340	H	8.594444275	11.643424034	13.015292168
H	10.635933876	3.313250065	14.494589806	H	7.240454197	10.523237228	13.156323433
H	9.819242477	4.115267277	15.841154099	H	7.796364307	11.417878151	14.586975098
C	7.027135849	5.449659824	8.104183197	H	10.095990181	10.758240700	15.665578842
C	5.805461884	6.008730412	7.655590057	H	11.146092415	9.632429123	14.780566216
C	5.814380646	6.780297756	6.489396572	H	10.752914429	11.210113525	14.081068039
H	4.889313698	7.230947971	6.140993595	H	7.512939930	9.551960945	16.352106094
C	6.988761425	6.987519741	5.774105072	H	6.467705250	9.311467171	14.936915398
H	6.976873398	7.586085320	4.866811275	H	6.865864754	7.940875530	15.976267815
C	8.184155464	6.434228897	6.227719784	H	9.829530716	8.295559883	16.422008514
H	9.093248367	6.606227398	5.661605835	H	9.012646675	6.816149712	15.867934227
C	8.234794617	5.664326668	7.395545483	H	10.364452362	7.460550308	14.934327126
C	4.500381470	5.829201698	8.429197311	B	10.171094894	6.250111580	11.419160843
H	4.640330315	5.040283203	9.171107292	O	10.832072258	6.456624985	12.690059662
C	3.327859879	5.403532982	7.527826786	O	11.152540207	6.368738651	10.382327080
H	2.448665619	5.168583870	8.138066292	H	9.625344276	5.083833218	11.355228424
H	3.576040030	4.518664360	6.932549953	C	12.248900414	6.380803108	12.456137657
H	3.037797928	6.199096203	6.832639694	C	12.371513367	6.859847546	10.962882042
C	4.157857418	7.111674786	9.205344200	C	12.692021370	4.921522617	12.638468742
H	4.963795185	7.380413055	9.891411781	C	12.957509041	7.273701668	13.473222733
H	3.238049269	6.980567455	9.787974358	C	13.544608116	6.256188869	10.190103531
H	4.019055367	7.960178852	8.527516365	C	12.409152985	8.392314911	10.840953827
C	9.547366142	5.044641495	7.870941639	H	12.430223465	4.592896461	13.646826744
H	9.582526207	5.125403881	8.961429596	H	12.179256439	4.271598339	11.923741341
C	9.621186256	3.542039633	7.534891605	H	13.772490501	4.805613041	12.507349014
H	8.836319923	2.976908445	8.041433334	H	14.033698082	7.318543434	13.272303581
H	10.586351395	3.131910324	7.852938175	H	12.554448128	8.287522316	13.451381683
H	9.522299767	3.378750324	6.455042839	H	12.816304207	6.870897293	14.481339455
C	10.798371315	5.760056019	7.340594292	H	14.499780655	6.503317356	10.667180061
H	10.940623283	5.589222908	6.266440868	H	13.455594063	5.170151711	10.122491837
H	11.678442955	5.381707668	7.865465641	H	13.559354782	6.657477379	9.171826363
H	10.755681992	6.838829517	7.517130375	H	13.374664307	8.796339989	11.163868904
C	8.985396385	8.125860214	10.051749229	H	12.260999680	8.664761543	9.791108131
H	9.224848747	7.478654385	9.206927299	H	11.621662140	8.859811783	11.436585426
C	7.724284649	8.905894279	9.740941048				
C	6.750988960	9.205696106	10.699665070				
H	6.825910568	8.789273262	11.697148323				
C	5.661977291	10.022228241	10.386618614				

=====

⁶H-TS

=====

Mn	8.061314583	5.186034203	11.114581108	H	4.605422974	5.158846378	9.204092979
N	6.559134483	4.337642670	12.270152092	C	3.398099184	5.259600639	7.436575413
N	6.998484612	4.705408096	9.315212250	H	2.489839792	5.002974987	7.993946075
N	9.021286964	7.305154324	11.273127556	H	3.763735294	4.354106426	6.943835258
C	5.360223770	2.246377230	12.803117752	H	3.113092899	5.969769955	6.652001858
H	4.685717583	2.788169384	13.470968246	C	3.940112114	7.172146797	9.000624657
H	6.110891819	1.762734652	13.436469078	H	4.647036552	7.559685707	9.734853745
H	4.795885563	1.470450521	12.282457352	H	2.976479053	7.011297703	9.498347282
C	6.039360046	3.189521790	11.824011803	H	3.797783613	7.947026253	8.239391327
C	6.076442719	2.776153564	10.478327751	C	9.517988205	5.037900448	7.854780197
H	5.663501263	1.791506410	10.287803650	H	9.576491356	5.064123631	8.948913574
C	6.413532257	3.507573366	9.315714836	C	9.540252686	3.549980402	7.455365658
C	6.029635429	2.818044424	8.012145996	H	8.723383904	2.998571396	7.923429489
H	4.943317413	2.704012871	7.945704460	H	10.481107712	3.087051153	7.774625301
H	6.460855484	1.811193109	7.998853207	H	9.455513954	3.437758207	6.367581844
H	6.377364159	3.357790232	7.132271290	C	10.783962250	5.737576485	7.337417126
C	6.327267647	4.739003181	13.620845795	H	10.898389816	5.630563736	6.251766205
C	5.282558441	5.661875725	13.863861084	H	11.663341522	5.289527416	7.808572769
C	5.015970707	6.030303001	15.184748650	H	10.789893150	6.802708626	7.586568832
H	4.206707001	6.721521378	15.398941994	C	8.840775490	8.073330879	10.004985809
C	5.787001133	5.537334919	16.237924576	H	8.916660309	7.373528004	9.171690941
H	5.564517498	5.833600998	17.260099411	C	7.553543568	8.858229637	9.876132011
C	6.854844570	4.684718609	15.974185944	C	6.595675468	9.001759529	10.882534027
H	7.470515728	4.328672886	16.796142578	H	6.668764114	8.436978340	11.804892540
C	7.144707203	4.266439438	14.669652939	C	5.514013290	9.873416901	10.714315414
C	4.480541229	6.228043079	12.695877075	H	4.790798664	9.985775948	11.515956879
H	5.170979023	6.302466393	11.846414566	C	5.351706028	10.575118065	9.522916794
C	3.337779999	5.285151958	12.267567635	H	4.507330894	11.246740341	9.392683983
H	3.718514442	4.327641964	11.906382561	C	6.273679256	10.390840530	8.488118172
H	2.753284454	5.735437393	11.457588196	H	6.143746376	10.908955574	7.541518688
H	2.660466433	5.093154907	13.108420372	C	7.363882542	9.546583176	8.668812752
C	3.923071384	7.630985737	12.974346161	H	8.079158783	9.406124115	7.862103462
H	3.114748478	7.610311985	13.714510918	O	9.504538536	9.309021950	12.655409813
H	3.510586500	8.054661751	12.053696632	B	8.856963158	8.115208626	12.498630524
H	4.703134537	8.303340912	13.346607208	O	8.113497734	7.723404408	13.570804596
C	8.333805084	3.349235535	14.409709930	H	9.673074722	8.778728485	9.887911797
H	8.292698860	3.028486252	13.364333153	C	9.092602730	9.862614632	13.936912537
C	8.317726135	2.090439558	15.296819687	C	8.467392921	8.609016418	14.678615570
H	9.117354393	1.404616356	14.995133400	C	8.080648422	10.970996857	13.629629135
H	7.365967751	1.553253174	15.229081154	C	10.329464912	10.444303513	14.615575790
H	8.481142998	2.337914944	16.352033615	C	7.208748341	8.913703918	15.481492996
C	9.654900551	4.117241859	14.587135315	C	9.470881462	7.826737881	15.530994415
H	9.727573395	4.953506947	13.888733864	H	8.555250168	11.710817337	12.978811264
H	10.504854202	3.451025486	14.400909424	H	7.209252834	10.578929901	13.100778580
H	9.746656418	4.506573200	15.608568192	H	7.746537685	11.472263336	14.542582512
C	6.999423027	5.488322735	8.121149063	H	10.084671974	10.811392784	15.617753983
C	5.791094303	6.076311588	7.672406197	H	11.122705460	9.698945045	14.698985100
C	5.823132038	6.893130779	6.535943031	H	10.709635735	11.284298897	14.026737213
H	4.903016090	7.358152390	6.191482067	H	7.433239460	9.626155853	16.282621384
C	7.006548882	7.126360416	5.846264362	H	6.420723438	9.333605766	14.853130341
H	7.011960983	7.763959885	4.965491772	H	6.828708649	7.992624283	15.926602364
C	8.188812256	6.535939217	6.289835930	H	9.788301468	8.402178764	16.405740738
H	9.105746269	6.718605995	5.739680290	H	8.987769127	6.906723499	15.869689941
C	8.215535164	5.711750031	7.420511723	H	10.345866203	7.546478748	14.939554214
C	4.455489635	5.861924648	8.382467270	B	10.399550438	6.761579514	11.368869781

O	11.008997917	6.613664627	12.596286774
O	11.272778511	6.762685776	10.310143471
H	9.684382439	4.570600510	11.209245682
C	12.409764290	6.309619904	12.339292526
C	12.607415199	6.876450062	10.880065918
C	12.582558632	4.791254044	12.424777985
C	13.241708755	7.006225586	13.412403107
C	13.578367233	6.089236736	10.008648872
C	12.949033737	8.372640610	10.862030983
H	12.299262047	4.458653450	13.425612450
H	11.928584099	4.287676334	11.708950043
H	13.622980118	4.503137589	12.245726585
H	14.311704636	6.886717319	13.211065292
H	13.011734009	8.072127342	13.468648911
H	13.026434898	6.559267998	14.387362480
H	14.582123756	6.094650745	10.447323799
H	13.251849174	5.055153847	9.887637138
H	13.635636330	6.547419548	9.017183304
H	13.962080956	8.561802864	11.230166435
H	12.879968643	8.736878395	9.833014488
H	12.239431381	8.940789223	11.471928596

=====

¶I

=====

Mn	-0.674343586	1.143901587	0.219904006
N	-0.871714473	2.432325363	-1.420056105
N	0.154675454	2.683257103	1.414235234
N	0.473219305	-0.976626039	0.155127764
C	-1.880796790	4.562279701	-2.207311630
H	-1.187197089	5.352399826	-2.512658596
H	-2.769371510	5.053321838	-1.797415853
H	-2.169294357	3.996420383	-3.092919588
C	-1.253584743	3.683184624	-1.132457852
C	-1.104738116	4.302025318	0.123394556
H	-1.511299014	5.306525707	0.185673088
C	-0.355011076	3.899922609	1.252356768
C	-0.176378146	4.964869022	2.323753834
H	0.117301732	5.917661190	1.873771548
H	0.568260849	4.680283070	3.066346645
H	-1.129948735	5.123995781	2.840253592
C	-0.693622708	2.067869186	-2.786012173
C	-1.545200944	1.103248358	-3.383540392
C	-1.351504326	0.798994243	-4.736581802
H	-1.999187827	0.074124217	-5.218002319
C	-0.347968787	1.412061810	-5.487048149
H	-0.225344568	1.164823532	-6.538188934
C	0.504653156	2.329065084	-4.876960278
H	1.307621837	2.780082941	-5.453973293
C	0.360533953	2.663404942	-3.525227308
C	-2.675932407	0.455599397	-2.584652424
H	-2.295427799	0.210673571	-1.584589005
C	-3.851670265	1.431932926	-2.384939194
H	-3.538553238	2.329294682	-1.848370194
H	-4.645724297	0.954642832	-1.799537778

H	-4.272774696	1.733124733	-3.352025032
C	-3.182897329	-0.866025507	-3.177018881
H	-2.371469498	-1.586381197	-3.311386347
H	-3.687264204	-0.720838606	-4.139977455
H	-3.909729958	-1.312377214	-2.493098021
C	1.373772264	3.599155188	-2.865453243
H	1.008970261	3.864051580	-1.871305823
C	1.574921131	4.910907745	-3.644346476
H	0.624097347	5.419648647	-3.830452919
H	2.220799446	5.591810226	-3.078634024
H	2.053401947	4.739258289	-4.615201950
C	2.719373465	2.875350952	-2.671236515
H	2.590031147	1.954530478	-2.096031904
H	3.160619259	2.614086151	-3.639587641
H	3.430816174	3.521441460	-2.144321918
C	0.955482423	2.366210461	2.552566290
C	0.351755112	1.955125093	3.761728048
C	1.185821891	1.591668248	4.827589989
H	0.737860501	1.276751280	5.766633511
C	2.571086168	1.614511609	4.703402042
H	3.199287176	1.327138186	5.542413712
C	3.151959896	1.982744694	3.489996910
H	4.233006954	1.965111375	3.391318083
C	2.363156796	2.348123550	2.396624327
C	-1.161747694	1.857846379	3.917421579
H	-1.622042656	2.195140362	2.984732151
C	-1.678309202	2.754442453	5.058200359
H	-1.371293426	3.796165466	4.919549942
H	-2.772898436	2.724099398	5.102773190
H	-1.299171805	2.423519850	6.032172203
C	-1.597366214	0.395878971	4.125950336
H	-1.296351194	-0.229665563	3.281893492
H	-1.167123675	-0.020303324	5.045510769
H	-2.688850164	0.333775699	4.205205917
C	2.982015133	2.706713438	1.049503922
H	2.255699396	2.418559790	0.279566735
C	3.190050364	4.228518963	0.926026821
H	2.242991924	4.765748978	1.012524724
H	3.636043072	4.484294891	-0.041444205
H	3.859261513	4.589556217	1.715924621
C	4.295877934	1.962678194	0.758241415
H	4.206311703	0.885009468	0.934038937
H	5.120183945	2.331983805	1.379375339
H	4.582684517	2.113680363	-0.287823051
C	1.402916074	-0.637277842	1.288022995
H	2.126232862	0.078783534	0.894348979
C	2.110286713	-1.815057397	1.915976167
C	3.187686920	-2.433182001	1.265168786
H	3.541725159	-2.030224085	0.317153394
C	3.820929766	-3.540020943	1.830047488
H	4.652800560	-4.013831139	1.308124423
C	3.389916420	-4.029594421	3.069276571
H	3.880866528	-4.891289711	3.514414072
C	2.332944155	-3.400561571	3.739290953
H	2.000262022	-3.771241903	4.708612919

C	1.695676088	-2.301621675	3.164672852
H	0.859590709	-1.824081063	3.672594309
O	1.077077270	-2.596949100	-1.632005453
B	1.132337093	-1.335869670	-1.104353905
O	1.907044053	-0.468834162	-1.834547520
H	0.829759061	-0.128584087	2.064109087
C	1.621863246	-2.523279428	-2.975609779
C	2.554497242	-1.256517053	-2.889479160
C	0.429987580	-2.330141068	-3.919510603
C	2.342032909	-3.833298683	-3.278167248
C	2.609019995	-0.443269759	-4.175595284
C	3.975117207	-1.571693420	-2.412246704
H	-0.072960809	-1.379474282	-3.729806185
H	-0.287716180	-3.137299061	-3.747129917
H	0.737957299	-2.352470160	-4.968906879
H	3.083280802	-4.071317196	-2.512692690
H	2.843182325	-3.781056404	-4.250513077
H	1.615658879	-4.650777817	-3.311411858
H	1.640164614	-0.012612329	-4.422286510
H	2.934484005	-1.082757115	-5.003979206
H	3.327566862	0.373057425	-4.076798439
H	3.972931147	-2.231247425	-1.542369366
H	4.469815731	-0.636410296	-2.133023739
H	4.558644295	-2.051320314	-3.203804970
O	-1.548079729	-2.255721331	-0.491246372
B	-0.686883509	-1.807896852	0.479019135
O	-0.933006644	-2.313510180	1.726934195
H	-2.093015671	0.437534362	0.894567549
C	-2.229880810	-3.404326916	0.082983702
C	-2.155256271	-3.103113651	1.629997492
C	-1.421661019	-4.640588284	-0.334106505
C	-3.642328978	-3.469186783	-0.484093308
C	-1.986265659	-4.337462902	2.511328936
C	-3.310268164	-2.233117104	2.132232904
H	-0.403434902	-4.597583771	0.061943755
H	-1.349995732	-4.658753872	-1.424960852
H	-1.897558212	-5.566245079	0.004352794
H	-4.166314125	-2.523440599	-0.339569837
H	-4.214718342	-4.268985748	-0.001953428
H	-3.600403070	-3.676300287	-1.557060480
H	-1.067290425	-4.876369476	2.274155855
H	-2.837609768	-5.016109467	2.390051365
H	-1.939110398	-4.034451485	3.561485291
H	-3.391344070	-1.318357348	1.539817810
H	-3.111002684	-1.942309499	3.166690350
H	-4.257364273	-2.780912161	2.105100870

=====

Borylimine

=====

C	-1.256090045	1.741418362	-1.601022363
C	-1.956302166	0.799060345	-0.856213093
C	0.095619567	1.536249876	-1.902118683
H	-3.004644871	0.936214685	-0.610662341
H	0.639956832	2.274415970	-2.484526157

C	-1.311098814	-0.362676173	-0.402533472
C	0.744332731	0.384155989	-1.454725981
H	1.792927742	0.223492607	-1.687826753
C	0.042260785	-0.561206639	-0.707341075
H	0.543470323	-1.460696936	-0.356769562
H	-1.758785844	2.638851881	-1.950369358
C	-2.039813757	-1.374974012	0.387694746
N	-3.264275789	-1.269014120	0.696009278
H	-1.426004171	-2.241373777	0.689876318
B	-4.144731522	-2.116240978	1.422656417
O	-4.462019444	-1.911773324	2.749378204
O	-4.847845554	-3.153677702	0.846082151
C	-5.891742229	-3.521429300	1.787581801
C	-5.290749073	-3.031945229	3.158041954
C	-7.152724266	-2.750715017	1.377448916
H	-8.011595726	-3.020643711	1.999200344
H	-6.992662907	-1.671405435	1.451499462
H	-7.387537956	-2.987267017	0.336319327
C	-6.131428242	-5.024596691	1.686050177
H	-6.855086803	-5.352262974	2.439860344
H	-6.533779621	-5.265675068	0.698181212
H	-5.206377029	-5.587509155	1.819227934
C	-4.357049465	-4.062868118	3.804555893
H	-4.911365509	-4.916911602	4.204921722
H	-3.622994661	-4.430681705	3.081907988
H	-3.815570354	-3.583339930	4.624298573
C	-6.316457748	-2.534684420	4.172037125
H	-7.013181686	-3.335536480	4.441423416
H	-5.804722786	-2.206090927	5.080958366
H	-6.885824680	-1.689618587	3.782346010

=====

Diborylamine

=====

C	-0.823808849	0.733582556	2.164133310
C	-1.428683043	-0.453747958	1.750603676
C	-0.400999933	1.672853589	1.220396042
H	-1.772031188	-1.180575371	2.480649948
H	0.069394454	2.597958803	1.542965531
C	-1.619883060	-0.717375040	0.387692004
C	-0.585096478	1.415634513	-0.139480114
H	-0.257748544	2.141458750	-0.879530013
C	-1.191486955	0.227678880	-0.552245021
H	-1.356681228	0.032448694	-1.607149482
H	-0.680845082	0.926690578	3.224268675
C	-2.341728926	-1.975405216	-0.055664703
N	-3.815310240	-1.815185666	0.006519103
H	-2.061645746	-2.814023733	0.585949183
B	-4.471486092	-2.155837774	1.226618886
O	-3.770060539	-2.637460232	2.321181059
O	-5.822835922	-2.040609121	1.463915825
C	-6.004778862	-2.185394049	2.894201279
C	-4.755175591	-3.050814390	3.302315712
C	-5.974573612	-0.771219134	3.490761518
H	-6.176712036	-0.779763103	4.566242695

H	-5.004562855	-0.295446098	3.318978310
H	-6.739118099	-0.167359278	2.995104313
C	-7.357456684	-2.842090845	3.151620150
H	-7.492233276	-3.044900656	4.219389915
H	-8.157501221	-2.171402454	2.825936317
H	-7.457410336	-3.778042555	2.599696875
C	-4.977010727	-4.555422306	3.105157137
H	-5.662205219	-4.964328289	3.853657007
H	-5.381062031	-4.761508942	2.110007286
H	-4.015672684	-5.068284512	3.195441246
C	-4.201986790	-2.771075964	4.696504116
H	-4.954664707	-2.988495111	5.461551189
H	-3.331754923	-3.407040596	4.882781982
H	-3.888501406	-1.730866194	4.798886299
O	-5.771629810	-0.768888295	-1.132314205
B	-4.444819450	-1.131750345	-1.077911139
O	-3.733592749	-0.751200080	-2.204432011
C	-6.019705772	-0.301712990	-2.482378483
C	-4.588027477	0.162130296	-2.939315081
C	-4.240163326	1.579940677	-2.464646816
C	-4.298571110	0.013176844	-4.429214954
C	-6.542340755	-1.501268029	-3.284293890
C	-7.071964741	0.801525950	-2.430507421
H	-4.800416470	2.338510752	-3.019703865
H	-4.449997425	1.697377086	-1.398023844
H	-3.171647072	1.753792763	-2.615609884
H	-4.990701199	0.622346520	-5.019980907
H	-3.280087233	0.351232469	-4.641554832
H	-4.383012295	-1.026322842	-4.749975204
H	-6.825404644	-1.215021253	-4.301957607
H	-5.788226604	-2.291488886	-3.339482307
H	-7.421927452	-1.906162977	-2.777010679
H	-7.218200684	1.243604541	-3.421830416
H	-8.025839806	0.382642299	-2.097756386
H	-6.787907600	1.589588881	-1.731373310
H	-2.059412718	-2.225398064	-1.081311107

Table S5. Vibrational frequencies (in cm⁻¹) of the optimized structures.

=====

1

=====

11.03	22.80	29.53	32.25	41.25	43.83
44.77	45.51	49.29	50.77	52.16	53.51
57.04	59.97	62.65	66.68	68.59	73.85
80.41	81.97	83.79	88.85	95.42	99.01
100.14	102.14	106.26	107.70	115.05	128.19
129.34	130.56	132.77	140.08	142.59	144.03
147.08	147.64	154.53	156.66	160.12	163.38
169.65	172.08	185.01	185.58	196.49	198.86
204.26	205.25	210.53	225.69	233.20	239.21
239.98	243.06	247.57	249.46	252.02	255.09
257.18	258.31	262.84	265.56	267.79	270.69
272.87	275.02	277.78	282.52	289.47	290.88
292.97	294.50	295.16	299.39	301.23	302.34
304.08	305.57	307.90	313.87	314.60	315.71
321.82	323.78	331.70	334.28	339.16	341.06
353.49	354.31	372.98	375.24	439.14	439.47
448.46	451.25	453.42	454.40	455.77	456.93
458.54	461.46	463.38	468.36	469.37	511.92
512.85	534.39	535.50	535.60	537.11	552.60
552.99	553.52	553.98	560.86	561.26	575.18
576.59	603.23	604.06	607.90	614.40	616.86
630.70	635.14	643.60	644.61	653.19	655.50
662.03	662.28	663.44	664.72	709.36	710.80
723.15	724.09	774.68	774.92	780.37	782.22
785.56	787.49	810.97	811.42	817.63	818.18
822.37	822.93	824.70	824.84	844.16	860.99
861.47	865.52	866.11	900.15	900.72	901.60
901.91	911.85	917.34	917.56	920.48	920.56
942.04	946.72	948.71	949.08	949.59	949.99
951.47	951.67	952.60	952.79	957.18	958.41
961.73	963.34	966.31	966.51	967.25	967.81
968.36	968.72	974.90	976.48	976.67	977.30
983.83	984.67	985.03	985.61	1041.15	1041.88
1053.89	1054.15	1055.70	1056.70	1067.73	1068.20
1073.75	1074.93	1079.63	1081.10	1090.91	1091.86
1095.35	1096.59	1114.21	1125.89	1126.21	1131.77
1133.11	1133.81	1134.31	1135.79	1136.71	1140.00
1141.00	1145.73	1147.08	1154.01	1177.97	1178.96
1183.30	1183.87	1198.23	1198.57	1199.83	1200.27
1208.31	1209.06	1215.19	1215.41	1218.88	1219.49
1228.86	1229.71	1263.70	1264.46	1275.86	1276.77
1284.63	1284.72	1285.70	1285.73	1295.59	1296.30
1300.80	1301.49	1305.66	1306.23	1307.64	1307.85
1335.04	1341.83	1346.45	1350.42	1360.25	1361.28
1365.28	1365.94	1369.56	1370.05	1375.86	1376.79
1391.58	1391.96	1395.85	1396.05	1412.89	1414.11
1415.26	1415.47	1418.57	1419.07	1420.44	1420.77
1423.11	1423.39	1423.85	1423.94	1433.34	1434.47
1438.04	1438.69	1440.38	1440.77	1442.23	1442.91
1444.10	1450.51	1476.92	1477.08	1484.27	1484.35
1493.83	1494.42	1495.00	1495.46	1496.82	1497.13

1497.29	1497.66	1498.27	1498.88	1499.33	1499.57
1500.17	1500.50	1501.05	1501.90	1503.46	1503.93
1504.30	1505.40	1506.25	1506.64	1508.02	1509.39
1509.70	1511.25	1513.65	1514.08	1515.77	1516.79
1520.27	1520.44	1520.76	1521.36	1522.62	1522.93
1523.44	1524.94	1526.60	1526.83	1527.28	1528.17
1529.93	1530.91	1576.35	1578.27	1582.60	1583.79
1629.22	1629.81	1631.10	1631.15	1642.22	1642.81
1643.63	1643.85	3020.03	3023.06	3027.29	3029.69
3031.43	3031.50	3031.59	3033.39	3033.60	3034.17
3035.40	3038.87	3042.86	3044.00	3047.16	3047.47
3050.25	3051.32	3061.15	3063.02	3063.23	3064.84
3065.03	3066.57	3076.64	3077.39	3077.79	3080.88
3087.80	3094.50	3094.65	3095.26	3098.67	3102.82
3103.04	3103.12	3103.74	3104.01	3104.82	3105.39
3106.51	3107.70	3108.52	3109.69	3110.15	3110.99
3112.59	3113.83	3115.91	3117.06	3118.38	3118.97
3120.23	3122.87	3124.81	3126.29	3128.81	3129.47
3130.26	3139.70	3147.41	3147.44	3147.66	3148.18
3148.68	3150.25	3159.70	3166.84	3167.08	3169.44
3172.09	3172.11	3180.30	3181.32	3192.50	3194.70
3195.83	3195.87	3203.39	3204.58	3213.01	3213.81

=====

Benzonitrile

=====

147.54	164.50	391.27	410.40	465.19	562.02
571.91	636.93	703.56	774.22	778.02	860.82
942.75	982.85	1010.97	1015.48	1054.93	1113.18
1200.29	1211.95	1226.57	1336.82	1364.03	1486.06
1534.30	1631.94	1658.23	2348.24	3186.98	3197.80
3206.72	3216.86	3219.80			

=====

HBPIn

=====

95.70	228.82	243.61	285.01	290.30	295.54
321.92	332.61	361.17	372.12	398.15	449.25
513.84	523.49	583.27	668.40	748.54	806.40
867.88	905.29	937.65	947.08	965.30	978.10
1022.84	1031.37	1065.23	1144.61	1183.04	1191.86
1206.76	1244.56	1272.73	1302.26	1382.94	1415.80
1418.70	1428.67	1438.63	1485.12	1494.16	1497.12
1501.91	1517.89	1520.49	1523.19	1541.73	2713.89
3051.59	3054.19	3055.98	3060.39	3124.32	3124.83
3133.28	3133.59	3137.25	3137.53	3154.74	3154.92

=====

⁶A

=====

14.73	20.76	42.13	43.33	46.35	50.26
64.15	65.42	67.51	69.37	71.41	94.37
109.17	111.74	119.15	133.97	135.44	149.53
151.87	172.00	187.09	203.93	211.70	222.09
239.57	242.40	251.05	253.04	256.49	263.60
265.10	271.27	273.43	279.02	282.18	287.12
289.26	296.00	298.39	302.40	307.52	312.66
332.74	337.21	357.23	371.63	439.61	440.63

445.87	453.31	455.35	455.84	511.16	529.23
533.73	545.46	546.86	555.60	569.41	606.71
614.99	641.73	644.18	645.68	651.10	664.69
711.70	728.05	770.31	774.94	779.70	815.09
816.94	817.67	819.23	862.76	868.39	897.60
898.28	918.67	918.74	943.77	944.17	944.90
945.68	953.05	954.13	959.22	969.24	970.06
973.15	974.48	975.81	976.21	976.99	1043.62
1052.21	1057.08	1064.79	1074.11	1076.94	1090.06
1091.48	1125.66	1127.53	1132.08	1132.99	1134.68
1139.36	1177.50	1178.72	1197.16	1198.10	1204.61
1215.37	1215.77	1229.52	1262.64	1278.62	1284.65
1284.85	1303.54	1305.79	1306.10	1312.25	1359.92
1360.28	1361.02	1361.20	1367.22	1371.22	1393.65
1394.30	1416.35	1417.36	1418.17	1419.25	1420.56
1421.33	1437.38	1437.87	1439.40	1439.73	1443.95
1481.66	1483.96	1491.55	1491.67	1491.77	1492.36
1494.82	1497.95	1499.73	1503.61	1504.15	1504.20
1505.03	1507.08	1507.45	1508.95	1515.40	1517.19
1519.69	1520.77	1521.49	1522.74	1522.96	1524.91
1532.26	1575.79	1595.56	1632.20	1632.61	1645.50
1645.92	3024.55	3026.17	3026.36	3027.97	3037.94
3038.10	3038.25	3038.60	3051.49	3052.34	3071.00
3071.30	3073.56	3073.99	3094.32	3096.13	3097.24
3099.37	3102.92	3103.17	3104.07	3104.10	3110.21
3110.64	3110.76	3110.98	3111.23	3111.57	3114.03
3114.55	3114.68	3115.29	3149.47	3149.88	3174.00
3174.18	3186.11	3186.30	3199.45	3199.72	3213.64

=====

6B

=====

10.20	15.53	22.24	25.71	35.70	44.82
47.42	50.15	57.01	58.55	63.36	69.19
73.85	86.39	96.73	101.83	110.03	112.82
122.52	125.67	129.78	136.92	138.08	147.09
151.77	160.07	178.09	195.97	201.80	207.96
209.39	221.73	243.60	246.08	246.72	252.41
259.89	263.44	269.22	275.62	285.00	291.88
295.35	297.82	301.98	312.35	315.84	319.58
325.57	332.23	337.48	344.57	348.08	366.15
397.87	410.10	438.76	444.36	451.41	452.42
457.63	459.15	482.21	511.81	530.33	532.51
547.74	551.18	558.76	566.01	569.92	572.14
607.10	615.16	631.63	636.81	643.36	648.47
656.59	658.92	701.94	713.61	728.08	762.80
775.95	778.83	780.59	781.68	808.51	816.64
820.68	821.00	863.15	865.08	865.69	898.65
898.83	917.07	921.01	941.51	946.48	947.23
949.67	950.76	954.40	958.06	958.39	965.74
967.38	969.07	974.92	976.23	977.04	977.59
987.40	1013.48	1018.21	1039.70	1049.40	1052.31
1054.56	1063.43	1074.57	1078.23	1089.70	1093.48
1115.86	1128.44	1130.04	1130.46	1133.40	1135.45
1143.41	1177.71	1182.28	1197.85	1198.58	1202.91
1206.76	1213.73	1213.95	1217.26	1229.86	1232.23

1263.26	1275.92	1284.45	1284.90	1300.79	1302.18
1304.76	1307.42	1337.22	1338.60	1364.14	1365.02
1365.47	1367.65	1370.38	1373.30	1390.55	1394.19
1412.28	1413.06	1415.09	1417.02	1419.13	1419.93
1432.90	1435.85	1436.67	1437.06	1453.23	1468.65
1479.16	1484.17	1485.79	1489.91	1493.56	1496.51
1498.28	1499.14	1500.62	1502.21	1502.81	1503.60
1504.81	1506.35	1507.79	1508.81	1513.09	1516.45
1518.15	1519.19	1522.56	1524.07	1524.59	1526.24
1528.31	1531.76	1568.94	1596.41	1625.85	1630.47
1632.50	1644.64	1646.92	1652.13	2350.19	3024.41
3025.79	3031.90	3032.53	3033.25	3036.67	3036.97
3039.86	3048.47	3059.34	3063.37	3084.66	3085.43
3085.61	3093.43	3095.70	3096.15	3101.08	3102.96
3108.31	3108.73	3109.63	3110.43	3112.84	3114.09
3117.33	3117.96	3118.22	3121.67	3125.80	3127.87
3143.89	3147.97	3150.47	3168.50	3171.74	3178.28
3183.08	3188.65	3192.72	3195.43	3200.20	3206.37
3207.02	3208.81	3213.17			

=====

6B-TS

=====

-513.06	16.02	17.23	22.56	24.97	38.99
45.42	47.19	52.27	56.41	60.82	69.18
70.67	72.33	82.49	90.97	99.65	105.96
117.58	121.08	126.28	131.84	133.05	146.11
150.04	155.98	164.35	194.39	206.59	210.73
220.44	226.99	242.92	247.11	247.76	251.81
258.00	261.45	262.97	265.40	275.73	282.50
287.55	291.27	296.58	298.24	304.73	317.95
321.27	326.65	335.32	338.20	372.00	395.68
413.59	440.72	441.54	449.89	451.23	453.72
458.57	486.64	490.00	511.64	527.76	531.74
546.89	548.76	556.99	569.03	607.04	613.59
628.17	634.88	642.83	647.17	652.92	654.72
657.49	675.55	701.79	714.49	730.45	767.04
774.77	779.96	782.94	810.26	816.90	819.42
821.63	823.15	858.64	862.58	870.74	899.52
900.47	917.99	922.83	944.84	945.07	946.91
947.51	950.67	956.17	958.42	958.54	966.82
968.76	970.65	975.39	976.05	978.29	978.65
979.13	1005.06	1014.87	1040.46	1049.74	1053.56
1054.82	1062.17	1074.27	1077.78	1089.93	1093.32
1113.87	1129.22	1129.82	1130.77	1132.71	1135.51
1143.20	1179.48	1182.07	1196.50	1198.45	1199.49
1202.82	1205.49	1214.38	1216.43	1221.08	1229.32
1244.63	1261.64	1276.75	1283.98	1284.70	1301.07
1303.68	1307.13	1308.31	1343.28	1347.43	1360.53
1362.99	1364.21	1366.23	1366.47	1371.53	1392.76
1393.79	1411.94	1415.29	1416.16	1418.18	1418.63
1422.42	1432.87	1437.20	1438.37	1440.67	1451.21
1479.40	1482.45	1487.88	1488.57	1492.03	1497.78
1498.07	1499.91	1500.51	1501.45	1502.57	1503.97
1505.91	1506.28	1508.41	1509.24	1512.20	1517.17
1519.12	1519.83	1522.55	1522.79	1524.50	1525.92

1529.47	1531.08	1567.77	1602.98	1630.97	1631.72
1634.57	1644.26	1645.14	1656.88	2048.89	3025.55
3032.06	3033.11	3034.46	3036.34	3037.23	3037.53
3041.33	3055.29	3055.81	3067.51	3074.28	3075.77
3080.39	3098.55	3099.35	3099.68	3099.73	3102.55
3108.19	3109.14	3110.16	3110.69	3111.51	3112.40
3113.82	3116.00	3123.12	3128.62	3132.11	3134.33
3135.02	3149.21	3153.72	3170.52	3170.85	3180.27
3181.12	3187.30	3192.11	3196.54	3200.67	3201.07
3208.02	3210.01	3217.80			

=====

°C

=====

14.23	20.46	24.19	26.31	29.00	44.66
46.60	49.26	52.15	55.45	64.98	65.94
70.28	72.72	73.45	78.44	92.22	98.93
115.18	120.98	135.00	137.42	150.09	152.88
172.92	174.95	191.52	199.04	214.49	224.02
241.60	245.04	248.74	252.33	254.50	261.19
264.94	265.58	269.51	270.97	272.36	275.15
287.74	293.10	294.70	297.04	309.49	312.65
314.51	322.77	332.09	335.48	375.53	421.36
440.84	441.85	445.54	451.95	456.13	456.70
483.13	511.20	530.73	532.40	547.38	548.53
554.70	567.38	570.44	606.97	614.42	630.92
642.68	644.51	646.77	652.70	661.06	691.25
707.79	714.87	730.87	764.03	764.49	775.02
779.81	815.41	816.94	819.47	820.43	827.75
865.11	868.55	869.77	897.94	899.11	917.85
918.37	918.62	944.71	944.99	948.51	949.38
956.14	957.79	958.35	967.85	967.91	969.39
971.09	975.28	976.58	977.44	977.54	981.64
1005.19	1013.69	1043.93	1049.31	1051.30	1057.14
1064.70	1074.26	1077.09	1090.04	1091.75	1109.52
1126.94	1128.61	1132.82	1133.55	1134.06	1138.91
1179.01	1180.23	1190.44	1197.87	1198.07	1198.85
1203.49	1214.87	1215.84	1223.62	1227.77	1262.88
1277.87	1283.71	1285.12	1301.70	1302.71	1305.14
1309.03	1324.36	1358.83	1359.40	1360.94	1361.08
1363.24	1366.02	1370.18	1392.10	1393.67	1405.82
1416.25	1417.04	1418.75	1419.63	1420.53	1421.19
1437.45	1439.07	1439.41	1440.39	1446.97	1480.93
1482.90	1491.40	1492.23	1492.54	1493.29	1495.21
1497.56	1499.62	1501.50	1503.38	1504.00	1505.34
1506.14	1508.80	1509.28	1510.01	1516.29	1519.14
1519.59	1521.02	1522.41	1524.51	1524.76	1526.82
1530.39	1571.49	1595.15	1629.63	1632.24	1632.40
1642.61	1645.51	1652.00	1740.82	2869.57	3022.43
3024.84	3025.50	3028.08	3034.36	3035.12	3035.43
3037.35	3050.00	3050.30	3070.02	3071.64	3072.12
3078.30	3095.34	3098.94	3099.88	3100.61	3101.23
3101.71	3102.02	3104.57	3106.36	3107.30	3107.51
3108.76	3109.47	3109.54	3110.88	3111.69	3112.45
3114.44	3148.93	3149.37	3151.31	3163.06	3171.66
3172.21	3174.22	3183.43	3183.64	3192.54	3197.34

3197.89	3207.85	3211.54
---------	---------	---------

=====

2

=====

16.32	21.36	21.47	26.63	28.20	30.46
37.16	40.81	42.11	51.82	52.59	54.78
55.06	55.57	57.23	57.42	59.76	64.28
67.19	73.39	74.59	77.85	78.95	81.31
82.71	85.43	88.86	92.74	94.90	97.60
98.38	100.75	102.10	109.34	115.78	119.01
119.49	123.80	124.45	126.65	129.12	135.44
140.06	142.11	144.50	149.11	149.36	152.80
156.89	157.73	159.29	160.02	165.08	166.13
168.65	175.67	192.81	199.83	201.08	202.40
206.77	209.03	215.73	216.97	220.76	223.55
238.04	238.25	241.91	242.41	243.92	244.36
251.47	252.84	254.15	256.12	256.97	258.31
262.06	263.77	266.00	267.69	276.04	280.51
284.24	287.01	288.72	289.77	291.49	291.75
295.20	300.41	301.21	301.75	306.27	309.30
310.49	311.73	323.24	325.33	327.70	329.04
336.76	337.85	338.70	341.64	342.05	344.48
365.42	366.29	374.58	405.16	420.75	421.08
442.21	443.13	447.49	448.41	451.34	452.13
456.69	457.68	461.34	463.15	464.74	465.87
495.57	496.63	510.06	511.60	511.80	523.39
528.42	530.34	530.41	530.71	546.07	546.61
551.64	552.07	557.15	557.87	569.75	569.87
606.59	607.29	613.23	613.59	630.46	630.75
631.24	632.00	636.29	637.22	646.52	647.50
650.62	651.98	659.23	659.91	687.46	690.53
704.38	705.98	707.86	708.25	722.26	722.50
763.64	763.79	765.88	766.09	772.24	773.54
778.31	780.76	809.31	810.42	811.29	812.17
818.24	818.37	821.25	821.31	844.50	845.02
859.53	859.79	861.77	862.19	865.11	865.68
900.37	900.52	901.40	901.70	916.05	916.22
918.69	918.92	928.84	929.25	941.75	941.85
943.17	943.38	946.29	947.82	950.42	950.63
951.30	951.53	956.12	956.26	958.70	958.78
961.37	962.09	966.17	966.55	967.96	968.38
974.24	974.40	977.12	977.40	980.10	980.19
981.33	981.48	984.37	984.66	995.78	996.38
1010.22	1010.59	1015.70	1015.84	1037.47	1037.74
1050.29	1050.45	1051.94	1052.13	1056.27	1056.99
1060.36	1060.61	1072.35	1073.02	1076.49	1077.57
1090.94	1091.11	1094.65	1094.80	1118.36	1118.63
1126.76	1126.80	1130.68	1131.11	1131.72	1131.90
1132.35	1133.33	1137.43	1137.52	1140.59	1140.83
1175.83	1176.57	1177.61	1177.81	1192.35	1192.37
1198.09	1198.27	1198.86	1198.94	1204.98	1205.23
1205.28	1205.78	1215.17	1215.34	1216.79	1216.93
1226.88	1227.37	1228.53	1229.11	1261.24	1261.44
1271.76	1272.20	1285.01	1285.32	1286.47	1286.73
1297.63	1297.78	1300.81	1301.21	1306.01	1307.02

1307.30	1307.62	1334.34	1334.68	1343.76	1344.15
1349.84	1350.27	1359.96	1360.33	1360.59	1361.00
1362.95	1363.33	1368.62	1368.87	1369.12	1369.27
1388.86	1389.57	1391.85	1392.41	1410.99	1411.29
1413.56	1413.73	1416.02	1416.65	1417.07	1417.72
1418.27	1418.53	1418.67	1419.28	1430.80	1430.99
1434.42	1434.68	1439.11	1439.45	1439.98	1440.74
1443.39	1444.59	1455.20	1461.15	1478.14	1478.56
1479.36	1480.19	1488.06	1488.53	1494.83	1495.05
1495.47	1495.98	1497.19	1497.50	1497.72	1498.44
1498.76	1498.90	1499.19	1500.08	1500.18	1500.89
1501.24	1501.90	1502.68	1503.14	1504.19	1504.72
1506.17	1506.74	1507.45	1508.23	1511.49	1511.74
1511.80	1512.33	1515.96	1517.72	1518.40	1518.59
1519.29	1521.72	1522.05	1523.15	1523.96	1525.06
1525.82	1526.16	1526.60	1527.42	1528.72	1529.29
1534.71	1534.83	1572.80	1574.68	1592.00	1592.78
1628.40	1628.88	1630.78	1631.37	1634.43	1635.27
1641.25	1642.20	1643.99	1644.13	1654.83	1655.19
1694.95	1707.37	2976.36	2979.10	3031.51	3031.77
3033.37	3033.39	3033.97	3034.07	3034.19	3034.49
3036.58	3036.69	3037.84	3037.94	3047.36	3049.39
3049.64	3049.92	3055.65	3055.77	3061.39	3061.84
3065.66	3065.82	3069.05	3069.18	3091.52	3091.61
3093.45	3093.49	3093.60	3093.98	3095.07	3095.59
3099.19	3099.43	3103.62	3103.74	3108.53	3108.97
3109.27	3109.60	3113.46	3113.77	3116.02	3116.17
3128.73	3129.03	3129.71	3130.27	3132.95	3133.04
3135.12	3135.50	3136.38	3136.70	3136.86	3137.63
3140.46	3141.64	3143.08	3143.18	3153.36	3154.45
3154.84	3155.30	3155.57	3156.95	3157.42	3157.83
3168.50	3168.62	3168.95	3169.15	3169.36	3169.82
3178.62	3179.09	3184.96	3185.51	3185.77	3186.58
3189.26	3189.69	3196.84	3197.04	3198.41	3198.51
3200.82	3201.47	3205.74	3206.28	3233.69	3236.47

=====

⁶D

=====

27.32	29.72	34.17	40.69	42.27	45.92
49.27	53.27	59.03	61.24	70.35	71.56
74.19	80.83	82.94	89.96	95.51	98.96
108.43	117.06	118.67	127.47	129.79	130.71
143.30	151.98	155.08	157.58	164.29	170.07
177.76	186.57	199.09	205.49	216.02	225.46
234.51	239.63	240.94	245.88	252.17	254.05
262.41	263.23	265.85	269.46	273.87	285.10
287.74	289.53	291.71	296.09	302.83	307.68
317.95	318.80	321.03	323.47	326.11	328.67
332.31	335.43	339.22	355.06	367.89	376.95
382.34	408.93	410.70	421.52	435.70	445.78
448.57	452.45	454.88	460.38	480.44	487.30
508.57	512.51	523.94	532.08	534.46	543.10
552.21	557.48	560.54	570.57	579.33	603.28
612.86	629.03	632.94	638.96	644.46	653.38
654.19	659.55	664.77	689.37	711.09	713.86

729.52	767.64	770.55	773.39	778.29	791.08
808.08	812.76	821.26	821.47	833.56	852.30
860.74	863.77	865.21	881.84	896.42	899.30
901.32	920.47	923.71	933.06	934.10	943.41
946.87	947.42	948.82	949.66	950.78	956.10
957.88	962.93	964.09	971.28	971.90	976.87
977.81	979.17	979.68	983.07	984.50	999.77
1010.44	1016.81	1020.37	1034.37	1035.43	1047.67
1053.77	1055.35	1059.71	1063.00	1076.06	1078.42
1079.45	1092.50	1094.66	1122.57	1125.74	1129.01
1130.83	1134.43	1136.39	1140.94	1144.89	1176.76
1179.45	1188.81	1194.30	1195.07	1198.92	1199.10
1206.15	1212.79	1216.41	1218.00	1218.80	1230.88
1240.71	1248.86	1260.95	1267.61	1275.74	1285.47
1287.08	1298.29	1298.85	1303.05	1305.45	1307.26
1331.88	1338.72	1354.65	1362.84	1364.70	1368.03
1368.47	1371.46	1388.47	1395.76	1410.77	1410.98
1413.74	1415.31	1416.27	1416.74	1417.82	1418.80
1424.04	1424.56	1433.67	1434.57	1436.32	1438.85
1441.86	1456.02	1475.44	1480.93	1484.82	1485.67
1492.13	1493.45	1496.31	1497.46	1498.89	1499.37
1501.32	1502.22	1502.71	1503.77	1505.43	1506.12
1506.33	1507.16	1509.81	1510.37	1513.01	1515.12
1516.86	1520.24	1520.44	1522.01	1523.77	1525.56
1527.22	1528.13	1532.13	1535.47	1537.40	1543.70
1565.69	1599.74	1627.78	1633.48	1634.45	1642.42
1646.73	1657.62	1733.03	2454.14	3025.75	3029.98
3030.99	3033.39	3035.97	3036.91	3037.28	3037.64
3043.08	3043.37	3043.72	3047.38	3049.98	3051.48
3057.42	3061.32	3077.26	3093.75	3097.31	3097.49
3100.23	3101.30	3103.90	3104.61	3108.48	3112.06
3113.57	3115.46	3115.82	3119.42	3121.63	3123.61
3124.36	3125.25	3128.05	3129.50	3131.58	3135.52
3138.22	3143.46	3146.20	3154.70	3154.96	3155.73
3157.14	3162.43	3164.70	3171.50	3172.09	3173.95
3180.59	3185.90	3190.82	3192.28	3199.16	3200.27
3203.47	3208.49	3236.83			

=====

⁶E

=====

11.87	15.74	24.02	28.18	30.03	36.29
43.84	46.24	48.14	50.55	55.99	59.83
65.17	73.62	78.35	90.03	91.66	98.79
103.51	109.56	112.48	115.19	119.49	127.64
135.84	140.49	146.61	147.68	156.30	160.39
164.33	179.02	192.30	198.34	219.30	220.97
235.79	242.52	244.16	249.57	252.07	258.20
260.23	262.42	266.96	268.56	278.84	282.76
286.61	290.96	294.93	297.07	300.71	311.11
315.91	321.19	324.13	325.42	328.38	331.64
332.53	334.80	341.51	346.11	366.59	373.38
380.87	401.64	418.56	423.32	447.01	448.05
451.58	455.09	461.23	461.79	469.60	488.13
510.16	513.64	523.72	530.59	533.71	537.31
548.84	550.89	556.48	572.00	581.01	610.81

617.09	632.38	643.89	644.93	648.61	653.11
663.17	663.52	679.55	703.63	718.67	726.84
732.81	768.73	772.65	775.95	782.03	818.19
818.56	819.71	820.70	823.29	849.36	859.55
861.90	866.55	869.76	893.14	898.35	899.94
923.34	925.49	927.79	932.83	937.34	947.80
948.55	950.12	950.97	952.02	953.83	957.38
959.45	964.70	968.98	969.52	974.68	976.13
978.99	980.65	980.77	985.24	999.52	1009.86
1015.86	1019.86	1029.93	1030.31	1043.10	1049.60
1053.87	1057.34	1063.61	1074.59	1077.23	1084.27
1089.34	1092.14	1104.82	1123.98	1124.81	1127.35
1129.01	1130.20	1133.80	1139.38	1180.60	1184.01
1185.25	1192.70	1197.90	1199.51	1200.44	1203.42
1213.63	1214.97	1215.41	1223.28	1223.74	1242.71
1249.79	1256.88	1262.63	1274.87	1285.33	1286.65
1290.94	1298.88	1299.53	1302.77	1305.68	1338.68
1354.81	1357.99	1360.15	1361.57	1362.51	1366.11
1367.54	1382.48	1389.26	1390.72	1407.19	1411.83
1414.05	1414.09	1418.10	1418.83	1420.31	1422.76
1423.22	1424.06	1433.07	1438.26	1439.17	1439.41
1443.14	1444.79	1482.65	1484.26	1485.30	1490.16
1490.97	1492.50	1492.89	1494.20	1497.39	1498.72
1499.19	1499.37	1501.17	1502.54	1503.85	1504.04
1505.70	1506.37	1507.57	1509.63	1510.79	1516.52
1517.36	1518.17	1519.24	1519.42	1521.16	1522.10
1524.43	1525.58	1526.32	1527.72	1537.86	1541.11
1568.97	1586.14	1632.16	1632.80	1634.30	1645.62
1646.89	1656.45	1695.33	1771.55	3022.52	3027.36
3030.81	3032.05	3032.12	3034.77	3034.90	3036.50
3036.99	3039.03	3043.17	3044.20	3046.05	3060.78
3061.43	3064.93	3065.46	3067.05	3070.94	3092.10
3097.82	3099.03	3101.86	3102.20	3103.77	3103.99
3104.44	3105.77	3109.62	3109.97	3110.24	3110.38
3114.70	3115.86	3118.16	3123.22	3123.51	3123.63
3127.58	3133.88	3136.87	3138.21	3138.49	3138.83
3144.12	3150.55	3151.99	3166.77	3168.67	3170.41
3175.67	3179.53	3180.93	3187.99	3195.18	3196.48
3200.73	3206.60	3212.28			

=====

⁶E-TS

=====

-360.97	24.13	26.93	34.51	36.01	39.91
42.43	42.49	47.07	50.51	52.96	60.51
66.82	69.37	74.84	76.86	81.87	88.53
94.58	106.32	109.68	112.62	125.74	129.17
134.30	138.23	140.22	146.40	157.54	162.59
167.01	172.45	179.36	192.63	208.50	212.69
217.20	226.91	234.48	241.35	245.26	247.74
251.88	254.63	259.93	267.11	279.21	282.78
286.58	288.34	291.10	292.22	297.10	300.42
301.83	308.25	310.65	312.35	321.83	322.69
327.21	330.83	338.18	341.57	341.77	366.40
373.38	379.61	401.51	422.36	436.74	440.61
444.08	447.13	450.55	453.63	456.79	458.74

508.41	509.56	514.71	527.08	534.32	534.84
544.43	549.71	556.27	557.41	570.95	584.04
604.61	614.21	629.72	631.51	635.34	639.45
645.23	648.90	664.60	667.51	707.02	711.15
712.30	727.85	760.46	762.28	774.14	779.45
779.58	811.87	814.37	818.29	818.94	855.82
859.17	862.46	865.85	868.71	874.74	896.50
899.93	916.33	920.36	929.22	939.70	942.13
942.44	948.01	948.37	949.53	949.68	951.87
952.18	957.83	962.49	966.69	970.22	976.40
977.00	977.83	978.60	981.49	989.20	999.82
1010.01	1016.24	1022.25	1024.52	1036.60	1037.11
1048.22	1053.02	1055.97	1064.20	1074.41	1077.77
1093.29	1094.56	1123.69	1127.54	1130.89	1133.94
1134.10	1139.02	1141.31	1142.75	1176.02	1180.76
1185.88	1190.43	1196.15	1198.43	1198.55	1204.51
1213.01	1215.08	1215.83	1227.66	1237.19	1248.15
1263.62	1268.09	1270.74	1274.84	1285.55	1285.97
1286.41	1296.41	1301.70	1305.65	1310.06	1310.89
1333.71	1343.90	1353.26	1353.54	1365.55	1367.22
1370.77	1372.25	1375.67	1394.57	1398.32	1410.71
1413.43	1414.09	1415.18	1415.75	1416.85	1419.54
1421.05	1423.40	1426.89	1431.15	1434.39	1436.09
1436.39	1438.74	1453.11	1478.54	1482.56	1484.40
1485.98	1492.46	1492.71	1492.99	1495.32	1497.04
1497.26	1499.02	1500.13	1501.63	1502.35	1503.69
1504.38	1506.69	1506.85	1509.14	1510.49	1513.79
1517.36	1517.65	1518.53	1519.30	1519.79	1521.26
1522.97	1523.16	1523.91	1528.55	1532.28	1537.73
1542.37	1561.82	1597.12	1632.08	1632.81	1633.19
1645.74	1646.39	1657.64	1710.00	3028.18	3030.42
3031.66	3031.73	3034.75	3035.39	3036.70	3037.28
3043.59	3044.52	3048.56	3050.04	3051.18	3055.12
3056.42	3069.32	3079.75	3088.40	3097.57	3097.71
3099.98	3100.97	3101.09	3105.33	3108.96	3109.12
3109.78	3111.49	3112.17	3116.07	3117.25	3117.50
3118.57	3119.24	3122.33	3124.36	3126.76	3131.82
3132.38	3139.87	3143.51	3144.50	3145.33	3148.41
3153.46	3153.94	3161.97	3168.28	3170.42	3172.27
3183.17	3183.30	3185.51	3196.40	3196.59	3200.28
3202.63	3206.12	3252.20			

=====

⁶F

=====

14.51	25.71	32.25	34.52	38.62	39.30
41.65	47.00	51.03	56.31	61.65	65.02
70.15	72.52	75.60	80.64	86.70	97.70
102.94	103.93	111.08	120.53	123.39	132.21
134.96	137.29	139.73	148.69	154.12	161.32
166.25	167.51	187.49	192.91	209.30	211.40
216.63	233.96	237.24	244.73	248.07	251.47
253.78	258.67	264.99	274.59	281.76	282.33
286.15	287.29	289.65	291.22	294.00	295.46
300.46	301.43	308.20	319.32	320.67	330.38
335.53	336.44	339.79	345.67	363.18	367.45

380.53	393.86	409.70	422.42	425.63	441.55
444.91	449.69	451.19	454.16	458.33	477.03
482.31	498.69	511.24	523.68	527.95	532.97
543.41	544.60	549.14	557.55	564.75	569.83
583.39	606.39	614.24	631.69	634.66	642.52
644.50	647.87	662.60	667.66	679.65	709.98
710.99	714.45	726.91	761.32	773.09	776.41
779.00	810.27	813.75	818.00	819.42	845.35
855.39	858.37	860.67	869.20	876.28	898.06
899.62	917.11	918.98	934.95	942.46	944.72
945.03	947.00	948.55	949.05	951.03	951.62
957.00	958.13	961.06	966.27	967.78	975.79
976.97	978.37	979.22	981.07	991.26	1001.00
1013.99	1018.17	1026.04	1027.88	1033.14	1038.51
1047.38	1053.04	1055.40	1063.10	1072.96	1076.60
1092.13	1093.55	1123.62	1128.24	1131.38	1134.57
1135.21	1138.05	1140.76	1149.36	1178.12	1179.00
1182.60	1193.99	1195.66	1198.52	1198.87	1203.29
1212.45	1214.71	1216.03	1227.20	1244.68	1246.90
1261.54	1273.05	1275.39	1284.39	1286.04	1296.46
1296.96	1301.49	1305.34	1309.08	1344.76	1353.97
1355.66	1364.81	1367.01	1367.93	1371.22	1372.56
1374.92	1388.04	1393.18	1397.99	1409.96	1412.95
1413.74	1414.35	1416.58	1417.52	1417.72	1420.90
1421.39	1431.35	1431.72	1435.01	1436.46	1437.43
1441.59	1442.41	1459.85	1480.17	1481.63	1485.04
1487.89	1493.55	1494.46	1495.43	1497.05	1497.10
1498.23	1498.64	1501.18	1501.99	1503.38	1503.97
1504.73	1505.63	1506.67	1508.98	1510.67	1513.69
1516.85	1517.92	1519.74	1520.24	1520.40	1521.99
1522.88	1523.80	1526.88	1527.83	1533.23	1537.14
1543.74	1563.02	1601.84	1630.33	1631.82	1633.59
1644.74	1646.04	1658.13	1706.04	3025.37	3029.27
3029.90	3033.11	3033.48	3034.13	3035.06	3035.43
3039.48	3045.86	3047.40	3048.52	3053.77	3056.18
3057.28	3071.16	3082.97	3091.52	3095.25	3096.88
3097.54	3099.71	3100.11	3106.12	3106.67	3106.82
3109.67	3110.64	3111.83	3115.09	3115.78	3115.98
3120.79	3122.86	3124.50	3125.56	3131.17	3132.24
3135.56	3141.35	3142.75	3147.04	3147.42	3150.26
3157.04	3158.75	3165.81	3166.80	3167.33	3172.04
3180.53	3182.63	3184.81	3193.51	3195.30	3197.64
3199.15	3208.10	3278.63			

=====

⁶F-TS

=====

-246.33	22.08	37.08	39.46	41.62	47.56
48.78	51.30	53.06	57.52	61.17	66.85
71.25	72.95	80.04	86.50	89.14	93.58
95.46	100.70	108.27	116.85	121.66	127.73
132.57	135.61	139.00	147.40	152.28	158.57
164.75	175.40	185.93	198.23	208.89	217.66
227.82	236.24	238.59	242.70	244.45	247.11
255.81	258.39	263.55	264.62	272.83	274.19
279.68	282.79	290.52	293.16	293.81	301.04

305.39	309.94	310.87	313.06	323.17	329.22
331.70	333.49	341.24	343.58	363.75	366.98
376.26	383.36	399.34	417.20	428.59	443.40
446.43	450.93	454.71	458.40	460.42	471.01
490.51	509.70	524.15	528.46	537.84	548.12
551.69	554.71	557.59	558.48	571.52	586.09
592.90	607.76	615.61	630.75	636.79	641.02
650.03	656.29	657.79	664.09	678.10	700.95
711.96	712.34	727.18	765.31	773.32	778.66
784.17	813.52	816.23	819.97	821.27	856.16
862.22	862.84	865.60	866.63	874.18	900.05
900.60	918.31	921.61	932.80	942.46	944.40
945.68	945.79	949.45	950.56	951.51	952.51
957.90	959.32	966.32	967.35	968.41	976.91
977.67	978.42	979.01	979.27	985.62	998.13
1008.68	1016.88	1025.90	1026.57	1039.08	1040.04
1051.26	1052.27	1053.27	1063.25	1073.55	1077.10
1090.02	1093.23	1117.20	1126.14	1129.12	1131.22
1133.87	1134.55	1138.99	1141.22	1146.11	1179.41
1180.36	1184.71	1194.53	1197.48	1197.93	1198.23
1206.60	1207.59	1213.43	1214.74	1230.62	1242.08
1248.21	1259.93	1273.96	1274.73	1281.75	1283.18
1294.67	1300.45	1300.92	1305.26	1306.92	1334.40
1345.30	1354.71	1356.38	1362.99	1364.95	1365.45
1370.98	1372.83	1379.49	1395.12	1398.35	1411.83
1412.56	1414.66	1417.74	1418.30	1419.60	1420.46
1421.15	1423.07	1431.09	1434.52	1435.54	1436.85
1438.84	1441.34	1449.34	1479.73	1481.67	1483.91
1487.16	1488.81	1490.98	1493.89	1494.93	1495.13
1497.75	1498.89	1499.50	1501.38	1502.37	1503.37
1503.97	1505.09	1506.48	1508.06	1508.43	1510.53
1516.42	1517.22	1518.85	1519.12	1521.00	1521.25
1523.68	1523.98	1525.25	1525.93	1534.69	1537.72
1544.69	1556.53	1565.72	1595.30	1627.86	1628.82
1639.20	1642.14	1643.25	1656.97	3033.09	3033.26
3033.55	3034.99	3036.97	3037.25	3038.88	3040.84
3048.28	3051.98	3054.39	3058.30	3058.70	3059.41
3075.85	3080.32	3083.26	3084.93	3085.09	3094.73
3100.17	3103.54	3104.00	3108.52	3109.25	3109.85
3111.28	3111.47	3113.43	3115.38	3120.49	3121.60
3122.75	3123.91	3126.73	3129.11	3129.14	3130.23
3132.27	3132.68	3134.93	3148.57	3149.09	3151.93
3156.45	3165.06	3167.33	3168.93	3173.24	3176.83
3178.75	3185.28	3186.04	3193.36	3196.77	3201.52
3208.03	3214.47	3238.18			

=====

⁶G

=====

11.74	20.21	33.70	35.53	39.00	43.10
47.17	50.28	52.56	55.62	60.91	65.05
69.91	73.29	75.35	78.94	81.16	90.77
91.82	100.23	110.99	114.80	119.22	126.38
130.15	140.78	141.15	148.07	153.96	167.10
168.39	177.66	192.92	204.94	219.88	227.17
233.05	234.49	244.82	250.69	252.03	253.88

257.06	261.10	264.47	265.31	269.92	274.90
275.89	283.64	287.57	291.59	296.08	300.53
302.09	309.32	310.65	313.96	318.12	321.72
334.57	335.41	337.36	346.31	368.63	375.50
379.80	395.39	423.07	438.98	441.55	444.81
445.76	450.32	454.15	457.56	469.57	492.31
511.21	522.94	527.77	534.02	544.33	547.12
548.79	557.69	568.42	587.07	605.93	611.83
614.57	628.59	639.87	644.04	646.63	651.75
660.16	667.82	681.39	686.37	709.17	713.73
726.32	749.34	770.30	776.20	781.39	797.15
814.58	816.82	818.91	819.60	857.11	860.44
861.02	866.76	867.17	898.31	901.41	908.43
916.61	920.27	925.30	939.54	940.51	946.73
947.03	948.07	950.25	953.98	957.17	959.00
967.44	968.81	970.90	972.47	976.83	977.08
977.40	977.65	978.73	989.19	993.52	1007.87
1021.54	1031.26	1040.22	1043.47	1051.07	1054.58
1056.48	1065.18	1072.99	1075.88	1090.65	1092.05
1099.38	1128.05	1128.97	1130.43	1133.79	1136.31
1136.99	1137.40	1139.91	1176.31	1179.10	1190.20
1191.69	1192.46	1197.88	1199.50	1204.84	1212.88
1214.85	1216.07	1218.36	1229.11	1251.81	1261.91
1267.09	1276.59	1283.59	1284.42	1291.96	1298.29
1302.18	1303.04	1307.55	1309.28	1312.05	1328.99
1357.13	1357.87	1365.15	1366.06	1367.29	1369.31
1374.57	1394.88	1396.19	1396.79	1413.27	1415.18
1416.46	1417.34	1418.92	1419.00	1420.79	1423.22
1426.80	1436.71	1438.02	1438.13	1439.23	1439.79
1445.36	1468.45	1479.50	1483.63	1486.43	1489.30
1491.26	1491.86	1492.60	1493.41	1494.80	1496.74
1498.50	1499.05	1500.87	1502.10	1503.83	1504.75
1505.22	1505.80	1507.14	1508.92	1509.31	1510.77
1516.33	1517.32	1519.72	1519.96	1520.53	1520.67
1522.09	1522.44	1525.26	1526.23	1531.26	1539.44
1541.20	1574.49	1595.66	1629.30	1632.70	1638.29
1642.63	1645.15	1661.15	2998.16	3028.69	3030.07
3032.99	3035.30	3035.78	3036.69	3037.63	3038.89
3046.06	3048.03	3050.83	3051.68	3055.11	3057.58
3063.27	3064.91	3080.94	3083.51	3088.04	3098.80
3099.40	3103.28	3104.76	3108.20	3108.84	3109.16
3109.89	3110.01	3111.82	3112.35	3113.62	3114.21
3115.86	3116.22	3117.21	3118.80	3122.29	3124.58
3126.26	3129.48	3130.61	3130.75	3145.85	3147.54
3149.68	3149.99	3157.24	3163.94	3169.70	3171.46
3172.15	3181.90	3184.95	3186.53	3195.39	3195.88
3200.09	3207.24	3246.48			

=====

⁶H

=====

18.64	25.50	29.71	39.52	41.91	44.51
46.31	50.37	53.34	55.86	60.14	62.94
68.15	72.42	75.50	79.44	82.27	84.84
92.37	97.62	99.07	110.63	116.92	118.93
125.07	131.96	135.59	141.37	145.38	151.62

153.88	156.11	158.82	165.27	166.87	169.89
171.22	172.22	201.04	203.05	207.45	217.52
231.79	240.33	246.40	248.24	248.69	250.71
252.48	255.57	258.32	261.76	268.59	272.51
275.06	276.76	284.46	287.81	293.93	298.50
299.57	303.45	305.52	306.03	311.98	315.21
318.25	320.88	322.90	328.36	329.84	334.94
343.84	346.74	351.34	363.43	366.22	370.12
377.27	379.51	395.95	397.73	404.40	415.92
420.30	434.86	436.43	449.14	452.16	452.48
454.54	459.19	462.86	476.27	496.34	507.82
516.00	523.24	526.68	527.59	532.52	538.66
551.29	554.33	559.77	566.91	580.68	584.59
596.52	599.54	609.61	611.52	612.37	630.14
637.36	647.95	652.18	657.82	668.47	673.09
694.01	700.99	709.17	724.49	733.33	748.53
772.35	779.45	780.42	786.38	804.89	814.12
818.14	819.86	829.14	841.97	855.57	858.71
861.13	864.19	867.52	878.69	899.97	900.60
904.84	919.61	920.13	925.43	926.90	937.88
942.24	942.67	943.31	946.60	947.73	949.25
952.66	953.57	954.58	957.81	962.70	969.68
972.14	975.58	977.93	978.13	979.69	980.62
981.51	982.55	992.56	995.62	1013.38	1015.62
1022.40	1026.46	1029.34	1031.31	1034.14	1038.57
1050.00	1054.17	1057.10	1063.33	1066.19	1070.23
1072.32	1075.86	1091.39	1094.34	1112.74	1126.48
1129.46	1132.58	1133.77	1135.93	1138.22	1145.83
1150.49	1173.73	1181.54	1184.87	1186.42	1191.67
1195.98	1196.39	1197.92	1200.48	1204.98	1215.29
1218.14	1225.75	1227.58	1229.54	1230.88	1246.42
1251.17	1258.69	1261.24	1271.95	1274.12	1281.92
1284.76	1292.96	1296.50	1299.60	1302.44	1304.96
1306.69	1308.68	1311.69	1333.46	1339.70	1358.46
1360.19	1361.38	1361.65	1369.48	1369.96	1374.47
1376.75	1392.74	1394.18	1409.69	1409.99	1411.88
1413.21	1413.31	1415.57	1417.21	1418.86	1420.41
1421.53	1422.01	1423.06	1430.90	1432.08	1433.13
1435.40	1437.27	1441.62	1447.32	1457.39	1474.61
1484.51	1484.73	1487.58	1487.98	1492.15	1493.06
1495.83	1496.35	1496.81	1498.51	1498.70	1499.91
1500.55	1501.41	1501.69	1502.29	1503.13	1504.07
1504.98	1505.71	1506.39	1507.92	1509.47	1512.38
1514.12	1516.53	1518.64	1519.00	1520.16	1521.26
1522.11	1523.40	1523.55	1525.86	1527.61	1528.00
1529.15	1530.13	1537.92	1544.44	1546.46	1550.25
1571.16	1596.34	1628.62	1632.46	1640.85	1642.23
1644.09	1666.81	1940.01	3027.60	3033.38	3035.46
3035.68	3036.28	3037.11	3037.96	3039.29	3040.14
3041.54	3045.50	3047.52	3052.05	3054.35	3054.96
3055.19	3057.34	3058.22	3062.60	3065.58	3069.69
3087.99	3091.37	3091.88	3095.61	3096.00	3103.22
3104.10	3105.69	3106.77	3108.06	3111.00	3112.12
3113.22	3113.88	3116.03	3118.37	3120.00	3120.60
3124.50	3126.21	3127.18	3131.82	3132.81	3136.66

3139.15	3139.51	3140.40	3144.51	3144.62	3145.10
3147.71	3148.31	3150.56	3151.22	3157.57	3159.82
3164.86	3165.05	3165.42	3168.74	3170.40	3172.30
3179.34	3181.64	3188.46	3188.73	3190.78	3194.73
3199.22	3209.63	3220.02			

=====

⁶H-TS

=====

-110.90	23.16	27.35	29.94	35.10	40.86
43.16	46.52	48.70	50.75	58.44	61.82
62.41	66.22	67.94	75.61	76.31	80.77
85.73	87.73	97.70	102.98	107.37	110.43
123.27	126.93	130.33	134.65	135.93	142.11
145.79	154.71	155.89	159.07	161.49	164.24
168.59	176.20	189.32	201.92	205.15	211.53
222.45	227.30	234.87	239.95	243.44	247.53
247.99	252.48	256.19	258.40	261.65	263.95
271.39	273.31	277.35	280.48	281.94	288.53
298.01	301.66	304.02	304.50	308.22	313.25
314.88	317.91	326.43	327.15	328.30	331.56
335.67	345.20	347.65	350.44	354.41	359.38
363.54	372.11	381.19	383.54	398.36	404.46
419.45	432.19	434.92	440.81	443.32	451.29
455.74	456.89	460.42	460.95	474.57	503.10
507.27	516.93	520.64	523.34	528.61	531.08
537.74	549.79	552.93	562.34	563.89	566.30
582.99	584.98	586.27	596.38	608.30	615.06
625.24	626.22	636.07	643.13	650.49	654.29
671.71	675.01	696.90	706.57	719.20	720.98
731.51	753.00	770.16	777.26	780.80	802.65
809.05	812.55	817.17	818.82	843.91	848.34
852.71	860.09	863.72	867.40	868.07	891.83
899.29	899.76	915.58	917.40	921.29	938.60
940.03	942.83	944.21	945.04	947.86	948.52
948.78	950.83	952.93	954.28	955.30	958.13
966.19	968.65	977.13	977.24	978.15	980.04
981.30	981.80	982.87	990.14	999.94	1007.06
1014.16	1026.84	1027.89	1028.52	1029.77	1037.92
1041.33	1046.45	1053.86	1060.28	1060.96	1069.94
1075.59	1088.55	1090.85	1094.45	1126.09	1127.36
1130.36	1131.34	1132.32	1141.84	1146.98	1147.76
1151.41	1173.96	1175.48	1176.83	1189.95	1192.66
1194.29	1196.85	1198.16	1199.39	1204.09	1215.40
1216.98	1226.35	1230.27	1233.87	1245.81	1248.24
1255.30	1268.25	1272.94	1276.32	1280.88	1281.82
1284.42	1294.87	1295.67	1300.20	1302.47	1308.10
1308.69	1327.48	1337.56	1343.99	1347.42	1349.48
1357.24	1358.42	1363.19	1369.17	1376.37	1378.73
1378.89	1389.77	1393.63	1396.42	1406.94	1411.77
1412.52	1416.12	1417.36	1417.80	1418.01	1418.86
1419.43	1423.44	1425.29	1430.03	1431.85	1432.34
1435.04	1437.51	1438.14	1440.79	1443.19	1457.35
1472.93	1480.22	1483.90	1485.17	1488.37	1491.34
1492.82	1493.41	1494.23	1496.16	1496.28	1497.35
1498.90	1499.22	1500.49	1500.97	1501.57	1502.63

1503.55	1504.02	1504.84	1506.56	1508.03	1510.57
1512.75	1514.91	1518.11	1518.36	1518.81	1519.67
1521.44	1522.44	1522.53	1524.12	1524.60	1526.26
1526.73	1527.88	1530.62	1532.02	1543.33	1545.98
1547.52	1564.28	1592.04	1625.57	1629.60	1641.31
1643.23	1643.61	1668.15	3030.74	3034.19	3035.46
3035.59	3035.90	3036.38	3037.44	3039.09	3041.87
3045.44	3045.87	3050.37	3051.22	3051.42	3053.11
3054.63	3055.08	3057.54	3058.89	3061.78	3062.49
3076.45	3092.30	3095.01	3098.11	3098.62	3101.59
3106.43	3108.00	3109.78	3110.42	3112.35	3118.44
3120.65	3121.18	3121.61	3122.03	3125.17	3125.92
3127.55	3129.36	3130.12	3133.20	3133.61	3135.48
3137.74	3137.93	3144.46	3145.11	3145.77	3149.13
3149.85	3150.62	3150.89	3153.65	3154.33	3158.11
3161.17	3164.60	3167.04	3167.45	3170.98	3171.55
3182.25	3184.04	3185.36	3190.52	3194.65	3199.11
3205.07	3207.55	3219.64			

=====

⁶I

=====

10.59	25.16	31.18	33.98	36.24	38.82
42.55	42.69	45.77	48.76	52.34	55.34
55.92	65.27	68.19	72.57	76.35	79.53
83.44	84.88	90.52	95.24	102.49	102.83
108.11	118.74	121.69	126.16	130.31	133.93
139.46	143.13	145.66	147.64	153.92	159.98
162.52	179.14	192.32	199.13	211.28	217.22
220.32	222.08	236.40	241.08	243.26	246.21
251.05	254.96	259.46	267.23	269.52	271.83
277.11	277.79	281.93	292.84	295.06	296.01
298.46	303.05	303.85	307.99	310.42	316.36
322.13	325.55	327.41	329.44	334.98	338.96
342.04	345.00	355.33	359.40	362.27	363.11
370.27	377.40	384.91	390.92	400.43	404.17
419.89	421.14	433.26	444.25	449.38	455.14
457.24	459.84	462.35	466.82	475.59	482.95
504.87	508.67	509.81	525.65	527.68	528.65
534.95	542.43	554.69	558.77	561.80	568.54
584.84	586.58	604.48	608.29	611.62	629.94
635.55	636.95	644.63	652.56	653.12	660.58
674.59	677.08	691.98	710.33	714.77	728.54
730.68	773.79	774.92	780.57	783.80	810.41
811.86	820.59	821.58	836.54	841.18	848.54
857.60	860.96	867.36	869.64	870.99	884.10
900.63	901.91	919.78	921.62	933.17	938.58
941.87	943.71	944.82	945.05	945.76	948.07
950.92	951.86	952.31	958.02	959.42	960.39
964.27	970.92	972.67	975.17	977.46	978.15
979.27	980.33	981.70	986.03	991.77	1000.85
1017.11	1026.34	1026.53	1028.82	1032.67	1035.02
1045.24	1048.06	1052.57	1055.76	1060.60	1076.07
1077.80	1079.58	1092.67	1094.87	1124.58	1127.11
1129.55	1130.61	1131.91	1141.19	1146.69	1147.41
1149.79	1176.27	1178.10	1178.81	1190.69	1193.20

1193.63	1195.39	1198.15	1198.38	1207.81	1216.94
1217.88	1222.20	1235.16	1238.83	1246.30	1248.65
1261.35	1272.18	1274.10	1275.07	1278.26	1280.53
1284.67	1296.86	1298.60	1301.97	1302.79	1304.00
1309.70	1330.81	1347.87	1352.20	1355.62	1357.12
1359.31	1360.20	1370.25	1370.66	1375.71	1392.79
1395.90	1396.13	1405.31	1406.98	1410.23	1412.34
1413.37	1416.48	1416.96	1417.50	1418.40	1420.11
1421.32	1425.00	1430.81	1431.57	1434.36	1434.99
1436.23	1438.75	1441.27	1442.38	1444.75	1462.55
1474.75	1480.98	1484.74	1485.51	1486.00	1492.52
1492.99	1495.00	1495.42	1495.81	1497.34	1498.68
1500.06	1500.39	1501.08	1501.27	1501.90	1502.44
1503.40	1505.18	1505.97	1507.22	1508.28	1509.27
1511.80	1514.73	1515.40	1517.43	1518.49	1518.85
1519.87	1520.94	1521.61	1522.54	1523.71	1526.47
1527.66	1529.46	1533.80	1534.61	1540.88	1543.81
1545.76	1565.78	1601.41	1623.08	1630.72	1632.94
1638.95	1645.36	1662.10	3026.08	3028.44	3034.31
3034.43	3035.06	3035.36	3038.25	3039.75	3044.27
3047.35	3048.44	3051.15	3051.28	3051.70	3052.86
3054.70	3055.01	3056.45	3057.56	3061.19	3083.37
3092.77	3094.18	3098.37	3098.68	3100.25	3100.44
3106.10	3109.73	3111.92	3112.12	3112.66	3114.60
3115.74	3117.42	3119.37	3121.64	3122.27	3122.83
3127.37	3130.98	3131.54	3133.41	3135.10	3135.16
3137.02	3137.74	3139.62	3143.34	3143.47	3144.96
3146.68	3150.15	3151.11	3151.30	3152.64	3153.70
3155.47	3156.13	3165.33	3167.46	3170.81	3171.18
3175.71	3178.21	3181.02	3186.14	3188.01	3189.62
3190.36	3200.88	3208.51			

=====

Borylimine

=====

22.24	31.19	45.59	103.26	105.94	118.25
180.82	227.37	238.40	258.07	280.26	294.41
322.75	326.02	331.26	341.70	377.81	378.90
401.84	417.90	456.41	493.16	521.86	542.95
562.93	584.40	630.64	664.11	679.78	700.08
706.15	771.20	846.26	861.71	865.20	865.43
927.38	936.19	940.36	946.81	974.10	986.05

999.28	1004.19	1015.48	1017.54	1022.21	1034.80
1053.40	1113.13	1143.13	1185.83	1191.75	1195.35
1204.96	1237.25	1247.67	1270.45	1300.08	1335.27
1337.49	1363.71	1368.52	1414.73	1417.18	1427.14
1437.05	1461.87	1485.80	1493.35	1498.14	1501.65
1506.06	1518.28	1520.61	1523.94	1536.83	1541.50
1641.03	1660.18	1807.13	2976.58	3049.79	3051.94
3054.60	3058.72	3122.79	3123.37	3129.52	3131.15
3135.00	3135.74	3152.61	3153.73	3170.23	3180.35
3192.20	3203.84	3212.90			

=====

Diborylamine

=====

10.44	28.62	31.87	35.97	61.92	68.61
90.55	96.98	116.98	125.60	160.69	195.40
207.22	212.70	226.13	228.58	242.02	245.32
282.85	294.09	301.80	305.20	316.64	324.20
327.11	334.64	337.84	361.33	367.80	370.89
379.25	387.41	401.65	418.73	421.64	436.74
455.35	466.04	505.84	511.66	526.22	528.62
565.72	586.48	588.48	628.67	636.17	656.44
659.36	678.41	691.69	702.75	721.20	773.79
834.63	836.85	864.23	867.79	868.27	870.62
892.30	938.89	939.86	941.50	943.78	946.79
949.09	975.16	977.16	984.22	989.97	992.11
999.64	1018.06	1022.09	1022.41	1029.51	1032.83
1059.13	1060.53	1117.54	1122.45	1146.18	1147.53
1182.89	1191.76	1191.97	1195.30	1197.58	1220.42
1231.05	1250.01	1250.73	1267.61	1269.92	1270.44
1302.44	1303.94	1334.33	1342.64	1362.45	1372.41
1393.37	1414.56	1414.61	1416.87	1417.46	1427.09
1427.47	1436.64	1437.10	1468.94	1485.98	1486.46
1491.57	1492.99	1493.38	1497.89	1498.92	1500.77
1501.65	1501.95	1516.86	1518.64	1519.19	1522.71
1523.65	1523.91	1524.33	1540.64	1541.59	1543.42
1642.22	1663.88	3048.73	3049.23	3051.10	3051.83
3053.89	3054.00	3057.95	3058.21	3078.71	3121.13
3121.84	3122.34	3123.10	3127.90	3128.77	3129.28
3131.60	3132.32	3134.15	3135.41	3136.03	3137.13
3150.67	3151.69	3151.80	3152.37	3167.97	3178.21
3193.03	3205.34	3208.16			

References

1. Y. Li, Z. Li, F. Li, Q. Wang and F. Tao, *Tetrahedron Lett.*, 2005, **46**, 6159-6162.
2. T. K. Mukhopadhyay, M. Flores, T. L. Groy and R. J. Trovitch, *Chem. Sci.*, 2018, **9**, 7673-7680.
3. D. F. Evans, *J. Chem. Soc.*, 1959, 2003-2005.
4. E. M. Schubert, *J. Chem. Educ.*, 1992, **69**, 62.
5. J. R. Pilbrow, *Transition Ion Electron Paramagnetic Resonance*, Clarendon Press, Oxford, 1990.
6. R. D. Dowsing, J. F. Gibson, M. Goodgame and P. J. Hayward, *J. Chem. Soc. A*, 1969, 187-193.
7. R. D. Dowsing, J. F. Gibson, M. Goodgame and P. J. Hayward, *J. Chem. Soc. A*, 1970, 1133-1138.
8. A. Bencini and D. Gatteschi, *Electron Paramagnetic Resonance of Exchange Coupled Systems*, Springer-Verlag, New York, 1990.
9. S. Stoll and A. Schweiger, *J. Magn. Reson.*, 2006, **178**, 42-55.
10. R. G. Parr and Y. Weitao, *Density-Functional Theory of Atoms and Molecules*, Oxford University Press, 1994.
11. A. D. Bochevarov, E. Harder, T. F. Hughes, J. R. Greenwood, D. A. Braden, D. M. Philipp, D. Rinaldo, M. D. Halls, J. Zhang and R. A. Friesner, *Int. J. Quantum Chem.*, 2013, **113**, 2110-2142.
12. J. C. Slater and J. C. Phillips, *Phys. Today*, 1974, **27**, 49.
13. S. H. Vosko, L. Wilk and M. Nusair, *Can. J. Phys.*, 1980, **58**, 1200-1211.
14. A. D. Becke, *Phys. Rev. A*, 1988, **38**, 3098-3100.
15. A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648-5652.
16. C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785-789.
17. S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104.
18. P. J. Hay and W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 270-283.
19. P. J. Hay and W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 299-310.
20. W. R. Wadt and P. J. Hay, *J. Chem. Phys.*, 1985, **82**, 284-298.
21. T. H. Dunning, *J. Chem. Phys.*, 1989, **90**, 1007-1023.
22. A. A. Rashin and B. Honig, *J. Phys. Chem.*, 1985, **89**, 5588-5593.