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Electronic Supplementary Information

Super Electron Donors Derived From Diboron

Li Zhang and Lei Jiao*

Center of Basic Molecular Science (CBMS), Department of Chemistry, Tsinghua University, Beijing 100084, China

Leijiao@mail.tsinghua.edu.cn

Contents

1. General Information

Experimental. Air- and moisture-sensitive reactions were carried out in an oven-dried sealed tube (with a Teflon screw cap) or glassware sealed with a rubber septum under an atmosphere of dry argon. Air- and moisture-sensitive liquids and solutions were transferred by syringe. Reactions were stirred using Teflon-coated magnetic stir bars. Elevated temperatures were maintained using Thermostat-controlled silicone oil baths. Organic solutions were concentrated using a rotary evaporator with a diaphragm vacuum pump. Analytical TLC was performed on silica gel GF_{254} plates. The TLC plates were visualized by ultraviolet light (λ = 254 nm). Purification of products was accomplished by flash column chromatography on silica gel (Innochem SilicaFlashP60, 230-400 mesh).

Chemicals. SuperDry solvent methyl *tert*-butyl ether (MTBE), dimethyl sulphoxide (DMSO), 1,2-dimethoxyethane (DME) were purchased from J&K Scientific, which were stored in a glove box and were used without further purification. Reagent grade tetrahydrofuran (THF) and hexane were purified by MBRAUN SPS 800 solvent purification system and were further deoxygenated by three freeze-pump-thaw cycles before use. Other chemicals were purchased from various commercial sources and were used as received. Substrates 2-chloro-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (ClBpin),[1] *N*-tosylindole (**12a**), [2] *N*-methoxy-*N*-methylbenzamide (**12b**),[3] *N*-methoxy-*N*-methyl-4-(trifluoromethyl)benzamide (**12c**),[4] 2-oxo-1,2-diphenylethyl acetate (**12d**),[5] and 1-(allyloxy)-2-iodobenzene (**14**) [6] were synthesized following the published procedures.

Analytical. NMR spectra were recorded on a Bruker AVANCE III HD 400 (^{1}H at 400 MHz, ^{13}C at 100 MHz, ^{11}B at 128 MHz) nuclear magnetic resonance spectrometer. The ^{1}H NMR were calibrated against the peak of tetramethylsilane (TMS, 0 ppm). The ^{13}C NMR were calibrated against the peak of the solvent (77.16 ppm for $CDCl_3$ and 40.45 ppm for d_6-DMSO[7]). The EPR measurement was performed on a JEOL JES FA200 X-band EPR spectrometer (9.05 GHz). GC analysis was performed on a Shimadzu GC-2010 instrument equipped with a FID detector using nitrogen as the carrier gas. UV-Vis spectrum was obtained from Agilent Cary 8454 UV-Vis Diode Array System. Electrochemical experiments were performed on a CHI-660E electrochemical workstation. The X-ray crystal structure analyses were performed with a SuperNova X-ray Diffraction System equipped with Atlas CCD detector and 4-circle kappa goniometer. Structure solution and refinement were accomplished with OLEX2.

2. Investigation of the NMR-Visible Species

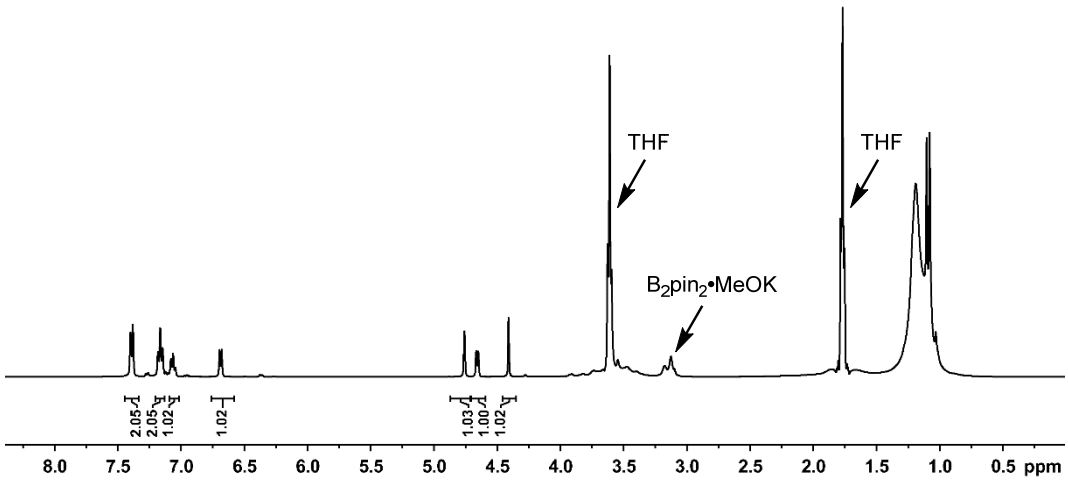
2.1 General

In the NMR study, non-deuterated THF, DME, and DMSO were utilized unless otherwise noted. The NMR spectra were recorded after ^{1}H gradient shimming without applying the ^{2}H-lock, and the undesired solvent signals were suppressed by the WET solvent suppression method.[8] The chemical shifts of the solvents utilized in the NMR experiments were calibrated against TMS (1.77 and 3.61 ppm for THF, 3.27 and 3.43 ppm for DME, and 2.54 ppm for DMSO), and for other ^{1}H NMR spectra, the chemical shifts were calibrated against the solvent peaks. For ^{13}C and ^{11}B NMR spectra, chemical shifts were calibrated by absolute δ referencing method[9] against solvent peaks in the corresponding ^{1}H NMR spectra. All measurements were performed under an argon atmosphere.

2.2 NMR Study of the Diboron/Methoxide/4-Phenylpyridine System

Experimental procedure: A 15 mL reaction tube was charged with B_2pin_2 (60.0 mg, 0.236 mmol), potassium methoxide (17.0 mg, 0.243 mmol), 18-crown-6 (63.0 mg, 0.239 mmol), 4-phenylpyridine (33.9 mg, 0.218 mmol), and 3 mL THF. The tube was sealed with a Teflon screw cap and the reaction mixture was allowed to react at room temperature for 2 h. During this time, the color of the solution gradually changed to purple. The NMR analysis indicated almost complete conversion of 4-phenylpyridine and the generation of a new species, which consisted of ca. 77% of pyridine-related species according to quantification by internal standard method.

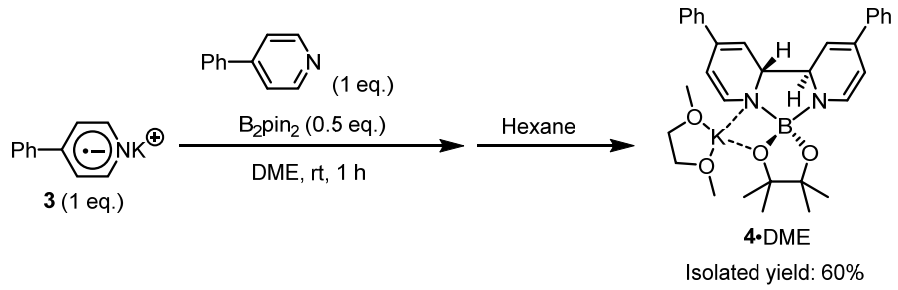
^{1}H NMR of diboron/methoxide/4-phenylpyridine system:



2.3 Synthesis and Characterization of Complexes 4·DME and 4·18-C-6

In order to synthesize complex **4** in better efficiency, a new kind of method was proposed and developed utilizing potassium as reducing agent to reduce 4-phenylpyridine. We found that, by the reaction between 4-phenylpyrdine radical anion (prepared by mixing potassium and 4-phenylpyridine) and B_2pin_2 in DME, complex **4** has been produced with better atom economy compared with the method shown in Scheme 2, since no MeOBpin was produced. This method is more suitable for the synthesis of complex **4** at a larger scale.

(1) Synthesis and characterization of complex **4**·DME



Isolated yield: 60%

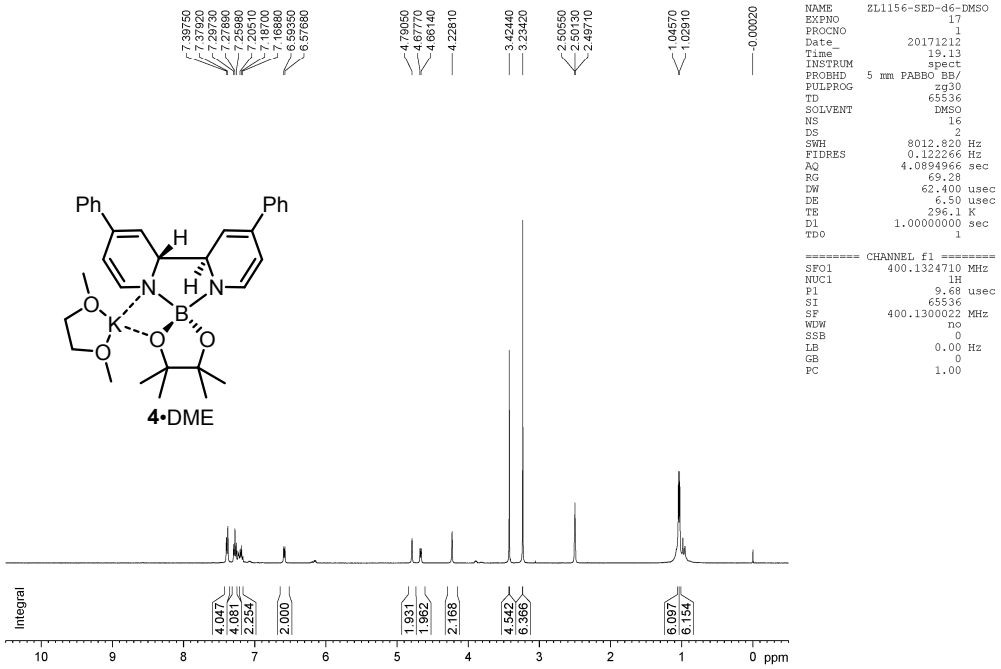
Experimental procedure: In a glove box, to a 50 mL flask charged with potassium (42.5 mg, 1.09 mmol) was added 4-phenylpyridine (339.0 mg, 2.18 mmol) and 15 mL DME. After reaction at room temperature for 10 min, B_2pin_2 (140.0 mg, 0.55 mmol) was added, and the resulting mixture was allowed to react at room temperature for 1 h. Then 30 mL of hexane was carefully added. After diffusion overnight, the mother liquid was removed and the crystals obtained were washed with hexane. After filtration, the residue solvent was removed under high vacuum, and the product **4**·DME could be obtained as yellow crystals in 60% yield (368.0 mg). Crystals suitable for X-ray diffraction analysis were obtained by applying a modified procedure, in which B_2pin_2 was added in the hexane layer to realize a reactive crystallization condition.

^{1}H NMR (400 MHz, d_6-DMSO): δ 7.40 (d, J = 7.2 Hz, 4H), 7.28 (t, J = 7.2 Hz, 4H), 7.19 (t, J = 7.2 Hz, 4H), 6.59 (d, J = 6.6 Hz, 2H), 4.79 (s, 2H), 4.67 (d, J = 6.6 Hz, 2H), 4.23 (s, 2H), 3.43 (s, 4H), 3.23 (s, 6H), 1.05 (s, 6H), 1.03 (s, 6H).

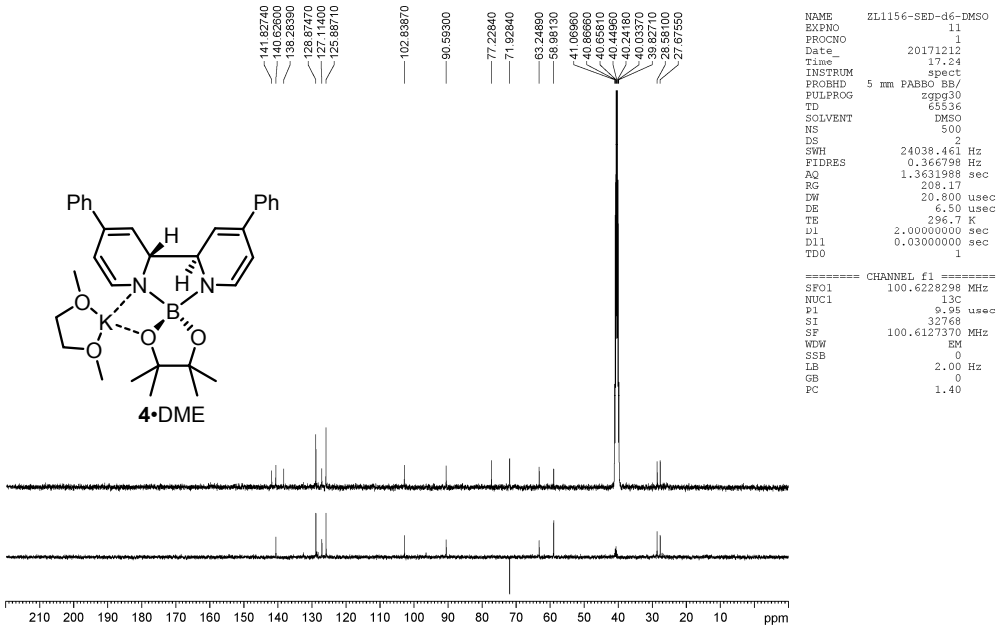
^{13}C NMR (100 MHz, d_6-DMSO): δ 141.8, 140.6, 138.3, 128.9, 127.1, 125.9, 102.8, 90.6, 77.2, 71.9, 63.2, 58.9, 28.6, 27.7.

^{11}B NMR (128 MHz, d_6-DMSO): δ 6.0.

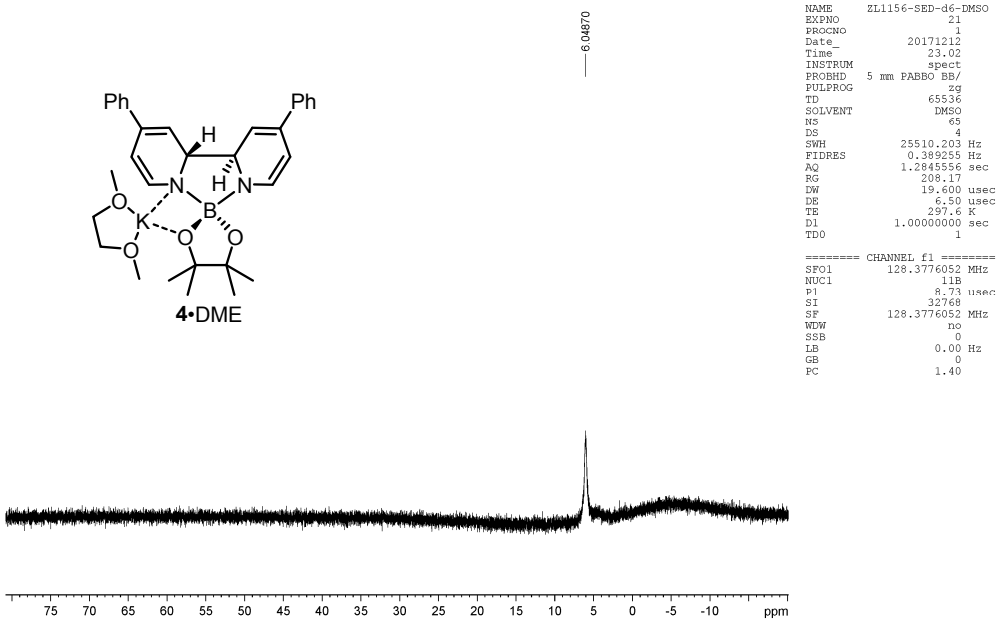
^{1}H NMR of complex **4**·DME in d_6-DMSO:



^{13}C NMR and DEPT135 of complex **4**·DME in d_6-DMSO:



^{11}B NMR of complex **4**·DME in DMSO:



NMR measurements of complex **4**·DME have also been done in THF for comparison with other spectra recorded in THF.

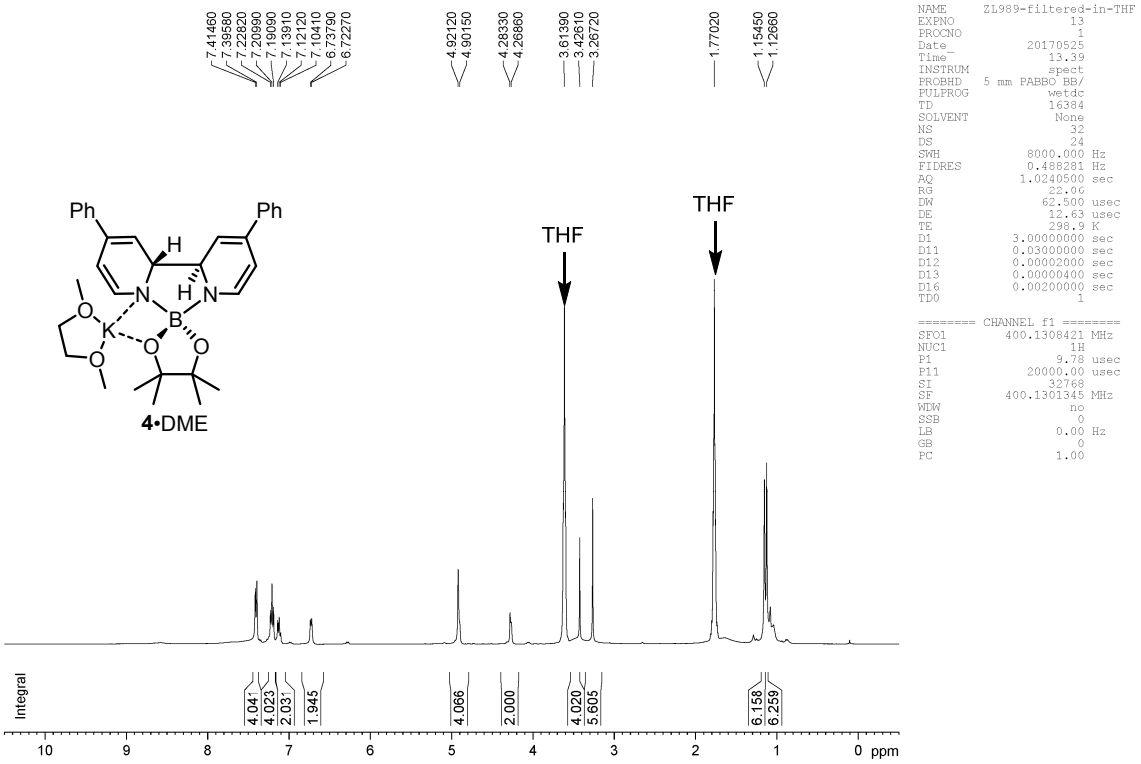
^{1}H NMR (400 MHz, THF): δ 7.40 (d, J = 7.5 Hz, 4H), 7.21 (t, J = 7.5 Hz, 4H), 7.13 (t, J = 7.2 Hz, 4H), 6.73 (d, J = 6.4 Hz, 2H), 4.97-4.87 (m, 4H), 4.30-4.24 (m, 2H), 3.43 (s, 4H), 3.27 (s, 6H), 1.15 (s, 6H), 1.13 (s, 6H).

^{13}C NMR (100 MHz, THF): δ 141.4, 138.7, 138.7, 127.6, 126.0, 125.4, 102.9, 92.3, 76.9, 71.8, 62.5, 57.9,

27.4, 26.4.

^{11}B NMR (128 MHz, THF): δ 6.0.

^{1}H NMR of complex **4**·DME in THF with solvent suppression:

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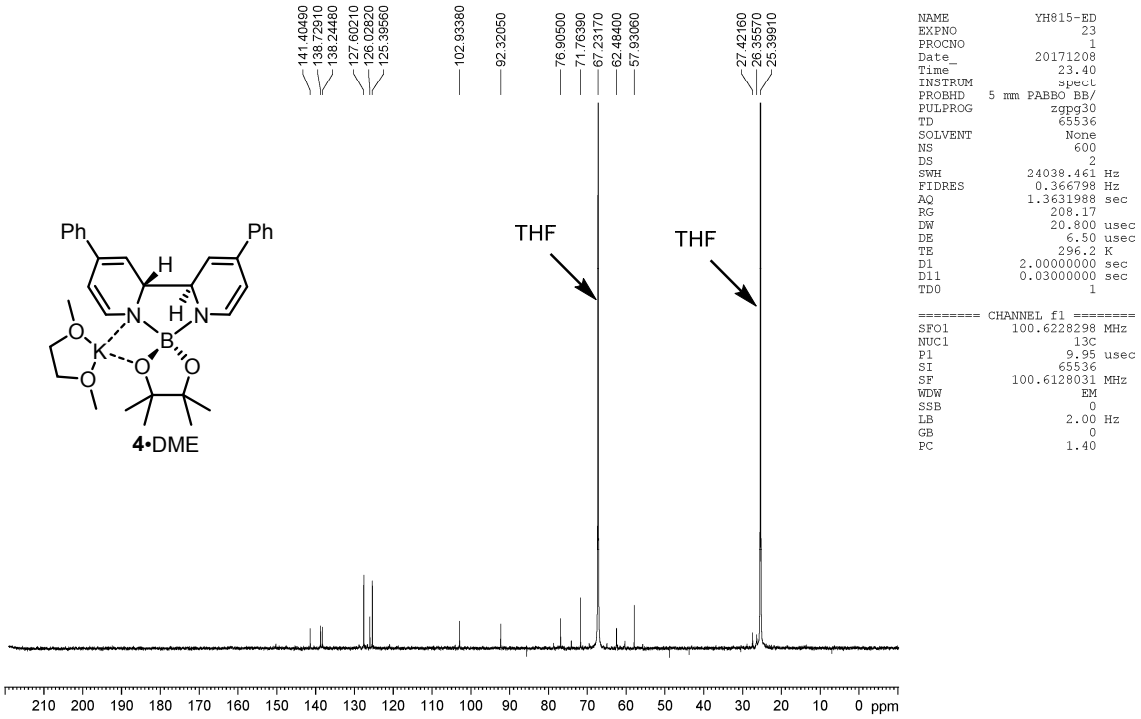
^{13}C NMR of complex **4**·DME in THF:

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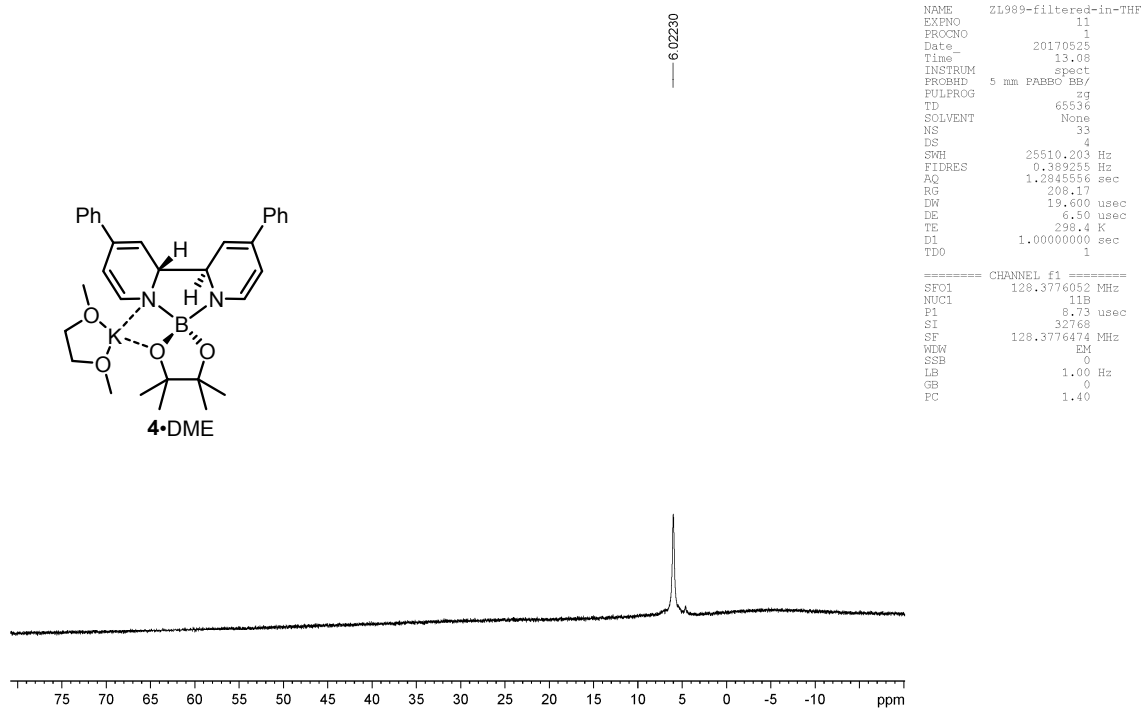
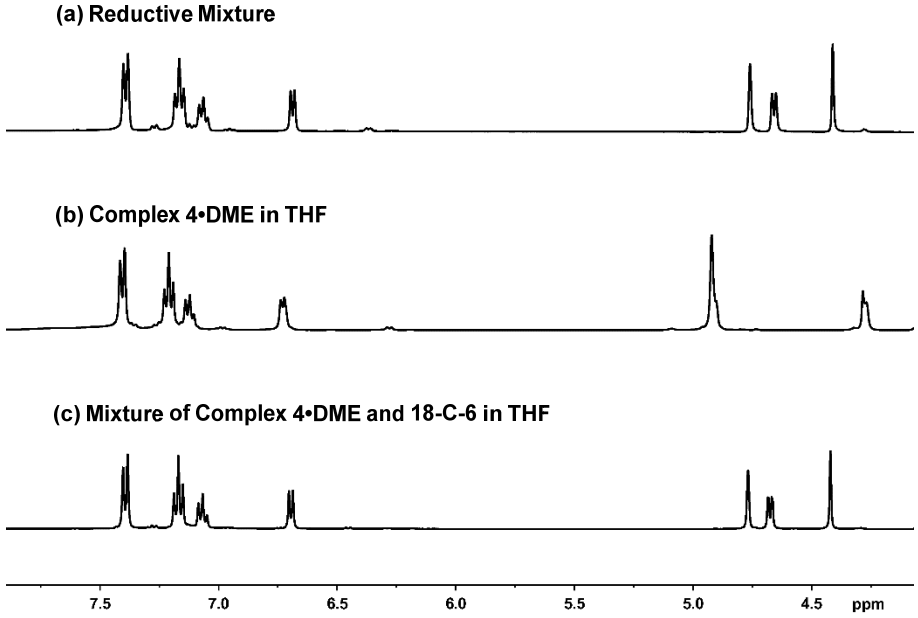
^{11}B NMR of complex **4**·DME in THF:



Comparison of the mixture of **4**·DME and 18-crown-6 in THF with reductive mixture:

Experimental procedure: In a glove box, to a 15 mL reaction tube charged with a solution of **4**·DME (11.2 mg, 0.020 mmol) in 1 mL of THF, 18-crown-6 (5.5 mg, 0.020 mmol) was added, and the resulting mixture was allowed to react at room temperature for 5 min. The ^{1}H NMR analysis of the resulting mixture indicated the generation of species identical with that in the reductive mixture. Based on the structure of **4**·DME elucidated by X-ray diffraction analysis, the NMR-visible species was proposed as a complex with the composition of **4**·18-C-6.

^{1}H NMR of the mixture of **4**·DME and 18-crown-6 in THF:



XRD of complex **4**·DME:

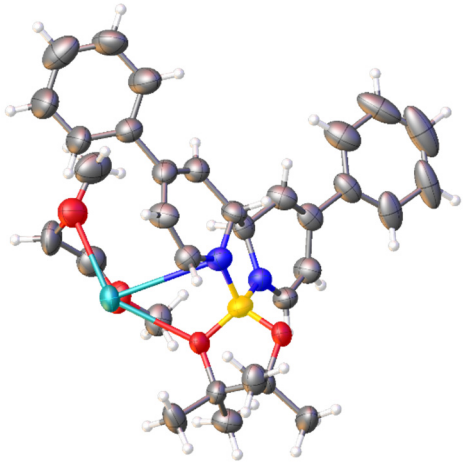
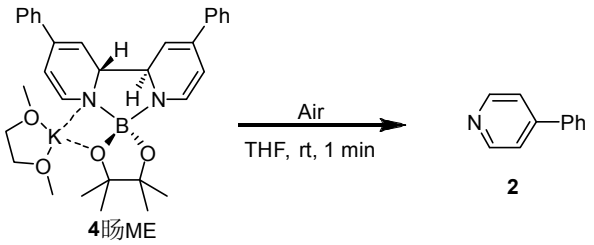


Figure S1. Ortep drawing of complex **4**·DME with 50% ellipsoids.

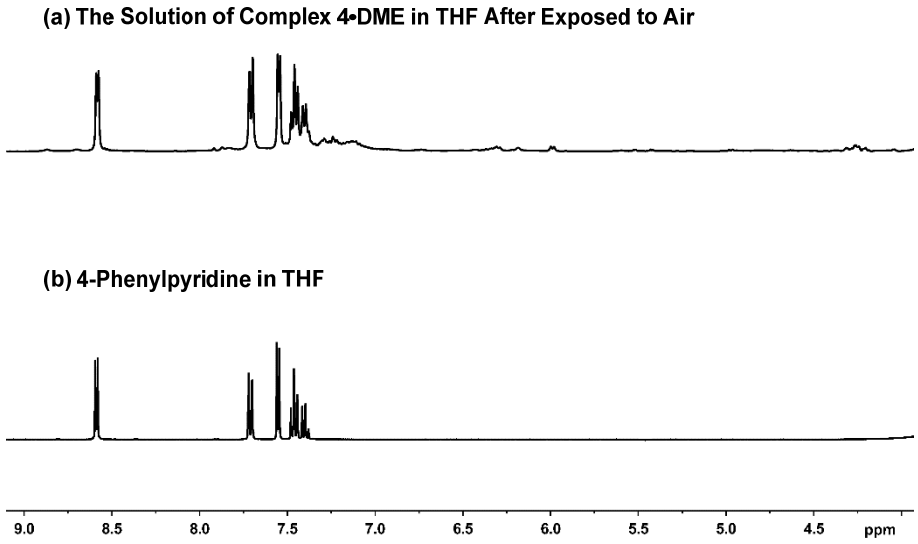
Molecular Formula	0.25($C_{64}H_{78}B_2K_2N_4O_8$), 0.25($C_{64}H_{73}B_2K_2N_4O_8$) $C_{32}H_{38}BKN_2O_4$
Formula mass	564.55
Crystal size/mm^3	1×0.3×0.1
Crystal system	monoclinic
Space group	*P* 1 2_1 1 (I.T.-No.: 4)
a /Å	12.3892(10)
b /Å	40.276(5)
c /Å	12.9956(7)
α	90
β	90.798(7)
γ	90
Volume /Å^3	6483.9(10)
ρ_{calcd} /g · cm^{-3}	1.157
T /K	175(1)
Radiation	CuK$_\alpha$, λ = 1.54184 Å
Measured reflns	17216
Indep. reflns	13676
param./restraints	1465/1
θ range	3.568° — 71.496°
GoF on F_2	1.000
R_{int}	0.0470
R_1 *[I > 2σ(I)]*	0.0683
*w*R2 (all data)	0.1833
max / min peaks /e Å^{-3}	0.242, -0.257
CCDC number	1585926

Decomposition pathway of complex **4**·DME:



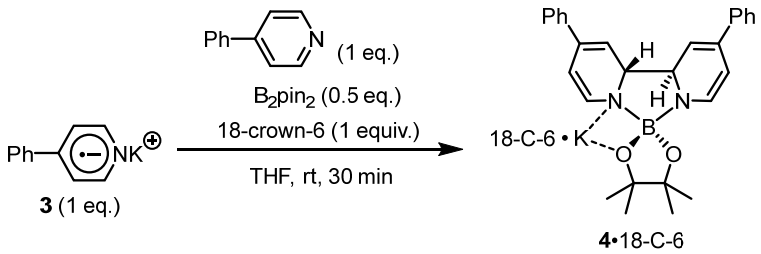
When the THF solution of complex **4**·DME was exposed to air, the yellow color of the solution immediately faded and the ^{1}H NMR spectrum showed that **4**·DME had been oxidized to 4-phenylpyridine. This result is in accordance with the electron donor character of complex **4**.

^{1}H NMR spectrum of the solution of **4**·DME in THF after exposed to air:



(2) Synthesis and characterization of complex **4**·18-C-6

The reaction between 4-phenylpyrdine radical anion (prepared by mixing potassium and 4-phenylpyridine) and B_2pin_2 in the presence of 18-crown-6 in THF could produce complex **4**·18-C-6.



Experimental procedure: A 15 mL reaction tube charged with potassium (4.3 mg, 0.110 mmol) was added 4-phenylpyridine (33.9 mg, 0.218 mmol) and 3 mL THF. After reaction at room temperature for 10 min. 18-crown-6 (28.0 mg, 0.109 mmol) and B_2pin_2 (140.0 mg, 0.55 mmol) were added successively, and the

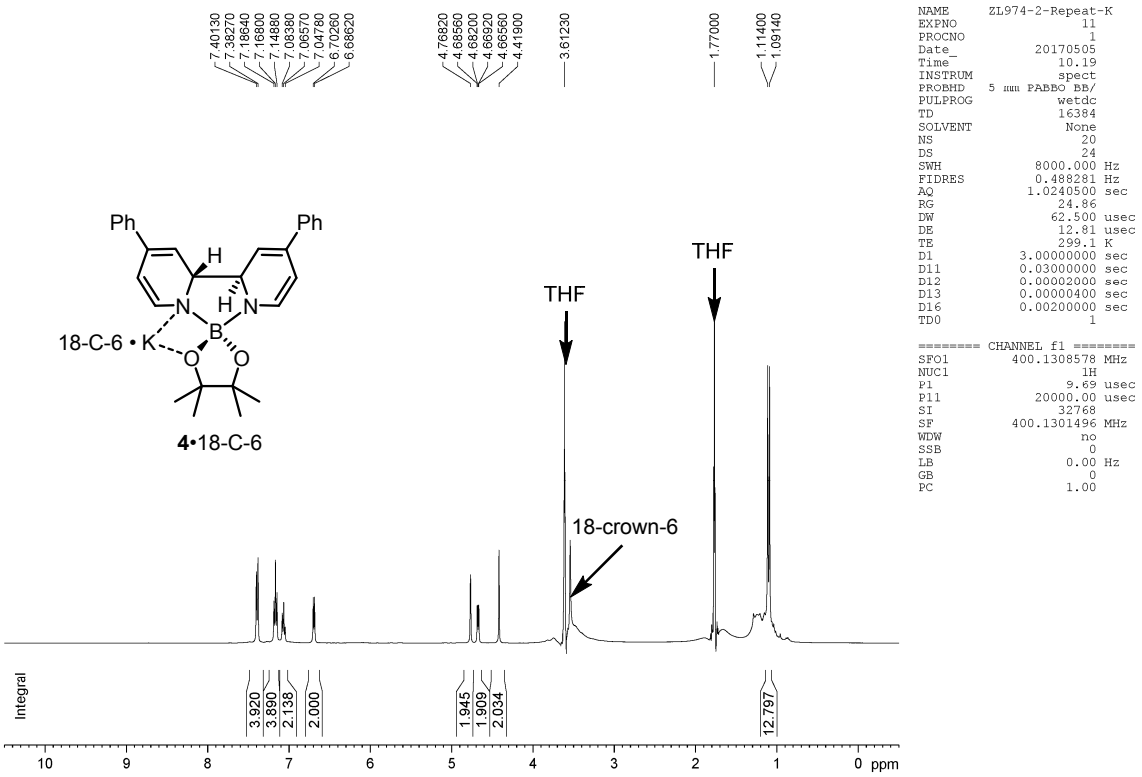
resulting mixture was allowed to react at room temperature for 30 min. NMR analysis indicated that the product generated in the mixture was identical to that in the diboron/methoxide/4-phenylpyridine system.

^{1}H NMR (400 MHz, THF): δ 7.39 (d, J = 7.5 Hz, 4H), 7.17 (t, J = 7.5 Hz, 4H), 7.07 (t, J = 7.5 Hz, 4H), 6.70 (d, J = 6.6 Hz, 2H), 4.77 (s, 2H), 6.68 (dd, J = 6.6 Hz, 1.8 Hz, 2H), 4.42 (s, 2H), 1.112 (s, 6H), 1.09 (s, 6H).

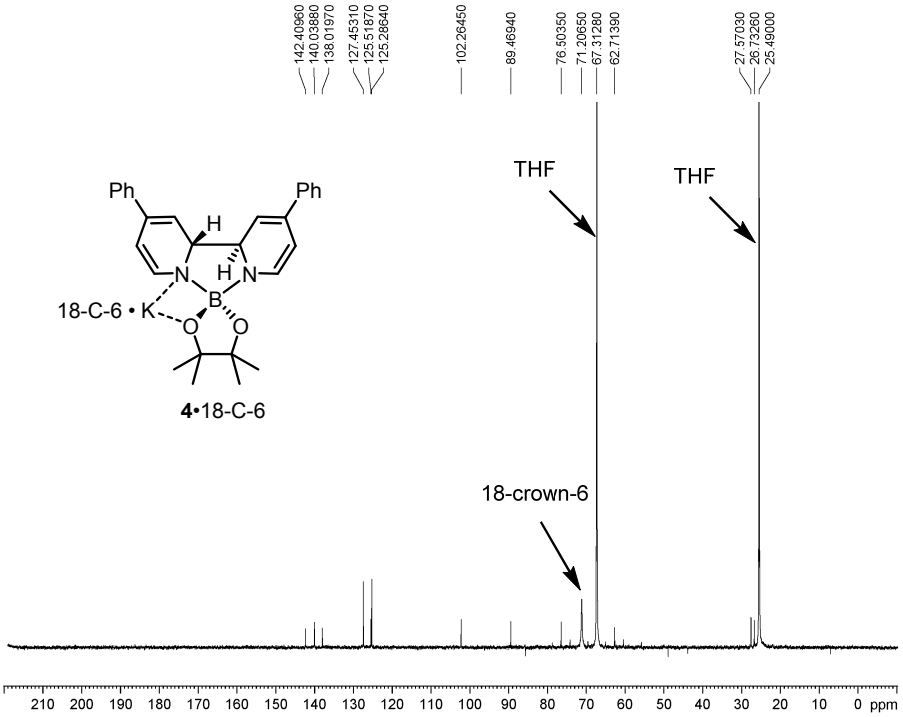
^{13}C NMR (100 MHz, THF): δ 142.4, 140.0, 138.0, 127.5, 125.5, 125.3, 102.3, 89.5, 76.5, 62.7, 27.6, 26.7.

^{11}B NMR (128 MHz, THF): δ 6.2.

^{1}H NMR of complex **4**·18-C-6 in THF with solvent suppression:



^{13}C NMR of complex **4**·18-C-6 in THF:

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TE                         299.9 K
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D11                   0.03000000 sec
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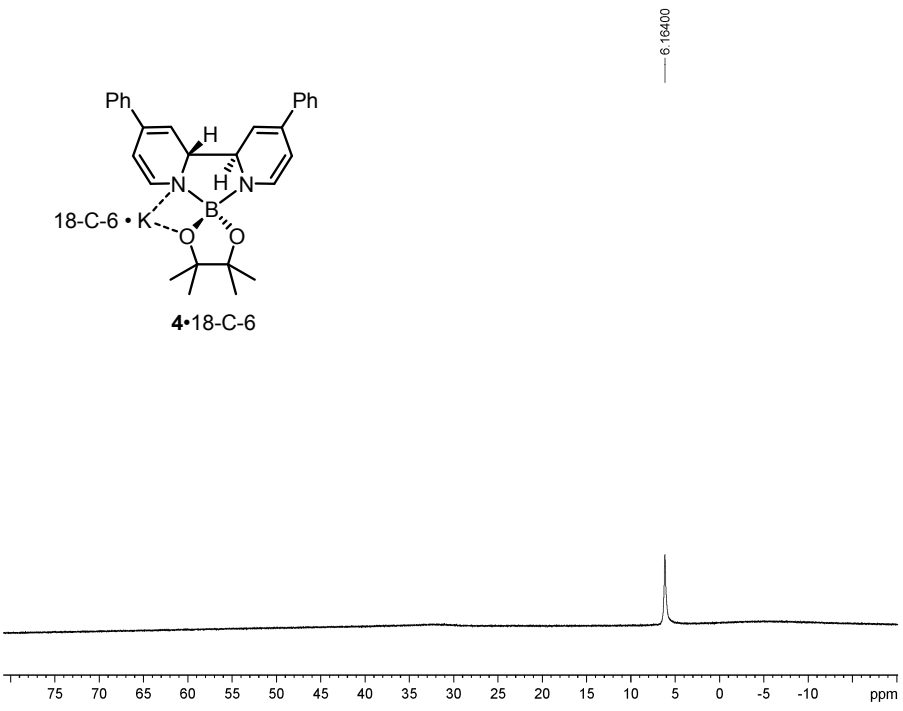
^{11}B NMR of complex **4**·18-C-6 in THF:

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```

2.4 Synthesis of Complex 4 in DMSO

(1) B_2pin_2/MeOK/4-phenylpyridine system in DMSO

Experimental procedure: A 15 mL reaction tube was charged with B_2pin_2 (2.6 mg, 0.010 mmol), potassium methoxide (0.7 mg, 0.010 mmol), 4-phenylpyridine (1.6 mg, 0.010 mmol), and 1 mL of DMSO. The tube was sealed with a Teflon screw cap and the reaction mixture was allowed to react at room temperature for 2 h. During this time, the color of the solution gradually changed to purple. NMR analysis indicated complete consumption of 4-phenylpyridine and formation of a major species.

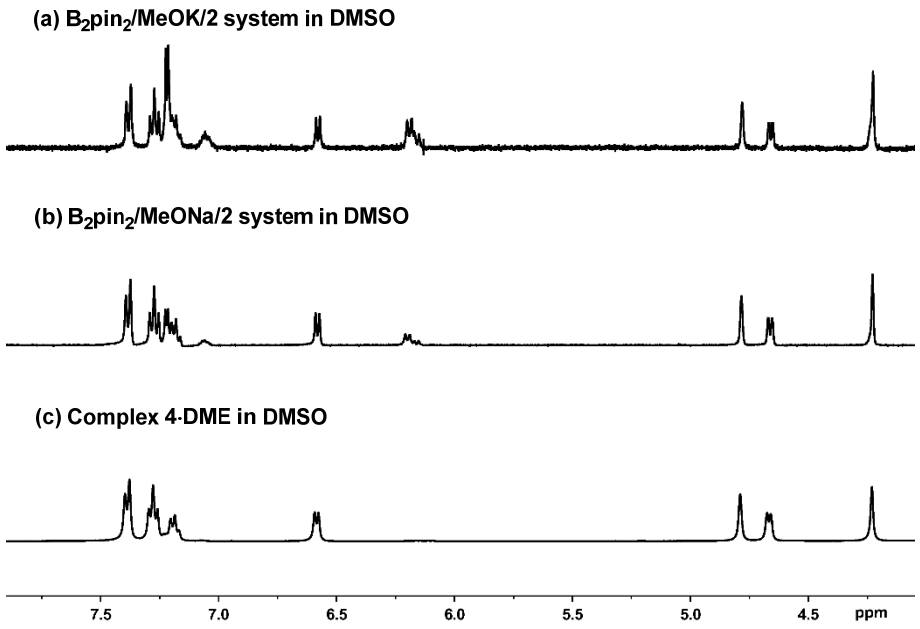
(2) B_2pin_2/MeONa/4-phenylpyridine system in DMSO

Experimental procedure: A 15 mL reaction tube was charged with B_2pin_2 (5.2 mg, 0.020 mmol), sodium methoxide (1.1 mg, 0.020 mmol), 4-phenylpyridine (3.1 mg, 0.020 mmol), and 1 mL of DMSO. The tube was sealed with a Teflon screw cap and the reaction mixture was allowed to react at room temperature for 2 h. During this time, the color of the solution gradually changed to purple. NMR analysis indicated complete consumption of 4-phenylpyridine and formation of a major species fully identical to that obtained in the B_2pin_2/MeOK/pyridine system.

(3) Complex **4**·DME in DMSO

To confirm the identity of the species generated in the above mentioned reaction systems, we compared the above ^{1}H NMR spectra with that of the independently prepared **4**·DME recorded in DMSO. The fully identical spectra indicated that the B_2pin_2/methoxide/pyridine system also produced complex **4** in DMSO.

^{1}H NMR of reaction mixture and complex **4**·DME in DMSO:



2.5 Electrochemical Study

To assess the redox character of complex **4**, we performed electrochemical study. Electrochemical experiments were performed on a CHI-660E electrochemical workstation by using a three-electrode system, in which glassy carbon (GC) electrode was used as the working electrode, platinum wire was used as the counter electrode, and a Ag^{+}/Ag electrode was used as the reference electrode. The experiments were conducted in a three-electrode cell under argon with a scan rate of 100 $mV \cdot s^{-1}$, employing anhydrous THF as the solvent and 0.1 M *n*-$Bu_4N^{+}PF_6^{-}$ as the supporting electrolyte. All measured potentials were relative to the potential of the $Fc^{+/0}$ couple. Both cyclic voltammetry (CV) and differential pulse voltammetry (DPV) experiments were conducted, and the peak potentials were read from the DPV plot (Figure S2).

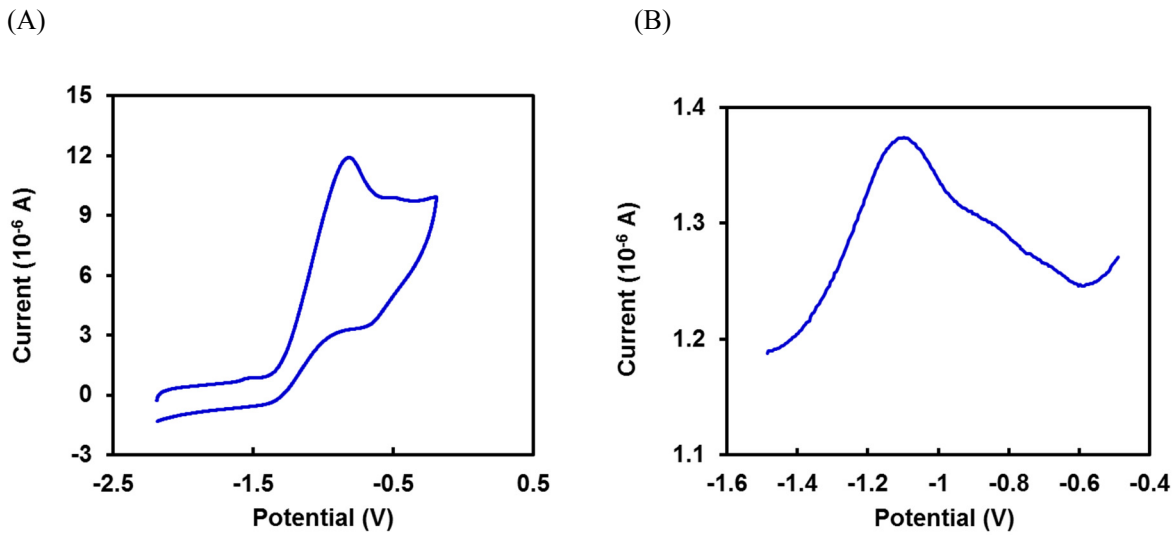
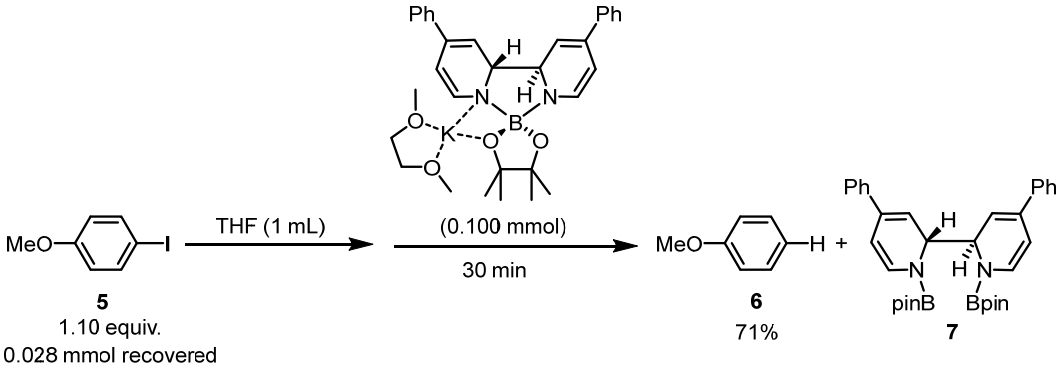


Figure S2. (A) CV of 2 mM electron donor **4**. (B) DPV of 2 mM electron donor **4**.

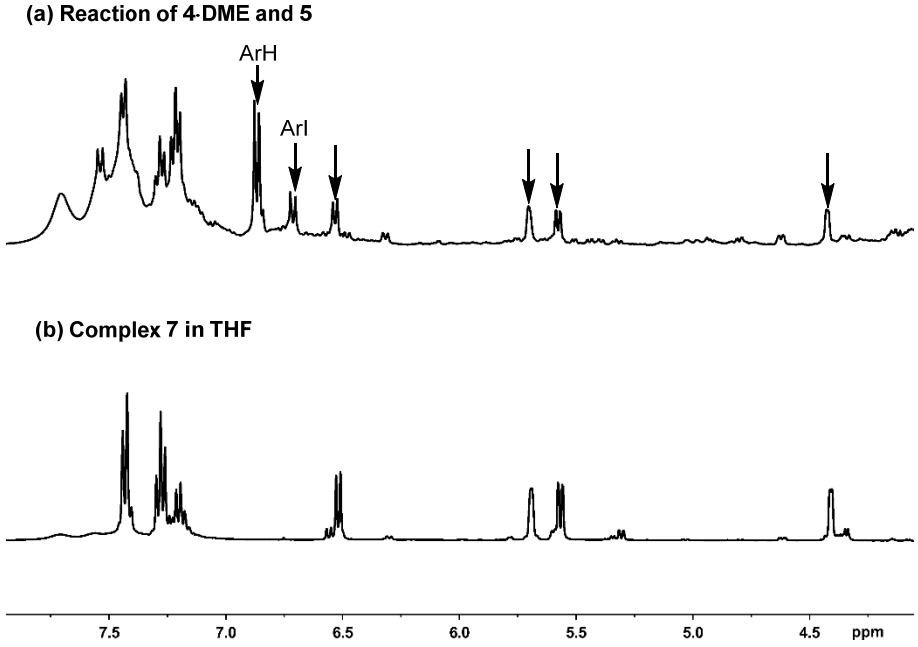
2.6 The Reaction between Complex 4·DME and MeOPhI

(1) NMR analysis of the reaction mixture

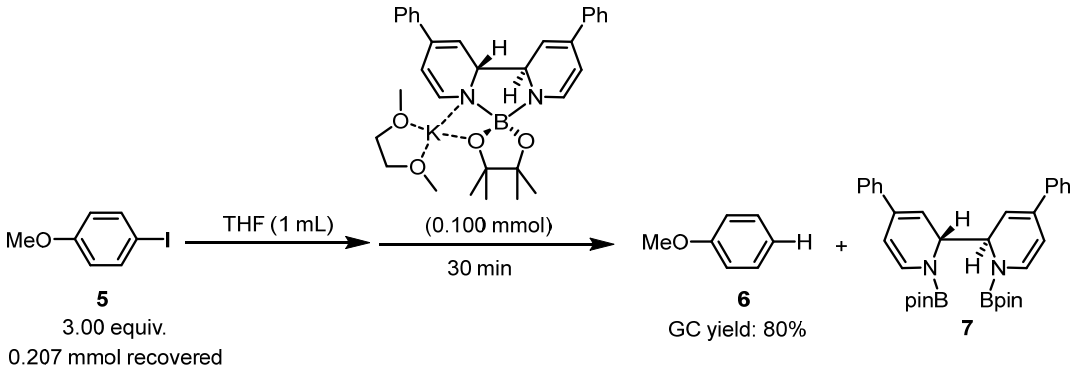


Experimental procedure: In a glove box, to a 15 mL reaction tube charged with a solution of 4-iodoanisole (25.7 mg, 0.110 mmol) in 1 mL of THF, electron donor **4**·DME (56.7 mg, 0.100 mmol) was gradually added. The tube was sealed with a Teflon screw cap and the reaction mixture was then allowed to react at room temperature for 1 h. The ^{1}H NMR analysis of the resulting mixture indicated complete consumption of **4**·DME and the production of both anisole and compound **7** (see Section 5.2 for independent preparation of compound **7** for comparison). GC analysis of the reaction mixture showed the 71% yield of anisole.

^{1}H NMR of the reaction between **4**·DME and MeOPhI in THF:



(2) GC analysis of the reaction mixture



Experimental procedure: In a glove box, to a 15 mL reaction tube charged with a solution of 4-iodoanisole (70.2 mg, 0.300 mmol) in 2 mL of THF, electron donor **4**·DME (56.7 mg, 0.100 mmol) was gradually added. The tube was sealed with a Teflon screw cap and the reaction mixture was then allowed to react at room temperature for 30 min. Then a standard solution of *n*-dodecane in toluene was added as the internal standard, followed by water. After shaking for 1 min, the organic layer was separated and analyzed by GC to obtain the yield of anisole.

3. Investigation of the EPR-Visible Species

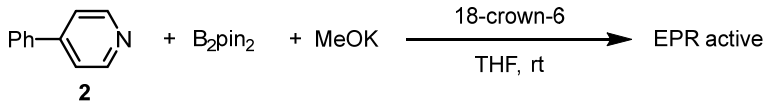
3.1 General

In order to gain more information on the radical species generated in the reductive mixture, we conducted detailed EPR study. The EPR measurement was performed on an X-band (9.05 GHz) EPR instrument JES FA200 (JEOL), and the measured spectrum were calibrated against the 3rd and 4th $^{55}Mn^{2+}$ signals (g = 2.033 and 1.981, respectively). All measurements were performed under Ar. Conditions for EPR measurement: microwave power (1 mW), central field (322.4 mT), magnetic width (5 mT), modulation width (0.1 mT), time constant (0.03 s), measurement time (4 min).

The structure utilized for the DFT calculation of the EPR spectrum was optimized at UB3LYP/6-31+G(d) level with the CPCM solvation model in THF. The calculation of the EPR spectrum was performed at the same level. The simulation of EPR spectrum was performed utilizing the EasySpin software.[10]

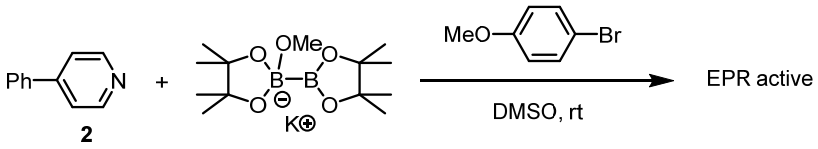
3.2 Preparation of EPR Samples in Figure 3

(1) EPR of the diboron/methoxide/4-phenylpyridine in THF



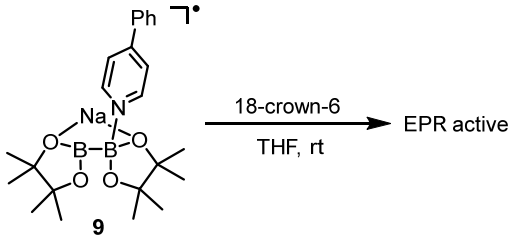
Experimental procedure: A 15 mL reaction tube was charged with B_2pin_2 (60.0 mg, 0.236 mmol), potassium methoxide (14.0 mg, 0.259 mmol), 18-crown-6 (63.0 mg, 0.239 mmol), 4-phenylpyridine (33.9 mg, 0.218 mmol), and 3 mL THF in a glove box. The mixture was allowed to react at room temperature for 2 h. A sample suitable for EPR analysis was prepared by diluting this solution with THF to a faint purple in color. A capillary was used to sample the solution and both ends of the capillary was sealed. The capillary was inserted into an EPR tube, which was subjected to EPR measurement. The obtained EPR spectrum is shown in Figure 3a.

(2) EPR of borylation reaction mixture in DMSO



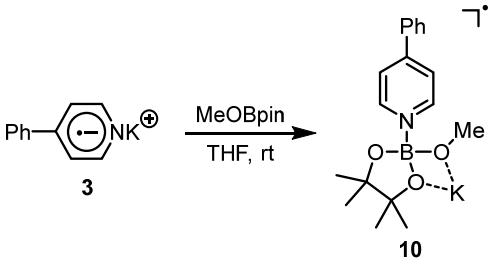
Experimental procedure: A 10 mL Schlenk tube was charged with B_2pin_2·MeOK ate complex (64.8 mg, 0.200 mmol), 4-phenylpyridine (15.5 mg, 0.100 mmol) in a glove box, then DMSO (1 mL) was added by syringe. After shaking up, 4-bromoanisole (18.7 mg, 0.100 mmol) was then added, a capillary was used to sample the solid liquid mixture and both ends of the capillary was sealed. The capillary was inserted into an EPR tube, which was subjected to EPR measurement. The obtained EPR spectrum is shown in Figure 3b. This spectrum was the EPR spectrum reported in our previous work.[11]

(3) EPR of the mixture of complex **9** and 18-crown-6



Experimental procedure: A 15 mL reaction tube was charged with compound **9** (4.7 mg, 0.0109 mmol, the synthetic procedure described in Section 3.5), 18-crown-6 (2.9 mg, 0.0109 mmmol) and THF (1.5 mL) in a glove box (the addition of 18-crown-6 to the mixture was to enhance the solubility of compound **9** in THF). A capillary was used to sample the solution and both ends of the capillary was sealed. The capillary was inserted into an EPR tube, which was subjected to EPR measurement. The obtained EPR spectrum is shown in Figure 3c.

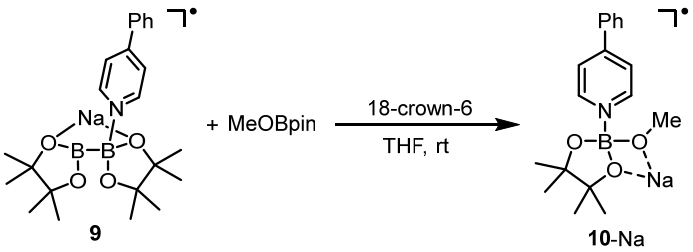
(4) EPR of independently prepared complex **10**



Experimental procedure: A 15 mL reaction tube was charged with 4-phenylpyridine (33.9 mg, 0.218 mmol), pottasium (8.5 mg, 0.217 mmol), and THF (3 mL) in a glove box. After 10 min, MeOBpin (36.0 mg, 0.214 mmol) was added. After 2 min, an aliquot of the reaction mixture was taken out and diluted with THF to faint purple in color. A capillary was used to sample the solution and both ends of the capillary was sealed. The capillary was inserted into an EPR tube, which was subjected to EPR measurement. The obtained EPR spectrum is shown in Figure 3d.

3.3 Exchange of Boron Lewis Acid between Complex 9 and Complex 10 in EPR

In order to further confirm the structure of **10**, we monitored the spectral change of complex **9** upon addition of MeOBpin. It was found that, after addition of MeOBpin, the broadened spectrum of complex **9** changed to a well-resolved spectrum similar to those shown in Figure 3a. This result indicated the exchange of the boron center between these two radical anion complexes.



Experimental procedure: A 15 mL reaction tube charged with compound **9** (4.7 mg, 0.0109 mmol),

18-crown-6 (2.9 mg, 0.0109 mmmol) and THF (1.5 mL) was added MeOBpin (3.7 mg, 0.0234 mmol) in a glove box. A capillary was used to sample the solution and both ends of the capillary was sealed. The capillary was inserted into an EPR tube, which was subjected to EPR measurement. The obtained EPR spectrum is shown in Figure S3.

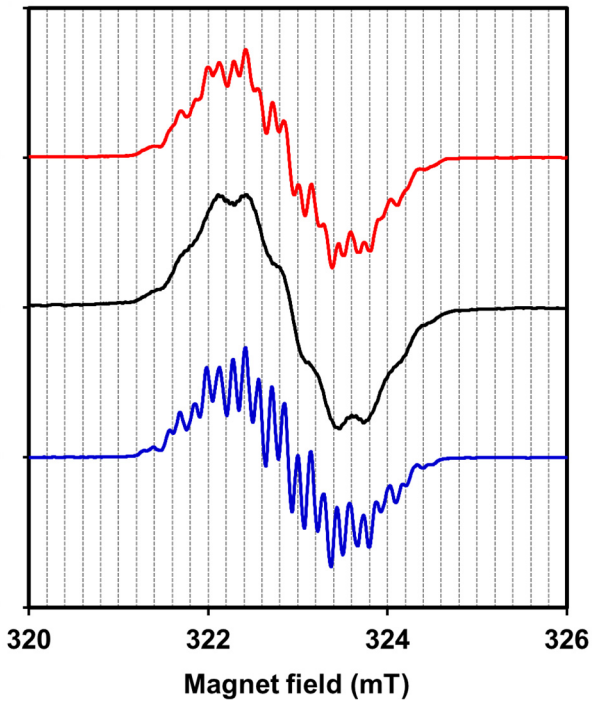


Figure S3. The exchange of boron Lewis acid in complex **9** monitored by EPR. Red line: EPR of the mixture of complex **9** and MeOBpin; black line: EPR spectrum of complex **9**; blue line: EPR of complex **10**.

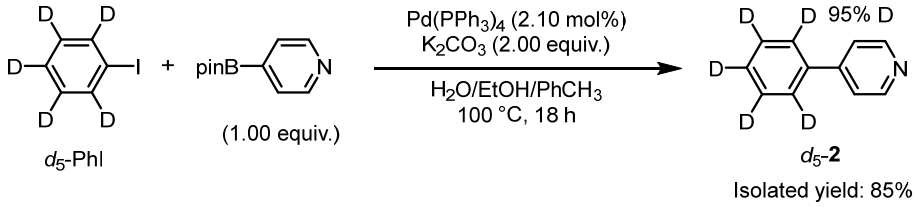
The obtained EPR spectrum has peaks all identical to those of complex **10**, however, the resolution was inferior. It is reasonable to attribute the slightly broadened EPR spectrum of reaction mixtures containing B_2pin_2 to the formation of a small fraction of complex **9**.

3.4 Synthesis and EPR study of Partially-Deuterated Complex 10

In order to further confirm the proposed structure as well as the coupling constants of the radical anion complex **10**, additional EPR study was conducted on partially-deuterated complex **10**. We employed d_5-**2**, in which the phenyl ring was deuterated, to synthesize complex **10**. By comparison of the determined EPR spectrum with the predicted one ($a(^1H)/a(^2H) \approx 6$), the identity of complex **10** could be further supported.

Deuterated iodobenzene was synthesized following the published procedure.[12] Deuterated 4-phenylpyridine (d_5-**2**) was synthesized following a modified condition of published procedure. [13]

(1) Synthesis of partially-deuterated 4-phenylpyridine d_5-**2**



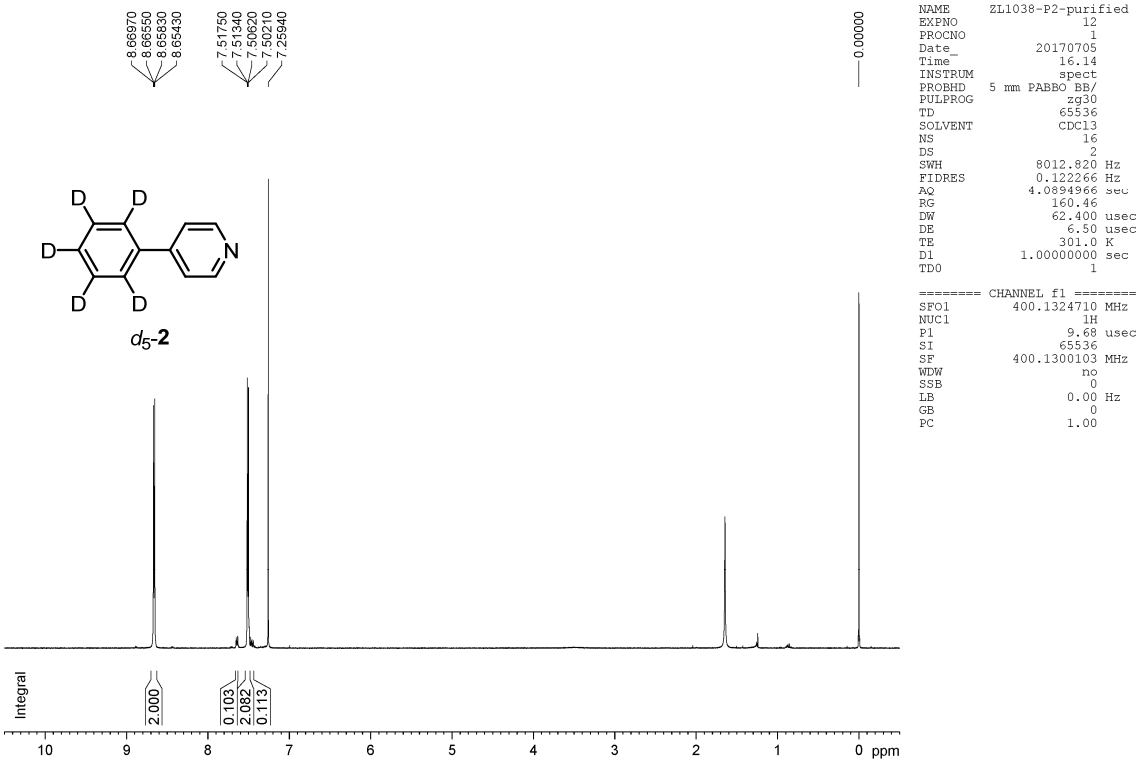
d_5-PhI

d_5-**2**

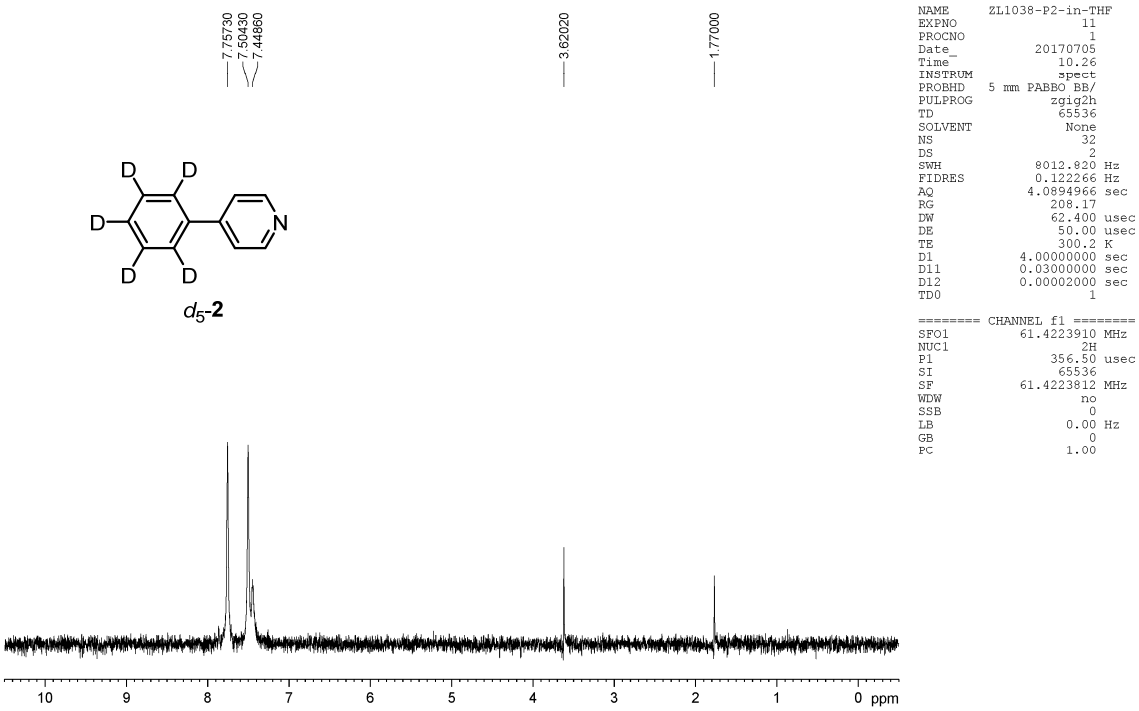
Isolated yield: 85%

Experimental procedure: A 15 mL reaction tube charged with 4-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolanyl)-pyridine (205.0 mg, 1.00 mmol), K_2CO_3 (276.0 mg, 2.00 mmol), and $Pd(PPh_3)_4$ (24.0 mg, 0.0207 mmol) was added water (1 mL), toluene (1.5 mL), and ethanol (0.5 mL). Deuterated iodobenzene (d_5-PhI, 209.0 mg, 1.00 mmol) was then added to the solution by syringe. The reaction mixture was refluxed under an argon atmosphere for 18 h. After cooling to room temperature, the reaction mixture was poured into water and then extracted with toluene. The combined organic phase was washed with brine and dried over Na_2SO_4. After evaporation, the crude mixture was purified by flash column chromatography on silica gel (eluted with 5:1 petroleum ether/EtOAc) to afford d_5-**2** in 86% yield (138.3 mg). The NMR data were in consistent with the reported data.[14] The ^{1}H NMR showed that the deuteration ratio is 95% and the deuterated positions are confirmed by ^{2}H NMR spectrum.

^{1}H NMR of d_5-**2** in $CDCl_3$:

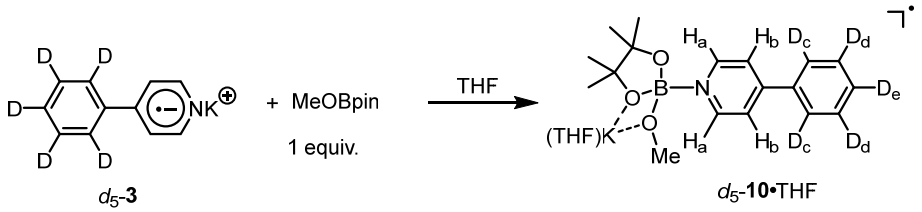


^{2}H NMR of deuterated d_5-**2** in THF:



d_5-**2**

(2) EPR study



d_5-**3** d_5-**10**•THF

Experimental procedure: A 15 mL reaction tube was charged with partially-deuterated 4-phenylpyridine d_5-**2** (34.8 mg, 0.218 mmol), potassium (8.5 mg, 0.217 mmol), and THF (3 mL) in a glove box. After 10 min, MeOBpin (36.0 mg, 0.214 mmol) was added. After 2 min, an aliquot of the reaction mixture was taken out and diluted with THF to faint purple in color. A capillary was used to sample the solution and both ends of the capillary was sealed. The capillary was inserted into an EPR tube, which was subjected to EPR measurement. The obtained EPR spectrum is shown in Figure S4.

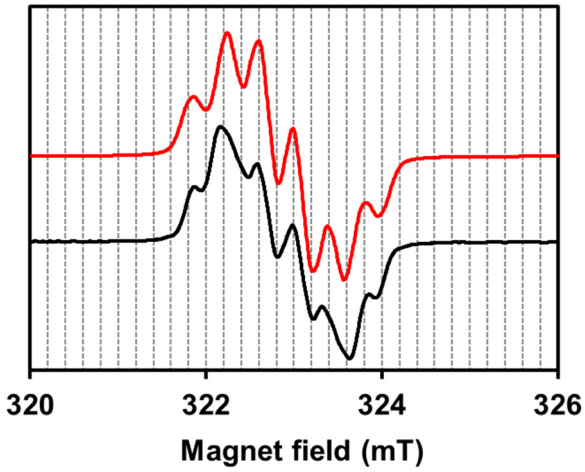
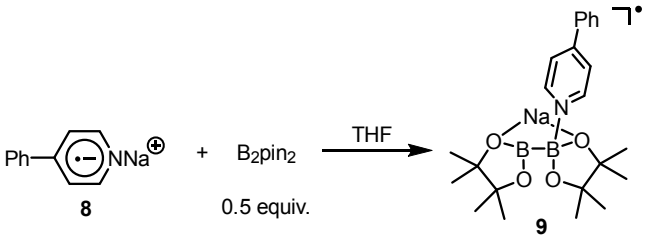


Figure S4. Predicted EPR spectrum and the experimental EPR spectrum. Red line: Predicted EPR spectrum utilizing hyperfine coupling constants derived from that in Table 1, $a(2D_c)$ = 1.6 MHz, $a(2D_d)$ = 0.6 MHz, $a(2D_e)$ = 1.7 MHz; black line: Experimental EPR spectrum of compound d_5-**10**.

The EPR spectrum resulted from of d_5-**10** are identical to that predicted using the hfcs derived from complex **10**. This further verified the structural assignment of complex **10**.

3.5 Synthesis and Characterization of Complex 9

(1) Synthesis of complex **9**



Isolated yield: 47%

Experimental procedure: A 35 mL reaction tube was charged with 4-phenylpyridine (155.0 mg, 1.00 mmol), sodium (23.0 mg, 1.00 mmol), and THF (10 mL) in a glove box, and the resulting mixture was allowed to react at room temperature for 30 min. Then B_2pin_2 (127.0 mg, 0.500 mmol) was added to the mixture and the color changed from blue to purple. Crystals started to precipitate in 5 min, and after 2 h, the crystals were filtered and dried under vacuum to afford complex **9** in 47% yield (205.0 mg).

Crystals of complex **9** suitable for X-ray diffraction analysis were obtained by applying a reactive crystallization protocol. Following the experimental procedure described above, after the preparation of radical anion **8**，a solution of B_2pin_2 in hexane was carefully added to the top to form a two layer system. After standing overnight at room temperature in the glove box, crystals of complex **9** were obtained and submitted to XRD analysis.

(2) XRD of complex **9**·THF

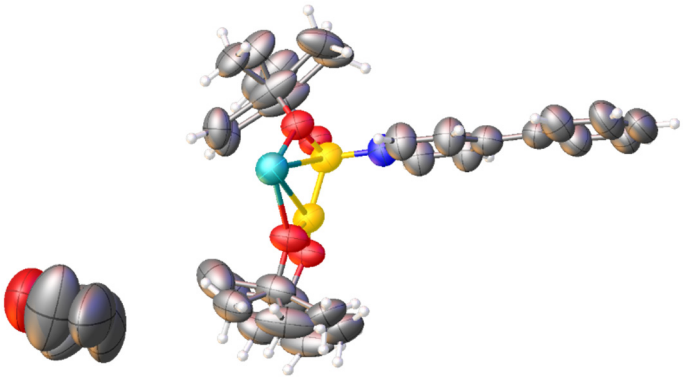
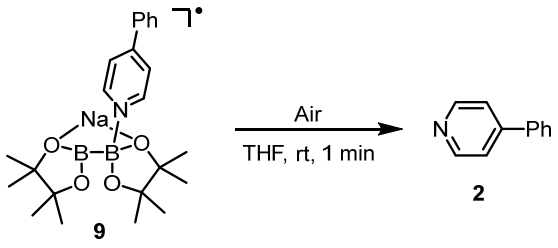


Figure S5. Ortep drawing of compound **9**·THF with 50% ellipsoids.

Molecular Formula	$0.5(C_{46}H_{48}B_4N_2Na_2O_8)$, C_4O
	$C_{27}H_{32}B_2NNaO_5$
Formula mass	495.14
Crystal size/mm^3	0.35×0.1×0.02
Crystal system	orthorhombic
Space group	Pbcm (I.T.-No.: 57)
a /Å	14.245(2)
b /Å	17.905(2)
c /Å	11.3809(9)
α	90
β	90
γ	90
Volume /Å^3	2902.9(6)
ρ_{calcd} /g · cm^{-3}	1.133
T /K	173.00(10)
Radiation	CuK_α, λ = 1.54184 Å
Measured reflns	8843
Indep. reflns	2355
param./restraints	214/0
θ range	3.965° — 61.167°
GoF on F_2	1.051
R_{int}	0.0556
R_1 *[I > 2σ(I)]*	0.0895
*w*R2 (all data)	0.2854
max / min peaks /e Å^{-3}	0.329, -0.222
CCDC number	1578447

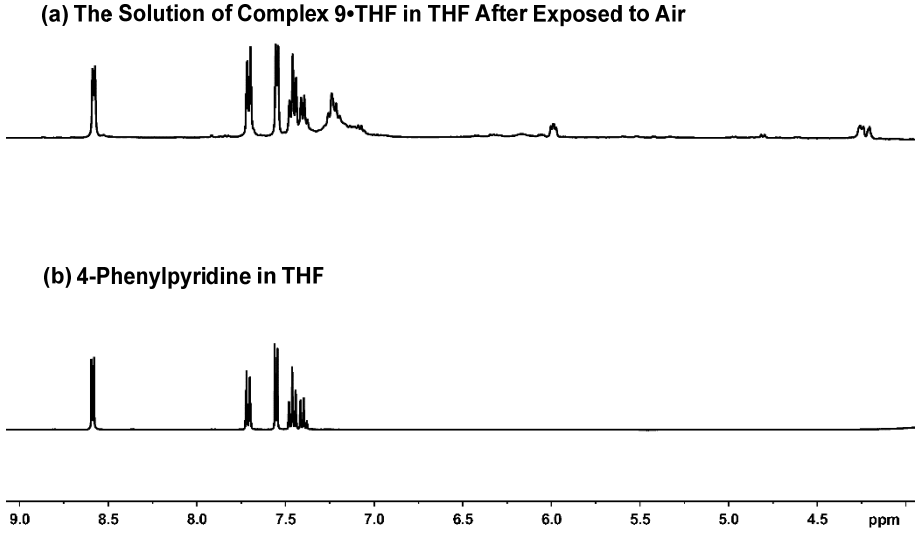
In this crystal structure, the occupancy of the methyl groups is not 100% but two 50% parts. Therefore, after one symmetry operation of the asymmetric unit, it collide with itself. Some hydrogen atoms on this part failed to be added because of this reason.

Decomposition pathway of **9**·THF:



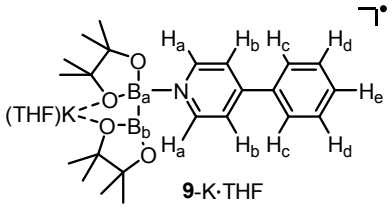
When the THF solution of **9**·THF was exposed to air, the purple color of the solution immediately faded and the ^{1}H NMR spectrum showed that **9**·THF had been oxidized to 4-phenylpyridine. This result is in accordance with the electron donor character of complex **9**.

^{1}H NMR spectrum of the solution of **9**·THF in THF after exposed to air:



(3) EPR simulation of complex **9**

The coupling constants of the complex **9** was also calculated based on the DFT calculation and EasySpin simulation. The DFT results showed that the couplings constants are very similar with that of complex **10**. Even though the EPR spectrum of complex **9** was broadening and relatively fewer information could be obtained, based on the experimental coupling constants of complex **10**, DFT calculation, as well as the XRD crystal structure, the EPR spectrum was solved.



9-K·THF

Table S1. Hyperfine coupling constants of complex **9**-K·THF (g = 2.0030)

hfcs/MHz	$a(^{11}B_a)$	$a(^{11}B_b)$	a(N)	$a(2H_a)$	$a(2H_b)$	$a(2H_c)$	$a(2H_d)$	$a(H_e)$
Exptl.	3.6	1.6	11.0	12.9	1.7	8.7	2.8	8.7
DFT	-3.8	3.3	12.7	-9.3	0.9	-9.7	3.8	-12.6

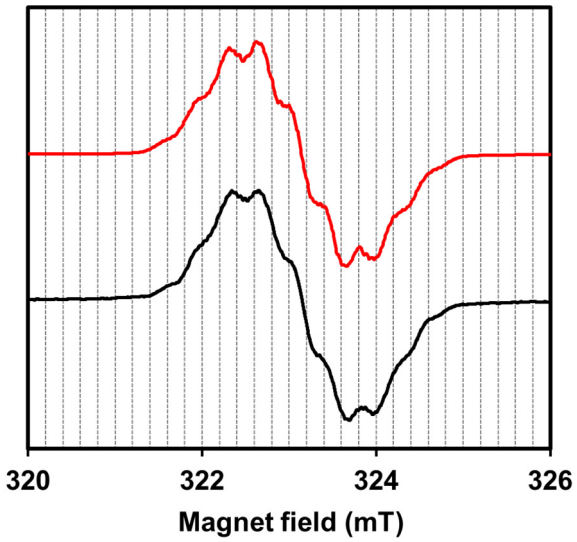


Figure S6. The experimental and simulated EPR spectra of complex **9**. Red line: simulated EPR spectrum of **9**; black line: EPR spectrum of complex **9** which is taken from Figure 3c.

Compared with the coupling constants of radical anion complex **10**, the couplings are very similar with that of complex **9** except a new boron center coupling which is not big. Because of the small coupling of this boron center, the spectrum is broadening.

3.6 EPR Simulation of Reaction Mixture

It was found that the resolution of the reaction mixture EPR spectrum was inferior than that of complex **10**, which could be attributed to the formation of some complex **9** in the reaction mixture because the reaction mixture contains B_2pin_2 and the exchange of boron center between complex **9** and complex **10** was observed. With the hyperfine coupling constants of complex **9** and complex **10** in hand, the EPR simulation of the

reaction mixture could be carried out utilizing EasySpin software by giving these two species different weights.

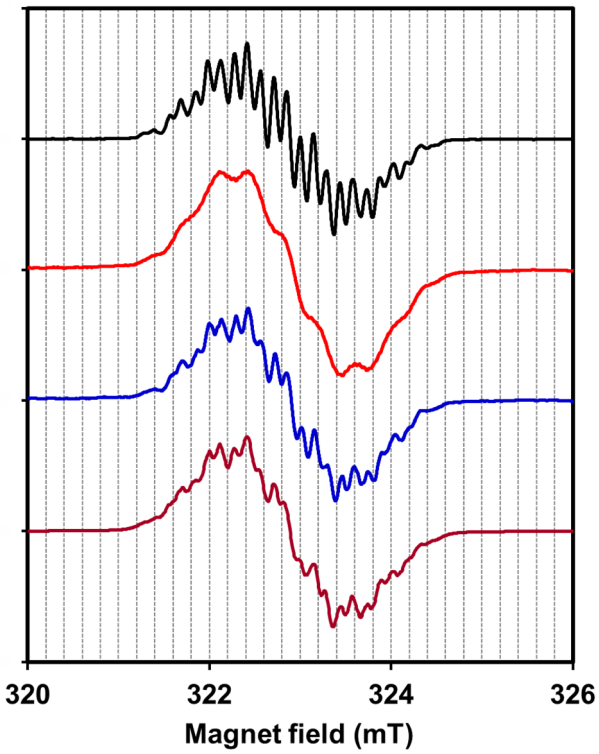


Figure S7. EPR Simulation of reaction mixture. Black line: EPR spectrum of complex **10** (taken from Figure 3d); red line: EPR spectrum of complex **9** (taken from Figure 3c); blue line: EPR spectrum of the B_2pin_2/MeOK/**2**/18-C-6 mixture (taken from Figure 3a); brown line: simulated EPR spectrum of reaction mixture with a combination of the simulated spectra of **9** (weight = 70%) and **10** (weight = 30%).

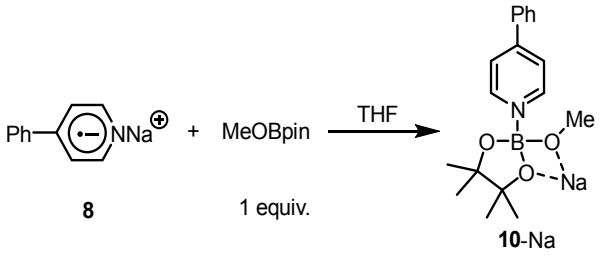
The simulated weighted average EPR spectrum (Figure S7), with 70% of complex **9** and 30% of complex **10**, well reproduced that of the reaction mixture. This verified that the EPR-visible species in the reaction mixture are complexes **9** and **10**.

3.7 The Effect of Cations on the EPR Spectra

It was found that, different cations (K^+ or Na^+) did not alter the EPR signals. This indicated that the study performed with either potassium or sodium methoxide made no difference in the elucidation of structures of these radical species.

(1) EPR of radical anion species utilizing sodium

Experimental procedure: A 15 mL reaction tube was charged with 4-phenylpyridine (33.9 mg, 0.218 mmol), sodium (5.0 mg, 0.217 mmol), and THF (3 mL) in a glove box. After 10 min, MeOBpin (36.0 mg, 0.214 mmol) was added. After 2 min, an aliquot of the reaction mixture was taken out and diluted with THF to faint purple in color. A capillary was used to sample the solution and both ends of the capillary was sealed. The capillary was inserted into an EPR tube, which was subjected to EPR measurement. The obtained EPR spectrum is shown in Figure S8.



8 10-Na

(2) Comparison between K^+- and Na^+-containing complex **10**

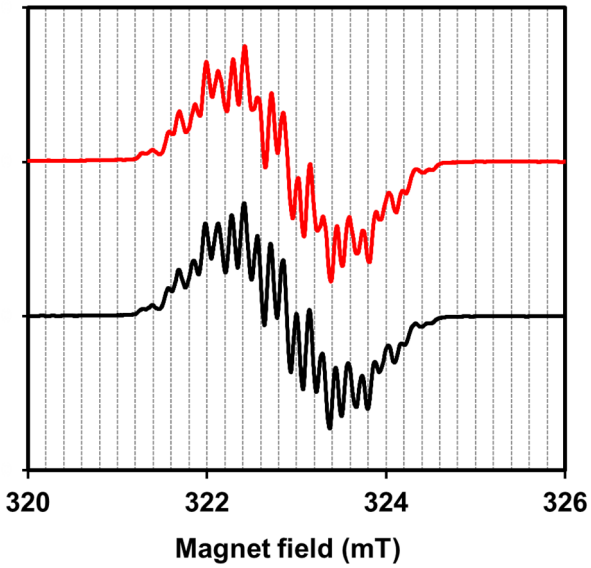
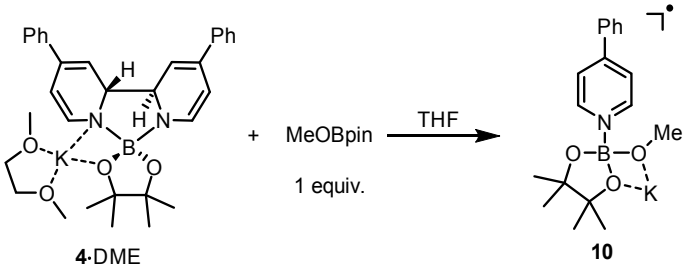


Figure S8. Comparison of radical anion species with different cations. Red line: EPR spectrum of complex **10**-Na (sodium is cation); black line: EPR spectrum of complex **10** (potassium is cation) which is taken from Figure 3d.

3.8 The Production of Radical Anion Complex 10 from Ate Complex 4

It was found that complex **10** could be produced by mixing **4**·DME and MeOBpin. The EPR spectrum was compared and it was identical to that shown in Figure 3d.

(1) Preparation of **10** by mixing **4**·DME and MeOBpin



4·DME **10**

Experimental procedure: In a glove box, to a 15 mL reaction tube charged with a solution of **4**·DME (5.7 mg, 0.01 mmol) in 1 mL of THF, MeOBpin (1.6 mg, 0.01 mmol) was added. A capillary was used to sample the solution and both ends of the capillary was sealed. The capillary was inserted into an EPR tube, which was subjected to EPR measurement. The obtained EPR spectrum is shown in Figure S9.

(2) Generation of complex **10** after adding MeOBpin to **4**·DME solution

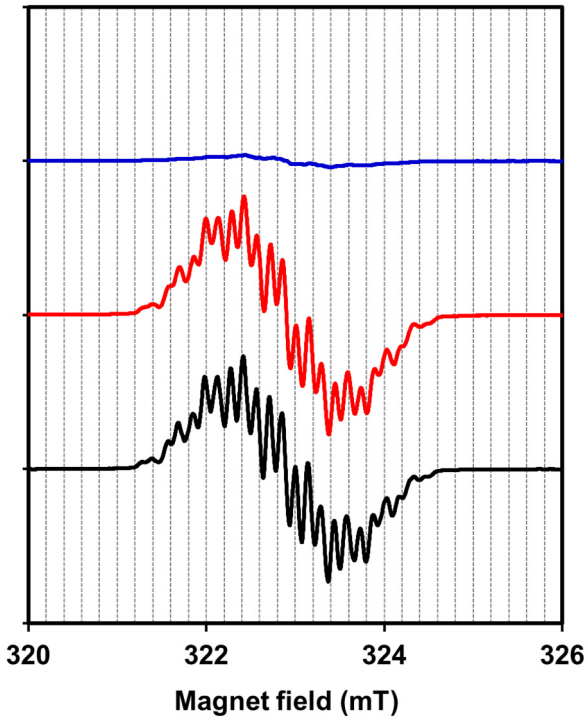


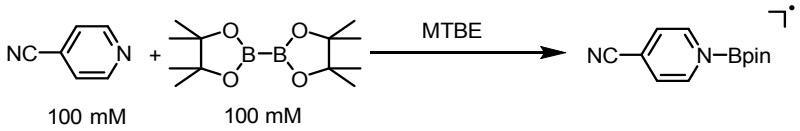
Figure S9. The reaction between complex **4** and MeOBpin. Blue line: EPR spectrum of **4**·DME; Red line: EPR spectrum of the mixture of **4**·DME and MeOBpin; black line: EPR spectrum of complex **10** which is taken from Figure 3d.

3.9 EPR Study on the Diboron/Methoxide/4-Cyanopyridine System

In the EPR study mentioned before, the radical species produced in the diboron/methoxide/pyridine system was the complex of pyridine radical anion and boron Lewis acid. In order to further investigate the universality of this mechanism, additional EPR study on a different pyridine additive was carried out.

It has been established previously that, 4-cyanopyridine cleaves the diboron without alkoxide to form pyridine-stablized boryl radical. Therefore we chose the diboron/4-cyanopyridine system as a suitable model to see whether or not a different radical species, the pyridine radical anion-borate complex, could be produced in the presence of methoxide.

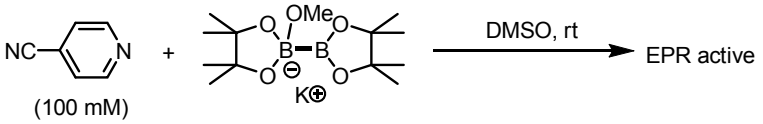
(1) EPR of diboron/4-cyanopyridine system



Experimental procedure: A 15 mL reaction tube was charged with 4-cyanopyridine (10.5 mg, 0.100 mmol) and B_2pin_2 (25.3 mg, 0.100 mmol) in a glove box, then MTBE (1 mL) was added by syringe. After 5 min, a capillary was used to sample the solution and both ends of the capillary was sealed. The capillary was inserted into an EPR tube, which was subjected to EPR measurement. The obtained EPR spectrum is shown in Figure S10 which is identical to that reported by Li and co-workers.[15]

(2) EPR of diboron/methoxide/4-cyanopyridine system

Experimental procedure: A 15 mL reaction tube was charged with 4-cyanopyridine (10.5 mg, 0.100 mmol) in a glove box, then DMSO (1 mL) was added by syringe. After dissolvation, a capillary was used to sample the solution and one end of the capillary was charged with ate complex B_2pin_2·MeOK. Then both ends of the capillary was sealed and the two components were allowed to react in the capillary at room temperature. The capillary was inserted into an EPR tube, which was subjected to EPR measurement. The obtained EPR spectrum is shown in Figure S10.



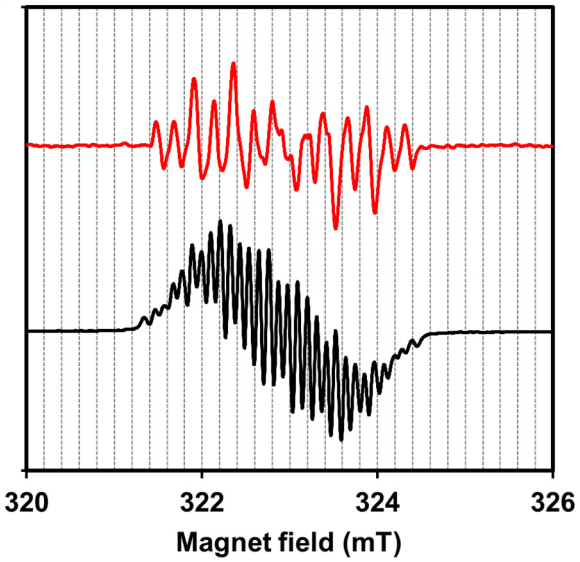
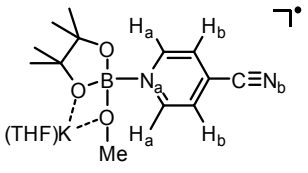


Figure S10. EPR spectra of the two reaction systems. Red line: the diboron/4-cyanopyridine system; black line: the diboron/methoxide/4-cyanopyridine system.

It was clear that the diboron/methoxide/4-cyanopyridine system exhibited a distinct EPR spectrum to that of the diboron/4-cyanopyridine system, confirming that in the presence of methoxide, different radical species was generated.

(3) Simulation of EPR Spectrum

Simulation and DFT calculation of the EPR spectrum of the diboron/methoxide/4-cyanopyridine system were performed based on the proposed radical anion-borate complex (Table S2 and Figure S11).



16·THF

Table S2. Hyperfine coupling constants of complex **16**·THF (g = 2.0032)

hfcs/MHz	$a(^{11}B_a)$	$a(N_a)$	$a(N_b)$	$a(2H_a)$	$a(2H_b)$
Exptl.	4.1	15.3	9.2	9.5	2.7
DFT	-5.7	14.7	7.9	-10.5	-2.3

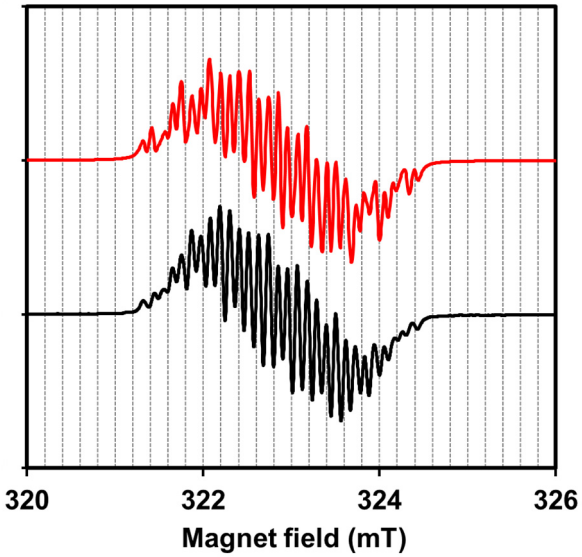


Figure S11. The simulated (red) and experimental (black) EPR spectrum of the diboron/methoxide/4-cyanopyridine system.

The above results confirmed the identity of the radical species in the diboron/methoxide/4-cyanopyridine system, which showed that in the presence of methoxide, the cleavage of diboron by pyridine indeed proceeds via the heterolytic cleavage pathway.

4. UV-Vis Spectroscopic Study

4.1 Preparation of the UV-Vis Samples

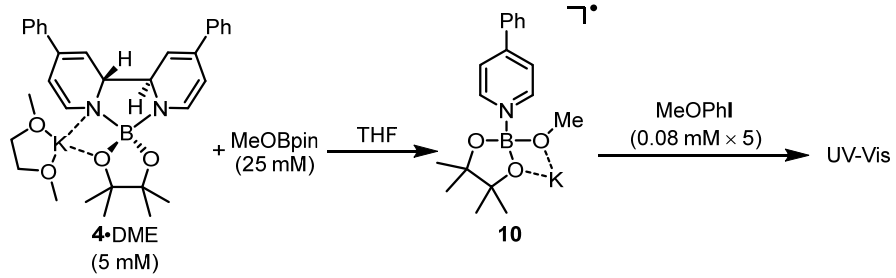
(1) UV-Vis of complex **4**·DME

Experimental procedure: A 15 mL reaction tube was charged with complex **4**·DME (1.2 mg, 2.1 μmol) and 2 mL THF in a glove box. After dissolvation, the solution was transferred to the cuvette with 1 cm optical path utilizing an oven-dried glass Pasteur pipette. The UV-Vis spectrum of complex **4**·DME was shown in Figure 4a.

(2) UV-Vis of complex **9**

Experimental procedure: A 15 mL reaction tube was charged with complex **9**·THF (0.5 mg, 1 μmol), 1 mL THF and 18-crown-6 (0.3 mg, 1 μmol) in a glove box. After dissolvation, the solution was transferred to the cuvette with 1 mm optical path utilizing an oven-dried glass Pasteur pipette. The UV-Vis spectrum of complex **9** was shown in Figure 4a.

(3) UV-Vis of complex **10** and the spectral change during addition of electron acceptor



Experimental procedure: A solution containing complex **10** was prepared by mixing electron donor **4**·DME (14.2 mg, 0.0250 mmol), THF (5 mL), and MeOBpin (19.8 mg, 0.125 mmol) in a reaction tube. ^{1}H NMR analysis showed that the conversion was incomplete (ca. 20%) and the mixture contained both complexes **4** and **10**. The mixture was transferred to the cuvette utilizing an oven-dried glass Pasteur pipette. The UV-Vis spectrum of the mixture were shown in Figure 4a. The mixture in the reaction tube was then added 4-iodoanisole (0.1 mg each time, 0.4 μmol× 5 times), and after each addition, an aliquot of the reaction solution was transferred to the cuvette for UV-Vis measurement. The obtained UV-Vis spectrum were shown in Figure 4b.

4.2 TD-DFT Calculation of UV-Vis Spectrum

In order to further confirm the structure of radical anion complex **10**, the UV-Vis spectra of complexes **9**·THF and **10**·THF were computed. The structures were optimized at the UB3LYP/6-31+G(d) level with the CPCM solvation model (THF as the solvent). The UV-Vis spectra were computed by time-dependent density functional theory (TDDFT, NStates = 50) at the UB3LYP/TZVP level with the CPCM solvation model (THF as the solvent). The parameters int=ultrafine and scf=tight were applied. The computed UV-Vis spectra were plotted using a 0.333 eV half-width at half-height.

The calculated UV-Vis spectrum of complex **9**·THF (two absorptions at 356 and 509 nm) fits the experimental spectrum (two absorptions at 381 and 573 nm), albeit a small blue shift were observed (Figure S12). The calculated UV-Vis spectrum of complex **10**·THF (two absorptions at 351 and 500 nm nm) also in

agreement with the experimental spectrum (two absorptions at 377 and 567 nm) (Figure S13). These results further confirmed the proposed structure of compound **10**.

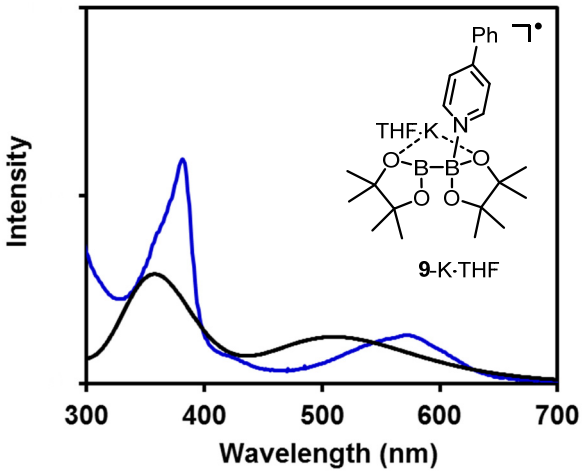


Figure S12. The comparison between the calculation and experimental results. Blue line: UV-Vis spectrum of the solution of **9**; black line: calculated UV-Vis spectrum of complex **9**-K·THF.

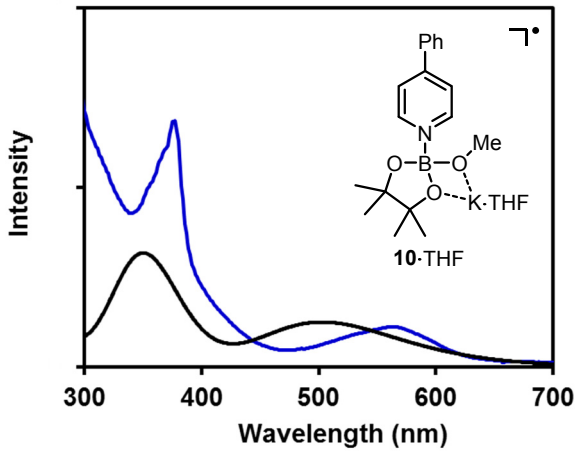
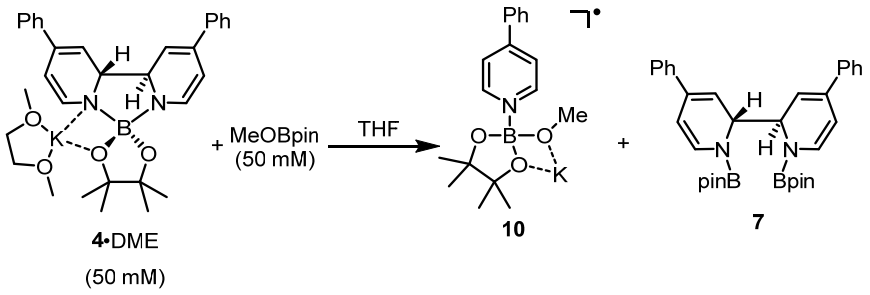


Figure S13. The comparison between the calculation and experimental results. Blue line: UV-Vis spectrum of the mixture of complex **4**·DME and MeOBpin; black line: calculated UV-Vis spectrum of complex **10**·THF.

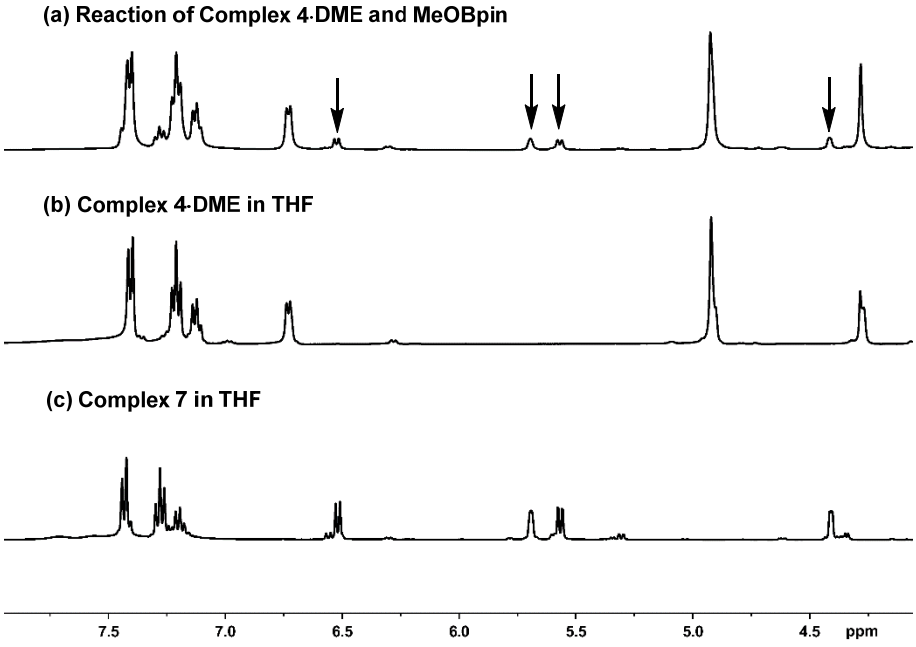
5. Interconversion of the Boryl-Pyridine Species

5.1 Production of Radical Anion Complex 10 and Boryl-Bipyridine Compound 7 from Complex 4



Experimental procedure: A 15 mL reaction tube was charged with complex **4**·DME (28.4 mg, 0.05 mmol) and THF (1 mL). Then MeOBpin (8.5 mg, 0.05 mmol) was added to the mixture and the color of the mixture gradually changed from yellow to purple. After 5 min, the mixture was analyzed by NMR, which showed incomplete conversion of **10** and the formation of a new species **7**. Based on the integral of corresponding signals of **10** and **7** in ^{1}H NMR spectrum, the conversion was estimated to be ca. 20%. EPR analysis of a diluted sample showed the formation of intense signals identical to the previously acquired EPR spectrum of **10** (see Section 3.8 for details). Both NMR and EPR results confirmed the formation of radical species **10** and boryl-bipyridine compound **7** from complex **4** after treatment with a boron Lewis acid.

^{1}H NMR of reaction between compound **4·DME** and MeOBpin:

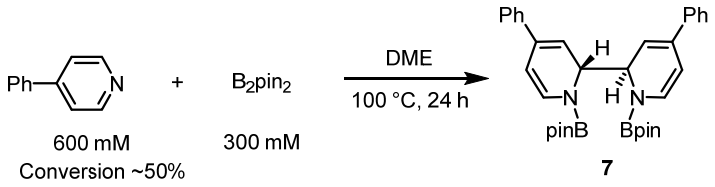


5.2 Independent Synthesis of Compound 7

Compound **7** could be synthesized by two methods. First, the reaction of B_2pin_2 and 4-phenylpyridine via a [3,3]-sigmatropic rearrangement pathway.[16] Second, the reaction of Cl-Bpin and complex **4**·DME via nucleophilic substitution reaction because chloride anion is good a leaving group compared with methoxide

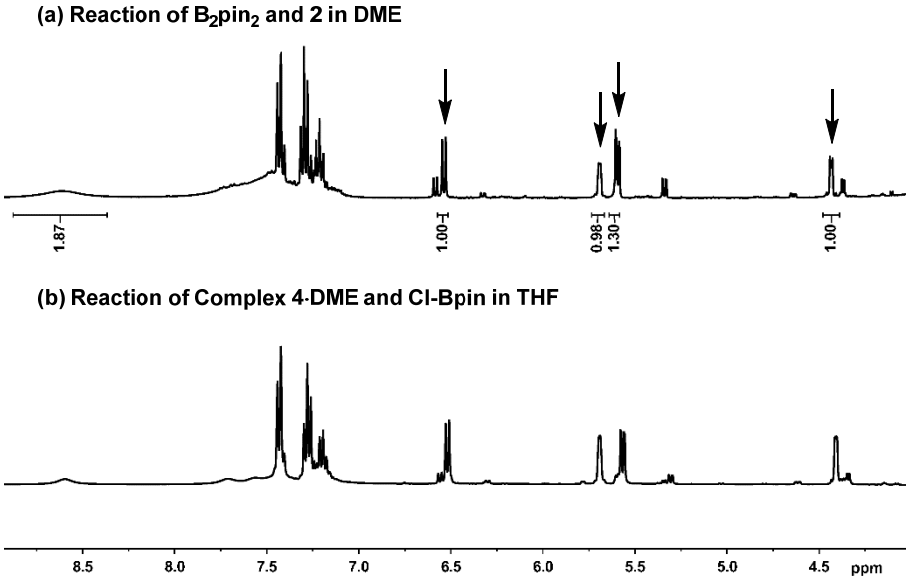
anion.

(1) [3,3]-sigmatropic rearrangement

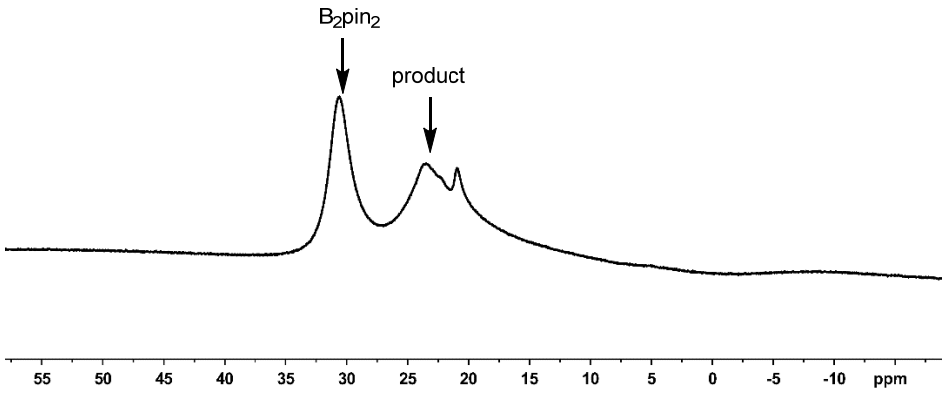


Experimental procedure: A 15 mL reaction tube was charged with a magnetic stir bar, 4-phenylpyridine (93.0 mg, 0.600 mmol), B_2pin_2 (76.3 mg, 0.299 mmol), and 1 mL of DME in a glove box. The tube was sealed with a Teflon screw cap and the reaction mixture was stirred in an oil bath at 100 °C for 24 h. The reaction mixture was then cooled to room temperature and analyzed by NMR, which showed that about 50% compound **7** was produced.

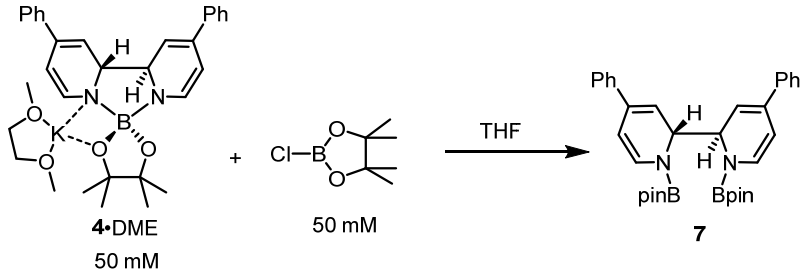
^{1}H NMR of synthesized compound **7** in DME by [3,3]-sigmatropic rearrangement:



^{11}B NMR of synthesized compound **7** in DME by [3,3]-sigmatropic rearrangement:



(2) Nucleophilic substitution reaction



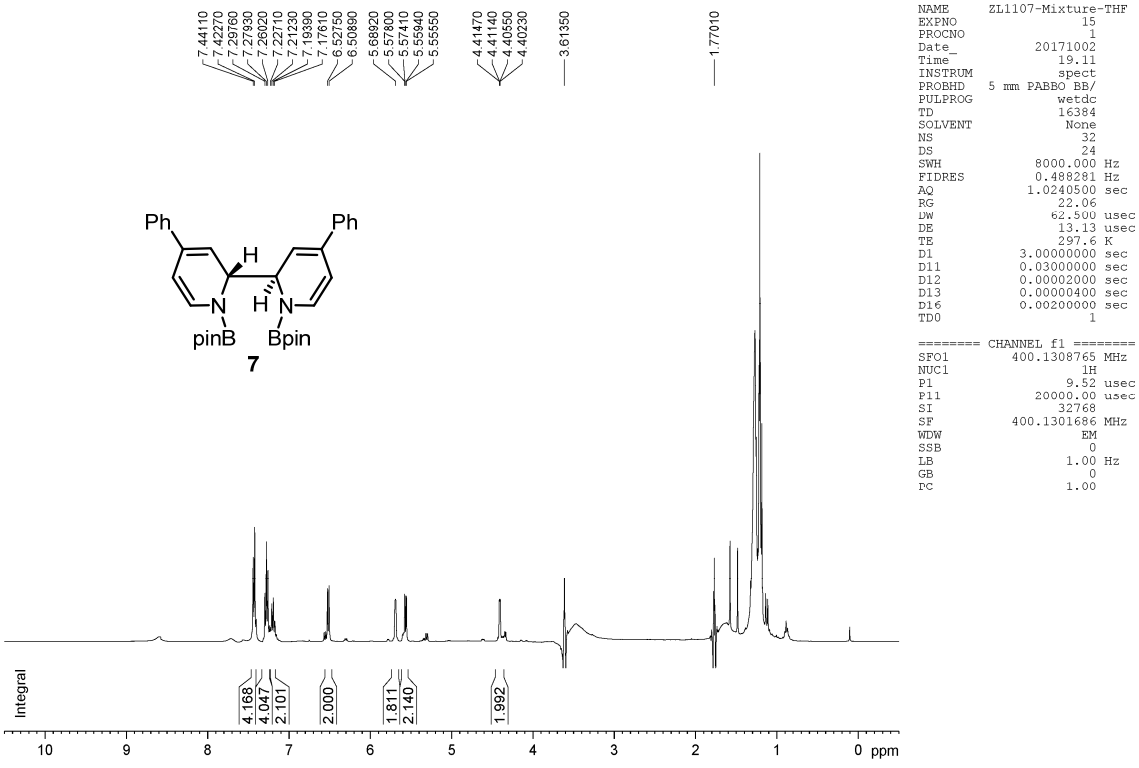
Experimental procedure: A 15 mL reaction tube was charged with a magnetic stir bar, electron donor **4**·DME (28.3 mg, 0.050 mmol), ClBpin (8.8 mg, 0.054 mmol), and THF (1 mL) in a glove box. After reacted for 5 min at room temperature, the solvent was removed under high vacuum. Then fresh THF (0.5 mL) was added and the resulting solution was analyzed by NMR, which showed that only compound **7** could be observed. This was used as an authentic sample to confirm the formation of **7** in other reactions.

^{1}H NMR (400 MHz, THF): δ 7.43 (d, J = 7.5 Hz, 4H), 7.28 (t, J = 7.5 Hz, 4H), 7.20 (t, J = 7.5 Hz, 4H), 6.52 (d, J = 7.5 Hz, 2H), 5.69 (s, 2H), 5.57 (d, J = 7.5 Hz, 2H), 4.41 (s, 2H), 1.27 (s, 24H).

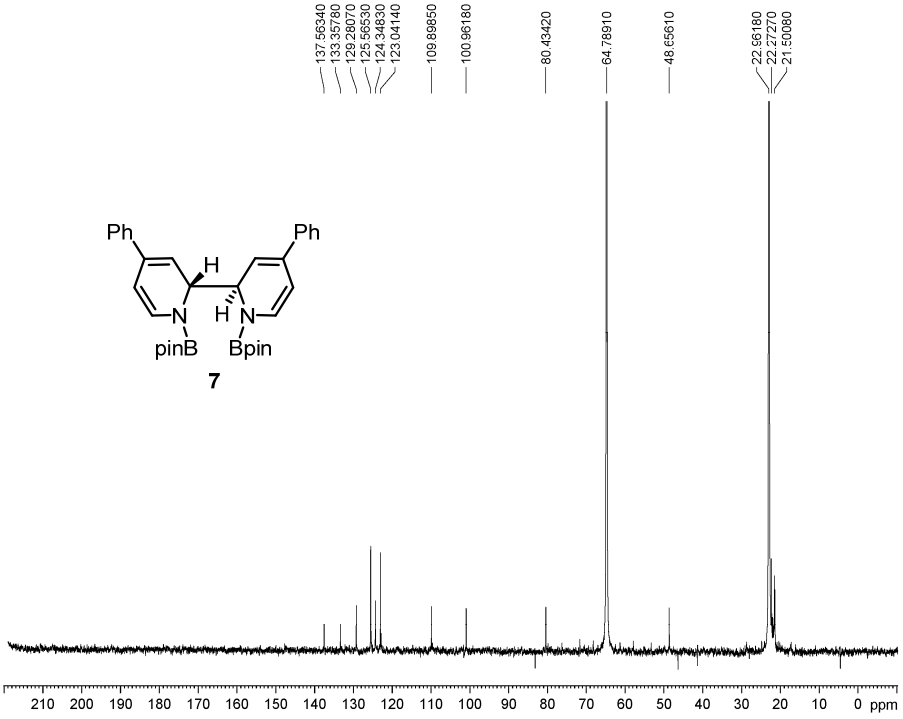
^{13}C NMR (100 MHz, THF): δ 137.6, 133.4, 129.3, 125.6, 124.3, 123.0, 109.9, 101.0, 80.4, 48.7, 22.3, 21.5.

^{11}B NMR (128 MHz, THF): δ 24.1.

^{1}H NMR of synthesized compound **7** in THF by nucleophilic substitution reaction:



^{13}C NMR of compound **7** in THF by nucleophilic substitution reaction:

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PROCNO                         1
Date_                   20171002
Time                       17.37
INSTRUM                    spect
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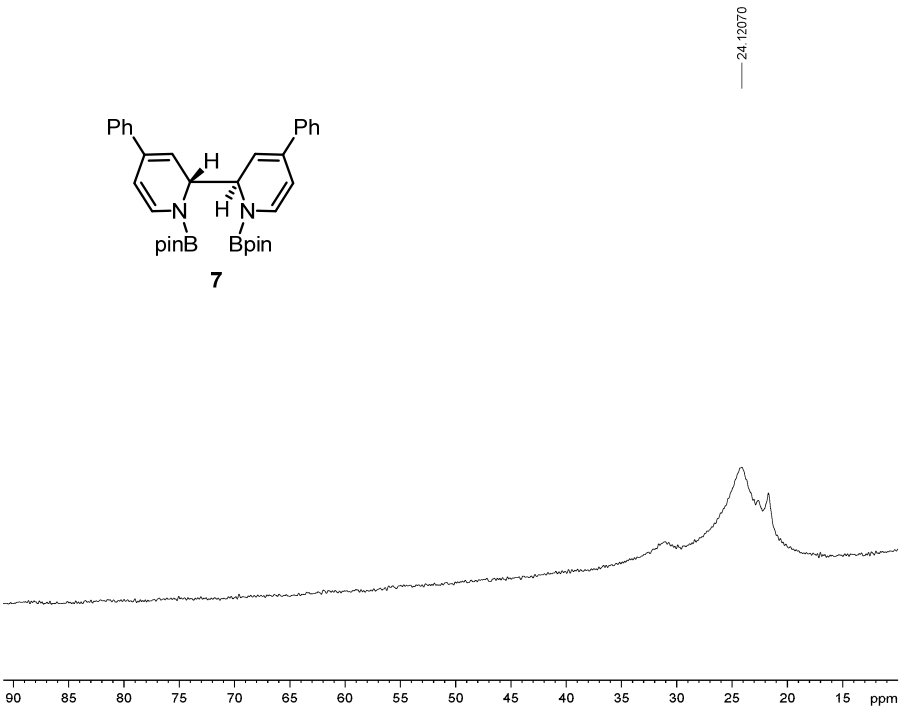
PULPROG                   zgpg30
TD                         65536
SOLVENT                     None
NS                           500
DS                             2
SWH                    24038.461 Hz
FIDRES                 0.366798 Hz
AQ                     1.3631988 sec
RG                        208.17
DW                        20.800 usec
DE                         6.50 usec
TE                        297.6 K
D1                     2.00000000 sec
D11                    0.03000000 sec
TD0                            1

======== CHANNEL f1 ========
SFO1                100.6228298 MHz
NUC1                        13C
P1                         9.95 usec
SI                        32768
SF                  100.6128114 MHz
WDW                          EM
SSB                           0
LB                         3.00 Hz
GB                            0
PC                         1.40
```

^{11}B NMR of compound **7** in THF by nucleophilic substitution reaction:




```
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PROCNO                         1
Date_                   20171120
Time                       9.53
INSTRUM                    spect
PROBHD   5 mm PABBO BB/
PULPROG                       zg
TD                         65536
SOLVENT                     None
NS                           128
DS                             4
SWH                    25510.203 Hz
FIDRES                 0.389255 Hz
AQ                     1.2845556 sec
RG                        208.17
DW                        19.600 usec
DE                         6.50 usec
TE                        295.8 K
D1                     1.00000000 sec
TD0                            1

======== CHANNEL f1 ========
SFO1                128.3776052 MHz
NUC1                        11B
P1                         8.73 usec
SI                        32768
SF                  128.3776016 MHz
WDW                          EM
SSB                           0
LB                         1.00 Hz
GB                            0
PC                         1.40
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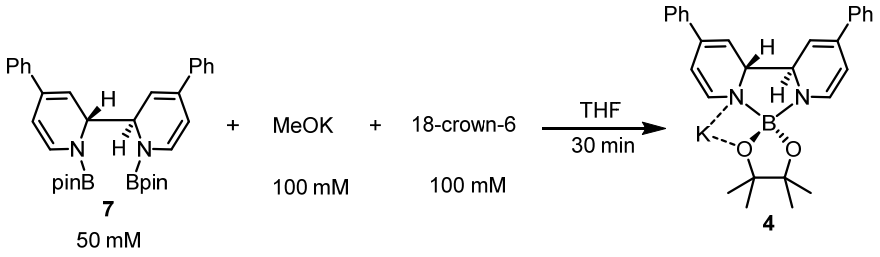
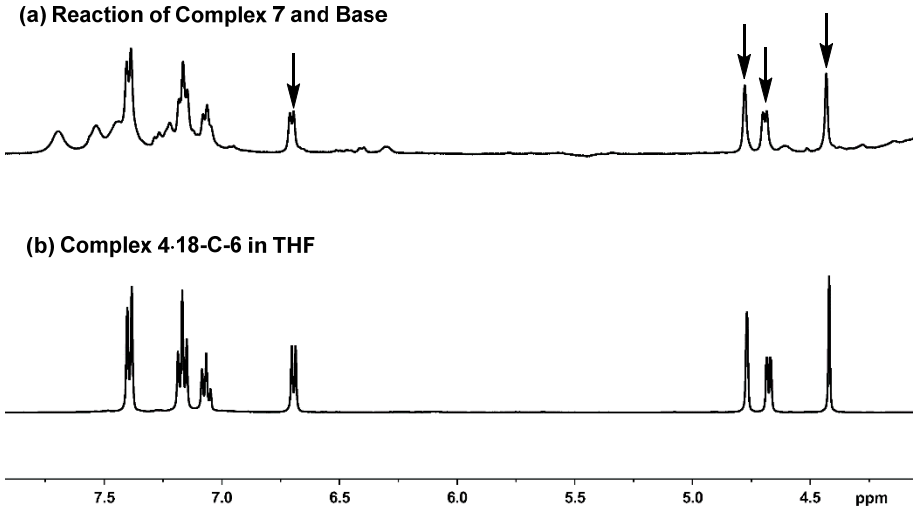
5.3 Transformation of Compound 7 to Complex 4



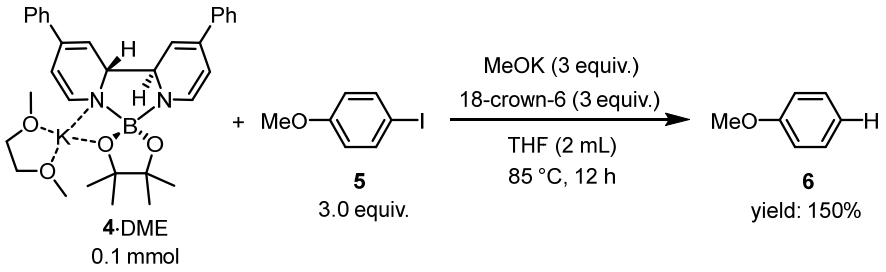
Experimental procedure: To a solution of the synthesized compound **7** (0.05 mmol, freshly prepared by nucleophilic substitution method described above) in THF was added pottasium methoxide (7.0 mg, 0.100 mmol) and 18-crown-6 (26.4 mg, 0.100 mmol). After reacted at room temperature for 30 min, the resulting solution was analyzed by NMR, which showed that compound **7** was completely consumed and complex **4** was generated as the major product.

^{1}H NMR of reaction between compound **7** and MeOK:



5.4 Transformation of Compound 7 to Complex 4 in the Reaction System

We proposed that the conversion of compound **7** to complex **4** by methoxide is important in the transformation network, because it regenerates a super electron donor to fully make use of the reductive power of complex **4**. To further confirm this, we performed the reaction between **4** and iodoarene **5** in the presence of excess potassium methoxide. Previously it was known that one equivalent of **4** could reduce one equivalent of **5** to give anisole (**6**) (80% yield was observed, see Section 2.6). In the presence of base, **4** is observed to reduce more amount of iodoarene **5** (150% yield), indicating that the transformation of compound **7** to complex **4** by methoxide occurred in the reaction system.

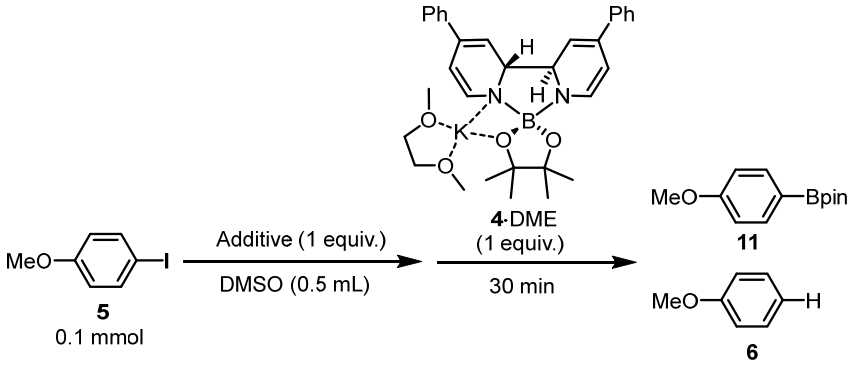


Experimental procedure: A 15 mL reaction tube was charged with a magnetic stir bar, 4-iodoanisole (70.2 mg, 0.300 mmol), MeOK (21.0 mg, 0.300 mmol), 18-crown-6 (79.2 mg, 0.300 mmol), and 2 mL of THF in a glove box. Complex **4**·DME (56.7 mg, 0.100 mmol) was then gradually added to the mixture. The tube was sealed with a Teflon screw cap and the reaction mixture was stirred in an oil bath at 85 °C for 12 h. The reaction mixture was then cooled to room temperature, and a standard solution of *n*-dodecane in toluene was added as the internal standard, followed by water. After shaking for 1 min, the organic layer was separated and analyzed by GC to obtain the yield of anisole.

6. Competition Experiments

6.1 Possible Borylation Species

Because the reaction between complex **4**·DME and iodoarene **5** did not produce any borylation product **11**, we performed additional experiments to investigate the real borylation species. In these experiments, different additives were added to the reaction mixture of **4**·DME and **5**. It was found that, the diboron (or its related species) was directly involved in the borylation process with the aryl radical.



Experimental procedure: A 15 mL reaction tube was charged with 4-iodoanisole (23.4 mg, 0.100 mmol), the additive (0.100 mmol), and 0.5 mL of DMSO in a glove box. Complex **4**·DME (56.7 mg, 0.100 mmol) was then gradually added to the mixture. The tube was sealed with a Teflon screw cap and the reaction mixture was allowed to react at room temperature for 30 min. Then a standard solution of *n*-dodecane in toluene was added as the internal standard, followed by water. After shaking for 1 min, the organic layer was separated and analyzed by GC. The results were summarized in Table S3.

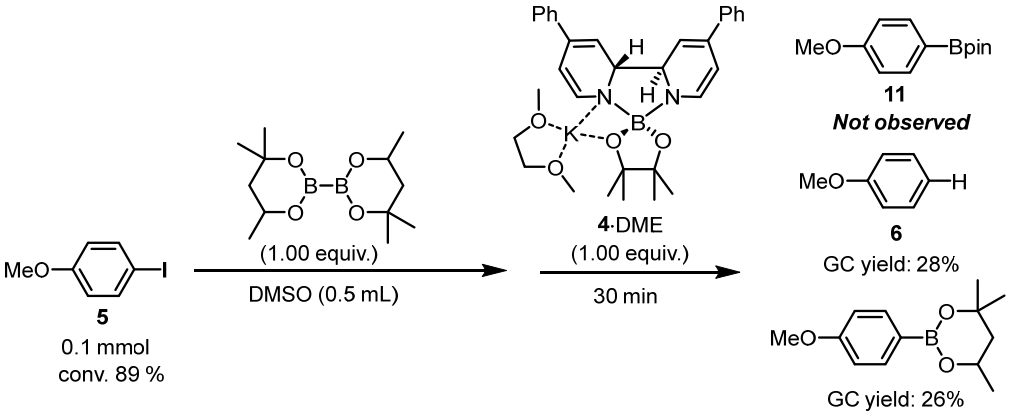
Table S3. Preliminary exploration of the borylation species

Entry	Additive	Conv. (%)	ArBpin (%)	ArH (%)
1	None	89	0	41
2	MeOBpin	95	0	43
3	B_2pin_2	94	29	28

The results excluded complex **4**, compound **7**, and MeOBpin as the borylation reagent. Either diboron or its pyridine complex might act as the borylation reagent.

6.2 Crossover Experiment

A crossover experiment employing bis(hexylene glycolato)diboron as the additive was carried out to further confirm the indispensable role of diboron in the carbon-boron bond formation event.

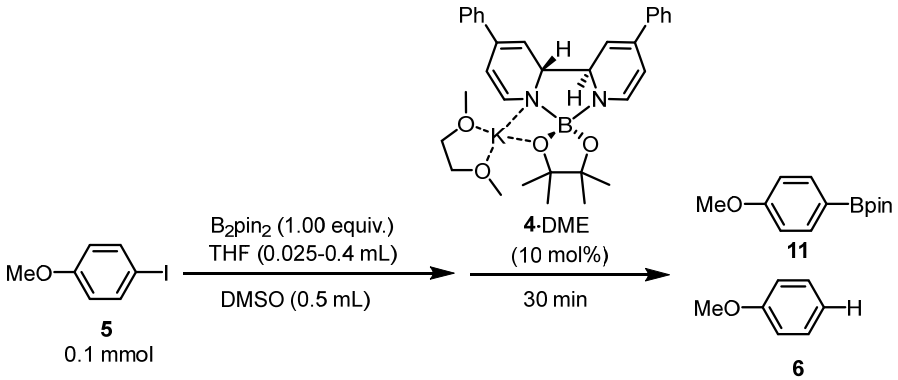


Experimental procedure: A 15 mL reaction tube was charged with 4-iodoanisole (23.4 mg, 0.100 mmol), bis(hexylene glycolato)diboron (25.4 mg, 0.100 mmol), and 0.5 mL of DMSO in a glove box. Complex **4**·DME (56.7 mg, 0.100 mmol) was then gradually added to the mixture. The tube was sealed with a Teflon screw cap and the reaction mixture was allowed to react at room temperature for 30 min. Then a standard solution of *n*-dodecane in toluene was added as the internal standard, followed by water. After shaking for 1 min, the organic layer was separated and analyzed by GC.

In this experiment, the only borylation product was the one with the hexylene glycol substituent, while no trace of the pinacol boronate **11** was observed. This means that the borylation reagent is only related to the diboron, rather than the SED complex or its related species.

6.3 The Establishment of the Kinetic Competition System

In the borylation reaction of 4-iodoanisole (**5**) in the presence of 10 mol% of electron donor **4**·DME and B_2pin_2, we achieved a kinetic competition scenario by adding a small amount of hydrogen atom donor THF (0.025-0.4 mL) to the DMSO solvent (0.5 mL). The observed product distribution ArH/ArBpin correlated well with the amount of THF added, which confirmed the kinetic competition between hydrogen atom transfer and borylation pathways and provided us with a probe to figure out the real borylation species (Table S4 and Figure S14).



Experimental procedure: A 15 mL reaction tube was charged with 4-iodoanisole (23.4 mg, 0.100 mmol), B_2pin_2 (25.4 mg, 0.100 mmol), THF (0.025-0.4 mL), and 0.5 mL of DMSO in a glove box. Complex **4**·DME (5.7 mg, 0.010 mmol) was then added to the mixture. The tube was sealed with a Teflon screw cap and the reaction mixture was allowed to react at room temperature for 30 min. Then a standard solution of *n*-dodecane in toluene was added as the internal standard, followed by water. After shaking for 1 min, the organic layer was separated and analyzed by GC. The results were summarized in Table S4.

Table S4. Determined [ArH]/[ArBpin] Ratio as a Function of [THF]

Entry	THF (mL)	Conv. (%)	ArBpin (%)	ArH (%)	ArH/ ArBpin
1	0	23.3	6.55	1.53	0.23
2	0.025	16.0	6.46	2.26	0.34
3	0.05	17.0	5.50	3.04	0.55
4	0.1	8.7	4.42	3.51	0.79
5	0.2	11.9	3.58	4.76	1.32
6	0.3	10.2	3.02	4.97	1.65
7	0.4	12.4	2.67	5.92	2.21

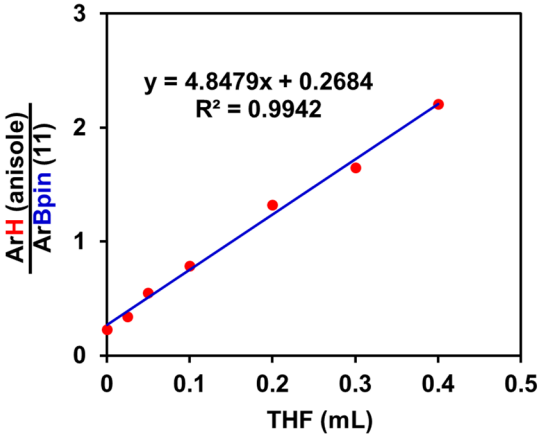
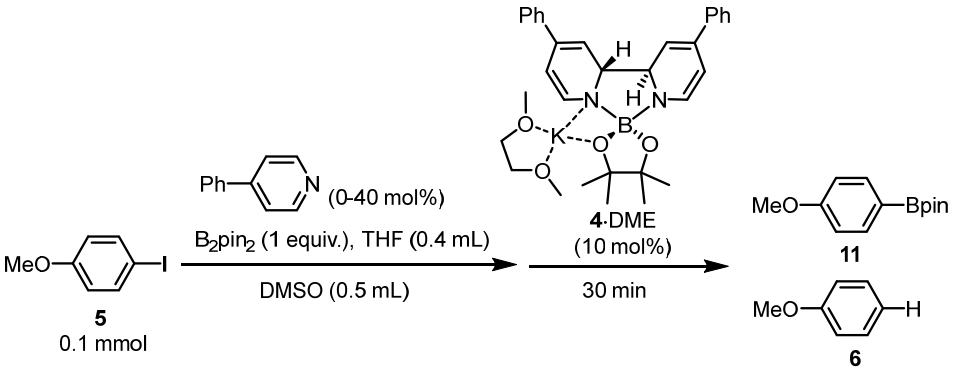


Figure S14. The relationship between the product distribution and the amount of THF added.

The product distribution ArH/ArBpin correlated well with the amount of THF added which is typical scenario of competition kinetics. It indicated that the aryl radical reacted simultaneously with the hydrogen atom donor (THF) and the boryl species, and the two pathways were in competition.

6.4 The Effect of 4-Phenylpyridine on the Borylation Process

We hope to figure out whether or not the pyridine-diboron complex is the key borylation species. In these experiments, a fixed amount of THF (0.4 mL) was utilized as hydrogen atom donor, 10 mol% electron donor **4**·DME was employed as reactant, 4-iodoanisole was used as the substrate, and different amounts of 4-phenylpyridine (0-40 mol%) was added.



The experiments were conducted following the experimental procedure described in Section 6.3, except that 0.4 mL of THF and 0-40 mol% of 4-phenylpyridine were used. The results were summarized in Table S5.

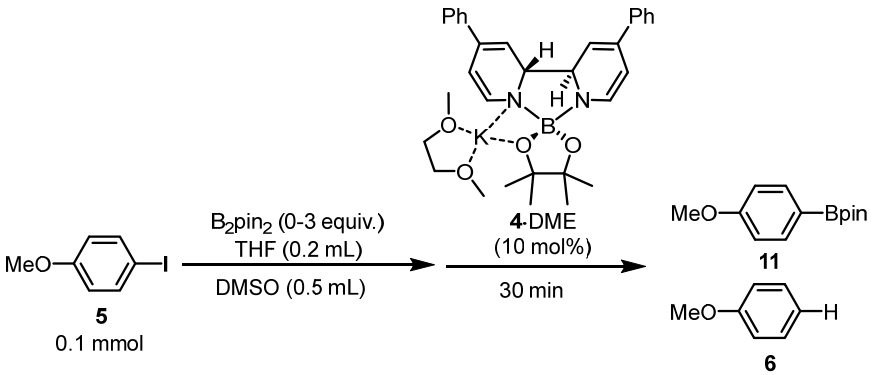
Table S5. Determined [ArBpin]/[ArH] Ratio as a Function of [**2**]

Entry	PhPy (mol%)	Conv. (%)	ArBpin (%)	ArH (%)	ArBpin/ ArH
1	0	12.4	2.67	5.92	0.45
2	10	12.5	1.93	4.95	0.39
3	20	12.7	2.20	5.16	0.43
4	40	10.1	2.49	5.43	0.46

The plot shown in Figure 8a in the main text was constructed using the data shown above. The product distribution ArBpin/ArH did not change as a function of [4-phenylpyridine], which excluded the complex between 4-phenylpyridine and diboron as the borylation reagent.

6.5 The Effect of Diboron on the Borylation Process

We hope to figure out whether or not the diboron is the key borylation species. In these experiments, a fixed amount of THF (0.2 mL) was utilized as hydrogen atom donor, 10 mol% electron donor **4**·DME was employed as reactant, 4-iodoanisole was used as the substrate, and different amounts of diboron (0-3 equiv.) was added.



The experiments were conducted following the experimental procedure described in Section 6.3, except that 0.2 mL of THF and 0-3 equiv. of B_2pin_2 were used. The results were summarized in Table S6.

Table S6. Determined [ArBpin]/[ArH] Ratio as a Function of [B_2pin_2]

Entry	B_2pin_2 (equiv.)	Conv. (%)	ArBpin (%)	ArH (%)	ArBpin/ ArH
1	0	10.0	0	7.00	0
2	0.5	14.9	2.00	5.76	0.35
3	1	11.9	3.58	4.76	0.75
4	2	10.8	5.90	4.00	1.48
5	3	12.9	6.99	3.00	2.33

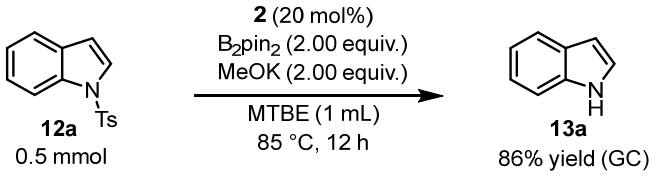
The plot shown in Figure 8b in the main text was constructed using the data shown above. The product distribution ArBpin/ArH has a perfect linear relationship with [B_2pin_2], which indicated diboron is the real borylation reagent.

7. Synthetic Applications

7.1 Reductive Cleavage of Various Substrates

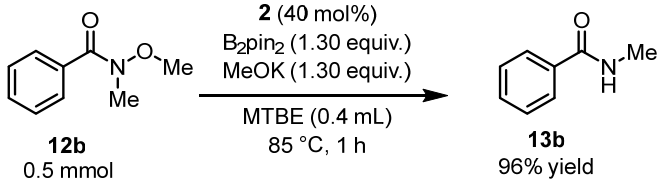
General procedure: A 15 mL reaction tube was charged with a magnetic stir bar, substrates **12** (0.500 mmol), MeOK (0.65 mmol), B_2pin_2 (0.65 mmol), 4-phenylpyridine (20-40 mol%), and MTBE in a glove box. The tube was sealed with a Teflon screw cap and the reaction mixture was stirred in an oil bath at 85 °C. Upon completion, the reaction mixture was cooled to room temperature, and 5 mL of water and 10 mL of diethyl ether was added. After extraction, the organic layer was separated and 2 drops of acetic acid was added to the aqueous phase to adjust to a neutral pH. After extraction of the aqueous phase with 3×10 mL ether, the combined organic extracts were washed with brine, dried over Na_2SO_4, and concentrated. The crude product was purified by flash column chromatography on silica gel to afford the desired product.

Indole (13a)



This reaction was carried out following the general procedure using **12a** (135.0mg, 0.500 mmol), MeOK (45.5 mg, 0.650 mmol), B_2pin_2 (165.0 mg, 0.650 mmol), 4-phenylpyridine (15.5 mg, 0.100 mmol), and 1 mL MTBE and reacted for 12 h. The yield of indole was determined by GC.

***N*-Methylbenzamide (13b)**

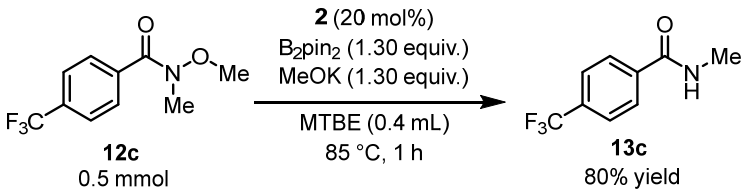


This reaction was carried out following the general procedure using **12b** (83.0 mg, 0.500 mmol), MeOK (45.5 mg, 0.650 mmol), B_2pin_2 (165.0 mg, 0.650 mmol), 4-phenylpyridine (31.0 mg, 0.200 mmol), and 0.4 mL MTBE and reacted for 1 h. Product **13b** was obtained as colorless oil in 98% yield (66.1 mg) using 5:1 petroleum ether/EtOAc as the eluent.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78-7.74 (m, 2H), 7.49-7.39 (m, 3H), 6.19 (brs, 1H), 3.02 (d, J = 4.8 Hz, 3H)

The NMR data were in consistent with the reported data.[17]

***N*-Methylbenzamide (13c)**

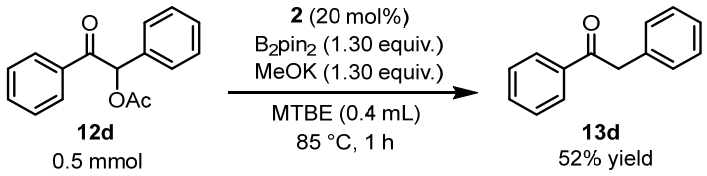


This reaction was carried out following the general procedure using **12c** (117.0 mg, 0.500 mmol), MeOK (45.5 mg, 0.650 mmol), B_2pin_2 (165.0 mg, 0.650 mmol), 4-phenylpyridine (15.5 mg, 0.100 mmol), and 0.4 mL MTBE and reacted for 1 h. Product **13c** was obtained as colorless oil in 80% yield (81.0 mg) using 5:1 petroleum ether/EtOAc as the eluent.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.87 (d, J = 8.1 Hz, 2H), 7.68 (d, J = 8.1 Hz, 2H), 6.37 (brs, 1H), 3.03 (d, J = 4.9 Hz, 3H)

The NMR data were in consistent with the reported data.[18]

Deoxybenzoin (13d)



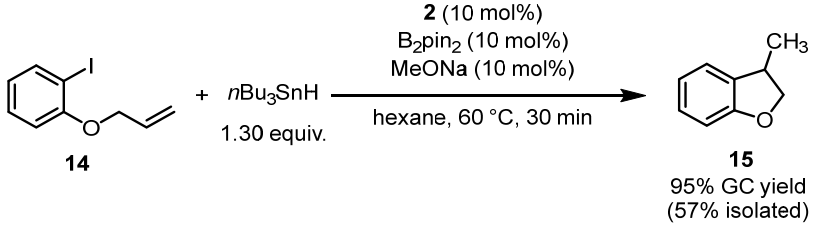
This reaction was carried out following the general procedure using **12d** (127.0 mg, 0.500 mmol), MeOK (45.5 mg, 0.650 mmol), B_2pin_2 (165.0 mg, 0.650 mmol), 4-phenylpyridine (15.5 mg, 0.100 mmol), and 0.4 mL MTBE and reacted for 1 h. Product **13d** was obtained as colorless oil in 52% yield (50.9 mg) using 50:1 petroleum ether/EtOAc as the eluent.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01 (d, J=7.6 Hz, 2H), 7.55 (t, J=7.6 Hz, 1H), 7.47 (t, J=7.6 Hz, 2H), 7.36–7.22 (m, 5H), 4.29 (s, 2H).

The NMR data were in consistent with the reported data.[19]

7.2 Initiation of Radical Chain Cyclization Reaction

3-Methyl-2,3-dihydrobenzofuran (15)



Experimental procedure for GC: To a 15 mL reaction tube charged with a magnetic stir bar, MeONa (1.1 mg, 0.020 mmol), B_2pin_2 (5.8 mg, 0.023 mmol), and 4-phenylpyridine (3.1 mg, 0.020 mmol) was added dry hexane (1 mL) under argon. Substrate **14** (0.200 mmol) and nBu$_3$SnH (76.0 mg, 0.261 mmol) was then added to the reaction tube. The reaction mixture was stirred in an oil bath at 60 °C under a balloon pressure of dry argon for 30 min. The reaction mixture was cooled to room temperature. A solution of n-dodecane in toluene was added as the standard, followed by water. After stirred for 5 min, the organic layer was separated and analyzed by GC to obtain the yield of **15**.

Experimental procedure for distillation: To a 25 mL round-bottom flask charged with a magnetic stir bar, MeONa (12.1 mg, 0.224 mmol), B_2pin_2 (58.1 mg, 0.228 mmol), 4-phenylpyridine (31.2 mg, 0.201 mmol) was added dry hexane (10 mL) under argon. Substrate **14** (2.000 mmol) and nBu$_3$SnH (760.0 mg, 2.610

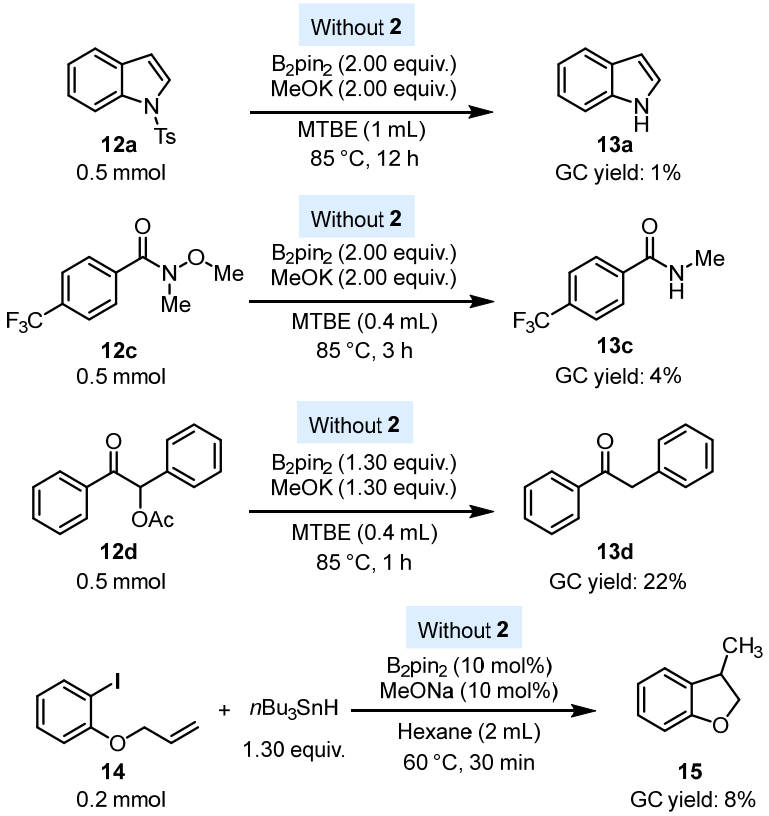
mmol) was then added to the flask. The reaction mixture was stirred in an oil bath at 60 °C under a balloon pressure of dry argon for 30 min. The reaction mixture was cooled to room temperature. The reaction mixture was then concentrated under reduce pressure (500 mbar). Product **15** was obtained as colorless liquid in 57% yield (153.7 mg) from 1-(allyloxy)-2-iodobenzene (**14**, 520.0 g) after vacuum distillation (95-100°C, 20 mbar).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.18–7.08 (m, 2H), 6.90–6.83 (t, J = 7.2 Hz, 1H), 6.81–6.76 (d, J = 7.4 Hz, 1H), 4.68 (t, J = 8.8 Hz, 1H), 3.70 (dd, J = 8.8, 7.5 Hz, 1H), 3.61–3.48(m, 1H), 1.33 (d, J = 7.1 Hz, 3H).

The NMR data were in consistent with the reported data.[20]

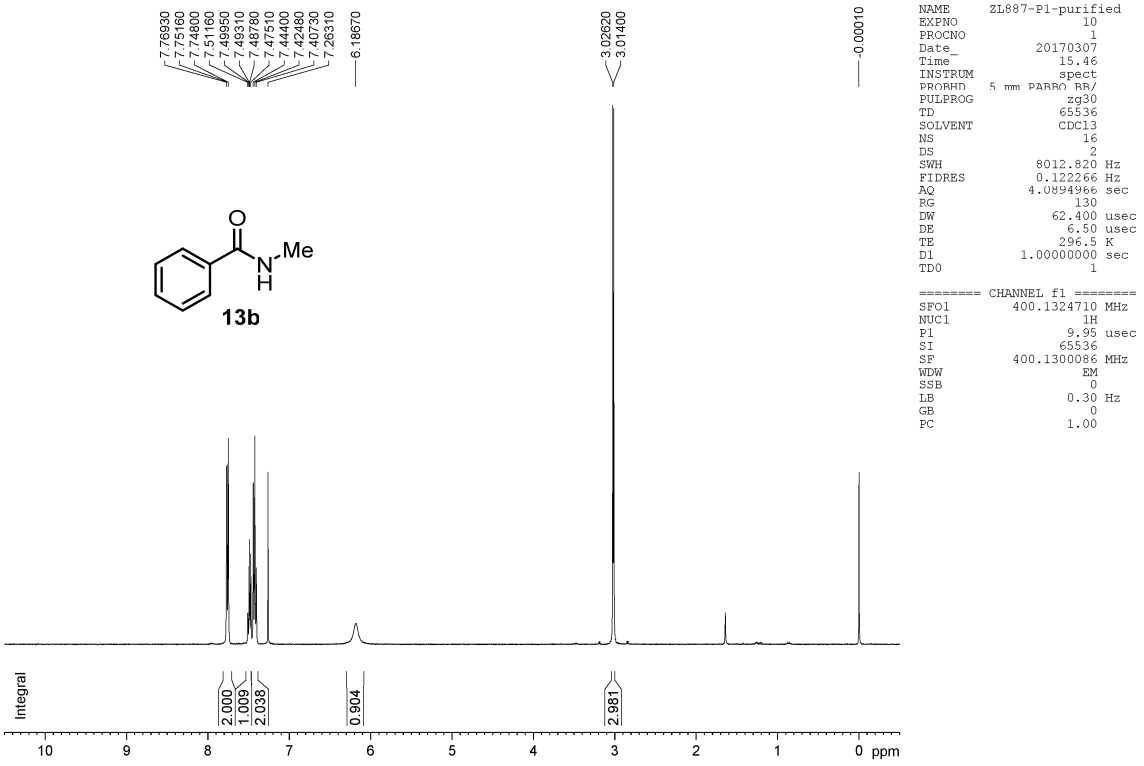
7.3 Control Experiments in the Absence of Pyridine 2

Control experiments of substrates shown in Scheme 11 and Scheme 12 without pyridine additive were carried out. For substrates **12a** and **12c**, reduction product could hardly be observed in the absence of **2**. For substrates **12d**, small amount of **13d** was observed, but when the reaction was added pyridine additive **2**, the yield of **13d** has improved a lot. For substrate **14**, product **15** was only obtained in 8% yield. These results further illustrate the importance of pyridine additive in these reduction or radical chain reaction, and confirmed that the real species that work is the SEDs generated in situ in the reaction mixture.

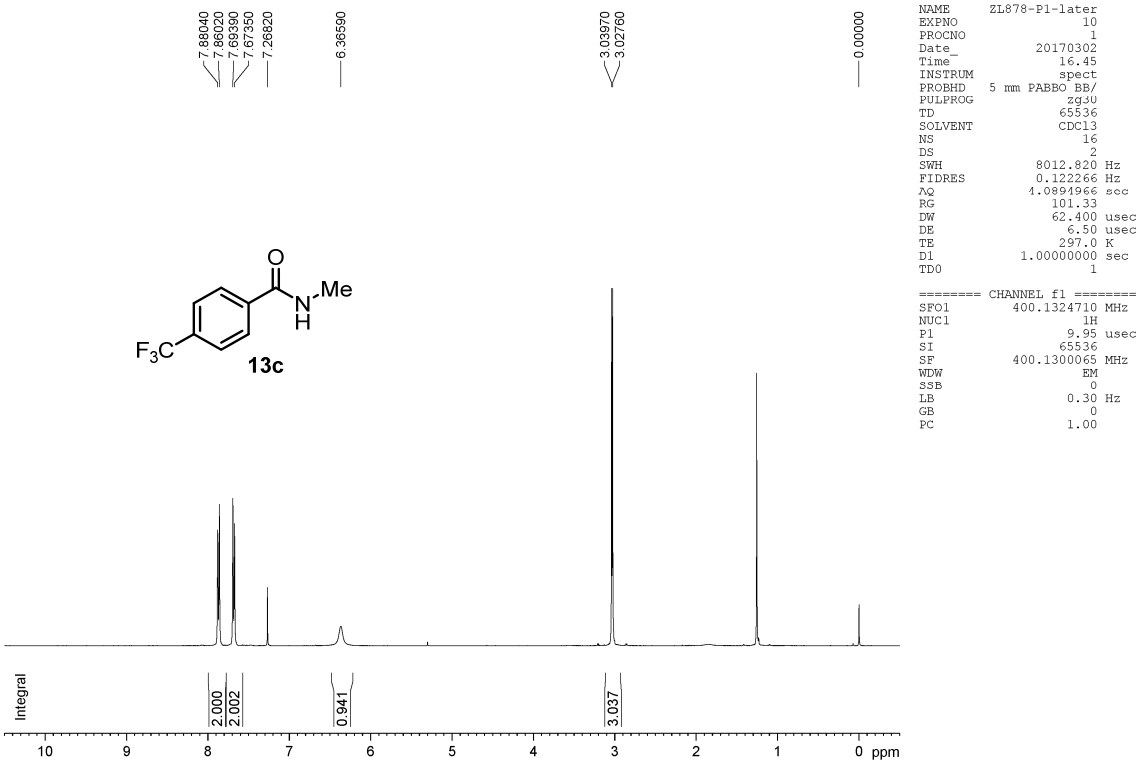


7.4 NMR Spectra

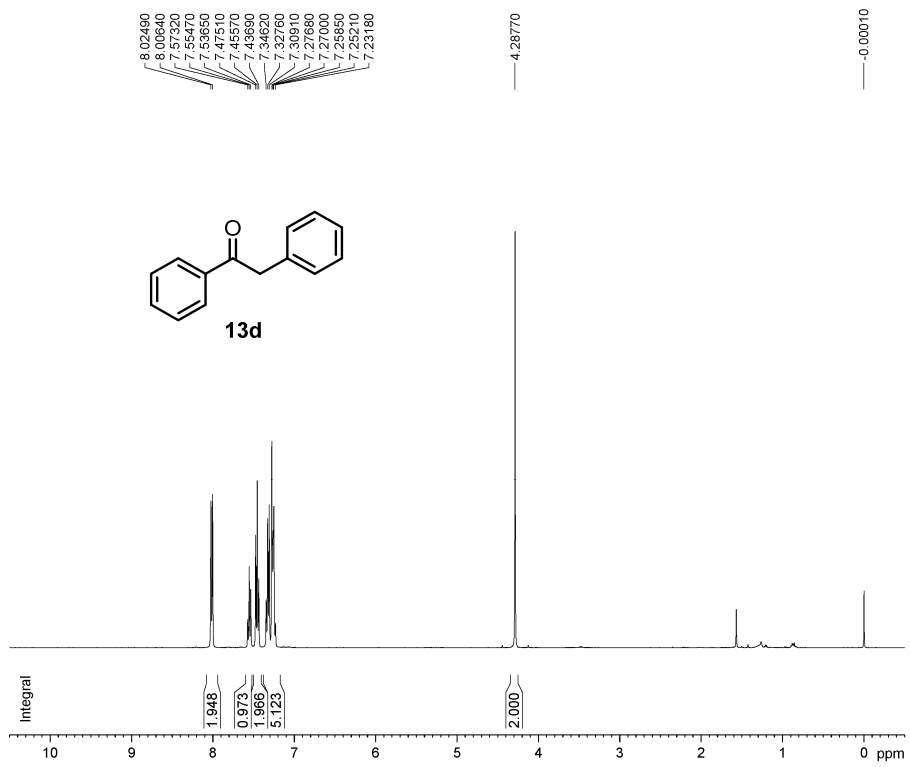
^{1}H NMR in $CDCl_3$:



^{1}H NMR in $CDCl_3$:



^{1}H NMR in $CDCl_3$:

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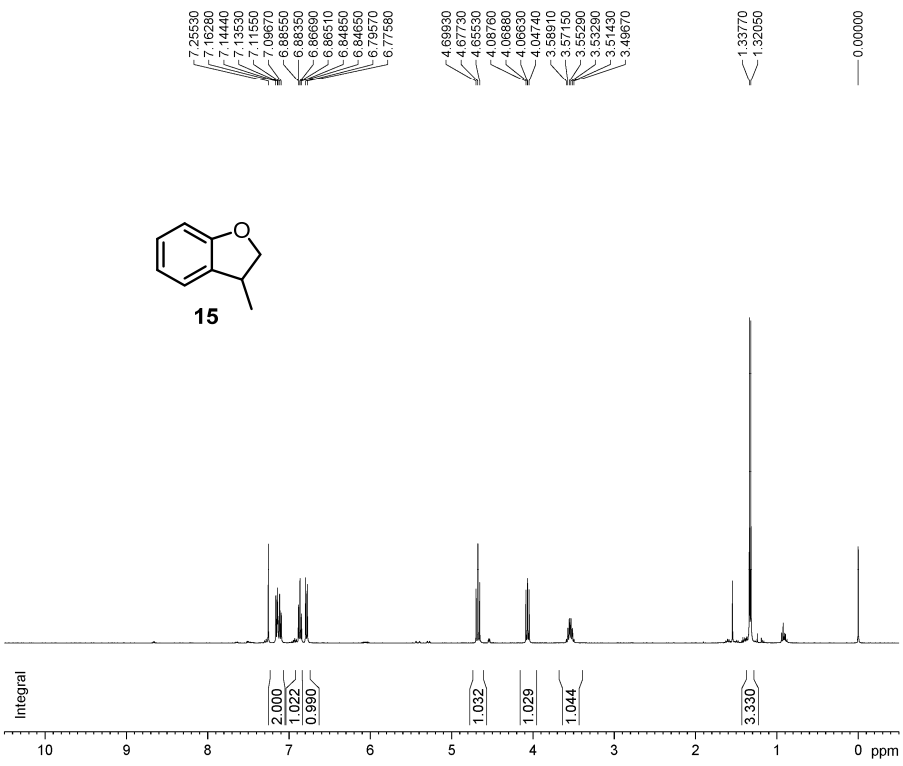
EXPNO                       10
PROCNO                       1
Date_                 20170312
Time                      8.47
INSTRUM                  spect
PROBHD     5 mm PABBO BB/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                  8012.820 Hz
FIDRES               0.122266 Hz
AQ                   4.0894966 sec
RG                      101.33
DW                      62.400 usec
DE                       6.50 usec
TE                      295.6 K
D1                   1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                     1H
P1                    9.95 usec
SI                   65536
SF            400.1300129 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

^{1}H NMR in $CDCl_3$:

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PROCNO                       1
Date_                 20170927
Time                     18.15
INSTRUM                  spect
PROBHD     5 mm PABBO BB/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                  8012.820 Hz
FIDRES               0.122266 Hz
AQ                   4.0894966 sec
RG                      101.33
DW                      62.400 usec
DE                       6.50 usec
TE                      297.9 K
D1                   1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                     1H
P1                    9.68 usec
SI                   65536
SF            400.1300115 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

8. DFT Computational Study

8.1 General Information

All calculations were performed with the Gaussian 09 program.[21] Density functional theory calculations using the M06-2X functional[22] were used to locate all the stationary points involved. For the integration grid in the DFT calculations, the parameter int=fine was applied. The default convergence criteria for geometry optimization was used. The 6-31+G(d) basis set was applied for all elements except iodine, which used the basis set of LANL2DZ. The keyword "5D" in Gaussian 09 program was used to specify that five (instead of six) *d*-type STO orbitals were used as basis sets in all elements of the calculations. A "broken-symmetry" guess was used for calculations on open-shell systems. Frequency calculations at the same level had been performed to confirm each stationary point to be either a minimum or a transition structure. To obtain more accurate energies, single-point energy calculations were performed on all optimized structures applying the 6-311+G(d,p) basis set for all elements except iodine, which used the basis set of LANL2DZ.

Solvation energies were evaluated by a self-consistent reaction field (SCRF) using the CPCM approach, where universal force field (UFF) was used to define the atomic radii. Solvation effect was taken into account during geometry optimization and single-pont energy with dimethylsulfoxide as the solvent. The reported energies are zero-point energy-corrected Gibbs free energies in solution ($\Delta G_{\text{sol 298K}}$).

8.2 The [3,3]-Sigmatropic Rearrangement Mechanism Described in Scheme 7

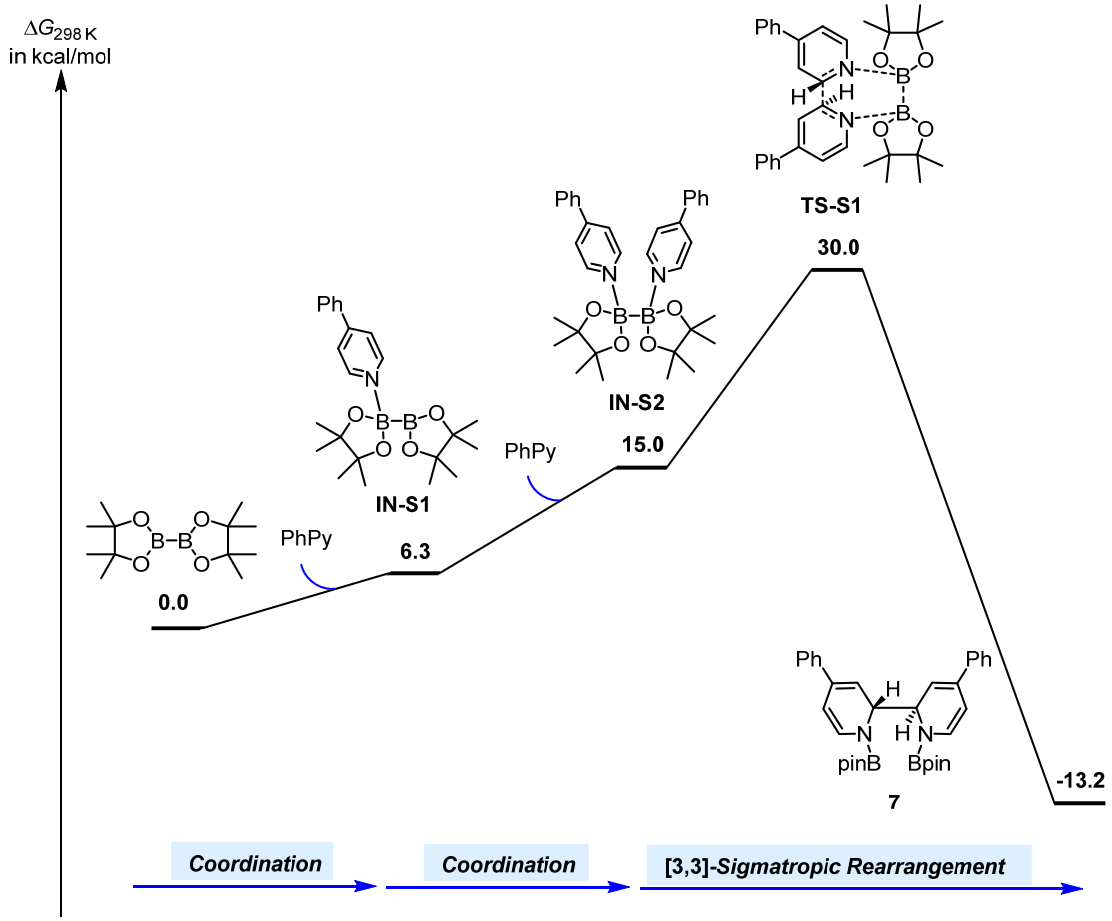


Figure S15. Additional calculation for the [3,3]-sigmatropic rearrangement mechanism.

The cleavage of B-B bond could also follow [3,3]-sigmatropic rearrangement pathway proposed by Tang et. al.[16] The whole potential surface was also calculated and the overall activation free energy barrier is higher than that of the heterolytic cleavage pathway shown in Figure 5. IRC calculation was performed to confirm the located transition state was related to a [3,3]-sigmatropic rearrangement rather than the homolytic cleavage.

8.3 Transformation from Complex 4 to Complex 10 and Compound 7

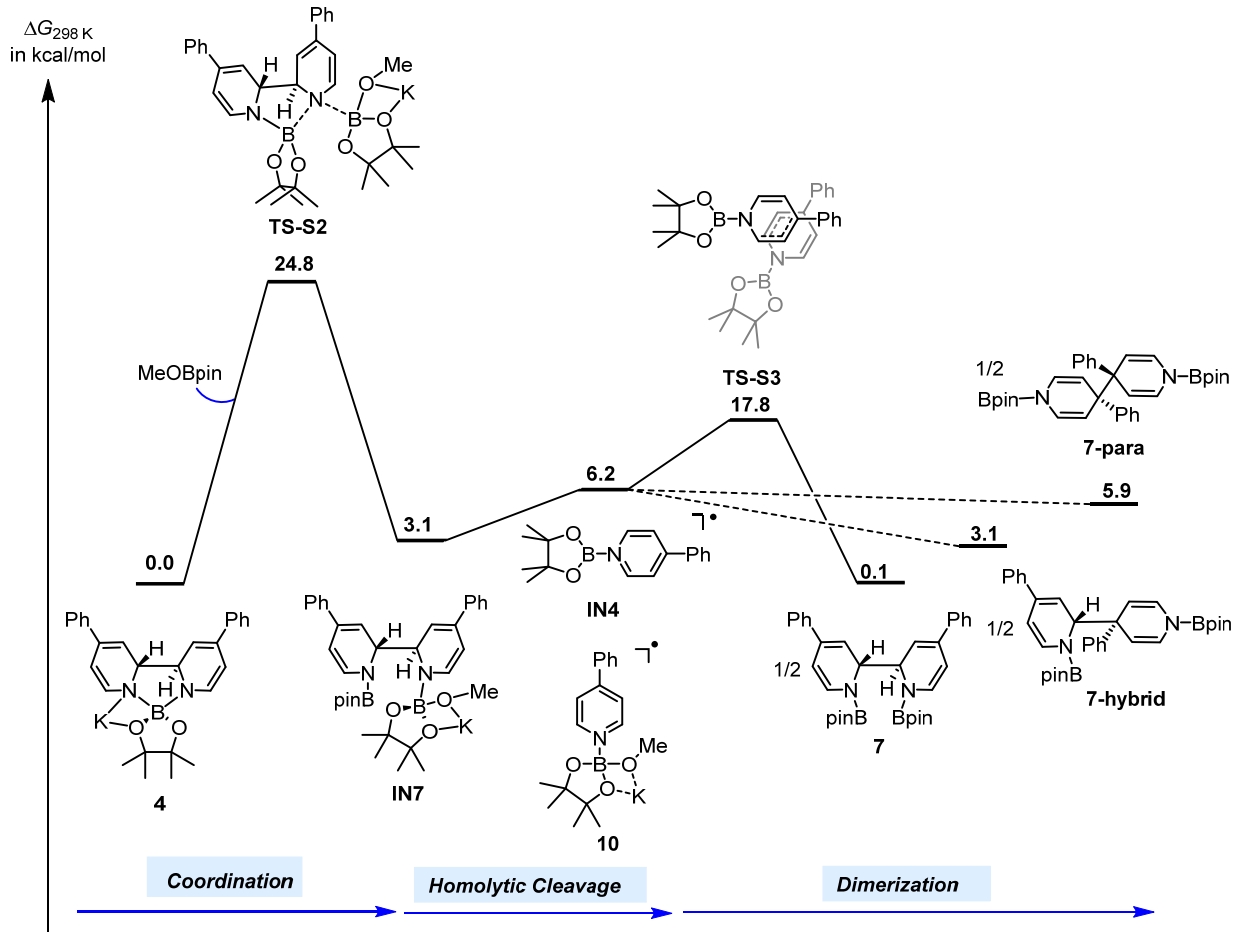
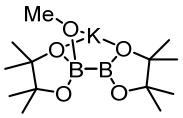


Figure S16. Plausible mechanism for transformation from complex **4** to complex **10** and **7**.

The computed free energies and the corresponding discussions were included in the main text (Scheme 8). For the dimerization of **IN4**, we calculated the dimerization products (**7**, **7-hybrid**, **7-para**) with different configurations and regioselectivities. It was found that the 2,2'-dimer **7** is the most stable, and the activation energy barrier is rather low.

8.4 Coordinates and Energies of Stationary Points in the Potential Energy Surface

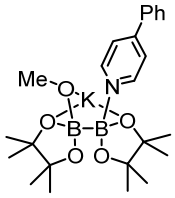
IN1 (B_2pin_2·MeOK)



G_{sol} = -1537.223977 Hatree

O	1.69546900	-0.68140900	-1.30466100
B	0.85986900	0.36786900	-0.67318000
O	1.54993200	0.59154400	0.65134300
B	-0.81513600	-0.06438700	-0.44687500
O	-1.68684700	0.74051600	0.29851800
O	-1.50122600	-1.18002900	-0.90552600
C	2.23761600	-0.60308200	0.97334000
C	2.73391800	-1.09633700	-0.42822200
C	-2.79532000	-1.23317100	-0.26301500
C	-3.03787300	0.25934000	0.11640600
C	1.25568500	-1.59600200	1.61393100
C	-3.81348200	-1.81460800	-1.23150100
C	-3.82685700	0.47260300	1.39855400
C	-2.65296400	-2.13902600	0.95943600
C	-3.65328100	1.07066500	-1.02298000
C	3.35383600	-0.29731800	1.96543600
C	2.90288500	-2.61108900	-0.52724300
C	4.05137200	-0.42858800	-0.83921500
O	0.82450500	1.65384900	-1.40863500
C	2.05470800	2.24009500	-1.76262200
H	0.76894800	-1.10873200	2.46670000
H	0.47899100	-1.90232600	0.90479500
H	1.76468900	-2.49647000	1.97536800
H	-3.57418100	-2.86380400	-1.43132300
H	-4.82055000	-1.77065600	-0.80158000
H	-3.81547500	-1.27538200	-2.18178700
H	-3.95403200	1.54489900	1.57852900
H	-4.82202200	0.02145100	1.31483200
H	-3.31690900	0.03627400	2.26051400
H	-3.61347100	-2.28304100	1.46448700
H	-2.28293700	-3.11610400	0.63318900
H	-1.93729800	-1.72463800	1.67740700
H	-4.70043500	0.79803100	-1.18852800
H	-3.61014200	2.13318500	-0.76412700
H	-3.10048800	0.92127300	-1.95644900
H	2.92092500	0.00703000	2.92514300
H	3.97791400	-1.18170200	2.14104900
H	3.99180800	0.51444600	1.60585100
H	1.94758400	-3.12560000	-0.39317800
H	3.29608500	-2.87389600	-1.51597900
H	3.60928200	-2.98051200	0.22613400
H	4.90183800	-0.83105200	-0.27629300
H	4.22450000	-0.61880400	-1.90456200
H	4.01335800	0.65296800	-0.68610800
H	1.85456500	3.15707200	-2.32828400
H	2.65326700	2.50307000	-0.87711600
H	2.65697700	1.56720700	-2.38739800
K	0.01828600	2.76009200	0.98720300

IN2



G_{sol} = -2016.325955 Hatree

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B	1.57916500	-0.90214500	0.47468000
O	1.16908300	-2.01914200	-0.42145500
B	0.86654000	0.64225200	0.00541000
O	1.10990800	1.81772000	0.87118600
O	1.18201200	1.10078500	-1.34535900
C	2.29871400	-2.84192300	-0.66439100
C	3.48281500	-1.81906600	-0.64054500
C	1.11645000	2.51965700	-1.38534300
C	1.52045600	2.93176900	0.07302600
C	2.12001900	-3.55497600	-2.00204800
C	2.07869900	3.01718800	-2.46209000
C	0.83883700	4.19921600	0.58025300
C	-0.29845700	2.98209700	-1.77209400
C	3.03760700	3.08634200	0.22852000
C	2.42742200	-3.89409400	0.44600400
C	3.63368600	-1.09061000	-1.98154500
C	4.82622600	-2.43051800	-0.25042800
N	-0.83261800	0.45674600	0.00566000
C	-1.63791600	1.04994700	0.89470300
C	-3.00424800	0.81740700	0.92158400

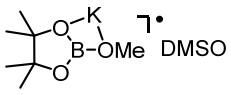
C	-3.57552200	-0.06061700	-0.00869900
C	-2.71503100	-0.66516700	-0.93434400
C	-1.35798900	-0.38646300	-0.89395500
C	-5.03169600	-0.33814500	-0.01371400
C	-5.74713500	-0.40800500	1.18920200
C	-7.11535600	-0.67017200	1.18350400
C	-7.78759900	-0.86097400	-0.02411300
C	-7.08344600	-0.79093900	-1.22664500
C	-5.71418000	-0.53459400	-1.22171800
O	1.38787400	-1.27054500	1.93468600
C	0.08306000	-1.30426300	2.43328200
H	3.02712300	-4.10517700	-2.28154200
H	1.29687400	-4.27535700	-1.92949300
H	1.88400900	-2.84500400	-2.79951700
H	1.70729500	2.71541900	-3.44771100
H	2.15734100	4.11085300	-2.45002000
H	3.07616900	2.59064200	-2.32979400
H	1.17511000	4.41335000	1.60080000
H	1.09255300	5.06127600	-0.04833500
H	-0.24869100	4.08946800	0.59747700
H	-0.32364700	4.06230200	-1.95597600
H	-0.58754800	2.47014600	-2.69656500
H	-1.04700700	2.75248600	-1.01066900
H	3.42553100	3.93653700	-0.34182100
H	3.27510800	3.26988500	1.28335000
H	3.55767300	2.18020600	-0.10291200
H	1.48193800	-4.44453900	0.51605700
H	3.22732900	-4.61408300	0.23532300
H	2.61495300	-3.41447700	1.40975100
H	2.67886200	-0.65188400	-2.28414000
H	4.35523300	-0.27412900	-1.85585400
H	4.00418900	-1.75447200	-2.77148200
H	5.11535400	-3.22616200	-0.94840000
H	5.60447200	-1.65875900	-0.27781200
H	4.79437100	-2.84829900	0.75949800
H	-1.14701800	1.73432000	1.57970300
H	-3.61771200	1.34159300	1.64691000
H	-3.09047100	-1.37083500	-1.66779600
H	-0.64203200	-0.84978400	-1.56426200
H	-5.22889800	-0.28067600	2.13577600
H	-7.65483100	-0.73169300	2.12386300
H	-8.85423600	-1.06407500	-0.02796100
H	-7.60031300	-0.93109300	-2.17117300
H	-5.17741000	-0.46309000	-2.16387700
H	0.05285000	-1.93293700	3.33297500
H	-0.28156800	-0.30319700	2.71729300
H	-0.63241500	-1.72416800	1.70705900
K	3.06880300	0.70930100	2.48100700

4-Phenylpyridine

G_{sol} = -479.1262172 Hatree

C	-1.47716300	-1.12922700	0.38567600
C	-2.86809500	-1.07864500	0.36725400
N	-3.56927300	0.00000000	0.00000000
C	-2.86809400	1.07864500	-0.36725500
C	-1.47716300	1.12922600	-0.38567600
C	-0.74587000	0.00000000	0.00000000
C	0.73814400	0.00000000	0.00000000
C	1.45060300	-1.15056600	-0.36420300
C	2.84384500	-1.14997300	-0.36568200
C	3.54455400	0.00000000	0.00000000
C	2.84384400	1.14997300	0.36568200
C	1.45060300	1.15056500	0.36420300
H	-0.97613600	-2.03337600	0.71784100
H	-3.44701900	-1.94825100	0.66849300
H	-3.44701800	1.94825200	-0.66849400
H	-0.97613600	2.03337600	-0.71784100
H	0.91217000	-2.04389600	-0.66910100
H	3.38260900	-2.04630800	-0.65809300
H	4.63041700	0.00000000	0.00000000
H	3.38260900	2.04630900	0.65809300
H	0.91217000	2.04389600	0.66910100

IN3



G_{sol} = -1679.222784 Hatree

B	-2.06819400	1.13778400	-0.46034700
O	-1.54585900	-0.17143700	-0.77375800
C	-2.30064500	-1.13326900	-0.01985600
C	-3.66388100	-0.39963700	0.18476000
O	-3.26127000	0.96612300	0.31722200
C	-4.41831100	-0.81979000	1.43904800
C	-4.58457700	-0.52737500	-1.03297500
C	-2.39481600	-2.43135100	-0.80825300
C	-1.57068900	-1.37701600	1.30358100
O	-1.07483600	2.03312500	0.04460200

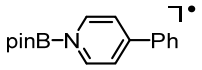
C	-1.49078100	3.32882300	0.40970800
H	-5.36935500	-0.27965100	1.49449500
H	-4.63853300	-1.89377900	1.41823800
H	-3.84432500	-0.59671600	2.34186900
H	-5.00212400	-1.53662300	-1.11871300
H	-5.41255500	0.18027700	-0.91890400
H	-4.05161500	-0.28285400	-1.95764000
H	-1.40312300	-2.88877800	-0.89054900
H	-3.05679300	-3.14414800	-0.30226000
H	-2.77661500	-2.25627600	-1.81739300
H	-2.06258100	-2.15231000	1.90164800
H	-0.54892700	-1.70915900	1.09005200
H	-1.51846400	-0.45653700	1.89449000
H	-0.61747100	3.88644900	0.75910400
H	-1.93121900	3.85199200	-0.45382200
H	-2.23816600	3.29759200	1.21207100
K	1.05333500	0.63839500	-0.84572900
S	4.71892400	-0.35269500	0.67297300
O	3.35918000	-0.09253000	0.01629000
C	5.82205400	0.90403200	-0.00480500
H	5.49282500	1.86865900	0.38479200
H	6.84420400	0.69935800	0.32230300
H	5.74755200	0.88679000	-1.09496200
C	5.40349100	-1.77388400	-0.20374100
H	4.78950200	-2.63909200	0.05075100
H	5.36171100	-1.57815400	-1.27813100
H	6.43209000	-1.93780600	0.12593000

DMSO

G_{sol} = -553.111396 Hatree

S	0.00000000	0.21291500	-0.45189300
O	0.00000300	1.49452000	0.38194700
C	1.35701400	-0.79163900	0.19196600
H	1.33978500	-1.77399000	-0.28648100
H	2.28685000	-0.27593000	-0.05377000
H	1.24723400	-0.88166900	1.27580500
C	-1.35701700	-0.79163400	0.19196700
H	-2.28684900	-0.27591800	-0.05376900
H	-1.33979500	-1.77398500	-0.28648400
H	-1.24723800	-0.88166900	1.27580500

IN4

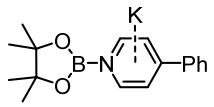


G_{sol} = -890.186703 Hatree

C	1.69582400	1.20631000	-0.01846700
C	0.33677700	1.19330400	-0.02435300
N	-0.38886900	0.00000000	0.00000000
C	0.33677700	-1.19330400	0.02435300
C	1.69582400	-1.20631000	0.01846800
C	2.46707600	0.00000000	0.00000000
C	3.92264500	0.00000000	0.00000000
C	4.66211100	1.15302700	0.35158000
C	6.05264800	1.15091300	0.34953300
C	6.76376800	0.00000000	0.00000000
C	6.05264800	-1.15091300	-0.34953300
C	4.66211100	-1.15302700	-0.35158000
B	-1.82945100	0.00000000	0.00000000
O	-2.57043000	1.15104300	0.02140400
C	-3.94403600	0.74637600	-0.23747900
C	-3.94403600	-0.74637600	0.23747900
O	-2.57043000	-1.15104300	-0.02140400
C	-4.87834300	-1.65776200	-0.53892700
C	-4.17486700	-0.89195100	1.73866300
C	-4.87834300	1.65776200	0.53892700
C	-4.17486700	0.89195100	-1.73866300
H	2.18051600	2.17565000	-0.06136600
H	-0.25974600	2.09691200	-0.05660100
H	-0.25974600	-2.09691200	0.05660100
H	2.18051600	-2.17565000	0.06136600
H	4.14332700	2.05698300	0.65569100
H	6.58654800	2.05412000	0.63237700
H	7.84938400	0.00000000	0.00000000
H	6.58654800	-2.05412000	-0.63237700
H	4.14332700	-2.05698300	-0.65569100
H	-4.81774500	-2.67314700	-0.13597200
H	-5.91296400	-1.31196000	-0.44065500
H	-4.61759100	-1.68916100	-1.59909400
H	-5.20967300	-0.65468200	2.00284400
H	-3.97147100	-1.92696100	2.02844600
H	-3.50893900	-0.23619800	2.30946300
H	-4.81774500	2.67314700	0.13597100
H	-5.91296400	1.31196000	0.44065500
H	-4.61759100	1.68916100	1.59909400
H	-5.20967300	0.65468200	-2.00284400

H	-3.97147100	1.92696100	-2.02844600
H	-3.50893900	0.23619800	-2.30946300

IN5



G_{sol} = -1490.170948 Hatree

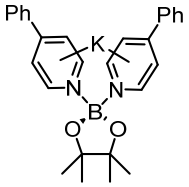
C	1.56662800	-0.84573000	-1.18616400
C	0.21592300	-0.82449500	-1.24307700
N	-0.52277100	0.22161800	-0.59280100
C	0.21481700	1.43941500	-0.40606100
C	1.56517300	1.41820000	-0.34491900
C	2.33861700	0.20532100	-0.54694700
C	3.74750600	0.12453000	-0.32339000
C	4.51172000	-1.04662400	-0.62510300
C	5.88307800	-1.11163800	-0.41481400
C	6.59596400	-0.03039600	0.11844800
C	5.87175400	1.12401800	0.44274500
C	4.50045100	1.20358400	0.23842100
B	-1.91245400	0.13600300	-0.36651400
O	-2.67220800	-0.97916300	-0.68035400
C	-3.95723400	-0.78454800	-0.04452600
C	-4.04925600	0.77502500	0.04495500
O	-2.66150800	1.15566100	0.19808400
C	-4.84004300	1.29490500	1.23396400
C	-4.55400600	1.41058500	-1.24906500
C	-5.03555400	-1.43495400	-0.89483600
C	-3.89042400	-1.44847300	1.32971700
H	2.06511900	-1.66545600	-1.69871900
H	-0.37647800	-1.55749700	-1.77949500
H	-0.37808900	2.34501900	-0.33973800
H	2.06312400	2.37454300	-0.20059400
H	4.01268800	-1.92436500	-1.02600500
H	6.40778100	-2.03115000	-0.66784300
H	7.66699200	-0.08888000	0.28497800
H	6.38664600	1.98128600	0.87283000
H	3.99057500	2.11824400	0.52755900
H	-5.87078700	0.92540600	1.19785800
H	-4.38933600	0.98459200	2.17953400
H	-4.86889600	2.38861000	1.20661900
H	-4.40604200	2.49311100	-1.19124900
H	-4.00339800	1.03283900	-2.11734200
H	-5.62021200	1.21529900	-1.39968300
H	-6.02820600	-1.21584800	-0.48620200
H	-4.99601400	-1.08342900	-1.92824500
H	-4.89879400	-2.52079400	-0.89365800
H	-3.63771700	-2.50513400	1.20048600
H	-3.12175800	-0.98375700	1.95710500
H	-4.85118200	-1.38333700	1.84946100
K	0.87551100	-0.70289300	1.86929500

MeOBpin

G_{sol} = -526.1989461 Hatree

B	1.17853800	-0.39880900	-0.11903500
O	0.18138200	-1.27528800	-0.47877600
C	-1.06163700	-0.69181600	-0.01550300
C	-0.71407600	0.83533100	0.03611400
O	0.70734300	0.81509900	0.32490600
C	-1.43046900	1.61136300	1.12807900
C	-0.88653400	1.52840000	-1.31315900
C	-2.17266300	-1.05374400	-0.98638500
C	-1.34619900	-1.28002700	1.36463700
O	2.49028200	-0.72976100	-0.20256000
C	3.46573600	0.25270600	0.13518600
H	-1.13550000	2.66419700	1.08417200
H	-2.51514900	1.55446100	0.98609500
H	-1.18567700	1.22483400	2.11992600
H	-1.94421200	1.62798000	-1.57496800
H	-0.44927000	2.52949200	-1.25407000
H	-0.37920200	0.97706200	-2.11189400
H	-2.35750600	-2.13161000	-0.94733300
H	-3.09974200	-0.53831500	-0.71289200
H	-1.91119400	-0.78493200	-2.01234900
H	-2.30255800	-0.92357700	1.75881000
H	-1.39041100	-2.36995400	1.28130400
H	-0.55600400	-1.02029500	2.07728600
H	4.44658300	-0.20672000	0.00981500
H	3.38426500	1.12149100	-0.52427900
H	3.34588800	0.57625200	1.17317100

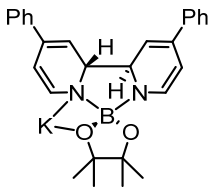
IN6



G_{sol} = -1969.28303 Hatree

N	-1.47184200	1.17227600	0.00629800
C	-0.84051600	1.51161200	-1.17026500
C	0.32060500	2.24334700	-1.20552300
C	0.97142000	2.66801500	-0.01149300
C	0.34130900	2.23818700	1.19188700
C	-0.82642200	1.51648900	1.17267100
C	-0.81847100	-1.58019400	-1.15053000
N	-1.46515900	-1.24388500	0.02334200
B	-2.46697600	-0.04470000	0.01757700
C	0.36117700	-2.27714000	-1.17840200
C	-0.80291300	-1.55942200	1.19444000
C	0.38135300	-2.24866500	1.21895200
C	1.03139500	-2.67580600	0.01968700
O	-3.30964800	-0.01741000	-1.15114300
C	-4.64063600	-0.30326200	-0.70913500
C	-4.63230800	0.24168200	0.75604800
O	-3.30369800	-0.06554200	1.19057200
C	-5.62810900	-0.43807300	1.68556900
C	-4.82649900	1.75970900	0.80789800
C	-5.63091700	0.39161300	-1.63334600
C	-4.85818200	-1.81807200	-0.75993300
C	2.20861500	3.44429500	-0.02063000
C	3.04850700	3.51098200	1.11544400
C	4.23238100	4.24198300	1.10133000
C	4.63057000	4.93347400	-0.04497800
C	3.81554500	4.87913000	-1.17946000
C	2.62993500	4.15303400	-1.16979900
C	2.29433300	-3.39872300	0.01765100
C	3.05534100	-3.57896100	1.20060600
C	4.26817100	-4.25925700	1.19224400
C	4.78680000	-4.78979800	0.00789700
C	4.05593700	-4.62164900	-1.17203500
C	2.84179400	-3.94517900	-1.17091800
H	-1.35357100	1.21073800	-2.07702700
H	0.73217000	2.48012300	-2.18165200
H	0.73915900	2.51735300	2.16233800
H	-1.34236700	1.24001500	2.08552600
H	-1.34177900	-1.30787200	-2.06052000
H	0.76733500	-2.51704200	-2.15567600
H	-1.31981700	-1.28447400	2.10749200
H	0.78709500	-2.49376700	2.19498400
H	-5.57508500	0.01773800	2.68009900
H	-6.65169200	-0.32071200	1.31126200
H	-5.41165100	-1.50476800	1.78505700
H	-5.85426000	2.04413100	0.55781100
H	-4.61053100	2.10718200	1.82380100
H	-4.14301800	2.26605800	0.11850700
H	-6.65450300	0.28717900	-1.25523700
H	-5.58795000	-0.06325400	-2.62881100
H	-5.40079800	1.45551400	-1.73208300
H	-4.17684800	-2.33427000	-0.07577000
H	-5.88815300	-2.08742900	-0.50242100
H	-4.65480000	-2.16834300	-1.77747000
H	2.78561700	2.96689400	2.01798900
H	4.85323700	4.26325300	1.99291300
H	5.55407800	5.50387700	-0.05452600
H	4.10091200	5.41816500	-2.07890300
H	2.00886600	4.15864800	-2.06032200
H	2.70130900	-3.17271300	2.14288900
H	4.81697300	-4.37088800	2.12395600
H	5.73352600	-5.32084100	0.00428500
H	4.43330700	-5.02833200	-2.10680700
H	2.30180300	-3.85768900	-2.10826900
K	2.25425400	-0.00801000	-0.07892000

4



G_{sol} = -1969.300595 Hatree

N	-1.16049700	0.88159300	-0.53100900
C	-2.36340900	1.02984900	0.07615800
C	-3.27093700	0.02894500	0.25945200
C	-2.92565900	-1.30924800	-0.20540200
C	-1.70278400	-1.53816000	-0.73427200
C	-0.64811700	-0.46788200	-0.81101500
C	0.52762100	-0.61852100	0.18478500
N	1.04541900	0.74837900	0.27309000
B	0.05987900	1.82641800	-0.26886300

C	1.61049900	-1.58192700	-0.21234000
C	2.30122500	0.92490600	0.74426400
C	3.20021900	-0.09713500	0.86723800
C	2.87936200	-1.35854100	0.20183600
O	-0.29237300	2.88862000	0.68195300
C	0.01660800	4.16563000	0.12223200
C	0.08853400	3.85634900	-1.41052600
O	0.60280900	2.53009600	-1.42804300
C	1.02679700	4.77066300	-2.18882600
C	-1.29606200	3.87845700	-2.06979200
C	-1.07247500	5.15683900	0.51580000
C	1.35973800	4.63574200	0.68488200
C	-3.94137300	-2.39245500	-0.11906300
C	-3.57454500	-3.70785800	0.19970100
C	-4.52947600	-4.72091900	0.26434700
C	-5.87343000	-4.43649100	0.01739500
C	-6.25286100	-3.13007100	-0.29258700
C	-5.29619400	-2.11784800	-0.35447700
C	3.97485900	-2.32875600	-0.06564900
C	4.99054900	-2.52462700	0.88088200
C	6.01071600	-3.44838800	0.65682700
C	6.03912600	-4.18983100	-0.52437000
C	5.03832100	-3.99802900	-1.47855700
C	4.01901700	-3.07495700	-1.25220000
H	-2.57404700	2.04517000	0.40945500
H	-4.22405700	0.22973800	0.73333100
H	-1.44386600	-2.51652600	-1.13413600
H	-0.19042600	-0.46355500	-1.81524700
H	0.09368400	-0.92228900	1.16607300
H	1.33649600	-2.47943100	-0.76377900
H	2.57778900	1.95175000	0.98096300
H	4.20116100	0.10339600	1.22978400
H	1.00187000	4.50362700	-3.25086200
H	0.71813100	5.81852100	-2.09522600
H	2.05719700	4.67632700	-1.83720100
H	-1.68940200	4.89793000	-2.14554200
H	-1.20924600	3.46590200	-3.08052800
H	-2.01366800	3.26696400	-1.51539500
H	-0.93279800	6.11523300	0.00232300
H	-1.03251400	5.34140600	1.59505400
H	-2.06536300	4.77013900	0.27123000
H	2.17813800	3.99502700	0.34344100
H	1.58343900	5.66609000	0.38761700
H	1.31948400	4.59457200	1.77906000
H	-2.53348500	-3.93267400	0.41653600
H	-4.22525500	-5.73217400	0.51931200
H	-6.61867700	-5.22461500	0.07321600
H	-7.29588500	-2.89786800	-0.48852800
H	-5.59959600	-1.10491300	-0.60582200
H	4.97310300	-1.96095800	1.80993900
H	6.78242900	-3.58993600	1.40804100
H	6.83470300	-4.90731900	-0.70207800
H	5.05639900	-4.56209400	-2.40677200
H	3.25719100	-2.91785800	-2.01102800
K	-0.22713000	1.54970500	2.95289000

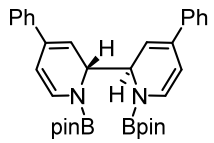
B_2pin_2

G_{sol} = -822.1193904 Hatree

O	1.61654600	1.13397600	-0.12185900
B	0.85263000	-0.00002400	0.00000100
O	1.61657100	-1.13400500	0.12186300
B	-0.85263000	-0.00002400	-0.00000100
O	-1.61657200	-1.13399900	-0.12192500
O	-1.61654600	1.13396900	0.12192000
C	2.99496800	-0.76585600	-0.15294100
C	2.99494900	0.76586000	0.15295000
C	-2.99494900	0.76586800	-0.15291000
C	-2.99496800	-0.76586400	0.15290100
C	3.24680000	-1.08203000	-1.62582700
C	-3.91639600	1.58980700	0.73105400
C	-3.91643100	-1.58978100	-0.73106600
C	-3.24676600	1.08212400	-1.62578100
C	-3.24679700	-1.08211500	1.62577100
C	3.91642800	-1.58982100	0.73098400
C	3.91639300	1.58984700	-0.73097200
C	3.24676900	1.08204000	1.62583700
H	3.03689200	-2.14123600	-1.80080300
H	2.59441200	-0.48982600	-2.27591900
H	4.28747300	-0.88574700	-1.90133100
H	-3.86407500	2.64223400	0.43630700
H	-4.95287900	1.25405800	0.61587800
H	-3.63815100	1.51174500	1.78439000
H	-3.86414000	-2.64220900	-0.43631600
H	-4.95290600	-1.25400400	-0.61589700
H	-3.63817800	-1.51172900	-1.78440100
H	-4.28744200	0.88587800	-1.90130100
H	-3.03683400	2.14133400	-1.80070000
H	-2.59438700	0.48993900	-2.27589900
H	-4.28746900	-0.88584600	1.90128700

H	-3.03688700	-2.14132900	1.80069100
H	-2.59440700	-0.48994400	2.27589200
H	3.86413000	-2.64223400	0.43618300
H	4.95290500	-1.25404500	0.61583000
H	3.63817800	-1.51182000	1.78432400
H	3.63815100	1.51183500	-1.78431300
H	3.86406500	2.64225900	-0.43617300
H	4.95287900	1.25409900	-0.61581000
H	4.28744600	0.88577800	1.90134400
H	3.03683800	2.14124100	1.80081200
H	2.59439100	0.48982200	2.27592700

7

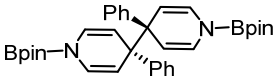


G_{sol} = -1780.3928268 Hatree

C	-2.06585900	-1.31813300	0.56659000
C	-0.82950000	-0.45943500	0.60863700
N	0.37254100	-1.29541000	0.68123100
C	0.39075400	-2.44403900	-0.09775900
C	-0.74649200	-3.01570900	-0.54615000
C	-2.03670100	-2.50539400	-0.07508200
C	-3.25333700	-3.34298400	-0.23050400
C	-4.50790000	-2.75224800	-0.44136500
C	-5.65345400	-3.53545600	-0.56467400
C	-5.56472600	-4.92638400	-0.48888100
C	-4.32095000	-5.52615300	-0.29034700
C	-3.17561300	-4.74125900	-0.16580800
B	1.48685500	-0.91501100	1.48888800
O	1.50103900	0.22123100	2.26139900
C	2.63242000	0.09173200	3.15853300
C	3.57538300	-0.87870300	2.36949400
O	2.63183100	-1.67179600	1.60160300
C	4.40059200	-1.80880300	3.24314600
C	4.46960600	-0.15013700	1.37139300
C	3.21350700	1.47254600	3.41194800
C	2.10649200	-0.51584100	4.45649400
H	-2.97584500	-0.94142800	1.02594700
H	-0.83533200	0.18919700	1.48989300
H	1.37239500	-2.86990000	-0.28242300
H	-0.69692900	-3.90192300	-1.16828500
H	-4.58117800	-1.67083100	-0.52763200
H	-6.61559800	-3.05959900	-0.73106700
H	-6.45716300	-5.53727500	-0.58830700
H	-4.24113000	-6.60767800	-0.22829200
H	-2.21417700	-5.21893100	0.00283200
H	5.02551300	-2.44618900	2.61043400
H	5.05920400	-1.22870700	3.89885000
H	3.76686700	-2.44951800	3.86057200
H	5.22874100	0.44943800	1.88350100
H	4.98078100	-0.89307900	0.75010600
H	3.88493000	0.50614300	0.71596900
H	2.48996200	2.07774500	3.96686500
H	4.12816100	1.39893800	4.01018200
H	3.44649400	1.98449800	2.47523000
H	2.89856400	-0.59765600	5.20683500
H	1.31799800	0.12979600	4.85423700
H	1.68297700	-1.51116400	4.28482500
C	-1.98409200	1.38183700	-0.63787000
C	-0.78791200	0.46719500	-0.64928800
N	0.45011900	1.24961900	-0.66652200
C	0.49654400	2.36100900	0.16571400
C	-0.63019100	2.97426600	0.58522200
C	-1.92254800	2.54680800	0.04172900
C	-3.10521800	3.43441300	0.17927100
C	-4.38796000	2.89114500	0.34308400
C	-5.50457600	3.71727900	0.45001000
C	-5.35799800	5.10445800	0.40380000
C	-4.08573900	5.65703200	0.25251800
C	-2.96909600	4.82913400	0.14522100
B	1.56376000	0.85000300	-1.46335700
O	1.48568600	-0.13149900	-2.42380300
C	2.83885800	-0.36160300	-2.88873800
C	3.54094900	0.99626700	-2.55175800
O	2.80682600	1.43809700	-1.37937300
C	3.33154700	2.05553200	-3.63191200
C	5.01455700	0.87847000	-2.20415100
C	3.39328500	-1.53323200	-2.08368700
C	2.80072500	-0.70161800	-4.36925000
H	-2.89146300	1.06448300	-1.14491700
H	-0.79185800	-0.17409000	-1.53585900
H	1.48987800	2.71530200	0.42565300
H	-0.56614700	3.82952800	1.24835000
H	-4.50598800	1.81204900	0.40549300
H	-6.48903000	3.27730100	0.58071100
H	-6.22746000	5.74949100	0.48973800
H	-3.96133300	6.73541700	0.21409200

H	-1.98441200	5.26994700	0.01374900
H	3.67698600	3.02105200	-3.25105300
H	3.89900000	1.81727400	-4.53654100
H	2.27285100	2.14774100	-3.89737300
H	5.57157000	0.47129600	-3.05523700
H	5.41837000	1.86946800	-1.97459200
H	5.17421800	0.23042200	-1.34031200
H	2.75831200	-2.40781300	-2.25504700
H	4.41411600	-1.78146400	-2.39017300
H	3.39134000	-1.31172600	-1.01003300
H	3.81783000	-0.78651300	-4.76707400
H	2.29878100	-1.66337900	-4.51180400
H	2.26231200	0.05771000	-4.94072500

7-para

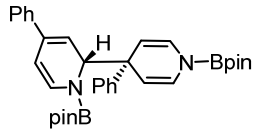


G_{sol} = -1780.374402 Hatree

C	-1.23147000	0.84557400	-1.07782200
C	-2.56702200	0.81602600	-1.15587700
N	-3.39814200	0.63314500	-0.04587000
C	-2.76257500	0.54898600	1.19873900
C	-1.43467800	0.59343000	1.34975300
C	-0.44707900	0.68623400	0.20670400
C	0.50561100	1.88515000	0.36656300
C	1.34605900	2.27357300	-0.68761000
C	2.25137200	3.32356200	-0.54407600
C	2.33134200	4.02605200	0.65858100
C	1.48337200	3.67176500	1.70565500
C	0.58131100	2.61668200	1.55747700
B	-4.81672700	0.50427900	-0.17574400
O	-5.47469000	0.60785000	-1.37659100
C	-6.83469000	0.15993700	-1.13054200
C	-7.00033400	0.43319800	0.40249500
O	-5.64430600	0.25846100	0.89208500
C	-7.91267200	-0.54271000	1.12520100
C	-7.40537800	1.87311500	0.70729900
C	-7.77997800	0.94714800	-2.02123600
C	-6.88482200	-1.32649300	-1.47480900
H	-0.68454200	0.99767600	-2.00313300
H	-3.08870900	0.93032900	-2.10052900
H	-3.43431600	0.43682400	2.04346200
H	-1.05128700	0.48749100	2.36038700
H	1.30871800	1.74896400	-1.63588100
H	2.89300400	3.59398000	-1.37835300
H	3.03686400	4.84386100	0.77264200
H	1.51919900	4.21670600	2.64497200
H	-0.06716500	2.37002100	2.39167100
H	-7.97157400	-0.27320800	2.18411600
H	-8.92336800	-0.50054500	0.70505500
H	-7.54263500	-1.56755600	1.04919900
H	-8.44256100	2.06167200	0.41422600
H	-7.31183300	2.04657800	1.78330700
H	-6.75931500	2.58666100	0.18480300
H	-7.59576900	0.68964000	-3.06863000
H	-8.82032800	0.69832500	-1.78596300
H	-7.64015200	2.02365600	-1.90044800
H	-7.89791400	-1.72404500	-1.36265100
H	-6.57281000	-1.45963200	-2.51484300
H	-6.20986400	-1.90581500	-0.83550300
C	1.23145800	-0.84575800	-1.07773300
C	2.56700800	-0.81615200	-1.15579500
N	3.39812300	-0.63312700	-0.04580800
C	2.76255600	-0.54888300	1.19879400
C	1.43466100	-0.59336400	1.34981500
C	0.44706400	-0.68631000	0.20677600
C	-0.50559300	-1.88523500	0.36677200
C	-1.34585000	-2.27396500	-0.68744100
C	-2.25113000	-3.32396700	-0.54379100
C	-2.33124900	-4.02617000	0.65902400
C	-1.48344700	-3.67159500	1.70613600
C	-0.58141600	-2.61650300	1.55784000
B	4.81670400	-0.50423400	-0.17569700
O	5.47466500	-0.60788400	-1.37653900
C	6.83465400	-0.15991500	-1.13053200
C	7.00031000	-0.43304400	0.40252700
O	5.64428000	-0.25829700	0.89210700
C	7.91263100	0.54294400	1.12514600
C	7.40538400	-1.87292800	0.70745100
C	7.77996000	-0.94717500	-2.02116400
C	6.88474500	1.32648800	-1.47492400
H	0.68453200	-0.99798500	-2.00302400
H	3.08869800	-0.93053200	-2.10043700
H	3.43429500	-0.43661500	2.04350600
H	1.05126700	-0.48734800	2.36044000
H	-1.30837700	-1.74959800	-1.63583900
H	-2.89261500	-3.59462300	-1.37810400
H	-3.03674800	-4.84398600	0.77317500
H	-1.51938200	-4.21631900	2.64557600

H	0.06693000	-2.36961400	2.39206800
H	7.97155700	0.27352400	2.18408100
H	8.92332100	0.50077700	0.70498700
H	7.54256200	1.56777300	1.04907100
H	8.44257000	-2.06149100	0.41439400
H	7.31184200	-2.04630200	1.78347300
H	6.75933300	-2.58653100	0.18501500
H	7.59574000	-0.68976000	-3.06857900
H	8.82030400	-0.69830200	-1.78591500
H	7.64016500	-2.02367600	-1.90028500
H	7.89782500	1.72407700	-1.36279500
H	6.57273300	1.45953100	-2.51497000
H	6.20976800	1.90584500	-0.83567000

7-hybrid

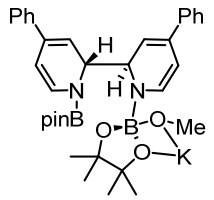


G_{sol} = -1780.3833583 Hatree

C	-3.99157700	0.02187700	0.29970200
C	-3.23734200	-1.06977400	0.52590000
N	-1.98919400	-1.24931400	-0.06766100
C	-1.28675500	-0.07257600	-0.59715200
C	-2.27266500	0.92118200	-1.15259500
C	-3.53161400	1.00774000	-0.67865700
C	-4.46500600	2.07035300	-1.13140100
C	-5.30513700	2.70468000	-0.20579800
C	-6.15964900	3.73101100	-0.60625900
C	-6.19427100	4.13450500	-1.94134300
C	-5.36756700	3.50396500	-2.87245700
C	-4.51215300	2.47969100	-2.47109500
B	-1.46255500	-2.56821400	-0.22602600
O	-2.01198000	-3.67314500	0.38553600
C	-1.38808000	-4.83118500	-0.22665300
C	-0.02691100	-4.24403200	-0.72924400
O	-0.37507900	-2.86496000	-1.01256800
C	0.51242400	-4.88533600	-1.99637800
C	1.04562400	-4.22593700	0.35775800
C	-1.25993300	-5.93062300	0.81373100
C	-2.29737600	-5.27993900	-1.36827200
H	-4.96795900	0.11041500	0.76201000
H	-3.57884400	-1.89749700	1.14015900
H	-0.62444000	-0.41954700	-1.39750700
H	-1.91089100	1.62032600	-1.90168000
H	-5.27382500	2.40743400	0.83973700
H	-6.79719200	4.21699300	0.12678700
H	-6.86272200	4.93077900	-2.25512500
H	-5.39505300	3.80369700	-3.91620000
H	-3.88558600	1.97959900	-3.20508700
H	1.46577200	-4.41985700	-2.26462700
H	0.68754300	-5.95496300	-1.83771700
H	-0.17983000	-4.76256400	-2.83233400
H	1.40957700	-5.23600600	0.56980600
H	1.88857500	-3.61823000	0.01484200
H	0.66412700	-3.79398700	1.28939600
H	-2.25566700	-6.28354500	1.09885600
H	-0.70200800	-6.77913100	0.40304500
H	-0.74919800	-5.57620200	1.71185300
H	-1.91524700	-6.18803900	-1.84440000
H	-3.29152700	-5.49280800	-0.96432900
H	-2.39470500	-4.49961500	-2.13053400
C	0.37112600	1.77737100	-0.15085100
C	1.69496500	1.90492000	-0.30531400
N	2.61686900	0.92941800	0.08751400
C	2.07948500	-0.24676400	0.62300300
C	0.76962000	-0.43664300	0.81592600
C	-0.30469800	0.57713200	0.48331800
C	-1.11234900	0.98007200	1.72842400
C	-1.80436600	2.19784000	1.77959500
C	-2.60376700	2.52965700	2.87280600
C	-2.72128700	1.65375300	3.95186800
C	-2.02006300	0.44935200	3.92734800
C	-1.22691700	0.12004800	2.82802200
B	4.02632300	1.10906000	-0.08307800
O	4.58021500	2.27601600	-0.54618900
C	5.97788300	1.98295300	-0.81111100
C	6.24882700	0.77101300	0.14399300
O	4.94596700	0.13080600	0.20264800
C	6.59916600	1.20234300	1.56554000
C	7.26597000	-0.22914700	-0.37744500
C	6.08428700	1.60984200	-2.28757000
C	6.80468200	3.22200000	-0.51354500
H	-0.24626900	2.59405500	-0.50890700
H	2.13526800	2.78758500	-0.75741300
H	2.81151900	-1.00999200	0.86713900
H	0.46928000	-1.40016200	1.21270300
H	-1.74213900	2.89873500	0.95330500
H	-3.13629100	3.47701600	2.87849400

H	-3.34178500	1.91241100	4.80497700
H	-2.09005000	-0.24103400	4.76338100
H	-0.70053700	-0.82892700	2.83737900
H	6.58366500	0.32257100	2.21545900
H	7.59806400	1.64662500	1.60913300
H	5.87620500	1.92898800	1.95098200
H	8.23408300	0.25923100	-0.53199100
H	7.40133500	-1.03008500	0.35555700
H	6.94169000	-0.67377700	-1.32087900
H	5.69972500	2.43813800	-2.88985400
H	7.12399500	1.42696900	-2.57500000
H	5.49615400	0.71464600	-2.51594400
H	7.87290700	2.99807600	-0.60704900
H	6.55737000	4.00863500	-1.23284800
H	6.61192000	3.60028700	0.49280800

IN7



G_{sol} = -2495.4945805 Hatree

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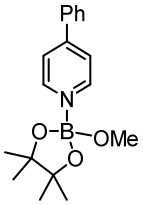
C	-1.33913900	0.59280100	-1.69560800
C	-0.11231100	1.05471200	-0.96231300
N	-0.30241100	2.41002200	-0.40364400
C	-1.58365700	2.83764500	-0.07050100
C	-2.69394600	2.21506600	-0.50627100
C	-1.55307300	-2.10684800	0.31024400
C	-0.37292300	-2.21067300	-0.37135300
N	0.60903700	-1.27522900	-0.35242300
C	0.29454200	0.05728600	0.18387900
C	-0.77229000	-0.01231400	1.24706900
C	-1.71254600	-0.98757300	1.22579900
B	0.82617200	3.23176700	-0.11410700
B	2.09297300	-1.66059200	-0.69646700
O	2.13809800	-2.82206500	-1.59176100
C	2.87250200	-3.87916300	-0.98637200
C	3.68034200	-3.15143700	0.14145000
O	2.77696900	-2.12247300	0.53822600
C	1.88730700	-4.90912000	-0.42247900
C	3.74510900	-4.55727200	-2.03834800
C	4.01099400	-4.02696800	1.34451300
C	4.97533300	-2.52554300	-0.39038000
O	2.76278800	-0.48537500	-1.23926400
O	2.09978400	2.94147400	-0.54326700
C	2.98584800	3.83301400	0.17462100
C	2.04515500	5.03990900	0.50354500
O	0.75115200	4.39534600	0.62179800
C	1.94481900	6.04217600	-0.64422000
C	2.36186600	5.75350500	1.80695400
C	4.16977200	4.17340000	-0.71426400
C	3.45067800	3.08582700	1.42339000
C	-3.78828600	0.49821500	-2.03654900
C	-4.88632500	1.30561900	-2.36806700
C	-6.02922400	0.75409300	-2.94550000
C	-6.09978200	-0.61745400	-3.19292100
C	-5.01755800	-1.43281100	-2.85725500
C	-3.87464500	-0.88054700	-2.28216400
C	-2.88288400	-0.95557200	2.14115600
C	-2.77057200	-0.51891700	3.46834100
C	-3.88967500	-0.46191700	4.29744800
C	-5.14271200	-0.84244300	3.81418000
C	-5.26629100	-1.28136300	2.49554700
C	-4.14537300	-1.34079900	1.66814600
C	2.64514600	-0.29946900	-2.62325600
H	-1.20352500	-0.21128000	-2.41489900
H	0.74688600	1.09023500	-1.63815500
H	-1.62178500	3.73216600	0.54403300
H	-3.66956000	2.58075000	-0.20678900
H	-2.28547600	-2.90429900	0.26232300
H	-0.12489100	-3.10696200	-0.93396200
H	1.22064500	0.48140300	0.59709100
H	-0.83839100	0.81490900	1.94967700
H	2.40084000	-5.79845000	-0.04113700
H	1.20767800	-5.22195400	-1.22276700
H	1.28114700	-4.48766900	0.38666200
H	3.11017300	-5.07168800	-2.76822100
H	4.35651100	-3.82596800	-2.57293700
H	4.40747000	-5.30165200	-1.58062900
H	3.11107700	-4.42680400	1.82050900
H	4.63955400	-4.87457300	1.04799000
H	4.56225700	-3.44014000	2.08745100
H	5.38960700	-1.86666700	0.38079300
H	5.72202100	-3.29210300	-0.62499300
H	4.78343500	-1.92540900	-1.28389700
H	1.72447700	5.53881300	-1.59161200
H	1.13431600	6.74515300	-0.43048500

H	2.87386800	6.60933100	-0.75756800
H	1.66253600	6.58295400	1.94968400
H	2.27832300	5.08011700	2.66296600
H	3.37725700	6.16375700	1.77958800
H	3.84397700	4.55543500	-1.68445700
H	4.80411900	4.92620400	-0.23396400
H	4.77213800	3.27497500	-0.88138500
H	3.93126900	2.15182500	1.11617500
H	4.17230700	3.67566300	1.99687100
H	2.60492200	2.83794600	2.07448700
H	-4.84040900	2.37681200	-2.18954600
H	-6.86570600	1.39698600	-3.20444000
H	-6.99251200	-1.04765400	-3.63730100
H	-5.06799800	-2.50388600	-3.03282800
H	-3.04621800	-1.52075900	-1.98837500
H	-1.79555300	-0.23552900	3.85714100
H	-3.78134900	-0.12681000	5.32513800
H	-6.01431200	-0.80128700	4.46069700
H	-6.23750800	-1.57631600	2.10817700
H	-4.25132600	-1.66825300	0.63617100
H	3.31864100	-0.96819300	-3.18000400
H	2.90479200	0.73753000	-2.86725700
H	1.62103000	-0.49002700	-2.98383100
K	0.96254000	-2.29640900	2.50820800

IN8



G_{sol} = -1005.3165569 Hatree

O	2.48336400	0.00028500	1.19655500
B	1.93003900	0.88680300	0.19850900
O	2.49963600	0.49412200	-1.07128000
C	3.42922900	-0.57223300	-0.85987100
C	2.98287800	-1.15576800	0.52461900
C	4.83967700	0.01981400	-0.81254900
C	3.33486500	-1.55930500	-2.01713200
C	4.11536800	-1.75637400	1.34694900
C	1.85827600	-2.18983200	0.38878900
H	5.00759400	0.60135300	-1.72530600
H	4.96130600	0.68652700	0.04616000
H	5.60308000	-0.76378700	-0.75654500
H	3.68970200	-1.08235500	-2.93716900
H	3.95937000	-2.44047100	-1.82910200
H	2.30500100	-1.88851900	-2.17843100
H	4.86636200	-1.00195700	1.59417200
H	3.71554100	-2.16324000	2.28192800
H	4.60355300	-2.57288700	0.80254200
H	2.23356800	-3.13419700	-0.01939300
H	1.43864400	-2.38521000	1.38153300
H	1.05179700	-1.83553300	-0.26012300
C	-1.69994500	0.31768000	-1.15288000
C	-0.33157800	0.51771700	-1.07196400
N	0.29498800	0.62129800	0.10716700
C	-0.40809900	0.53269700	1.24494200
C	-1.77744900	0.33212600	1.24146900
C	-2.45761400	0.21892500	0.02106600
C	-3.92169600	-0.00269100	-0.02455000
C	-4.69947300	0.59019800	-1.02787500
C	-6.07640200	0.38336100	-1.06665000
C	-6.69089300	-0.42436200	-0.10914200
C	-5.92246400	-1.02177300	0.89040600
C	-4.54671000	-0.80944600	0.93548000
H	-2.16227600	0.21239800	-2.12811300
H	0.30684500	0.57572700	-1.94647200
H	0.16497400	0.62176600	2.16146900
H	-2.30761000	0.28391300	2.18632700
H	-4.23175200	1.23645100	-1.76576400
H	-6.66923900	0.85807700	-1.84254500
H	-7.76380100	-0.58775000	-0.14204700
H	-6.39261300	-1.65866400	1.63349100
H	-3.95355600	-1.29467700	1.70573100
O	1.95814600	2.27965600	0.53814600
C	3.23733700	2.85899000	0.65336600
H	3.83324600	2.36738500	1.43450200
H	3.78997100	2.79889300	-0.29398500
H	3.11416700	3.91281000	0.92020800

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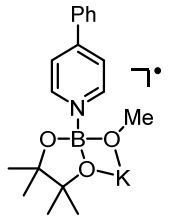
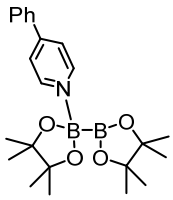


G_{sol} = -1605.303073 Hatree

O	2.26671500	-0.80024900	1.31164400
B	1.72521800	0.34578700	0.60087900
O	2.36189200	0.32165000	-0.72349200
C	3.25191200	-0.79160000	-0.81181200
C	2.76665500	-1.72549200	0.35376500
C	4.68136500	-0.28861300	-0.59873500
C	3.13990300	-1.41495100	-2.19913300
C	3.87867600	-2.55083600	0.99198200
C	1.63700400	-2.66905800	-0.07896100
H	4.87868000	0.52082400	-1.31013800
H	4.81629500	0.10255800	0.41323900
H	5.41770000	-1.08189900	-0.76680500
H	3.52144800	-0.71409700	-2.94964300
H	3.73217100	-2.33536800	-2.26182900
H	2.10139900	-1.65091400	-2.44652500
H	4.64097000	-1.91080900	1.44373900
H	3.45737200	-3.18839000	1.77672900
H	4.35957200	-3.19985400	0.25059600
H	2.00454300	-3.45468600	-0.74791800
H	1.22033300	-3.14536000	0.81506200
H	0.82936700	-2.13271300	-0.58506400
C	-1.80315700	-0.02097700	-0.98291800
C	-0.45055200	0.09847900	-0.83145500
N	0.15564000	0.26786200	0.38941100
C	-0.67178500	0.29486000	1.48781500
C	-2.02864000	0.17336100	1.40464000
C	-2.69685200	0.01121700	0.14171500
C	-4.12873100	-0.11593400	0.01650600
C	-4.76507500	-0.27428200	-1.24668900
C	-6.14317600	-0.39821900	-1.36261300
C	-6.96943700	-0.37273300	-0.23282500
C	-6.36888100	-0.21779100	1.02215700
C	-4.99169400	-0.09267100	1.14809500
H	-2.17560300	-0.14729400	-1.99328100
H	0.22482800	0.05499700	-1.67975100
H	-0.16903400	0.42033100	2.44111100
H	-2.58515800	0.20524800	2.33455600
H	-4.17142000	-0.29992700	-2.15449800
H	-6.58099200	-0.51738400	-2.35081100
H	-8.04646000	-0.47030300	-0.32757400
H	-6.98468300	-0.19497700	1.91801900
H	-4.57774300	0.02503200	2.14416700
K	1.69989400	2.91288100	-1.10048900
O	1.90180900	1.60098500	1.32327300
C	3.19492100	1.89440100	1.79961100
H	3.61500300	1.05405000	2.36589100
H	3.88744200	2.12950500	0.97655300
H	3.13235500	2.76869200	2.45494300

IN-S1

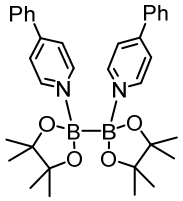


G_{sol} = -1301.23549 Hatree

O	1.52331700	1.59883400	-1.15226400
B	1.24088100	0.81027000	0.03479700
O	1.49801300	1.66850700	1.18075200
B	1.97222000	-0.75673400	0.01206500
O	3.26450200	-1.02790000	0.42617400
O	1.35611500	-1.90888300	-0.45044700
C	2.05551900	2.89702900	0.70868600
C	1.53422900	2.97528800	-0.76146800
C	2.35902200	-2.94688100	-0.56372800
C	3.44450400	-2.46399200	0.44787300
C	3.58117600	2.78239800	0.77284900
C	1.72901900	-4.28975500	-0.23078300
C	4.87478900	-2.79484000	0.05291000
C	2.84835700	-2.93797200	-2.01133200
C	3.17156700	-2.92581800	1.87886200
C	1.58832300	4.03944200	1.60200000
C	2.44229100	3.74727300	-1.71040000
C	0.11328400	3.54619500	-0.84939000
H	3.87197100	2.53384600	1.79890700
H	3.93822800	1.98548500	0.11225700
H	4.07343400	3.72006300	0.49306500
H	0.98801300	-4.54665600	-0.99430700
H	2.49104000	-5.07716600	-0.21657500
H	1.22982300	-4.26859200	0.74070700

H	5.56227800	-2.42499500	0.82001600
H	5.00829500	-3.87920600	-0.03061200
H	5.14349200	-2.33463700	-0.90079800
H	3.58009700	-3.73203700	-2.19033400
H	1.99311100	-3.09987800	-2.67454600
H	3.30491200	-1.97601700	-2.26757800
H	3.33892800	-4.00173000	1.99069800
H	3.85011100	-2.39827700	2.55615600
H	2.14269400	-2.69832200	2.17735700
H	2.01251000	3.91966900	2.60465000
H	1.92263100	5.00560500	1.20602400
H	0.49893600	4.05560700	1.69151400
H	3.41765600	3.26349600	-1.80505100
H	1.98397100	3.79484500	-2.70422200
H	2.59229800	4.77396900	-1.35648600
H	0.11109700	4.63011000	-0.69027400
H	-0.28554800	3.34485600	-1.84951800
H	-0.55812600	3.09263400	-0.11445800
C	-2.47839500	0.33561100	1.23432900
C	-1.12160900	0.61390800	1.19347700
N	-0.41559000	0.51943700	0.05906600
C	-1.02676900	0.13842300	-1.07066800
C	-2.38004100	-0.15158900	-1.10804000
C	-3.14196400	-0.05556200	0.06437700
C	-4.59372000	-0.35238500	0.06576500
C	-5.19246100	-0.96881500	1.17263700
C	-6.55754200	-1.24573200	1.17262700
C	-7.34183400	-0.90444400	0.07007900
C	-6.75381200	-0.28805300	-1.03497300
C	-5.38766500	-0.01680900	-1.03923100
H	-3.01358700	0.45338300	2.17032500
H	-0.56451700	0.94516500	2.06317500
H	-0.39460600	0.08056200	-1.95049900
H	-2.82792600	-0.46990200	-2.04323100
H	-4.58620300	-1.25501800	2.02760400
H	-7.00784600	-1.73285800	2.03211000
H	-8.40630400	-1.11849200	0.07206800
H	-7.35919700	-0.01277700	-1.89307500
H	-4.94123200	0.48152300	-1.89530000

IN-S2



G_{sol} = -1780.347979 Hatree

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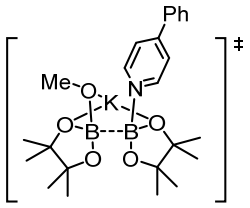
B	-1.94029800	0.54577700	-0.68360200
O	-1.81470800	-0.02300700	-2.02866000
B	-1.94000000	-0.54583500	0.68368600
O	-3.04463400	-1.49004800	0.74115600
O	-1.81437500	0.02290200	2.02877500
C	-2.89817500	0.45493500	-2.82346900
C	-3.29328700	1.78958200	-2.11406600
C	-2.89770200	-0.45522500	2.82365100
C	-3.29267300	-1.78992100	2.11424300
C	-4.02267200	-0.58343300	-2.76214900
C	-2.43531600	-0.62482200	4.26634900
C	-4.75685700	-2.17916800	2.27884600
C	-4.02236700	0.58296600	2.76246100
C	-2.40982300	-2.96457600	2.55614900
C	-2.43594100	0.62457500	-4.26621000
C	-4.75754900	2.17857900	-2.27853500
C	-2.41066000	2.96436100	-2.55607900
H	-3.62701300	-1.54786800	-3.09900900
H	-4.37820400	-0.70077900	-1.73338700
H	-4.86787400	-0.31520600	-3.40563700
H	-2.20486200	0.35546400	4.69809400
H	-3.22006300	-1.08761100	4.87693500
H	-1.53588200	-1.24371000	4.32547800
H	-4.94065100	-3.14209200	1.78934700
H	-5.01798300	-2.28285000	3.33888600
H	-5.41691300	-1.43394800	1.82741900
H	-4.86746800	0.31460200	3.40602100
H	-3.62682900	1.54745500	3.09930700
H	-4.37801200	0.70028400	1.73373500
H	-2.67177500	-3.30172900	3.56536400
H	-2.56261000	-3.79966600	1.86356900
H	-1.34811800	-2.70159000	2.54793500
H	-2.20541300	-0.35568300	-4.69797700
H	-3.22080000	1.08727200	-4.87672400
H	-1.53658800	1.24357300	-4.32542800
H	-5.41743300	1.43325900	-1.82701800

H	-4.94145400	3.14148800	-1.78904900
H	-5.01879900	2.28217700	-3.33855300
H	-2.67275300	3.30145000	-3.56528000
H	-2.56352200	3.79943600	-1.86349900
H	-1.34891500	2.70153800	-2.54794700
C	1.82639900	1.69307700	-0.82159700
C	0.60627200	1.10574600	-1.11804500
N	-0.51968400	1.44369100	-0.47450700
C	-0.47377900	2.38092400	0.48343700
C	0.70777500	3.01446200	0.83183800
C	1.89941100	2.66957500	0.17886900
C	3.18770600	3.30821500	0.53757700
C	4.37303800	2.56067300	0.53587700
C	5.58491900	3.15772800	0.87501200
C	5.62842300	4.51023200	1.21490800
C	4.45269300	5.26200200	1.21819600
C	3.23928300	4.66456700	0.88485400
H	2.70698500	1.39741200	-1.38253400
H	0.49058100	0.34677300	-1.88596000
H	-1.41838800	2.59444800	0.97211500
H	0.69937200	3.75303700	1.62666200
H	4.34414900	1.50210300	0.29141800
H	6.49418100	2.56441200	0.87883500
H	6.57362400	4.97627800	1.47669000
H	4.48012500	6.31650500	1.47554200
H	2.33119700	5.26108500	0.87178300
C	0.70806100	-3.01429600	-0.83188200
C	-0.47349000	-2.38077100	-0.48346200
N	-0.51935500	-1.44345500	0.47441400
C	0.60663500	-1.10539800	1.11782700
C	1.82676100	-1.69270900	0.82133900
C	1.89973100	-2.66930700	-0.17903100
C	3.18801700	-3.30795700	-0.53774900
C	3.23960400	-4.66433300	-0.88493100
C	4.45301100	-5.26177100	-1.21827200
C	5.62873300	-4.50998500	-1.21507800
C	5.58521900	-3.15745800	-0.87528000
C	4.37333800	-2.56039800	-0.53614800
H	0.69962700	-3.75295900	-1.62662600
H	-1.41813200	-2.59438600	-0.97202500
H	0.49096500	-0.34637500	1.88569500
H	2.70737400	-1.39695700	1.38218600
H	2.33153000	-5.26086900	-0.87179400
H	4.48044800	-6.31629300	-1.47554200
H	6.57393100	-4.97603700	-1.47685900
H	6.49446900	-2.56412500	-0.87917000
H	4.34444400	-1.50181000	-0.29176800

TS1

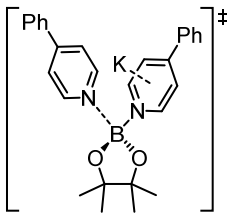


G_{sol} = -2016.305653 Hatree

O	-2.27704300	1.38180500	0.60403900
B	-0.87418200	1.11921800	0.40629300
O	-0.41154500	1.88797500	-0.69179400
B	-0.93509200	-0.96770300	-0.18613500
O	-1.56446800	-1.71343900	0.87590900
O	-1.67875000	-1.13878900	-1.38796200
C	-1.36419900	2.94302500	-0.89249600
C	-2.71205500	2.29643700	-0.41611400
C	-2.37359500	-2.38261300	-1.23063600
C	-2.68864600	-2.40976400	0.30398400
C	-1.34096500	3.35781200	-2.35589000
C	-3.60303200	-2.37778200	-2.12656900
C	-2.75726200	-3.80852400	0.90321700
C	-1.42389500	-3.51226600	-1.64429200
C	-3.96060100	-1.63535600	0.64645800
C	-0.94358000	4.12257500	-0.01098400
C	-3.41705600	1.52606700	-1.53168700
C	-3.68982500	3.28667400	0.20733200
N	0.51798200	-1.00118900	-0.24780100
C	1.28431700	-1.35008000	0.86186800
C	2.63873300	-1.14766900	0.89903800
C	3.35292400	-0.61876800	-0.20100500
C	2.57466100	-0.42753600	-1.37505000
C	1.22404500	-0.63608300	-1.39227200
C	4.79145500	-0.35381300	-0.14364100
C	5.44505300	-0.13915400	1.08940500
C	6.81558800	0.09450300	1.15722300
C	7.58860500	0.13975900	-0.00522900
C	6.95941700	-0.05744200	-1.23707100
C	5.59094900	-0.30167800	-1.30644100
O	-0.13763000	1.09019300	1.62632900
C	1.15000100	1.67306400	1.64138200
H	-2.11618700	4.10479600	-2.56212700
H	-0.36868800	3.80183100	-2.59447900

H	-1.49840800	2.49829300	-3.01238900
H	-3.29242700	-2.39132700	-3.17659600
H	-4.22299600	-3.26268300	-1.94204100
H	-4.20582000	-1.48185600	-1.95726500
H	-2.98406300	-3.74034500	1.97251700
H	-3.54986500	-4.39571200	0.42452800
H	-1.80901600	-4.33845000	0.78742600
H	-1.91366700	-4.49106600	-1.60448500
H	-1.09342400	-3.33203700	-2.67230500
H	-0.53771200	-3.53882500	-1.00016400
H	-4.84912900	-2.11036000	0.21889200
H	-4.09759300	-1.62031900	1.73381800
H	-3.88872100	-0.60675000	0.28254600
H	0.08444500	4.40237500	-0.26310100
H	-1.58808400	4.99434100	-0.16586900
H	-0.97437600	3.85101700	1.05012100
H	-2.75263200	0.78358500	-1.97850300
H	-4.28007300	0.99916300	-1.11041500
H	-3.78584800	2.21034600	-2.30344500
H	-3.96173200	4.06634300	-0.51395900
H	-4.60519000	2.76111600	0.49960600
H	-3.26878700	3.76314400	1.09579500
H	0.73033300	-1.77874300	1.68766900
H	3.16196300	-1.44856100	1.80322000
H	3.03614800	-0.10022100	-2.30257700
H	0.61529900	-0.47841800	-2.27425200
H	4.86514700	-0.13085200	2.00824000
H	7.28069600	0.25696000	2.12612300
H	8.65665000	0.32801900	0.04668600
H	7.54215100	-0.03183600	-2.15425400
H	5.14026400	-0.47793700	-2.27903200
H	1.67053200	1.32218300	2.53749600
H	1.73756800	1.38691600	0.76196800
H	1.07746400	2.76814200	1.67148100
K	-2.14865700	-0.00220100	2.97566200

TS2

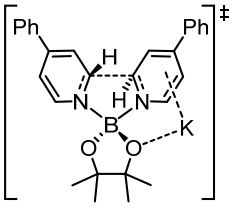


G_{sol} = -1969.275702 Hatree

N	-1.48013700	1.25015500	-0.05647800
C	-0.82534900	1.54142800	-1.18820100
C	0.34128100	2.29890000	-1.21980600
C	0.87948200	2.78980400	-0.01980700
C	0.21073100	2.44320400	1.16397400
C	-0.95088400	1.68125300	1.09606700
C	-0.74120200	-1.74621800	-1.17908200
N	-1.42831600	-1.44244800	0.01929000
B	-2.61655400	-0.62415600	0.01180300
C	0.44405600	-2.40259800	-1.19320300
C	-0.67249500	-1.61938500	1.20276400
C	0.51261600	-2.27609200	1.21806600
C	1.14832900	-2.79324700	0.01713100
O	-3.39478100	-0.46371600	-1.13757000
C	-4.76536200	-0.38637200	-0.69562000
C	-4.62852000	0.11723300	0.78353600
O	-3.35514800	-0.42941100	1.18007000
C	-5.69945000	-0.41255900	1.72697600
C	-4.56036900	1.64106800	0.88958100
C	-5.53453500	0.55371700	-1.61047500
C	-5.34530000	-1.79863300	-0.78391000
C	2.09907400	3.63356900	-0.00412000
C	3.01729800	3.54840900	1.05243400
C	4.16085700	4.34438000	1.06449900
C	4.40179900	5.24165900	0.02392000
C	3.49291400	5.33614200	-1.03086200
C	2.35221900	4.53706400	-1.04631800
C	2.42455900	-3.42146400	0.01393300
C	3.15299700	-3.70713200	1.21833600
C	4.40770000	-4.29980500	1.20422700
C	5.04322400	-4.65422300	0.00597800
C	4.35819700	-4.38911700	-1.18827200
C	3.10314200	-3.79700000	-1.19481800
H	-1.26688200	1.16122800	-2.10635800
H	0.82324800	2.49863200	-2.17208800
H	0.56278800	2.79678600	2.12796500

H	-1.50308300	1.42012400	1.99613100
H	-1.25898000	-1.46445800	-2.08967800
H	0.86563300	-2.61244200	-2.17243500
H	-1.13359000	-1.23331300	2.10570900
H	0.99265600	-2.37977100	2.18744700
H	-5.54026600	-0.00002100	2.72850200
H	-6.69609200	-0.10727100	1.38880000
H	-5.66993400	-1.50255800	1.79560500
H	-5.53817100	2.09245300	0.69148100
H	-4.25930000	1.90808000	1.90814800
H	-3.82728400	2.05596900	0.19425500
H	-6.55231500	0.70784300	-1.23466200
H	-5.60427200	0.11758800	-2.61216300
H	-5.03980200	1.52468100	-1.69039500
H	-4.80290700	-2.48582200	-0.12541700
H	-6.40624000	-1.81869100	-0.51523300
H	-5.24248900	-2.15705800	-1.81284000
H	2.85041800	2.84178100	1.86160200
H	4.86653900	4.25868400	1.88528100
H	5.29161400	5.86362200	0.03459000
H	3.66793200	6.03903400	-1.83979700
H	1.63990800	4.63461700	-1.86093500
H	2.71108400	-3.47180100	2.18216700
H	4.90256300	-4.49268000	2.15461900
H	6.02408400	-5.11897400	0.00300100
H	4.81462000	-4.65234300	-2.14106900
H	2.62421400	-3.62960500	-2.15506900
K	2.32545500	-0.16875600	-0.14828600

TS3

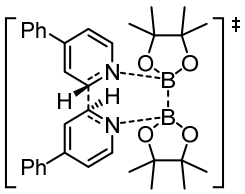


G_{sol} = -1969.260352 Hatree

N	-1.07193300	1.27109100	0.07613800
C	-2.20131900	1.72422400	0.67178800
C	-3.38203400	1.02729800	0.65062200
C	-3.43830600	-0.23800200	-0.01213800
C	-2.27243100	-0.72026000	-0.57088600
C	-1.06190600	-0.00892700	-0.41718900
C	2.18267800	0.48762400	1.66771600
N	0.79318400	0.62431700	1.49131400
B	0.35401000	1.78347600	0.54617000
C	2.86435700	-0.64425100	1.38013400
C	0.09086200	-0.63169100	1.43625300
C	0.76925900	-1.79806200	1.11123200
C	2.15474100	-1.83120000	0.88853000
O	0.24839300	3.10042300	1.14465700
C	1.02615500	4.03688700	0.40065900
C	1.21955600	3.32248100	-0.97792000
O	1.25536200	1.94463900	-0.59948200
C	2.51753400	3.67694900	-1.69330800
C	0.04134600	3.55524400	-1.93022700
C	0.27671500	5.36190400	0.31445600
C	2.35398100	4.25455600	1.13118900
C	-4.71083100	-0.99079000	-0.10322000
C	-4.71801400	-2.39356200	-0.07599000
C	-5.91381000	-3.10135800	-0.16842100
C	-7.12597900	-2.41971800	-0.28723800
C	-7.13175400	-1.02465600	-0.31129500
C	-5.93543600	-0.31648400	-0.21716500
C	2.84794300	-3.01020800	0.39354700
C	2.14889700	-4.09295800	-0.20175200
C	2.80468400	-5.22989300	-0.65695800
C	4.19658900	-5.34390600	-0.56563400
C	4.91058100	-4.28244300	-0.00634200
C	4.25781600	-3.14445000	0.46086200
H	-0.91763000	3.37516400	-1.43687200
H	-4.25793000	1.44560400	1.13341000
H	-2.25460500	-1.66321200	-1.10871800
H	-0.19076600	-0.27328000	-1.00616100
H	2.69437300	1.36123700	2.06959900
H	3.93189000	-0.66877100	1.58283400
H	-0.85305400	-0.69372700	1.98096500
H	0.18001100	-2.71543100	1.07306900
H	2.55914000	3.16714400	-2.66284400
H	2.57602200	4.75502400	-1.88184500
H	3.39205400	3.38180000	-1.10679900
H	0.04495800	4.57696800	-2.32476100
H	0.12855400	2.85966300	-2.77189300
H	-2.10434200	2.69338100	1.15114000
H	0.80392800	6.06736300	-0.33868600
H	0.20696900	5.81034100	1.31130700
H	-0.73758800	5.22191900	-0.06867800
H	2.95080400	3.33772800	1.14618700
H	2.94790200	5.04788600	0.66415100
H	2.14281000	4.54513200	2.16560800

H	-3.78203600	-2.93282600	0.04266000
H	-5.89969200	-4.18688500	-0.13731400
H	-8.05878600	-2.97130200	-0.35690100
H	-8.06959700	-0.48554400	-0.40840100
H	-5.95157000	0.76933200	-0.25578600
H	1.07203500	-4.02809800	-0.32931900
H	2.22379600	-6.03268600	-1.10508400
H	4.70808700	-6.22904200	-0.93130900
H	5.99383500	-4.33906300	0.07161300
H	4.85770200	-2.35024700	0.89431000
K	2.90434900	0.06645300	-1.52567000

TS-S1

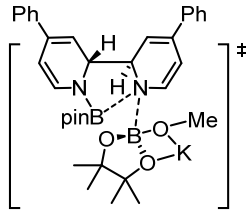


G_{sol} = -1780.324063 Hatree

O	-2.84097100	0.71329600	-1.35595800
B	-1.56805600	0.15609600	-1.10508800
O	-1.39443600	-1.05247700	-1.81118100
B	-1.56804500	-0.15609600	1.10509700
O	-2.84095800	-0.71329900	1.35596600
O	-1.39442500	1.05247200	1.81119900
C	-2.65740800	-1.36717200	-2.43082200
C	-3.34722800	0.03524400	-2.52210100
C	-2.65740400	1.36716600	2.43082900
C	-3.34721500	-0.03525300	2.52211300
C	-3.41247500	-2.33605300	-1.52308100
C	-2.38761400	2.02213600	3.77840900
C	-4.86532200	0.00063900	2.44835500
C	-3.41246900	2.33602500	1.52306300
C	-2.89263000	-0.83124900	3.74705600
C	-2.38760300	-2.02212600	-3.77840700
C	-4.86533400	-0.00066000	-2.44833500
C	-2.89265600	0.83124600	-3.74704500
H	-2.80139800	-3.23412400	-1.38152900
H	-3.60446100	-1.88436300	-0.54504300
H	-4.36333900	-2.64013500	-1.97311000
H	-1.91104900	2.99542300	3.62306600
H	-3.32603000	2.18643800	4.32058700
H	-1.72726100	1.41030700	4.39740700
H	-5.26281600	-1.01545500	2.53934300
H	-5.27838200	0.60257400	3.26581700
H	-5.20339000	0.41979200	1.49718300
H	-4.36332400	2.64013800	1.97308900
H	-2.80137900	3.23407900	1.38146400
H	-3.60446500	1.88428200	0.54505200
H	-3.28961900	-0.40832100	4.67552300
H	-3.25606700	-1.85923300	3.65226000
H	-1.79922800	-0.85838200	3.81531500
H	-1.91101700	-2.99540300	-3.62306900
H	-3.32601500	-2.18644500	-4.32058700
H	-1.72726200	-1.41027900	-4.39740100
H	-5.20339200	-0.41979300	-1.49715000
H	-5.26284000	1.01542700	-2.53934700
H	-5.27839300	-0.60262000	-3.26578000
H	-3.28965200	0.40832000	-4.67551100
H	-3.25609500	1.85922800	-3.65224100
H	-1.79925400	0.85838300	-3.81531300
C	1.99304400	1.38828700	-1.01426600
C	0.87984200	0.57779400	-1.19156300
N	-0.39158300	1.06456300	-1.04489300
C	-0.54043000	2.39202900	-0.70553300
C	0.53415500	3.21196400	-0.50953700
C	1.86234800	2.72543700	-0.64698100
C	3.03500600	3.59287300	-0.42192400
C	4.23717900	3.06206100	0.07443300
C	5.34702100	3.87775400	0.28007000
C	5.27833500	5.24350500	0.00102800
C	4.08831000	5.78456800	-0.48829200
C	2.97912900	4.96876900	-0.69742700
H	2.97091200	0.94571200	-1.18149700
H	0.95177900	-0.44269400	-1.54988500
H	-1.56490600	2.72951500	-0.61207000
H	0.34607600	4.24495200	-0.23506100
H	4.29534700	2.00631400	0.32642900
H	6.26442400	3.44766300	0.67140000
H	6.14248200	5.88016100	0.16577600
H	4.02508900	6.84476900	-0.71579500
H	2.06824600	5.40133300	-1.10204600
C	0.53416900	-3.21195600	0.50952000
C	-0.54041700	-2.39202300	0.70551800
N	-0.39157200	-1.06456100	1.04489100
C	0.87985300	-0.57779000	1.19156400
C	1.99305600	-1.38828100	1.01426400
C	1.86236100	-2.72542900	0.64697200
C	3.03502000	-3.59286500	0.42191700

C	2.97914200	-4.96876100	0.69741800
C	4.08832300	-5.78456000	0.48828600
C	5.27835000	-5.24349700	-0.00103000
C	5.34703700	-3.87774500	-0.28007000
C	4.23719500	-3.06205200	-0.07443500
H	0.34609200	-4.24494200	0.23503300
H	-1.56489300	-2.72950800	0.61204300
H	0.95178800	0.44269600	1.54989100
H	2.97092300	-0.94570700	1.18149800
H	2.06825700	-5.40132600	1.10203400
H	4.02510200	-6.84476100	0.71578800
H	6.14249800	-5.88015200	-0.16577600
H	6.26444100	-3.44765400	-0.67139600
H	4.29536300	-2.00630400	-0.32642900

TS-S2



G_{sol} = -2495.460077 Hatree

C	-3.96761800	0.93377000	-0.34881400
C	-4.14497300	-0.10573700	-1.35534100
C	-3.08370700	-0.94229300	-1.59501300
N	-1.84561300	-0.68059500	-1.13510700
C	-1.57024600	0.70064400	-0.78060800
C	-2.70724000	1.26792800	0.02452900
C	0.51214700	1.92804500	-0.05749000
C	-0.22202100	0.61468000	-0.04950400
N	0.53140500	-0.49049600	-0.70669300
C	1.15487600	-0.04089100	-1.88751900
C	1.49217500	1.23890500	-2.14221000
C	1.27605200	2.26271300	-1.11778800
B	-0.61711000	-1.62727700	-1.10283900
B	2.14416900	-0.87432700	0.70081700
O	2.02817000	-2.19278200	1.14744700
C	1.60528700	-2.16826700	2.52624200
C	2.00364800	-0.72278700	2.97553900
O	1.83654900	0.02908300	1.75825300
C	0.10111000	-2.39325000	2.63241600
C	2.33814500	-3.28166600	3.26384400
C	1.11821400	-0.11356600	4.05188000
C	3.47243900	-0.62753900	3.39766200
O	3.22282400	-0.46122300	-0.08793200
O	-0.71415300	-2.71338200	-0.15320600
C	-0.64739800	-3.96520600	-0.82099900
C	0.04654100	-3.59938500	-2.17267200
O	-0.39730500	-2.26426300	-2.39393200
C	-0.36153100	-4.46856900	-3.35508800
C	1.56978900	-3.58990500	-2.03527500
C	-2.06849400	-4.50341700	-1.01875800
C	0.14392000	-4.96015800	0.02530600
C	-5.15874700	1.51728300	0.32310900
C	-5.15989900	2.85722900	0.73928300
C	-6.26547400	3.40693200	1.38539600
C	-7.39971700	2.62863800	1.62086100
C	-7.41649300	1.29719100	1.20356800
C	-6.30838500	0.74899900	0.55896500
C	1.96135400	3.57728900	-1.22496200
C	3.20338100	3.68794800	-1.86875000
C	3.86749300	4.91295300	-1.93721200
C	3.29683100	6.05216200	-1.37156100
C	2.05592700	5.95800100	-0.73782100
C	1.39447000	4.73493900	-0.66821000
C	3.95910100	-1.35798800	-0.89191500
H	-5.12643500	-0.33897900	-1.75136100
H	-3.20887900	-1.87975700	-2.13430000
H	-1.43560700	1.29040400	-1.71370500
H	-2.50507400	1.92303900	0.87055300
H	0.37323700	2.60016500	0.78686500
H	-0.41316200	0.30370800	0.98188100
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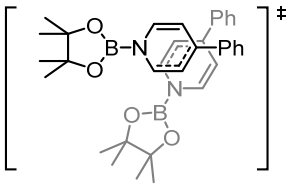
H	1.99105700	1.48636000	-3.07325500
H	-0.19947300	-2.40836500	3.68597800
H	-0.16138000	-3.34334800	2.16709500
H	-0.45731700	-1.61508400	2.10626400
H	1.98545600	-4.25123700	2.89673900
H	3.41812100	-3.22606800	3.10532500
H	2.13632200	-3.23172000	4.34000500
H	0.08388000	-0.02614300	3.71115600
H	1.13919300	-0.72292400	4.96235100
H	1.48418800	0.88726000	4.30399800
H	3.73189100	0.42209600	3.57468200
H	3.65723800	-1.17100000	4.32940700
H	4.13708600	-1.02929400	2.62447000
H	-1.43012700	-4.37691700	-3.56725800
H	0.19327900	-4.16153400	-4.24855900

H	-0.13240400	-5.52292000	-3.15988100
H	2.00713400	-3.12465400	-2.92615100
H	1.86068200	-3.01596600	-1.15044900
H	1.97970800	-4.60169400	-1.94257100
H	-2.64872400	-3.86627700	-1.69159300
H	-2.06283700	-5.52059700	-1.42688600
H	-2.57354700	-4.52470500	-0.04692200
H	-0.44273800	-5.25486600	0.90311100
H	0.36544600	-5.86875500	-0.54814900
H	1.07937200	-4.51274200	0.37056100
H	-4.29023900	3.47606700	0.53429000
H	-6.24581700	4.44822200	1.69474700
H	-8.26419200	3.05748800	2.11922300
H	-8.29326700	0.68159600	1.38477400
H	-6.32633500	-0.29311700	0.25131300
H	3.66383000	2.80573100	-2.30679700
H	4.83190800	4.97482000	-2.43295000
H	3.81005700	7.00738700	-1.42927900
H	1.59715200	6.84286700	-0.30622900
H	0.41742400	4.67620400	-0.19629000
H	4.02869200	-2.34442700	-0.41988500
H	4.96427000	-0.94651200	-1.01736100
H	3.49934700	-1.46571200	-1.88001100
K	3.66332700	1.95788700	1.01346800

TS-S3



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N	-0.33758400	1.90175100	-0.72640800
C	-0.23875900	0.53978000	-1.06046600
C	0.96786700	0.00577900	-1.48567100
C	2.18161000	0.66046200	-1.26283300
C	3.47743300	0.07290300	-1.60898000
C	4.67911600	0.79570900	-1.45774000
C	5.91180700	0.23789200	-1.78510800
C	5.99808800	-1.06877400	-2.26493200
C	4.82235700	-1.81072300	-2.40247200
C	3.58840600	-1.25271300	-2.08362400
B	-1.61245300	2.50875700	-0.48346700
O	-1.76857400	3.80543900	-0.06251000
C	-3.19043100	4.09096700	-0.16384200
C	-3.82271400	2.66258900	-0.05301900
O	-2.79294700	1.82631600	-0.64446900
C	-5.11396000	2.47791700	-0.83112500
C	-3.99476200	2.20027800	1.39179400
C	-3.58150000	5.04401000	0.95200700
C	-3.42054000	4.73588900	-1.52803400
H	2.93952400	2.63650100	-0.58868500
H	0.75138600	3.62055900	-0.20771500
H	-1.18282400	0.04972000	-1.27173600
H	0.93501500	-1.00651300	-1.87346800
H	4.66394100	1.81029700	-1.07413200
H	6.81373700	0.83076400	-1.65528700
H	6.95982500	-1.50328000	-2.52128200
H	4.86393800	-2.83370400	-2.76740800
H	2.70034200	-1.86262800	-2.21292700
H	-5.48384600	1.45782100	-0.68998700
H	-5.87897900	3.17218600	-0.46713200
H	-4.96517400	2.64722000	-1.89989400
H	-4.79807100	2.75057200	1.89076200
H	-4.24942100	1.13601500	1.39505400
H	-3.07033200	2.33531600	1.96395400
H	-3.10790900	6.01647700	0.78742000
H	-4.66694200	5.19029200	0.96251800
H	-3.26784700	4.66720300	1.92799300
H	-4.46640400	5.03166800	-1.65417600
H	-2.79594900	5.63057800	-1.60554800
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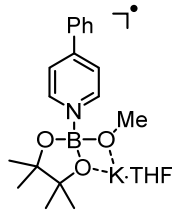
C	2.06971900	-2.02692700	0.78293800
C	0.86929200	-2.59461000	0.53926100
N	-0.33136400	-1.90994000	0.73267500
C	-0.23860400	-0.55000000	1.07765900
C	0.96546000	-0.01305600	1.50603100
C	2.18183900	-0.66213900	1.28147200
C	3.47453100	-0.07105800	1.63290800
C	4.67620400	-0.79863900	1.50793300
C	5.90621800	-0.23752200	1.83969600
C	5.98962700	1.07704700	2.29775700
C	4.81390500	1.82358900	2.40898700
C	3.58260600	1.26254800	2.08535800
B	-1.60428600	-2.51658300	0.47985300
O	-1.76656000	-3.83453600	0.13349100
C	-3.14936700	-3.96580800	-0.29769500

C	-3.84642000	-2.78796200	0.46364700
O	-2.77808700	-1.80905900	0.55537800
C	-4.24075300	-3.15532200	1.89183100
C	-5.02050400	-2.16374500	-0.27086800
C	-3.16236400	-3.77935200	-1.81277200
C	-3.65166600	-5.34860800	0.07826500
H	2.94919600	-2.62859800	0.59089000
H	0.76555900	-3.61792600	0.19527900
H	-1.18542800	-0.06653000	1.29246700
H	0.92861400	0.99652100	1.90076400
H	4.66268000	-1.82102400	1.14564400
H	6.80826900	-0.83466100	1.73238400
H	6.94921200	1.51401400	2.55796900
H	4.85344300	2.85296300	2.75576800
H	2.69445900	1.87713500	2.18934500
H	-4.53330000	-2.24457500	2.42269300
H	-5.08698400	-3.84887400	1.90190600
H	-3.40482700	-3.61540700	2.42931000
H	-5.79935700	-2.91278600	-0.45007200
H	-5.45104700	-1.36423900	0.33992200
H	-4.71285700	-1.73882900	-1.22916100
H	-2.50082000	-4.52301400	-2.26650700
H	-4.16862000	-3.91573900	-2.22010900
H	-2.80435900	-2.78238500	-2.09228000
H	-4.72067400	-5.43801700	-0.14288700
H	-3.11787500	-6.10432000	-0.50578800
H	-3.49418000	-5.55563000	1.13907900

8.5 Coordinates of Stationary Points for Spectroscopy Calculation

10·THF



O	2.99339700	-1.53034900	1.02968800
B	2.08379700	-0.44361000	0.69392800
O	2.58184900	0.09884400	-0.58688800
C	3.77518300	-0.59312900	-0.99439800
C	3.72328300	-1.92734900	-0.13786100
C	4.99049700	0.29112700	-0.66064300
C	3.73090800	-0.80998200	-2.51207200
C	5.09678600	-2.45273100	0.29683900
C	2.96504300	-3.07029800	-0.84316800
H	4.86386900	1.26635600	-1.14617600
H	5.08662600	0.45793800	0.41566300
H	5.92583300	-0.14849800	-1.02632600
H	3.76029300	0.15940900	-3.02451600
H	4.59410000	-1.39441700	-2.85352000
H	2.81950900	-1.32806300	-2.82226000
H	5.63069000	-1.72595100	0.91516000
H	4.96935800	-3.36861300	0.88598400
H	5.72096200	-2.69654100	-0.57168200
H	3.52445300	-3.45787500	-1.70266500
H	2.82694000	-3.89136500	-0.13017600
H	1.97602700	-2.75668600	-1.18833700
C	-1.33802000	-1.39145400	-0.93241700
C	-0.04607000	-0.96913900	-0.75734000
N	0.57133900	-0.90694300	0.47483500
C	-0.18580200	-1.32682200	1.55213800
C	-1.47871700	-1.76217300	1.44040000
C	-2.16063300	-1.81527300	0.17133800
C	-3.53297900	-2.24691400	0.02215000
C	-4.17288900	-2.32105800	-1.25378700
C	-5.49502000	-2.73373400	-1.39248000
C	-6.26300700	-3.09746100	-0.27414900
C	-5.66021900	-3.03457900	0.99293100
C	-4.33874000	-2.62314600	1.14110200
H	-1.72043400	-1.39186000	-1.94762600
H	0.56581800	-0.65349500	-1.59386700
H	0.31469700	-1.28500200	2.51261700
H	-1.97416800	-2.07207100	2.35428400
H	-3.62430400	-2.05430600	-2.15168200
H	-5.93420100	-2.77395500	-2.38762800
H	-7.29486100	-3.41933800	-0.38621500
H	-6.23028600	-3.30953200	1.87847200
H	-3.92403400	-2.58873400	2.14363000
K	1.14076500	2.42924200	-0.17782600
O	1.95361200	0.55736600	1.76052800
C	3.09287100	0.97483000	2.48904900
H	3.66158200	0.12051200	2.87742400
H	3.77269700	1.58918000	1.87759600
H	2.75190300	1.58443400	3.33470900
C	-2.51871400	5.92955500	-0.34804500

H	-2.61375900	6.13361000	-1.42136800
H	-2.80397000	6.83344400	0.19899800
C	-1.09687100	5.47236000	-0.01264100
H	-0.32941700	5.92129600	-0.65150100
H	-0.84573200	5.67436800	1.03743500
C	-3.35104900	4.69624300	0.04008100
H	-3.52145200	4.67382200	1.12314200
H	-4.32342600	4.65638400	-0.46031200
C	-2.43370200	3.54632400	-0.38274200
H	-2.54381400	2.64751700	0.23169000
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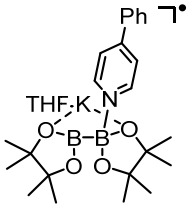
O	-1.07916800	4.03939900	-0.22397700

9-K·THF



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O	1.28767900	-0.56070600	-1.68682800
B	1.61791200	-1.33244600	0.89571500
O	2.26485000	-0.15719600	1.29447400
O	1.71367900	-2.28526700	1.89711700
C	1.89977600	-1.30041300	-2.75771200
C	1.22115700	-2.71862400	-2.63936400
C	2.63197200	-1.81903700	2.93324500
C	2.62341100	-0.26012200	2.71071500
C	3.41940800	-1.35016700	-2.50371800
C	2.10879300	-2.28150600	4.29295900
C	3.96708000	0.43491400	2.92656900
C	3.99208000	-2.47198400	2.64695400
C	1.52542600	0.46706500	3.49969500
C	1.63595700	-0.57226900	-4.08020800
C	2.09791600	-3.88210200	-3.11793700
C	-0.13693000	-2.79464400	-3.36780200
H	3.80537600	-0.32622200	-2.42682000
H	3.64854700	-1.87123700	-1.56846700
H	3.95738400	-1.84784900	-3.31904400
H	2.13170400	-3.37572300	4.34107000
H	2.73675800	-1.89524500	5.10465700
H	1.07950900	-1.95637600	4.46477200
H	3.86569200	1.50737200	2.72438300
H	4.30061900	0.32058800	3.96462300
H	4.74301500	0.03606400	2.26815300
H	4.73124500	-2.21520400	3.41379500
H	3.86951000	-3.56035400	2.64186200
H	4.38537400	-2.17180300	1.67005200
H	1.74309700	0.47646400	4.57324000
H	1.46559200	1.50585500	3.15639500
H	0.54563800	0.00277700	3.34810600
H	2.14191900	0.40133900	-4.07819600
H	2.02350800	-1.14688500	-4.93071700
H	0.56821000	-0.39808000	-4.23869300
H	3.01733400	-3.96072800	-2.53105100
H	1.54859800	-4.82525700	-3.01192100
H	2.36714900	-3.76796000	-4.17569700
H	-0.01314700	-2.80461100	-4.45778500
H	-0.63984400	-3.72424700	-3.07671000
H	-0.79150900	-1.96042400	-3.10170900
C	-2.79397500	0.02832100	-0.84561200
C	-1.46331100	-0.22255000	-1.06376000
N	-0.76033600	-1.20980000	-0.41104200
C	-1.47695000	-1.95896900	0.49890400
C	-2.80682700	-1.76104200	0.76148300
C	-3.57082800	-0.73482500	0.09781900
C	-4.97306700	-0.49541000	0.35338200
C	-5.71679300	0.50182600	-0.35218100
C	-7.06714300	0.72910200	-0.10307300
C	-7.76400300	-0.01773100	0.86144400
C	-7.05899700	-1.00492100	1.57045400
C	-5.70880200	-1.23946600	1.32817000
H	-3.24369000	0.83198300	-1.41947400
H	-0.88885800	0.34810700	-1.78407100
H	-0.91552700	-2.73646700	1.00682900
H	-3.26737500	-2.41654400	1.49304900
H	-5.22952500	1.10491200	-1.11211300
H	-7.58632000	1.49940900	-0.67067200
H	-8.81837800	0.16237100	1.05318700
H	-7.57096300	-1.59984500	2.32473700
H	-5.21310600	-2.01204500	1.90779600
K	1.97608200	1.82223600	-0.59416700
C	-0.17606300	6.36736000	-0.00588800
H	-0.12669400	6.51534700	1.07956900
H	-1.05144700	6.90343400	-0.38507900
C	-0.21939000	4.87450700	-0.34263800
H	-0.72569000	4.26787200	0.41476500
H	-0.69439700	4.69352900	-1.31597100
C	1.14005900	6.80745100	-0.66816400

H	0.99455600	6.96397600	-1.74385100
H	1.55326800	7.72640200	-0.24098500
C	2.04046100	5.59529500	-0.41962900
H	2.79973000	5.44511400	-1.19395400
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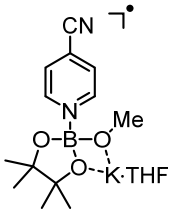
O	1.16295100	4.44286000	-0.41852900

16·THF



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O	-1.89614300	-0.72503200	-0.68055900
C	-3.30315600	-0.67471100	-0.97815700
C	-3.82634300	0.47555000	-0.01770500
C	-3.91312700	-2.05112400	-0.65879100
C	-3.48441500	-0.38876400	-2.47306700
C	-5.24665800	0.25611900	0.51587600
C	-3.75123100	1.87938400	-0.64828600
H	-3.37686400	-2.81798700	-1.23111700
H	-3.82130100	-2.29406700	0.40334500
H	-4.97273800	-2.10442400	-0.93470000
H	-3.08045300	-1.22123700	-3.06209200
H	-4.54567700	-0.28253900	-2.72949300
H	-2.96622800	0.52417800	-2.77861000
H	-5.32495500	-0.67168900	1.08849700
H	-5.51494900	1.08347400	1.18210500
H	-5.97963600	0.22837600	-0.30037700
H	-4.48553000	2.00687600	-1.45270000
H	-3.96352300	2.62019300	0.12998100
H	-2.75798000	2.10006300	-1.04810000
C	0.99077200	2.25650300	-0.98039000
C	-0.07806200	1.42124700	-0.79836100
N	-0.46366100	0.94076400	0.44613900
C	0.23614400	1.42748300	1.54250400
C	1.30846400	2.26656900	1.43273400
C	1.76954200	2.70166500	0.14033500
H	1.23816300	2.58965300	-1.98390900
H	-0.68164800	1.07868300	-1.62984300
H	-0.12027800	1.08025000	2.50408800
H	1.81045900	2.60784400	2.33263900
K	0.63996000	-1.70106700	-0.36136400
O	-1.04528600	-1.05869000	1.61976500
C	-1.84824800	-1.79413100	2.52430200
H	-2.67356400	-1.18524900	2.90897000
H	-2.27288400	-2.69678600	2.05531700
H	-1.21555300	-2.11220000	3.36248200
C	5.69233500	-2.06097100	-0.13020700
H	6.09023300	-2.34597300	-1.11167700
H	6.41107200	-2.37775300	0.63193800
C	4.30681600	-2.67827400	0.08713100
H	4.16974100	-3.63409700	-0.43089300
H	4.09117600	-2.82053400	1.15480500
C	5.38717400	-0.55460000	-0.09116600
H	5.29881900	-0.20243600	0.94323600
H	6.14408900	0.05546700	-0.59266400
C	4.03268900	-0.48810500	-0.79361200
H	3.40778400	0.34766900	-0.46808200
H	4.14503800	-0.44747100	-1.88550100
O	3.35178700	-1.72827700	-0.44775400
C	2.91502100	3.50184300	-0.01920200
N	3.88554900	4.14913400	-0.15797200

References

[1] Cui, Y.; Li, W.; Sato, T.; Yamashita, Y.; Kobayashi, S. *Adv. Syn. Cat.* **2013**, *355*, 1193-1205.
[2] Williams, C. W.; Shenje, R.; France, S. *J. Org. Chem.* **2016**, *81*, 8253-8267.
[3] Cutulic, S. P.; Murphy, J. A.; Farwaha, H.; Zhou, S. Z.; Chrystal, E. *Synlett* **2008**, *2008*, 2132-2136.
[4] Beutner, G. L.; Kuethe, J. T.; Yasuda, N. *Tetrahedron Lett.* **2009**, *50*, 781-784.
[5] Cutulic, S. P.; Findlay, N. J.; Zhou, S. Z.; Chrystal, E. J.; Murphy, J. A. *J. Org. Chem.* **2009**, 74, 8713-8718.
[6] Dahlén, A.; Petersson, A.; Hilmersson, G. *Org. Biomol. Chem.* **2003**, *1*, 2423-2426.
[7] Gottlieb, H. E.; Kotlyar, V.; Nudelman, A. *J. Org. Chem.* **1997**, *62*, 7512-7515.
[8] Smallcombe, S. H.; Patt, S. L.; Keifer, P. A. *J. Magn. Reson., Ser. A* **1995**, *117*, 295-303.
[9] Harris, R. K.; Becker, E. D.; De Menezes, S. M. C.; Granger, P.; Hoffman, R. E.; Zilm, K. W. *Pure Appl. Chem.* **2008**, 80, 59-84.
[10] Stoll, S.; Schweiger, A. *J. Magn. Reson.* **2006**, *178*, 42-55.
[11] Zhang, L.; Jiao, L. *J. Am. Chem. Soc.* **2017**, *139*, 607-610.
[12] Ghorai, D.; Choudhury, J. *ACS Catal.* **2015**, *5*, 2692–2696.
[13] Su, S. J.; Tanaka, D.; Li, Y. J.; Sasabe, H.; Takeda, T.; Kido, J. *Org. Lett.* **2008**, *10*, 941-944.
[14] Ma, R.; Liu, A. H.; Huang, C. B.; Li, X. D.; He, L. N. *Green Chem.* **2013**, *15*, 1274-1279.
[15] Wang, G.; Zhang, H.; Zhao, J.; Li, W.; Cao, J.; Zhu, C.; Li, S. *Angew. Chem., Int. Ed.* **2016**, *55*, 5985-5989.
[16] Chen, D.; Xu, G.; Zhou, Q.; Chung, L. W.; Tang, W. *J. Am. Chem. Soc.* **2017**, *139*, 9767-9770.
[17] Du, Y.; Hyster, T. K.; Rovis, T. *Chem. Comm.* **2011**, *47*, 12074-12076.
[18] Frings, M.; Bolm, C.; Blum, A.; Gnamm, C. *Eur. J. Med. Chem.* **2017**, *126*, 225-245.
[19] Imai, S.; Togo, H. *Tetrahedron* **2016**, *72*, 6948-6954.
[20] Pan, X.; Lacôte, E.; Lalevée, J.; Curran, D. P. *J. Am. Chem. Soc.* **2012**, 134, 5669-5674.
[21] Full citation of Gaussian 09: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J.; *Gaussian 09, revision B.01*; Gaussian Inc.: Wallingford, CT, 2010.
[22] (a) Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215-241. (b) Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res.* **2008**, *41*, 157-167.