

Supplementary Information

for

Direct Borylation of Tertiary Anilines via C-N Bond Activation

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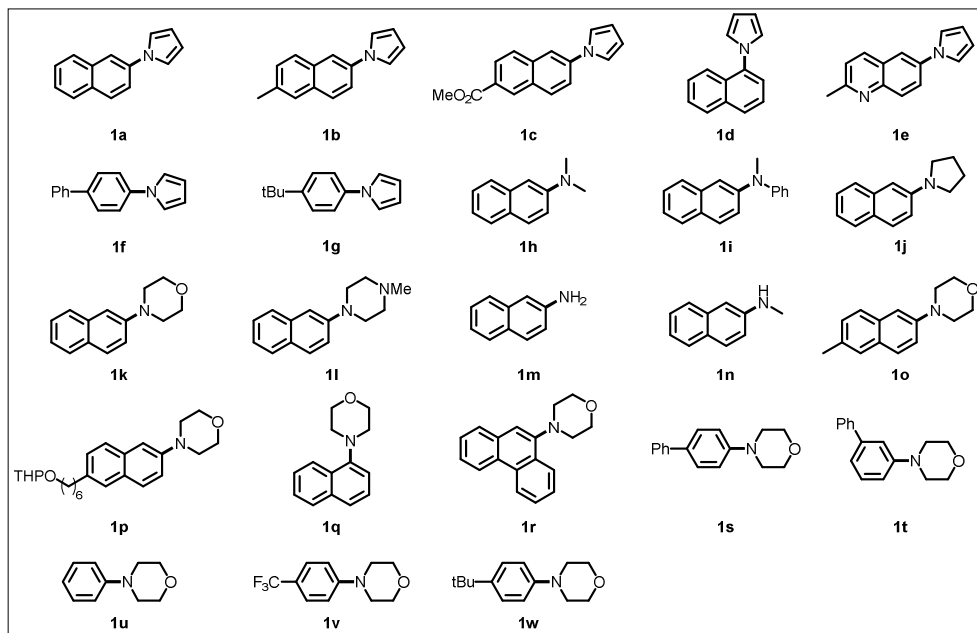
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(I) General considerations

All the reactions were carried out under nitrogen atmosphere using standard Schlenk technique and heated in the oil bath. The catalysts $\text{Ni}(\text{cod})_2$ was purchased from Strem without further purification. Phosphine ligands, such as PCy_3 , PPh_3 , and DCyPE , were purchased from Acros without further purification. NHC ligands, such as IMes: (1,3-bis(2,4,6-trimethylphenyl)imidazol-2-ylidene), SIMes: (1,3-bis(2,4,6-trimethylphenyl)-4,5-dihydroimidazol-2-ylidene), IPr: (1,3-bis(2,6-di-*i*-propylphenyl)imidazol-2-ylidene), SIPr: (1,3-bis(2,6-di-*i*-propylphenyl)-4,5-dihydroimidazol-2-ylidene) were purchased from Alderich without further purification. ItBu: (1,3-Di-*t*-butylimidazol-2-ylidene), IAd: (1,3-bis(1-adamantyl)imidazol-2-ylidene) were purchased from Strem without further purification. IMes^{Me} was prepared via the reported method.¹ THF, toluene were freshly distilled over sodium under N_2 with the use of diphenyl ketone as an indicator, B_2pin_2 (bis(pinacolato) diboron) was purchased from Beijing Ouhe technology Co., Ltd and used with strict recrystallization, B_2nep_2 (bis(neopentyl glycolato) diboron) was purchased from Beijing Zhongshenghuateng technology Co., Ltd (used for the borylation of pyrroles) and Ark(FoGang) Chemicals Industry Co. Ltd. (used for borylation of aniline derivatives) without further purification. PhCO_2Na , Na_2CO_3 , AcONa were purchased from Beijinghuagong Chemicals without further purification, CsF , KF , NaF were purchased from Alfa-Asea without further purification, MeONa , $^t\text{BuONa}$, EtONa , HCOONa , K_3PO_4 were purchased from J&K without further purification. ^1H NMR (400/500 MHz)/ ^{13}C NMR (100/125 MHz) were registered on Bruker 400/500 M spectrometers with CDCl_3 as solvent and tetramethylsilane (TMS) as internal standard. Data are presented as follows: chemical shift (ppm), multiplicity (s = singlet, d = doublet, t = triplet, dd = doublet of doublets, m = multiplet, br = broad), coupling constant J (Hz) and integration. Column chromatography was performed on silica gel 200-300 meshes. MS and HRMS were performed by the State-authorized Analytical Center in Peking University.

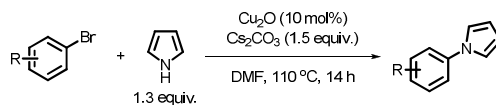
(II) Preparation of substrates

Substrate Scope

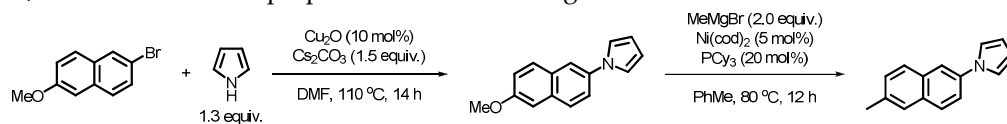


A, Substrates **1h**, **1m**, **1n** were purchased from J&K without further purification;

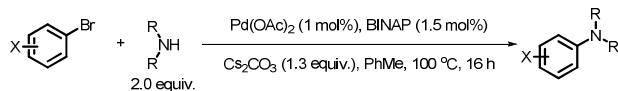
B, Substrates **1a**, **1c**, **1d**, **1e**, **1f**, **1g** were prepared from the commercially materials via the following method:



C, Substrates **1b** were prepared via the following methods:



D, Substrates **1i**, **1j**, **1k**, **1l**, **1o**, **1p**, **1q**, **1r**, **1s**, **1t**, **1u**, **1v**, **1w** were prepared via the following method:



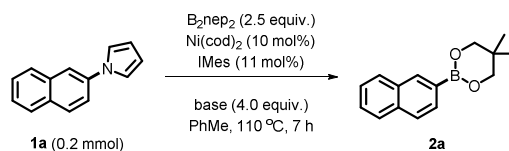
(III) General procedure of borylation of C-N bonds

Typical procedure A: (suitable for borylation of N-aryl pyrroles): In a nitrogen-filled glovebox, an oven-dried seal-tube equipped with a magnetic stir bar was charged with N-aryl pyrrole (0.2 mmol), B₂nep₂ (0.5 mmol), PhCO₂Na (0.8 mmol), then **the purple mixture** of catalyst Ni(cod)₂ (0.02 mmol, 5.6 mg) and ligand IMes^{Me} (0.022 mmol, 7.3 mg) in PhMe (1.0 mL) was added via syringe (**note: the Ni(cod)₂ and IMes^{Me} should be stirred in PhMe for 30 min**). The reaction was removed from the glovebox and maintained at 110 °C for 7 h in an oil-bath (**after addition of the mixture of catalyst and ligand, the reaction system will maintain purple, while will become yellow after heated at 110 °C in 2 min**). Then the reaction was purified by flash chromatography. Any deviations from this protocol are specified in the table footnotes.

Typical procedure B: (suitable for borylation of other substrates in table 2 and table 3): In a nitrogen-filled glovebox, an oven-dried seal-tube equipped with a magnetic stir bar was charged with aniline derivatives (0.2 mmol), B₂nep₂ (0.5 mmol), then **the purple mixture** of the catalyst Ni(cod)₂ (0.02 mmol, 5.6 mg) and ligand IMes^{Me} (0.07 mmol, 23.2 mg) in THF (1.0 mL) was added via syringe (**note: the Ni(cod)₂ and IMes^{Me} should be stirred in THF for 30 min**). The reaction was removed from the glovebox and maintained at 135 °C for 48 h in an oil-bath (**the reaction system will not become yellow after heated at 135 °C**). Then the reaction was purified by flash chromatography. Any deviations from this protocol are specified in the table footnotes.

(IV) Complementary experiments

Table S1: Effects of various bases^a



entry	bases	yield (conversion)
1	-	40% (75%)
2	CsF	6% (33%)
3	KF	49% (90%)
4	NaF	43% (94%)
5	Na ₂ CO ₃	21% (67%)
6	K ₃ PO ₄	4% (35%)
7	^t BuONa	<5% (23%)
8	EtONa	0% (7%)
9	PhONa	0% (11%)
10	HCO ₂ Na	45% (100%)
11	CH ₃ CO ₂ Na	37% (92%)
12	PhCO ₂ Na	54% (>95%)
13	PhCO ₂ K	49% (>95%)
14 ^b	PhCO ₂ Na	0%

Reaction conditions: **1a** (0.2 mmol), B₂nep₂ (0.5 mmol), Ni(cod)₂ (10 mol%, 5.6 mg), IMes (11 mol%, 6.9 mg), base (0.8 mmol), PhMe (1.0 mL), 110 °C, 7 h; ^a NMR yields were reported and dibromomethane was used as inner standard; ^b THF was used the solvent.

Table S2: Effects of various ligands^a

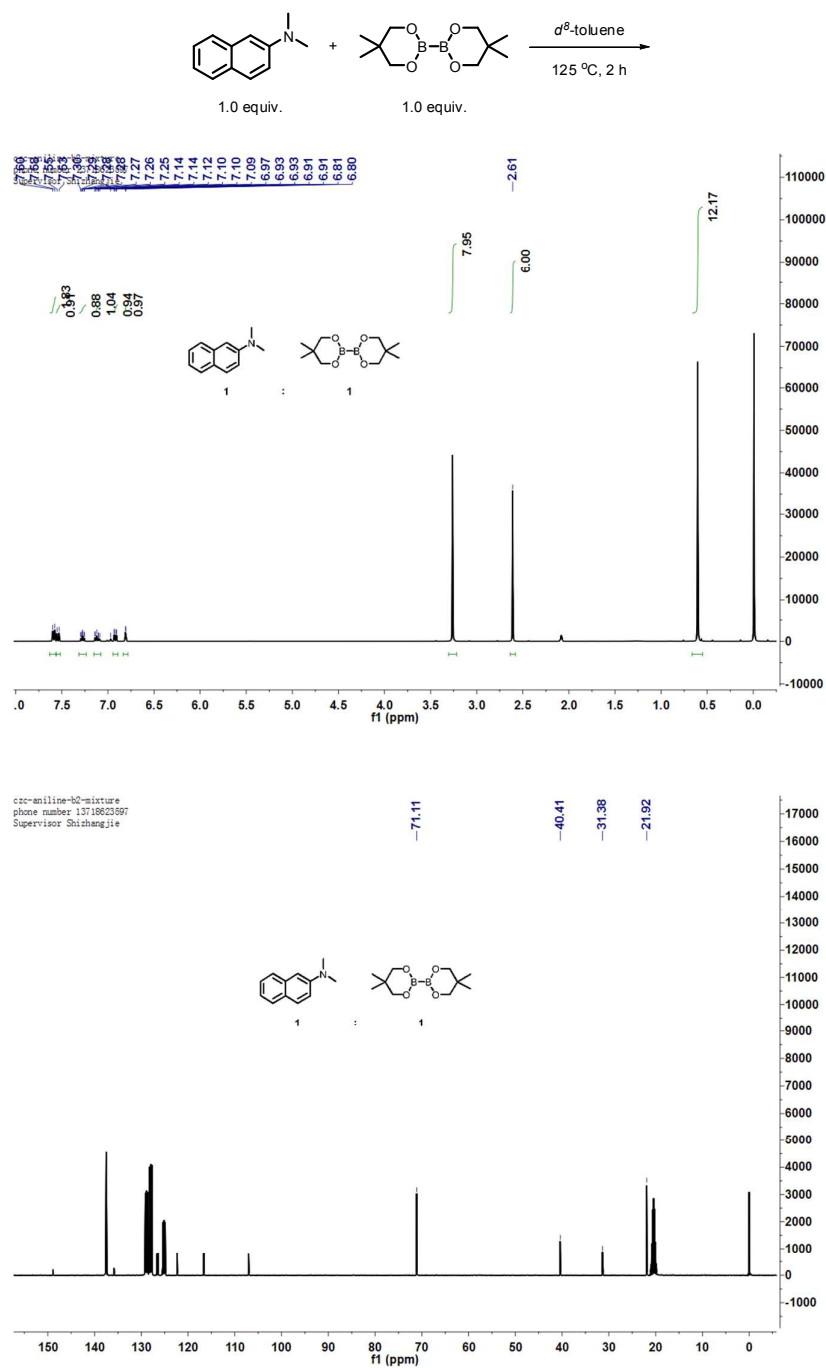
1a, 0.2 mmol
 $\xrightarrow[\text{PhCO}_2\text{Na (4.0 equiv.)}]{\text{B}_2\text{nep}_2 \text{ (2.5 equiv.)}, \text{Ni(cod)}_2 \text{ (10 mol\%)}, \text{ligand (11 mol\%)}, \text{PhMe, 110 }^\circ\text{C, 7 h}}$
 2a

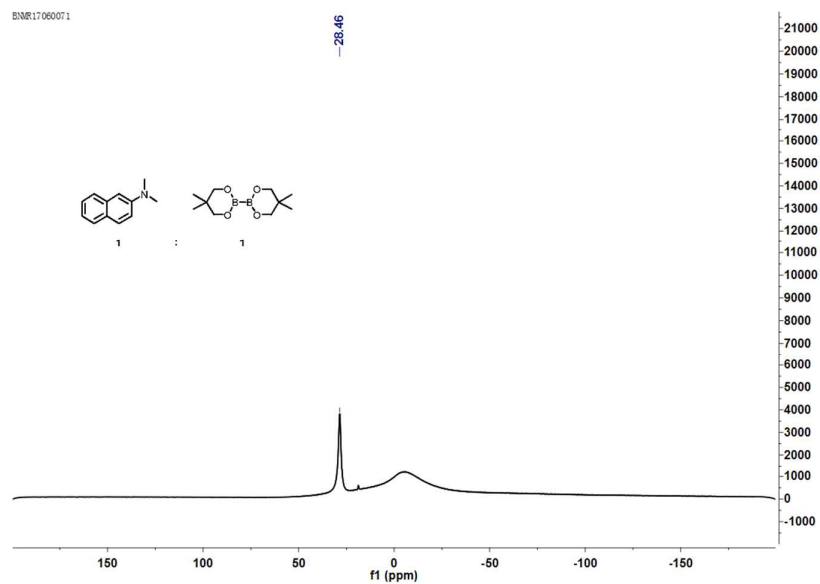
entry	ligand (loading)	yield (conversion)
1	PPh ₃ (40 mol%)	0% (0%)
2	PCy ₃ (40 mol%)	0% (0%)
3	DCyPE (20 mol%)	0% (0%)
4	IPr (11 mol%)	0% (0%)
5	SIPr (11 mol%)	0% (0%)
6	IMes (11 mol%)	53% (>95%)
7	SIMes (11 mol%)	0% (0%)
8	IAd (11 mol%)	0% (0%)
9	I ^t Bu (11 mol%)	18% (25%)
10	IMes ^{Me} (11 mol%)	67% (>95%), 62% ^c
11 ^b	IMes ^{Me} (11 mol%)	52% (90%)
12 ^d	IMes ^{Me} (HCl) (11 mol%)	<10% (20%)

Reaction conditions: **1a** (0.2 mmol), B₂nep₂ (0.5 mmol), Ni(cod)₂ (10 mol%, 5.6 mg), IMes (11 mol%, 6.9 mg), base (0.8 mmol), PhMe (1.0 mL), 110 °C, 7 h; ^a NMR yields were reported and dibromomethane was used as inner standard (isolated yields in the parenthesis); ^b B₂pin₂ (2.5 equiv.) was used to instead of B₂nep₂; ^c isolated yield; ^d ^tBuONa (11 mol%) was added.

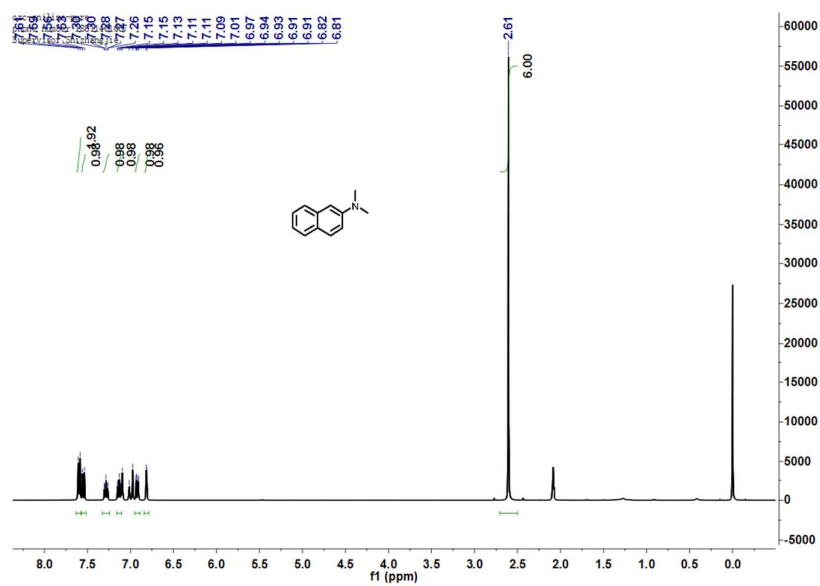
S3: Determination of the interaction between tertiary aniline and B₂nep₂

To determine the interaction of tertiary anilines and B₂nep₂ in the catalytic system, *N,N*-dimethyl (2-naphthyl) amine and B₂nep₂ were heated in *d*⁸-toluene at 125 °C for 2 h, and then detected by NMR spectroscopy and did not found the variation of chemical shift in ¹H-NMR, ¹³C-NMR, and ¹¹B-NMR. These results ruled out the Lewis acid-base interaction between *N,N*-dimethyl (2-naphthyl) amine and B₂nep₂.

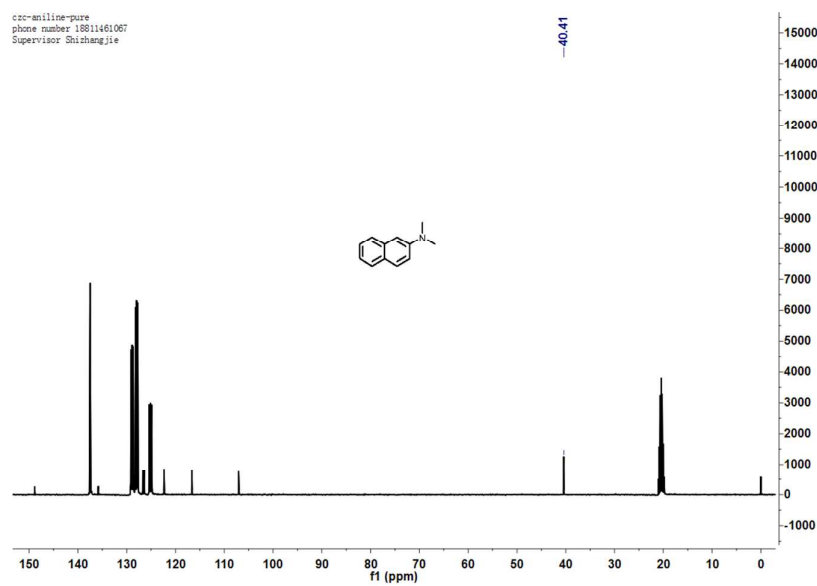




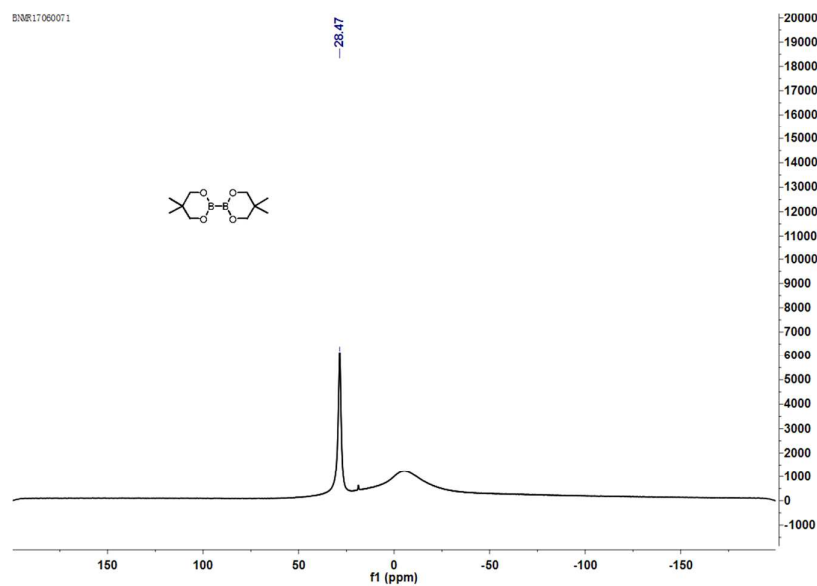
¹H-NMR of *N,N*-dimethyl (2-naphthyl) amine in *d*⁸-toluene



¹³C-NMR of *N,N*-dimethyl (2-naphthyl) amine in *d*⁸-toluene

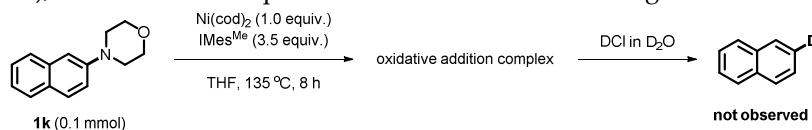


¹¹B-NMR of B₂nep₂ in *d*⁸-toluene



S4: Stoichiometric experiment

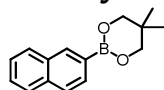
In a nitrogen-filled glovebox, an oven-dried seal-tube equipped with a magnetic stir bar was charged with compound **1k** (0.1 mmol, 21.3 mg), then the purple mixture of the catalyst $\text{Ni}(\text{cod})_2$ (0.1 mmol, 27.5 mg) and ligand IMes^{Me} (0.35 mmol, 116.4 mg) in THF (1.0 mL) was added via syringe. The reaction was removed from the glovebox and maintained at 135 °C for 8 h in an oil-bath. Then the reaction mixture was quenched with DCl (in D_2O), the deuterated naphthalene was not observed using GC-MS.



S5: Ni-catalyzed borylation of *N,N*-dimethyl (2-naphthyl) amine in 1 mmol scale

In a nitrogen-filled glovebox, an oven-dried seal-tube equipped with a magnetic stir bar was charged with *N,N*-dimethyl (2-naphthyl) amine **1k** (1.0 mmol, 213.3 mg), B_2nep_2 (2.5 mmol, 564.7 mg), then the purple mixture of catalyst $\text{Ni}(\text{cod})_2$ (0.1 mmol, 16.8 mg) and ligand IMes^{Me} (0.35 mmol, 116.0 mg) in THF (5.0 mL) was added via syringe. The reaction was removed from the glovebox and maintained at 135 °C for 48 h in an oil-bath. Then the reaction was purified by flash chromatography [$V_{(\text{petroleum ether})}:V_{(\text{ethyl acetate})} = 30:1$]. The product **2a** was obtained as white solid (133.7 mg, yield: 56%).

(V) Synthesis and analytical data for the products



5,5-dimethyl-2-(naphthalen-2-yl)-1,3,2-dioxaborinane, **2a**, white solid²

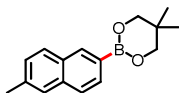
[CAS: 627906-96-1]

Procedure: In a nitrogen-filled glovebox, an oven-dried seal-tube equipped with a magnetic stir bar was charged with substrate **1a** (0.2 mmol, 38.7 mg), B_2nep_2 (0.5 mmol, 113.0 mg), PhCO_2Na (0.8 mmol, 115.3 mg), then the purple mixture of catalyst $\text{Ni}(\text{cod})_2$ (0.02 mmol, 5.6 mg) and ligand IMes^{Me} (0.022 mmol, 7.3 mg) in PhMe (1.0 mL) was added via syringe. The reaction was removed from the glovebox and maintained at 110 °C for 7 h in an oil-bath. Then the reaction was purified by flash chromatography [$V_{(\text{petroleum ether})}:V_{(\text{ethyl acetate})} = 30:1$]. The product **2a** was obtained as white solid in 29.8 mg (62% yield). This product can also be prepared from substrates **1h** (43% yield), **1i** (29% yield), **1j** (<10% yield), **1k** (65% yield), **1l** (13% yield), **1m** (0% yield), **1l** (0% yield) via general procedure B.

^1H NMR (400 MHz, CDCl_3) δ 8.35 (s, 1H), 7.97 – 7.72 (m, 4H), 7.62 – 7.36 (m, 2H), 3.83 (s, 4H), 1.05 (s, 6H).

^{13}C NMR (100 MHz, CDCl_3) δ 135.01, 134.83, 132.86, 129.89, 128.65, 127.63, 126.77, 126.59, 125.56, 72.38, 31.94, 21.92.

MS (EI) m/z : 240 (M^+).



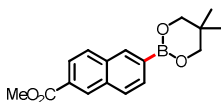
5,5-dimethyl-2-(6-methylnaphthalen-2-yl)-1,3,2-dioxaborinane, **2b**, white solid

Procedure: In a nitrogen-filled glovebox, an oven-dried seal-tube equipped with a magnetic stir bar was charged with substrate **1b** (0.2 mmol, 41.5 mg), B₂nep₂ (0.5 mmol, 113.0 mg), PhCO₂Na (1.0 mmol, 144.1 mg), then the purple mixture of catalyst Ni(cod)₂ (0.02 mmol, 5.6 mg) and ligand IMes^{Me} (0.022 mmol, 7.3 mg) in PhMe (1.0 mL) was added via syringe. The reaction was removed from the glovebox and maintained at 110 °C for 7 h in an oil-bath. Then the reaction was purified by flash chromatography [*V*_(petroleum ether):*V*_(ethyl acetate) = 30:1]. The product **2b** was obtained as white solid in 31.0 mg (61% yield). This product can also be prepared from substrates **1o** (29.0 mg, 57% yield) via general procedure B.

¹H NMR (400 MHz, CDCl₃) δ 8.30 (s, 1H), 7.86 – 7.69 (m, 3H), 7.59 (s, 1H), 7.29 (d, *J* = 8.1 Hz, 1H), 3.82 (s, 4H), 2.51 (s, 3H), 1.05 (s, 6H).

¹³C NMR (100 MHz, CDCl₃) δ 136.37, 135.07, 134.75, 131.13, 129.98, 128.45, 127.86, 126.63, 126.14, 72.36, 31.92, 29.69, 21.92.

HRMS (ESI) Anal. Calcd. (M+Na⁺) 277.1373, Found: 277.1363.



methyl 6-(5,5-dimethyl-1,3,2-dioxaborinan-2-yl)-2-naphthoate, **2c**, white solid.

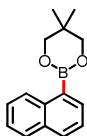
[CAS: 1268936-10-2]

Procedure: In a nitrogen-filled glovebox, an oven-dried seal-tube equipped with a magnetic stir bar was charged with substrate **1c** (0.2 mmol, 50.3 mg), B₂nep₂ (0.5 mmol, 113.0 mg), PhCO₂Na (0.8 mmol, 115.3 mg), then the purple mixture of catalyst Ni(cod)₂ (0.02 mmol, 5.6 mg) and ligand IMes^{Me} (0.022 mmol, 7.3 mg) in PhMe (1.0 mL) was added via syringe. The reaction was removed from the glovebox and maintained at 110 °C for 7 h in an oil-bath. Then the reaction was purified by flash chromatography [*V*_(petroleum ether):*V*_(ethyl acetate) = 10:1]. The product **2c** was obtained as white solid in 17.9 mg (30% yield).

¹H NMR (400 MHz, CDCl₃) δ 8.59 (s, 1H), 8.37 (s, 1H), 8.04 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.91 (t, *J* = 4.2 Hz, 3H), 3.98 (s, 3H), 3.84 (s, 4H), 1.06 (s, 6H).

¹³C NMR (125 MHz, CDCl₃) δ 167.31, 134.89, 134.66, 133.85, 130.79, 130.72, 128.86, 128.15, 127.95, 124.97, 52.21, 31.96, 21.92.

HRMS (ESI) Anal. Calcd. (M+Na⁺) 321.1274, Found: 321.1260.



5,5-dimethyl-2-(naphthalen-1-yl)-1,3,2-dioxaborinane, **2d**, white solid²

[CAS: 22871-77-8]

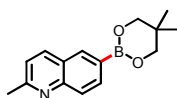
Procedure: In a nitrogen-filled glovebox, an oven-dried seal-tube equipped with a magnetic stir bar was charged with substrate **1d** (0.2 mmol, 38.7 mg), B₂nep₂ (0.5 mmol, 113.0 mg), PhCO₂Na (0.8 mmol, 115.3 mg), then the purple mixture of catalyst Ni(cod)₂ (0.02 mmol, 5.6 mg) and ligand IMes^{Me} (0.022 mmol, 7.3 mg) in PhMe (1.0 mL) was added

via syringe. The reaction was removed from the glovebox and maintained at 110 °C for 7 h in an oil-bath. Then the reaction was purified by flash chromatography [$V_{(\text{petroleum ether})}:V_{(\text{ethyl acetate})} = 30:1$]. The product **2d** was obtained as white solid in 23.5 mg (49% yield). This product **2d** can also be prepared from substrates **1q** (28.8 mg, 60% yield) via general procedure B.

^1H NMR (400 MHz, CDCl_3) δ 8.75 (d, $J = 8.3$ Hz, 1H), 8.03 (dd, $J = 6.9, 1.0$ Hz, 1H), 7.89 (d, $J = 8.1$ Hz, 1H), 7.86 – 7.78 (m, 1H), 7.54 – 7.39 (m, 3H), 3.89 (s, 4H), 1.10 (s, 6H).

^{13}C NMR (100 MHz, CDCl_3) δ 136.70, 134.32, 133.38, 130.89, 128.40, 128.32, 125.96, 125.20, 124.96, 72.48, 31.78, 21.94.

MS (EI) m/z : 240 (M^+).



6-(5,5-dimethyl-1,3,2-dioxaborinan-2-yl)-2-methylquinoline, **2e**, yellow solid³

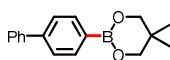
[CAS: 1352304-55-2]

Procedure: In a nitrogen-filled glovebox, an oven-dried seal-tube equipped with a magnetic stir bar was charged with substrate **1e** (0.4 mmol, 83.4 mg), B_2nep_2 (1.0 mmol, 225.9 mg), PhCO_2Na (1.6 mmol, 230.6 mg), then the purple mixture of catalyst $\text{Ni}(\text{cod})_2$ (0.04 mmol, 11.2 mg) and ligand IMes^{Me} (0.044 mmol, 14.6 mg) in PhMe (2.0 mL) was added via syringe. The reaction was removed from the glovebox and maintained at 110 °C for 7 h in an oil-bath. Then the reaction was purified by flash chromatography [$V_{(\text{petroleum ether})}:V_{(\text{ethyl acetate})} = 5:1$]. The product **2d** was obtained as yellow solid in 53.1 mg (52% yield).

^1H NMR (400 MHz, CDCl_3) δ 8.27 (s, 1H), 8.06 (d, $J = 8.5$ Hz, 2H), 7.97 (d, $J = 8.5$ Hz, 1H), 7.27 (d, $J = 6.9$ Hz, 1H), 3.83 (s, 4H), 2.75 (s, 4H), 1.06 (s, 6H).

^{13}C NMR (100 MHz, CDCl_3) δ 159.74, 149.29, 136.79, 134.57, 133.80, 127.47, 125.87, 121.84, 72.42, 31.94, 25.49, 21.91.

MS (EI) m/z : 255 (M^+).



2-(biphenyl-4-yl)-5,5-dimethyl-1,3,2-dioxaborinane, **2f**, white solid.

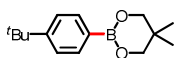
[CAS: 5123-05-7]

Procedure: In a nitrogen-filled glovebox, an oven-dried seal-tube equipped with a magnetic stir bar was charged with substrate **1f** (0.2 mmol, 43.9 mg), B_2nep_2 (0.5 mmol, 113.0 mg), PhCO_2Na (0.8 mmol, 115.3 mg), then the purple mixture of catalyst $\text{Ni}(\text{cod})_2$ (0.03 mmol, 8.4 mg) and ligand IMes^{Me} (0.033 mmol, 11.0 mg) in PhMe (1.0 mL) was added via syringe. The reaction was removed from the glovebox and maintained at 110 °C for 12 h in an oil-bath. Then the reaction was purified by flash chromatography [$V_{(\text{petroleum ether})}:V_{(\text{ethyl acetate})} = 30:1$]. The product **2f** was obtained as white solid in 29.3 mg (55% yield). This product **2f** can also be prepared from substrates **1s** (71% yield) via general procedure B.

^1H NMR (500 MHz, CDCl_3) δ 7.88 (d, $J = 7.6$ Hz, 2H), 7.65 – 7.57 (m, 4H), 7.43 (t, $J = 7.6$ Hz, 2H), 7.34 (t, $J = 7.3$ Hz, 1H), 3.78 (s, 4H), 1.03 (s, 6H).

^{13}C NMR (125 MHz, CDCl_3) δ 143.23, 141.17, 134.30, 128.68, 127.34, 127.16, 126.29, 72.30, 31.87, 21.87.

MS (EI) m/z : 266 (M^+).

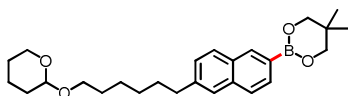


2-(4-tert-butylphenyl)-5,5-dimethyl-1,3,2-dioxaborinane, **2g**, white solid⁴
[CAS: 905966-37-2]

Procedure: In a nitrogen-filled glovebox, an oven-dried seal-tube equipped with a magnetic stir bar was charged with substrate **1g** (0.2 mmol, 39.9 mg), B₂nep₂ (0.5 mmol, 113.0 mg), then the purple mixture of catalyst Ni(cod)₂ (0.04 mmol, 11.2 mg) and ligand IMes^{Me} (0.044 mmol, 14.6 mg) in PhMe (1.0 mL) was added via syringe. The reaction was removed from the glovebox and maintained at 120 °C for 12 h in an oil-bath. Then the reaction was purified by flash chromatography [*V*_(petroleum ether):*V*_(ethyl acetate) = 30:1]. The product **2g** was obtained as white solid in 18.7 mg (38% yield). This product **2g** can also be prepared from substrates **1w** (39% yield) via general procedure B.

¹H NMR (500 MHz, CDCl₃) δ 7.74 (d, *J* = 8.2 Hz, 2H), 7.38 (d, *J* = 8.2 Hz, 2H), 3.75 (s, 4H), 1.32 (s, 9H), 1.01 (s, 6H).

¹³C NMR (125 MHz, CDCl₃) δ 153.72, 133.72, 124.51, 72.24, 34.76, 31.85, 31.21, 31.18, 21.87.
MS (EI) *m/z*: 246 (M⁺).



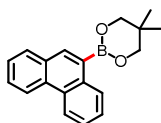
5,5-dimethyl-2-(6-(6-(tetrahydro-2H-pyran-2-yloxy)hexyl)naphthalen-2-yl)-1,3,2-dioxaborinane, **2h**, white solid.

Procedure: In a nitrogen-filled glovebox, an oven-dried seal-tube equipped with a magnetic stir bar was charged with substrate **1p** (0.2 mmol, 79.5), B₂nep₂ (0.5 mmol), then the purple mixture of the catalyst Ni(cod)₂ (0.02 mmol, 5.6 mg) and ligand IMes^{Me} (0.07 mmol, 23.2 mg) in THF (1.0 mL) was added via syringe. The reaction was removed from the glovebox and maintained at 135 °C for 48 h in an oil-bath. Then the reaction was purified by flash chromatography [*V*_(petroleum ether):*V*_(ethyl acetate) = 5:1]. The product **2h** was obtained as white solid in 56.9 mg (67% yield).

¹H NMR (400 MHz, CDCl₃) δ 8.30 (s, 1H), 7.84 – 7.70 (m, 3H), 7.58 (s, 1H), 7.30 (d, *J* = 8.4 Hz, 1H), 4.56 (s, 1H), 3.93 – 3.84 (m, 1H), 3.82 (s, 4H), 3.77 – 3.68 (m, 1H), 3.54 – 3.43 (m, 1H), 3.42 – 3.33 (m, 1H), 2.76 (t, *J* = 7.6 Hz, 2H), 1.90 – 1.77 (m, 1H), 1.77 – 1.66 (m, 3H), 1.65 – 1.57 (m, 3H), 1.54 – 1.46 (m, 3H), 1.46 – 1.36 (m, 4H), 1.05 (s, 6H).

¹³C NMR (101 MHz, CDCl₃) δ 141.23, 135.06, 134.76, 131.39, 129.93, 128.50, 127.16, 126.30, 126.07, 98.82, 72.38, 67.58, 62.32, 36.12, 31.93, 31.20, 30.76, 29.66, 29.14, 26.13, 25.48, 21.93, 19.67.

HRMS (ESI) Anal. Calcd. (M+NH₄⁺) 442.3123, Found: 442.3126.



5,5-dimethyl-2-(phenanthren-9-yl)-1,3,2-dioxaborinane, **2i**, white solid.³
[CAS: 1416371-19-1]

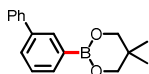
Procedure: In a nitrogen-filled glovebox, an oven-dried seal-tube equipped with a magnetic stir bar was charged with substrate **1i** (0.2 mmol, 52.7), B₂nep₂ (0.5 mmol), then

the purple mixture of the catalyst $\text{Ni}(\text{cod})_2$ (0.02 mmol, 5.6 mg) and ligand IMes^{Me} (0.07 mmol, 23.2 mg) in THF (1.0 mL) was added via syringe. The reaction was removed from the glovebox and maintained at 135 °C for 48 h in an oil-bath. Then the reaction was purified by flash chromatography [$V_{(\text{petroleum ether})}:V_{(\text{ethyl acetate})} = 30:1$]. The product **2i** was obtained as white solid in 30.8 mg (53% yield).

^1H NMR (400 MHz, CDCl_3) δ 8.84 – 8.78 (m, 1H), 8.74 – 8.63 (m, 2H), 8.34 (s, 1H), 7.92 (d, $J = 7.3$ Hz, 1H), 7.70 – 7.54 (m, 4H), 3.92 (s, 4H), 1.12 (d, $J = 2.3$ Hz, 6H).

^{13}C NMR (100 MHz, CDCl_3) δ 136.56, 134.52, 131.61, 131.16, 130.06, 129.21, 129.01, 127.35, 126.44, 126.31, 125.89, 122.65, 122.41, 72.57, 31.81, 21.96.

MS (EI) m/z : 290 (M^+).



2-(biphenyl-3-yl)-5,5-dimethyl-1,3,2-dioxaborinane, **2j**, white solid.

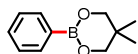
[CAS: 5630-18-2]

Procedure: In a nitrogen-filled glovebox, an oven-dried seal-tube equipped with a magnetic stir bar was charged with substrate **1t** (0.2 mmol, 79.5), B_2nep_2 (0.5 mmol), then the purple mixture of the catalyst $\text{Ni}(\text{cod})_2$ (0.02 mmol, 5.6 mg) and ligand IMes^{Me} (0.07 mmol, 23.2 mg) in THF (1.0 mL) was added via syringe. The reaction was removed from the glovebox and maintained at 135 °C for 48 h in an oil-bath. Then the reaction was purified by flash chromatography [$V_{(\text{petroleum ether})}:V_{(\text{ethyl acetate})} = 30:1$]. The product **2j** was obtained as white solid in 29.8 mg (56% yield).

^1H NMR (500 MHz, CDCl_3) δ 8.06 (s, 1H), 7.79 (d, $J = 7.3$ Hz, 1H), 7.68 – 7.60 (m, 3H), 7.45 – 7.37 (m, 3H), 7.31 (t, $J = 7.4$ Hz, 1H), 3.77 (s, 4H), 1.02 (s, 6H).

^{13}C NMR (125 MHz, CDCl_3) δ 141.39, 140.25, 132.73, 132.63, 129.37, 128.56, 127.96, 127.16, 126.97, 72.27, 31.83, 21.84.

MS (EI) m/z : 266 (M^+).



5,5-dimethyl-2-phenyl-1,3,2-dioxaborinane, **2k**, white solid.

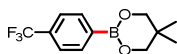
[CAS: 5123-13-7]

Procedure: In a nitrogen-filled glovebox, an oven-dried seal-tube equipped with a magnetic stir bar was charged with substrate **1u** (0.2 mmol, 32.7), B_2nep_2 (0.5 mmol), then the purple mixture of the catalyst $\text{Ni}(\text{cod})_2$ (0.02 mmol, 5.6 mg) and ligand IMes^{Me} (0.07 mmol, 23.2 mg) in THF (1.0 mL) was added via syringe. The reaction was removed from the glovebox and maintained at 135 °C for 48 h in an oil-bath. Then the reaction was purified by flash chromatography [$V_{(\text{petroleum ether})}:V_{(\text{ethyl acetate})} = 30:1$]. The product **2j** was obtained as white solid in 16.0 mg (42% yield).

^1H NMR (400 MHz, CDCl_3) δ 7.80 (d, $J = 7.5$ Hz, 2H), 7.41 (d, $J = 7.2$ Hz, 1H), 7.34 (t, $J = 7.4$ Hz, 2H), 3.76 (s, 4H), 1.01 (s, 6H).

^{13}C NMR (101 MHz, CDCl_3) δ 133.81, 130.64, 127.54, 72.28, 31.85, 21.88.

MS (EI) m/z : 190 (M^+).



5,5-dimethyl-2-(4-(trifluoromethyl)phenyl)-1,3,2-dioxaborinane, **2l**, white solid.⁴

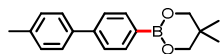
[CAS: 501374-30-7]

Procedure: In a nitrogen-filled glovebox, an oven-dried seal-tube equipped with a magnetic stir bar was charged with substrate **1v** (0.2 mmol, 46.3 mg), B₂nep₂ (0.5 mmol), then the purple mixture of the catalyst Ni(cod)₂ (0.02 mmol, 5.6 mg) and ligand IMes^{Me} (0.07 mmol, 23.2 mg) in THF (1.0 mL) was added via syringe. The reaction was removed from the glovebox and maintained at 135 °C for 48 h in an oil-bath. Then the reaction was purified by flash chromatography [*V*_(petroleum ether):*V*_(ethyl acetate) = 25:1]. The product **2l** was obtained as white solid in 38.7 mg (75% yield).

¹H NMR (500 MHz, CDCl₃) δ 7.90 (d, *J* = 7.8 Hz, 2H), 7.59 (d, *J* = 7.9 Hz, 2H), 3.78 (s, 4H), 1.03 (s, 6H).

¹³C NMR (125 MHz, CDCl₃) δ 134.07 (s), 132.24 (q, *J* = 32.0 Hz), 124.27 (q, *J* = 270.8 Hz), 124.14 (q, *J* = 3.7 Hz), 72.37 (s), 31.88 (s), 21.83 (s).

MS (EI) *m/z*: 258 (M⁺).



5,5-dimethyl-2-(4'-methylbiphenyl-4-yl)-1,3,2-dioxaborinane, **2m**, white solid.

[CAS: 1996626-86-8]

Procedure: In a nitrogen-filled glovebox, an oven-dried seal-tube equipped with a magnetic stir bar was charged with compound **6** (0.2 mmol, 50.7 mg), B₂nep₂ (0.5 mmol), then the purple mixture of the catalyst Ni(cod)₂ (0.02 mmol, 5.6 mg) and ligand IMes^{Me} (0.07 mmol, 23.2 mg) in THF (1.0 mL) was added via syringe. The reaction was removed from the glovebox and maintained at 135 °C for 48 h in an oil-bath. Then the reaction was purified by flash chromatography [*V*_(petroleum ether):*V*_(ethyl acetate) = 20:1]. The product **2m** was obtained as white solid in 37.6 mg (67% yield).

The product **2l** was prepared from **6** via general procedure B in 61% yield.

¹H NMR (400 MHz, CDCl₃) δ 7.86 (d, *J* = 7.5 Hz, 2H), 7.58 (d, *J* = 7.6 Hz, 2H), 7.52 (d, *J* = 7.6 Hz, 2H), 7.24 (d, *J* = 7.5 Hz, 2H), 3.79 (s, 4H), 2.39 (s, 3H), 1.03 (s, 6H).

¹³C NMR (101 MHz, CDCl₃) δ 143.20, 138.30, 137.18, 134.30, 129.44, 127.02, 126.12, 72.33, 31.91, 21.91, 21.10.

MS (EI) *m/z*: 280 (M⁺).

(VI) Density Functional Theory Calculations

Computational Studies. All calculations were performed with the ORCA program package (Version 4.0.1.2).⁵ For geometry optimizations, the GGA BP86 density functional⁶ in combination with triple- ζ quality def2-TZVP(-f) basis sets⁷ for Ni, B, C (in the C–N bond in *N,N*-dimethyl-2-naphthylamine), N (in the C–N bond in *N,N*-dimethyl-2-naphthylamine), and def2-SV(P) basis sets for the remaining elements. The resolution of the identity⁸ (RI, for BP86) and RI plus chain of spheres⁹ (RIJCOSX, for B3LYP) approximations were used to accelerate the calculations with the auxiliary basis set SARC/J. All the geometries were fully optimized without symmetry constraints. Harmonic vibrational frequencies were computed to verify the nature of stationary points. All minimum optimized structures reported in this paper had positive eigenvalues of the Hessian matrix, whereas the transition states (TSs) had only one negative eigenvalue. Zero-point energies, thermal corrections, and entropy terms for the optimized geometries were obtained from the frequency calculations. Final single point energies were computed by the B3LYP density functional^{6,10} with the large and flexible def2-TZVPP basis set⁷ on all elements. To account for solvation effects, the conductor-like polarizable continuum model (C-PCM)¹¹ was employed in the geometry optimizations, frequency calculations and the final single point calculations, for which tetrahydrofuran ($\epsilon = 7.25$) used in experiments was chosen as the solvent. To consider dispersion forces for the germanium corrole reaction systems, all calculations were conducted including semiempirical van der Waals (VDW) corrections.¹²

In this paper, we chose the reaction complex in which reactants/products weakly interacted with each other as the reference point to compute the activation barrier and the Gibbs free energy change (if the counting of molecules changed after the reaction). Based on previous researches,¹³ for substrate binding in solution choosing the reference point as infinitely separated reactants could lead to an error of ~13 kcal/mol for calculated entropy terms, because only when all reactants entered into the same solvent cage could the reaction easily occur. In fact, a series of pre-equilibria between reactants had been set up before the actual reaction took place.¹⁴ Thus, we could reasonably calculate the reaction barrier and free energy change with respect to the lowest-energy reactant complex. However, this approximation might slightly underestimate the entropy contributions as the individual translational entropy for each reactant was completely neglected.

DFT calculation results

Computational studies were conducted using density functional theory (DFT) in order to get more insights to the aforementioned mechanism and the calculated potential energy surface was shown in following **Figure S1**. The coordination of *N,N*-dimethyl-2-naphthylamine **1h** was endothermic (11.8 kcal/mol) due to its relatively poor frontier orbital matching with Ni(0) center comparing to that for cyclooctadiene, which could act as a soft base. However, the following C–N bond oxidative addition, in which only a small activation energy barrier (8.5 kcal/mol) was observed, was energetically favored with a Gibbs free energy change of -11.7 kcal/mol. The dimethylamino group (-NMe₂) in **int. 2** (**Figure S1**) showed stronger Lewis basicity than that for the free *N,N*-dimethyl-2-naphthylamine, as indicated by the calculated Mulliken charges on amino nitrogen atoms (-0.15 for *N,N*-dimethyl-2-naphthylamine *vs.* -0.48 for the dimethylamino group in **int. 2**), thus facilitating the coordination of B₂nep₂ (-7.0

kcal/mol). In addition, no complexation of B_2nep_2 with free N,N -dimethyl-2-naphthylamine was observed by ^{11}B NMR spectroscopy (details see SI). The calculated B-B bond (1.736 Å) in **int. 3** was slightly longer than that in free B_2nep_2 (1.707 Å). As a result of the surrounding steric hindrance, the uncoordinated $Bnep$ moiety in **int. 3** was found to sit on top of the naphthyl group *via* the “Ni-N-B” linkage (**Figure S2a**), with a B-C distance of 3.120 Å. Similar core framework (B-C distance: 1.866 Å, B-B distance: 2.016 Å, **TS2**, **Figure S2b**) was seen in the transition state for the subsequent product formation process. Although a relatively high activation energy (35.6 kcal/mol), which was in accordance with the requisite high reaction temperature (135 °C) and long reaction time (48 h), was found, the whole product formation process was significantly exothermic with a large Gibbs free energy change of -32.2 kcal/mol, thus provided the major contribution to the whole driving force of the catalytic borylation reaction. Further Gibbs free energy descending (-11.0 kcal/mol) was observed for the catalyst regeneration process. This is an unusual proposed example to facilitate the concerted reductive elimination on Ni-center through a cyclic five-membered transition state.

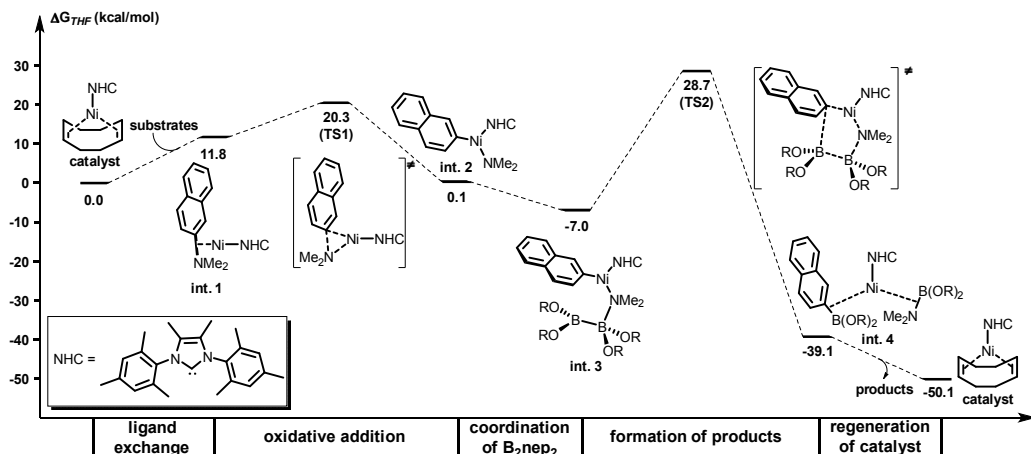


Figure S1. Computational study of catalytic cycle for the nickel catalyzed C-N bond borylation

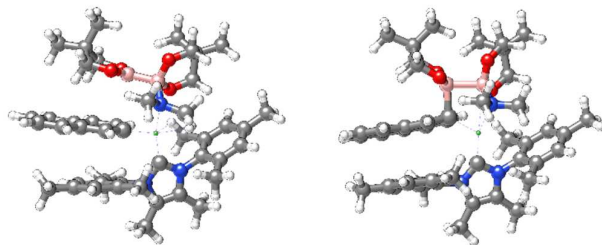


Figure S2. Calculated structures for **int. 3** (left, **a**) and **TS2** (right, **b**)

Calculated Structures:

(IMes^{Me})Ni(cod):

C	-0.21208485419699	0.14487447952265	-0.87857179375920
C	0.44039992139923	1.26611380921097	-0.41359369561495
C	-1.56827169764562	1.10723309283050	0.73965552057365
N	-0.40575819444080	1.83150136431088	0.55427685375414
N	-1.42775278987303	0.07385483300026	-0.16495996359899
C	-2.39416343904766	-0.97588896996985	-0.24328138659045

C	-3.55870846883823	-0.78056355064241	-1.01800905589234
C	-2.18985026840731	-2.14775323442989	0.51740111639203
C	-4.53521324515605	-1.79320274585202	-1.01164725664919
C	-3.19215109138429	-3.13762269666555	0.49161857274141
C	-4.37370499672405	-2.97587199570707	-0.25888848146998
H	-5.45280503029725	-1.65056849844742	-1.60185394106231
H	-3.05159519851162	-4.05282693473841	1.08542384786777
C	-0.17559599812414	2.98477001014374	1.36881128228299
C	-0.70971636823407	4.22898935679464	0.95858187883949
C	0.49495457039929	2.82808769662777	2.60336899485939
C	-0.54194478190423	5.33407787688593	1.81262159544798
C	0.64102501226327	3.96320901514474	3.42448693382779
C	0.13254491508802	5.22222352217217	3.04731391981905
H	-0.95609981305961	6.30676556630420	1.50940606569662
H	1.15365360982737	3.85605061887948	4.39157811838474
C	1.00921172712412	1.47242834746936	3.02669446848014
H	0.20132699334331	0.71666584109713	2.96921776835141
H	1.82822542427034	1.11741027401924	2.36920827081791
H	1.39236744878629	1.50049948950694	4.06275402807354
C	-1.46004841940031	4.33873118248345	-0.34657687528734
H	-0.81170951045306	4.09659650277065	-1.21223975186621
H	-2.30399486140585	3.62000514542396	-0.36550649397739
H	-1.85885486958221	5.35881269564202	-0.49232601372807
C	0.31919436742229	6.43267733152154	3.93563654084420
H	1.16196038696433	7.06210015415722	3.58025477513544
H	-0.58253154819802	7.07556062171215	3.94174047602618
H	0.54371672203139	6.14097015699027	4.97856328624208
C	-0.94405960129575	-2.30107749666145	1.35755843216306
H	-0.03717811309768	-2.41636800721082	0.73049753145152
H	-0.77960367663421	-1.40198249449311	1.98470995637842
H	-1.01353308989432	-3.18343529502236	2.01976169929246
C	-3.74337261463981	0.49768942243319	-1.79892972926096
H	-3.63111129516314	1.37603221088748	-1.13328483704913
H	-2.97921072753434	0.60399379658572	-2.59510944649373
H	-4.74029264376975	0.53457514063400	-2.27517284398359
C	-5.45997964625713	-4.02915740090971	-0.24378367066160
H	-6.34912072858370	-3.67527981170010	0.31700628681283
H	-5.80268001508328	-4.27355359544793	-1.26776445028963
H	-5.11459079038308	-4.96395301510505	0.23493053524270
C	1.75141027991062	1.88135735191345	-0.77741812076146
H	1.62596196752694	2.90176710525546	-1.19363022279591
H	2.41770618707807	1.97288034687213	0.10485314580275
H	2.27270780801562	1.26846923291266	-1.53455874311629
C	0.14986587740310	-0.84563791725423	-1.93528507586924
H	0.18941847817295	-1.88010612663770	-1.53925348880370
H	-0.58534549565181	-0.84678274574981	-2.76592933596009
H	1.14164456408302	-0.61105969280548	-2.36239026935280
Ni	-2.76574832192758	1.60112752535726	2.07269873877532
C	-4.98208108087415	-0.06103775393496	2.65365224788905

H	-5.60344700415638	0.08581244839901	3.55749802299245
H	-5.21027221079587	-1.07903900379811	2.28228942536628
C	-3.50998411338408	-0.00854924108481	3.03844352798731
H	-2.91449256612743	-0.86730835634885	2.71447373026579
C	-2.95594090612007	0.82256314272519	4.01802919408014
H	-1.94913564222141	0.55514481923085	4.36694676944610
C	-3.69742971000910	1.82541261745078	4.87804143232996
H	-2.94261677130846	2.51598862633718	5.30641816883563
H	-4.19258042726667	1.34012077638933	5.75204600678862
C	-4.72386543960942	2.65064477164548	4.06385101854536
H	-5.69310780739981	2.11968257351741	4.01132437388657
H	-4.93382829535184	3.60443057323817	4.58961037589907
C	-4.21112573019409	2.93603228975940	2.66227915844396
H	-3.74859997475554	3.92324736882498	2.51143615339180
C	-5.41100984662969	0.96170735807691	1.54279777085204
H	-6.49728812903623	1.17933745192558	1.66495765841149
H	-5.30719996042834	0.47328000025797	0.55677196336162
C	-4.59877522277441	2.24182226102719	1.50663171680397
H	-4.56037814786650	2.75263243433853	0.53747179794022

(IMes^{Me})Ni(N,N-dimethyl-2-naphthylamine):

C	-0.47445462993854	0.50582671155225	-0.86300030832721
C	0.16484723377789	1.66121633541345	-0.46421165840855
C	-1.46940124491142	1.20734993772596	1.10603647997277
N	-0.45817804786595	2.06609585320266	0.73092790665905
N	-1.45547467753557	0.25213491720401	0.10808528725699
C	-2.47429820397845	-0.75443719419993	0.04846433626399
C	-3.68843593828458	-0.45023940096728	-0.61429154584622
C	-2.25397432858113	-2.00006472496541	0.67352069538687
C	-4.69761884523329	-1.42919133662330	-0.62248143225727
C	-3.29438013093849	-2.95003438853527	0.63913748438701
C	-4.52220927322702	-2.68394949490079	0.00168041310677
H	-5.65176916803661	-1.20266281459524	-1.12079082542177
H	-3.14217850689916	-3.92167071430922	1.13118902674843
C	-0.24925923186857	3.33308501507126	1.36416468099962
C	-0.84992096431989	4.47383158454915	0.78612350561691
C	0.52191973116437	3.40779533304241	2.54323972729285
C	-0.60957243060200	5.72203780217759	1.38927876950487
C	0.70876140173094	4.67426255701737	3.12987379815710
C	0.16663554062854	5.84448625158675	2.55877610736640
H	-1.07333868734537	6.61711972929192	0.95107801396169
H	1.29684314873465	4.74831421089015	4.05657751580437
C	1.09202844136950	2.15216188327473	3.15613828319723
H	0.27383016263429	1.45037530321084	3.42199118965494
H	1.74676796828364	1.61320593834644	2.44219213563694
H	1.67917577080652	2.37889792201505	4.06483941784203
C	-1.77345644868592	4.33416152122084	-0.39771567366285
H	-1.26750787457329	3.89638664473058	-1.28058892106741

H	-2.61518538021086	3.66050232629821	-0.14226609620286
H	-2.19993759653670	5.31047949140505	-0.68488642725274
C	0.41805940082437	7.20034560327348	3.18136889245732
H	1.33224342729865	7.66926732350017	2.76113563478291
H	-0.42079285719035	7.89657871824281	2.98934574196880
H	0.56394655868140	7.12441844824801	4.27568519701422
C	-0.96199781757372	-2.26187736606525	1.40610726491174
H	-0.07997080096070	-2.11190301422804	0.75325544986747
H	-0.85289930205468	-1.55095465471516	2.25162098826287
H	-0.92801103355275	-3.29219611126366	1.80418578585543
C	-3.89978207849621	0.91056713371774	-1.23145524869451
H	-3.88638261480156	1.69151682448385	-0.44228398634809
H	-3.09713080807304	1.17092340317624	-1.94918314683227
H	-4.86998796045826	0.96474051386474	-1.75840858673434
C	-5.63344418914266	-3.71061002270132	-0.01988187543456
H	-6.56599718452071	-3.30221201073670	0.41800344268570
H	-5.87655775855615	-4.02057698937446	-1.05559913285048
H	-5.36083287705913	-4.61834933549075	0.54937770163873
C	1.31874293421784	2.40465072745102	-1.05234491649480
H	1.05994606944250	3.45749686925041	-1.27932729246571
H	2.18358071159458	2.42795298791749	-0.35839603037974
H	1.64771939220496	1.92515868886731	-1.99072843784071
C	-0.26610665933310	-0.39210494632412	-2.03743062083066
H	0.00505656327277	-1.42106545987522	-1.72612364630966
H	-1.18365413428301	-0.47285535206530	-2.65515125676222
H	0.54422570456155	-0.00834863552499	-2.68379327531566
Ni	-2.73206964402099	1.24531397298505	2.39532240888111
C	-5.77956744066592	5.71428045181426	-0.48582767973471
C	-5.86998177976020	4.44356574747310	0.08363450234847
C	-5.10135439375389	4.09171877913295	1.23595878538099
C	-4.21339333261282	5.08894725755929	1.79675065235249
C	-4.15674113198338	6.38041965777350	1.20507438835786
C	-4.92229328940085	6.69675114492526	0.08010654933664
H	-5.85043942758669	2.05935227827595	1.38335031292002
H	-6.37386856257011	5.95647527941701	-1.37839885219358
H	-6.53564905834052	3.68634361330616	-0.35692038805608
C	-5.17549577876103	2.79825926688766	1.82884732383809
C	-3.40940975503439	4.71971909831149	2.92102536280589
H	-3.48384875080272	7.13080871463575	1.64529280784172
H	-4.85920737865358	7.69719213462738	-0.36975528757984
C	-3.45664566889550	3.44300308369783	3.45827548061676
C	-4.33036941263965	2.44497356478348	2.89562836384690
H	-2.70610235479346	5.45282010978666	3.33680890225423
H	-2.82740372040856	3.20040037341259	4.32094335518663
N	-4.33525954045358	1.12282368592055	3.49511185086388
C	-4.35868335288178	1.06350378385276	4.97246197210801
H	-5.36018638584889	1.35658365728900	5.35699390850925
H	-4.13595767893861	0.02871908396257	5.28644899040247
H	-3.59729162275624	1.72767355184274	5.40673378421619

C	-5.29702914836937	0.16168876881435	2.91994726823187
H	-5.14778470738438	0.08246813522739	1.82949266109671
H	-5.10018256330358	-0.82861598278252	3.36469120411419
H	-6.34634031497936	0.46214543330931	3.13733576953210

TS1:

C	-0.48844104412532	0.21435349525176	-0.93110316595701
C	-0.03238695186968	1.47853357915797	-0.62192162694292
C	-1.80012381447153	1.02788500617194	0.79383296231412
N	-0.84520645721924	1.94716955580968	0.42592331324115
N	-1.55603860750079	-0.03183451053099	-0.05477264455359
C	-2.36189995933861	-1.21618651976339	-0.02352555999211
C	-3.56225154331857	-1.24219063256161	-0.77141765629851
C	-1.94639495025936	-2.30716035140790	0.77049742167542
C	-4.34772091184708	-2.40768585463311	-0.71555746086222
C	-2.76448813881574	-3.45452171452398	0.79335589250758
C	-3.96609645253303	-3.52415468615200	0.05970844166979
H	-5.28675076622468	-2.44289191357791	-1.28657579326375
H	-2.45641603834719	-4.31334735755171	1.40705155392840
C	-0.71945760153404	3.25263905382211	1.00375059137462
C	-1.36765020851767	4.33685522465531	0.37690894524951
C	0.06695228230462	3.41411123605827	2.16503495780272
C	-1.18297058523764	5.61988825436244	0.92603612055653
C	0.22916685982478	4.71466123983122	2.67315458089210
C	-0.38056302400963	5.83029709452255	2.06267127311528
H	-1.70806268513935	6.47136736220338	0.47167420793495
H	0.83508778213998	4.85847499490665	3.58009774629988
C	0.67317381230453	2.20986695962692	2.84361829053086
H	-0.12322887187184	1.50035551950979	3.14725772665424
H	1.35057320817219	1.65156972877035	2.16635904638225
H	1.24701558881558	2.50318565094519	3.74146447773714
C	-2.23595719772117	4.11524740252247	-0.83607873338027
H	-1.63204022343961	3.88581514738644	-1.73828587430122
H	-2.91982229501534	3.26139967258529	-0.67409810355060
H	-2.84694287056380	5.01021489492322	-1.04781307982519
C	-0.20394790866798	7.21330089333699	2.64697790909575
H	-0.60613533040246	7.26423683578264	3.67826236417520
H	0.86658150961838	7.49554410477419	2.70559423018507
H	-0.73016933541310	7.97670096640991	2.04589189126002
C	-0.68266626863347	-2.21606008092597	1.59122297981296
H	0.21195134422365	-2.05765916081854	0.95700367405024
H	-0.73096243249252	-1.35533019129634	2.28920691608796
H	-0.52389456139255	-3.13650849701657	2.18207874636433
C	-3.98591943252765	-0.03145924669884	-1.56692660183510
H	-4.11791353549724	0.84032179040858	-0.89219451312620
H	-3.21826342093217	0.25928622497646	-2.31095380979234
H	-4.93665878832009	-0.21347647318704	-2.09969000772356
C	-4.84648031516962	-4.75338462528120	0.12088740663448

H	-5.73428380407186	-4.57454541186069	0.76139195316765
H	-5.22311473291348	-5.03321602067814	-0.88161152638220
H	-4.30489706005353	-5.62100230296081	0.54109831889565
C	1.08537571350820	2.29250786534229	-1.18434397471824
H	0.72416299523627	3.24796387823689	-1.61341226354112
H	1.83227049333526	2.54967521505671	-0.40684671883558
H	1.60413743779997	1.73544330156784	-1.98439836126520
C	-0.04813404750992	-0.78237249154581	-1.95149047442597
H	0.25774019274202	-1.73991196391868	-1.48557741634288
H	-0.86009986785255	-1.01705676241761	-2.66885552538336
H	0.81197355824055	-0.39520974288359	-2.52648825277456
Ni	-3.17807352194736	1.05822445040916	1.99243627125233
C	-5.02929933751540	7.18976321430278	0.78939155190701
C	-5.10427927329804	5.80166390057442	0.71604195578165
C	-4.47994570267582	4.97291220082559	1.70198777755007
C	-3.75998029431434	5.61893824267674	2.77743784409177
C	-3.72098603362251	7.03962349796440	2.83901773200963
C	-4.33660120097024	7.82082658323926	1.86261535127103
H	-5.06815350431486	3.08722359222370	0.80867922846888
H	-5.51039950052306	7.80465667290424	0.01508461719032
H	-5.64339808116855	5.31972207668336	-0.11363229026755
C	-4.51993520765756	3.55210569711815	1.63886315708474
C	-3.07280329389839	4.78798489122170	3.71543204765461
H	-3.17320588760709	7.51434331292839	3.66604693375980
H	-4.28604507244763	8.91767316556869	1.91502312278860
C	-3.09443318556195	3.40909000859030	3.60610714217510
C	-3.81197894659842	2.75668642358078	2.54942615934769
H	-2.48766455329274	5.26539491598388	4.51556639987814
H	-2.51468296140507	2.80560672224167	4.31516060910302
N	-4.66493771361426	1.15488001111978	3.09132202815858
C	-4.69101208763685	1.12172271817417	4.54830581006065
H	-5.20823755484584	2.01040099041860	4.98163786347609
H	-5.23069095938628	0.21099000496536	4.88693716976459
H	-3.66860591979333	1.07355842160999	4.95925547960442
C	-6.00399408962013	1.11963898387351	2.51469260227741
H	-5.94886297704476	1.05554393154809	1.41347702042382
H	-6.54517269729788	0.22107005753646	2.88153247057670
H	-6.60066517943656	2.02343067499378	2.78647815008874

(IMes^{Me})Ni(2-C₁₀H₇)(NMe₂):

C	-0.37844900477013	-0.05687854953197	-0.31288858340043
C	0.33030756565408	1.06236745913832	0.06671592542913
C	-1.78286772911327	1.24442219069884	0.96699612105418
N	-0.54377581448848	1.83017101107879	0.85767117643947
N	-1.65630094502019	0.07191423306335	0.26430583666708
C	-2.67551439535011	-0.93434476428042	0.25092546748948
C	-3.80315796942684	-0.76423788674133	-0.58291446831057
C	-2.53890708547355	-2.03586107270336	1.12320149702492

C	-4.81055017372890	-1.74422825280040	-0.53009722131515
C	-3.56382354691338	-3.00197518375628	1.12410511694673
C	-4.70704681616986	-2.87248774818638	0.31275471598607
H	-5.70077733550817	-1.62546003358269	-1.16579874901274
H	-3.47928553947862	-3.86195758148893	1.80447129017411
C	-0.18699365581815	2.99760438449269	1.60988099370500
C	-0.59788966599884	4.27013785044759	1.15238829953110
C	0.52863052757156	2.82439719119900	2.81677575689422
C	-0.29438110404449	5.38552335268909	1.95450978273151
C	0.81073858044989	3.97254869684841	3.58332712950769
C	0.40496364464806	5.25830671525019	3.17371118044678
H	-0.61682353813326	6.38142253848063	1.61803295627940
H	1.34959400658438	3.85382410886014	4.53450215136643
C	0.95489559365790	1.45040730138193	3.27780402983704
H	0.12769172361004	0.72162899464927	3.18407995254268
H	1.80310126049737	1.06180745300037	2.67895399917908
H	1.27563013584600	1.47237034672133	4.33434683295118
C	-1.35659571713802	4.41203957732201	-0.14416839370463
H	-0.82207658938643	3.92321898819663	-0.98227168524322
H	-2.34952097983963	3.92203657215974	-0.06635720789779
H	-1.51295161663393	5.47514579664572	-0.39914254573869
C	0.72619150154977	6.47996675474847	4.00591417497759
H	1.56350858037863	7.05548453013625	3.55956567076063
H	-0.14086268303420	7.16637098459485	4.06701130366781
H	1.02329584866690	6.20501973954864	5.03465078693505
C	-1.37670527219453	-2.12165439530238	2.08123653131386
H	-0.40037685496289	-2.18153088938429	1.56170378052498
H	-1.34589631042578	-1.21968671259303	2.72550024426083
H	-1.46953624477258	-3.00489034560980	2.73862117141685
C	-3.92122789192769	0.45196131259777	-1.46838947601354
H	-4.00769945976373	1.37088439928559	-0.84896484564562
H	-3.02229436215607	0.58456210312029	-2.10188834243956
H	-4.80757997421770	0.38725213429113	-2.12537227715308
C	-5.81464452548272	-3.90223943128079	0.35013869040488
H	-6.75603353778408	-3.46149318760578	0.73530783999266
H	-6.03592817297772	-4.29390141777167	-0.66212454612573
H	-5.55391335530428	-4.75862029915742	0.99889584007335
C	1.70424182172550	1.53070258987281	-0.28170243689876
H	1.67474017515178	2.48983332084433	-0.83682942247627
H	2.32800321903190	1.69436025771090	0.61889176999964
H	2.21726110056350	0.78610680629021	-0.91642794115775
C	-0.02093792509103	-1.20143404465121	-1.20171265661787
H	-0.10277370667722	-2.17432207159247	-0.67845157344970
H	-0.68631233417218	-1.25098062073770	-2.08636437405081
H	1.01782704384477	-1.09881576148181	-1.56190971630458
Ni	-3.26184578262749	2.01402538695035	1.70646767592867
N	-4.53171560431598	3.24491515333658	1.53360651084596
C	-4.37161119919632	4.59951140501696	2.04269660060781
H	-3.32658799636625	4.77079966228161	2.36223902846238

H	-4.62316518606916	5.35610813565995	1.26104188547248
H	-5.04281158698510	4.79616788152280	2.91298633010848
C	-5.89830902081685	2.98582917382976	1.10804901679089
H	-6.20514234787743	3.67520969310025	0.28531935571760
H	-6.00096043435163	1.94684324309780	0.74416727501038
H	-6.62536628978395	3.13534880758831	1.94274954983447
C	-3.97420511852192	-0.23168073227458	3.26196112955585
C	-3.94366393840675	-1.06945906299500	4.36955096783781
C	-3.07293514563049	-0.80369470415935	5.47103980768812
C	-2.23772850675785	0.37592891590605	5.41392785272174
C	-2.29529707125217	1.21051952730807	4.25704137545431
C	-3.13384897003183	0.92149714530546	3.18594707840071
H	-3.62822465954362	-2.55134592017584	6.65179957754287
H	-4.63723266787584	-0.47271158596797	2.42017274272178
H	-4.58460930939479	-1.96344397258004	4.40342049641520
C	-2.99322294521748	-1.65349808407429	6.61516224803514
C	-1.36366483236502	0.65106803286503	6.51188029618340
H	-1.64498264983634	2.09615231254275	4.21988920570258
C	-1.30916882056453	-0.19639959821726	7.61416921359906
C	-2.13013680606198	-1.36060087252585	7.66796227179411
H	-0.73164757368847	1.55024918397866	6.46688193141804
H	-0.63186470100903	0.03071935783345	8.44977281830812
H	-2.07981542150509	-2.02420346027897	8.54257111428705

Reaction complex_(IMes^{Me})Ni(2-C₁₀H₇)(NMe₂)+B₂nep₂:

C	-1.27642440382849	-0.39944525242697	-0.23080454737161
C	-0.28521265783967	0.01444031047857	0.63181591536867
C	-2.20011588241353	1.18506036127341	1.18080800002660
N	-0.87435955229394	0.96520670847381	1.48517078910177
N	-2.42378456262022	0.32546323048884	0.12600543466873
C	-3.67833793404958	0.23852891942378	-0.56046661779809
C	-3.87214530052336	1.01724477770536	-1.72512552253043
C	-4.67304142038198	-0.62790234489986	-0.05866351184748
C	-5.11380687883499	0.92146938624269	-2.38026204206361
C	-5.89369291198885	-0.70072039302288	-0.75666394028760
C	-6.13569077908689	0.06821796947563	-1.91311642158492
H	-5.28486675085180	1.52705285458264	-3.28197522602631
H	-6.67916409244279	-1.37366379412534	-0.38370359663229
C	-0.13704572721206	1.67106182801449	2.49374031549668
C	0.25544145673781	3.00361694833248	2.23599310494560
C	0.17632927225973	1.01804471556136	3.70503236478626
C	0.99326955530447	3.67638860614519	3.22559106102388
C	0.90772342748238	1.73794138169877	4.66832592986932
C	1.33420114976057	3.05963598703351	4.44598169844753
H	1.29699317354937	4.71722540815698	3.04334555347541
H	1.13016831749027	1.25665024880933	5.63100660388593
C	-0.25085230818044	-0.40509611903352	3.97390476789495
H	-1.17357246192646	-0.66560346127751	3.42599916252416

H	0.53515800062562	-1.12939555283363	3.67475455405674
H	-0.44345657791063	-0.55362555260410	5.05159616752554
C	-0.16498831401784	3.69555335196239	0.96342468167656
H	0.03033497435723	3.07068176421186	0.06969050075468
H	-1.26202691750209	3.88215691087532	0.97884786730853
H	0.35488622196962	4.66228377747567	0.83892970350752
C	2.14743101082601	3.79158853316670	5.48847394511075
H	3.23445658145329	3.60836357617247	5.34852195647109
H	1.98599741342470	4.88502132324262	5.43600531304961
H	1.87931991609415	3.45878565617134	6.50787699469522
C	-4.42079545941456	-1.42865609983813	1.19448337857115
H	-3.48241631179824	-2.01293528814126	1.12433911062087
H	-4.30920395808093	-0.75653352089478	2.06825685342962
H	-5.25258884882543	-2.12602314010563	1.39953898589552
C	-2.77155746205893	1.91379084657425	-2.24216280626264
H	-2.32817505404815	2.52280068984921	-1.43137479591110
H	-1.94058955241237	1.32358665697522	-2.67923660387353
H	-3.14714449169140	2.59636979969642	-3.02551206885157
C	-7.46673720695366	0.00464326628237	-2.62765831985583
H	-8.07197761659253	0.91057145228760	-2.41695203892173
H	-7.33506212794901	-0.04876634797204	-3.72593359021044
H	-8.06086753745033	-0.87128264949302	-2.30614337159284
C	1.16194101504746	-0.34315672769874	0.70495987430046
H	1.79977698748155	0.56033361289849	0.63704226353369
H	1.42440644641467	-0.85653330445037	1.65023831354275
H	1.43203037047660	-1.01522379038758	-0.12885805547470
C	-1.28122329326472	-1.40738991693543	-1.33141080203247
H	-1.99738317315064	-2.22854652381261	-1.12712803506494
H	-1.57123646547415	-0.95902830813624	-2.30201265487417
H	-0.27858560408832	-1.85368679411400	-1.45032310807485
Ni	-3.42749823936527	2.44295765428061	1.80438431717517
N	-4.79642752827061	3.68094574413198	1.94442763766604
C	-4.67575308492335	3.83867201232920	0.51212537647825
H	-5.63897379968639	3.71654576399981	-0.03902508654060
H	-4.16838584408719	4.77199505284460	0.16772893834497
H	-4.06691929937868	2.96413743100310	0.07196141666889
C	-4.77239753108508	4.91781851885504	2.69871649325108
H	-5.72156380525401	5.48555610792381	2.55566505629470
H	-4.68500412282427	4.68527908285728	3.77499671713819
H	-3.93251024142143	5.60451646830116	2.41411364980230
C	-3.14732903541411	1.22478082721731	4.35675745898512
C	-2.70159649634632	1.13200272790165	5.66821251393061
C	-2.00681157037105	2.21439161120357	6.28251108774558
C	-1.82798062987226	3.42901711128864	5.52240061655061
C	-2.30161010489827	3.48281229219063	4.18046572234172
C	-2.92789184454137	2.39890294742240	3.58437389345743
H	-1.62690184082553	1.21709565432195	8.18297854595271
H	-3.68168409805312	0.38009423623461	3.90603098783542
H	-2.87303726635856	0.21320359709458	6.24830592848631

C	-1.49902705267669	2.15007015983228	7.61433498760497
C	-1.18022290311516	4.53784454411138	6.14784310922170
H	-2.13409237528842	4.40915576882656	3.61353550060631
C	-0.71757486086514	4.45503278769597	7.45582844913428
C	-0.86843374298489	3.24591296366442	8.19602847223615
H	-1.04702358271203	5.46206818760734	5.56730037143021
H	-0.22162455606231	5.31908681995315	7.91984139520306
H	-0.48953074666060	3.18400360273333	9.22503054343983
C	-6.73528714453811	0.92595313362506	2.37449395613321
C	-8.06064641590397	1.64999962808585	2.08287753954344
C	-7.88213429628892	3.11808861992061	2.51070322194010
H	-5.92859321617088	1.30931675349096	1.71641323569509
H	-6.84499002433146	-0.16183484224404	2.20033329592125
H	-7.16551194363820	3.62069641530568	1.83237038062213
H	-8.85259156882732	3.65156977489080	2.47815341344313
C	-9.21308802442865	0.99296558157084	2.86853436614388
H	-10.16976555648768	1.51731895098050	2.67278933290747
H	-9.33639669544656	-0.06738466183453	2.56995877981556
H	-9.02953822324027	1.01868365961555	3.96032368243727
C	-8.34045446750977	1.59784855591205	0.57365737990472
H	-8.48423766863677	0.55368986417608	0.23496728510318
H	-9.25866072770052	2.16498117015804	0.31902574398072
H	-7.49591262364655	2.02263020265910	-0.00402577277975
O	-6.30153634096356	1.09848762813453	3.72839681655013
O	-7.36428411649879	3.25333408519488	3.84136222725110
B	-6.52792122809776	2.29483539543169	4.36933520841460
C	-4.76598641164279	4.14711056789171	7.44700395529815
C	-5.32869975532426	3.27239191075498	8.58160543159915
C	-5.19307658187379	1.80730748830248	8.12746304956601
H	-3.67049010230303	4.01165305134539	7.36122794284576
H	-4.96190703590711	5.21872424224646	7.65121383664254
H	-4.12350223534617	1.52301791905047	8.07731084669960
H	-5.69567369130073	1.12935668184467	8.84488349946828
C	-6.80849561869996	3.61568410926907	8.84747906116958
H	-7.21523305261743	2.98689604229062	9.66405372030128
H	-6.91518502380991	4.67745935961416	9.14584480986405
H	-7.43700370940311	3.45323770870233	7.95091321600091
C	-4.48807798242628	3.49208053985938	9.85038344329979
H	-4.56050746040471	4.54469510649240	10.19068626534882
H	-4.84490860349132	2.84561227741504	10.67679167479729
H	-3.41980960788414	3.26549303609131	9.66607629588799
O	-5.36225205795114	3.84489631674080	6.17580199359431
O	-5.78181004098165	1.57301654930430	6.83890561876033
B	-5.82336709653105	2.57860257434936	5.89605787696524

(IMes^{Me})Ni(2-C₁₀H₇){Me₂NB(nep)B(nep)}:

C	-1.20406420486938	-0.41906393710128	-0.12809676095088
C	-0.17306592601413	0.00338939185331	0.68320278837481

C	-2.07025725544997	1.13136324237718	1.34731998782260
N	-0.72873722932275	0.93477661950059	1.57752119217266
N	-2.34241251870584	0.28159313997143	0.29856837646307
C	-3.61201540603583	0.21980963284727	-0.36575913398448
C	-3.79111018944394	1.00124438959700	-1.53100797075506
C	-4.63635824485025	-0.59512234038904	0.16339263491605
C	-5.03872468936972	0.93773726898061	-2.18063503828828
C	-5.85531991594926	-0.64589622728497	-0.53793494322485
C	-6.07945507541875	0.11530616123951	-1.70327955251854
H	-5.20059884103823	1.54940735728882	-3.07942856572217
H	-6.66437729346109	-1.27793221832081	-0.14532077805528
C	0.04910982250286	1.64101077570596	2.55588151429683
C	0.40554913352842	2.98103360741477	2.29175179607587
C	0.42335271570982	0.98274059606812	3.74785276961072
C	1.15531969015413	3.66653811021661	3.26448783457528
C	1.16161098276320	1.71543548379569	4.69422737162968
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H	1.42841624396156	4.71547405498411	3.08109611000759
H	1.42955713509299	1.23189480727210	5.64430062622251
C	0.04794424307332	-0.45528630830024	4.01440683286836
H	-0.86628767389904	-0.74903665469177	3.46941539539025
H	0.85925090375437	-1.14825672999617	3.70871855656372
H	-0.13403682065938	-0.61462012915298	5.09237706976319
C	-0.07014350692425	3.67010387137325	1.03720984665575
H	0.12180829866762	3.06058389578472	0.13221477306458
H	-1.17122257441858	3.82379935133342	1.08169157760439
H	0.41559385544965	4.65385510304024	0.90855530112204
C	2.33744869398924	3.80278225148286	5.51423928837947
H	3.38499409436642	3.43981235138237	5.55615529885693
H	2.36510250449143	4.88781574019035	5.30211210031886
H	1.89689393436499	3.66362906576793	6.51930711633138
C	-4.45522989399025	-1.31017563293790	1.47796342966262
H	-3.43255722846520	-1.71425817121011	1.59665450726940
H	-4.62670185279969	-0.58756436902993	2.30372816584769
H	-5.18010506547938	-2.13691054216401	1.58755206055429
C	-2.68569031657960	1.90195099923196	-2.02930173088395
H	-2.30235620214849	2.55004321116681	-1.21676194579216
H	-1.81802504722677	1.32420459078076	-2.40529561495058
H	-3.04135026213734	2.54951944314556	-2.85055174125550
C	-7.42714863699650	0.08237571338418	-2.38752753999464
H	-8.18459120459929	0.62224604901578	-1.78280356444565
H	-7.39159159770428	0.56012115367839	-3.38344306767600
H	-7.79369241203932	-0.95473546663220	-2.51125036916394
C	1.27977350292235	-0.33683814959117	0.68187376768381
H	1.90211780241425	0.57690208112421	0.61265960678055
H	1.58918453838687	-0.87352540129896	1.59967572387148
H	1.52049936706131	-0.98074981694138	-0.18235514546652
C	-1.25198104478373	-1.42100302809509	-1.23310798050247
H	-1.94028278749739	-2.25559813341093	-0.99281803536131

H	-1.60467575067506	-0.97376257330916	-2.18286320715998
H	-0.24931822968613	-1.84712470673369	-1.40971524962110
Ni	-3.30464267530435	2.32099193371698	2.05813543311068
N	-4.70385478219197	3.61251280859860	2.29659424709234
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H	-5.95298663501999	3.25818655856585	0.56415283918811
H	-4.48786039716029	4.27875379628689	0.25970108635024
H	-4.38138834184619	2.49076605699910	0.46298782030789
C	-4.36225521031904	5.00202880599789	2.64664860772263
H	-5.22717280435638	5.66690072852763	2.44231593568750
H	-4.13602655752412	5.04549843154457	3.72316175317069
H	-3.48888634674108	5.35616466237395	2.06429455378491
C	-2.82684626904541	1.10431464586847	4.54462109568598
C	-2.39015381245472	1.02873992764839	5.85989625795077
C	-1.76080728953162	2.14413082160925	6.48732630591124
C	-1.58247675376225	3.35209165950649	5.71676677393883
C	-2.02715464728532	3.38509076124295	4.36303506350065
C	-2.63893213495632	2.28949730222835	3.78041462747285
H	-1.47926319355616	1.20109542513336	8.43206865975592
H	-3.32830888734552	0.24446948889964	4.08526784469836
H	-2.53452875208736	0.10454119729174	6.43879212102312
C	-1.33606177046727	2.12299517393120	7.84905384440864
C	-0.98705971743106	4.48624851262865	6.34734313226708
H	-1.86482456846400	4.30693914731042	3.78974697853357
C	-0.59154074249894	4.44021375662649	7.67923852881908
C	-0.76650239201256	3.24745061038442	8.43982699653129
H	-0.84816007790957	5.40219007093900	5.75539180248473
H	-0.13901361779560	5.32456042839836	8.14928555772975
H	-0.45222320394912	3.21944431549852	9.49195225201876
C	-7.06707787595856	1.10888370035042	1.99875369199023
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H	-6.90684718179417	1.30141949301135	0.90913428840816
H	-7.13978494228366	0.00243121490917	2.10501105164918
H	-8.04151676777732	3.52277993470490	1.19482997715192
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C	-8.76207298056253	1.38766281356487	3.85847882972846
H	-9.69480159706668	1.89767434999634	4.17508580724338
H	-8.92124913298125	0.29369199515039	3.95235064664625
H	-7.95200744024395	1.67684296786921	4.55384577975688
C	-9.50926607407727	1.30606571235693	1.44356324335001
H	-9.65405518372659	0.20742809758843	1.49278747786351
H	-10.47829495686236	1.78431882560024	1.69333143927002
H	-9.26457831929357	1.56649559509845	0.39335186910413
O	-5.97308664321252	1.54995858005576	2.76417227279991
O	-7.10750468624129	3.74638207755679	3.06007617909797
B	-5.86990705031467	2.94643778444255	3.23309772456993
C	-4.79729320804747	4.20544344061851	6.96271343766697
C	-5.67833144566586	3.21844711365612	7.74669678848495

C	-5.47244586379402	1.84234648210602	7.09041190171743
H	-3.72567908665154	3.98123067331354	7.13405131715897
H	-4.98557432556023	5.24500542553848	7.30195561238761
H	-4.43448548125003	1.49307995935932	7.27162322308832
H	-6.16533233815089	1.09569424314794	7.52989929153509
C	-7.16137717956099	3.63007936463573	7.66262994296263
H	-7.79714635649344	2.92635726150131	8.23597877760282
H	-7.31297522512760	4.64621799821832	8.07886307464524
H	-7.52104448970954	3.63524257636471	6.61573211052448
C	-5.20982033071199	3.16707999093339	9.20883060556630
H	-5.33373053328291	4.15331868712172	9.70033721777453
H	-5.79647742923442	2.42581651309491	9.78720270609048
H	-4.13868474305852	2.88790905893542	9.27644229376399
O	-5.05293100216595	4.16392051829961	5.55370381533364
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B	-5.45739047676998	2.99476011310157	4.91826213620123

TS2:

C	-0.98202525354243	-0.20464941738809	-0.07248335519097
C	-0.01511998787498	0.18594258260873	0.82872159811853
C	-1.97868913510638	1.23353961831102	1.43903054584884
N	-0.65326992989334	1.04514683365198	1.74988514213549
N	-2.16157107652438	0.43959240576616	0.32713210602830
C	-3.39163560842627	0.43311809905574	-0.41401050972977
C	-3.50682608320613	1.30344048785269	-1.52382743574460
C	-4.43629155864557	-0.44273371541787	-0.03849613694716
C	-4.70364599552561	1.27765799415470	-2.26459727460440
C	-5.61865797003073	-0.42230375245689	-0.80225997261180
C	-5.77316056942849	0.42833648709097	-1.91706075474467
H	-4.81000215060810	1.95423605698929	-3.12507406903401
H	-6.44384901101543	-1.08974019586608	-0.51409943692393
C	0.03982153924975	1.68562159808223	2.82928370852133
C	0.27138304063307	3.08211920462523	2.76322969270058
C	0.52914274902602	0.90198197504904	3.89602950740160
C	1.05937717550109	3.66707553458148	3.76860154093684
C	1.32658142537842	1.53386612754122	4.87086781672330
C	1.61742650067180	2.90658511919382	4.81717969950667
H	1.24947246229079	4.74989793929569	3.72700444501436
H	1.70379119673360	0.93675379799155	5.71214935481127
C	0.21464747531914	-0.56926763545386	4.02464980968228
H	-0.69002581716563	-0.84696590634203	3.45591821448542
H	1.05227500864243	-1.20537177033173	3.67233793914186
H	0.03967808600645	-0.82207308166145	5.08628387400773
C	-0.31371043852581	3.91593732532716	1.65134876143599
H	-0.05498405811791	3.50844688474001	0.65396353568513
H	-1.42746465943062	3.90374625015115	1.70740303015389
H	0.04164256935557	4.96107544096399	1.70720162951980
C	2.51351485623207	3.55446378807167	5.84704611104367

H	3.53737767713242	3.70589071254934	5.44587823500079
H	2.13159163157753	4.54833306766049	6.14734406485802
H	2.59701497319521	2.93104054991820	6.75575768792176
C	-4.31936498023669	-1.32351349194358	1.17877956976827
H	-3.27794106742759	-1.63946913378018	1.36820285415243
H	-4.65552148145721	-0.75484284747546	2.06668487548401
H	-4.95637277603951	-2.22184108175841	1.08589445190664
C	-2.40116652892345	2.27852606152926	-1.85094222085404
H	-2.26078730480395	2.99817219571805	-1.01742911557915
H	-1.42483121705574	1.77670546943134	-1.99506518057717
H	-2.63496971294010	2.85240169903422	-2.76565639166670
C	-7.07160492436617	0.44929085740706	-2.69251000544936
H	-7.87553487904647	0.93532469156559	-2.10287602909583
H	-6.97018617929809	1.00779453892121	-3.64108958882035
H	-7.41930354480220	-0.57458105229869	-2.92927538310697
C	1.44690342035405	-0.11428302701950	0.86829970424173
H	2.03588759623011	0.80835768951325	1.03349849966318
H	1.72033194139432	-0.82589432041856	1.67110846720046
H	1.76858977890908	-0.55583347717558	-0.09216578615392
C	-0.93350416401987	-1.12578705787424	-1.24623721713691
H	-1.59142823347291	-2.00519236335749	-1.09745053419804
H	-1.26807889301967	-0.62720178220181	-2.17753404252460
H	0.09413872331004	-1.49536098694439	-1.40595971794898
Ni	-3.39239162482025	2.32301848608252	1.94974337391740
N	-5.00177298764772	3.39340307504154	1.81466706761814
C	-5.63369348599138	3.14363989462086	0.49586478147337
H	-6.60413371276442	3.67931697377091	0.40506915715061
H	-4.96387447224595	3.49684240757878	-0.31245222537320
H	-5.80055587703223	2.06239106911748	0.36538818875544
C	-4.72993188642361	4.84181883010675	1.93840759461661
H	-5.67504940047998	5.42417483377910	1.88445075100811
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H	-4.06688985224798	5.16345014263681	1.11113619313451
C	-3.43718562896757	0.88944349557466	4.26264874826403
C	-2.66116071275533	0.40596549352085	5.28864345066248
C	-1.83309178207315	1.27676490059340	6.07661881321345
C	-1.77205406511223	2.66999030607831	5.70559974331220
C	-2.51837302644961	3.12761283602018	4.58203702725781
C	-3.42165971463462	2.28975159376188	3.88160493592663
H	-1.15262347497852	-0.23710013635356	7.47956897797637
H	-4.14163941539735	0.23624570245684	3.74022158682152
H	-2.69628860394157	-0.66316573040718	5.54799193214035
C	-1.10209544442160	0.82802952273702	7.20607082947029
C	-0.98064408346472	3.55262786374864	6.50106064262858
H	-2.45134093782739	4.19022918386116	4.31821242371096
C	-0.29278118472040	3.09021231245787	7.62003471090489
C	-0.34268623428974	1.71581043079624	7.97440208019378
H	-0.93456490318652	4.61415226061069	6.21922927367689
H	0.30111580679524	3.78886750559802	8.22561433165045

H	0.20729921147280	1.35403536914549	8.85423727775228
C	-7.23163909670257	0.72959833942660	2.45486617524406
C	-8.38424046052340	1.31961336041094	3.28939593702923
C	-8.36667665663539	2.84192567294291	3.04922259351712
H	-7.46565320521031	0.84797101626251	1.36904531760365
H	-7.13910160026938	-0.35964723015625	2.64884812060271
H	-8.73393589716997	3.04566995446533	2.01539886448583
H	-9.06323404928217	3.34710560990352	3.75128786906609
C	-8.19182826624300	0.99398599344326	4.78112567261679
H	-9.00794467648221	1.44127334986616	5.38396325691751
H	-8.20858472400882	-0.10373624143015	4.94233407092075
H	-7.22778455457799	1.38638231471670	5.15410221763092
C	-9.72264634317216	0.74984676606446	2.78788448287050
H	-9.76257059960290	-0.34824960912712	2.93740725795943
H	-10.57214259915924	1.19491094630122	3.34389873496029
H	-9.87788167324323	0.95493997530777	1.70920060326877
O	-5.97849629029140	1.32515234072322	2.73625988961343
O	-7.08651741137019	3.44485562353667	3.19115881776178
B	-5.87652858374340	2.73190413902351	2.93734029447281
C	-4.87890975490040	4.98458288494654	6.20737866832727
C	-5.83681232805916	4.21435434524772	7.13437217594254
C	-5.42136807590022	2.73493809450696	7.04340107635490
H	-3.84022908856848	4.92073256440080	6.60657300338860
H	-5.15908605350721	6.05646399683346	6.16094326226251
H	-4.42185375541787	2.59297763307918	7.51234856979216
H	-6.14446533477589	2.09570084372317	7.59079984826254
C	-7.29137173559448	4.39226727529960	6.65871811361241
H	-7.98544405272473	3.80328686047652	7.29032767929138
H	-7.59249074286407	5.45762496961383	6.71594628460126
H	-7.40993554178088	4.05816331939794	5.61091890322957
C	-5.66827191624003	4.70581141477821	8.58037156314339
H	-5.95915708549136	5.77150196904957	8.67353030709661
H	-6.30557005772720	4.12122564811852	9.27330241714927
H	-4.61799021364026	4.60988864354491	8.92116138376487
O	-4.89679876117339	4.47882325420207	4.87660750559900
O	-5.36431320925550	2.26342703890758	5.70172698941329
B	-4.91157081297965	3.08945648024548	4.67121769144463

(IMes^{Me})Ni {(nep)B-2-C₁₀H₇}[Me₂NB(nep)]:

C	-1.32524831145823	1.47588064545582	0.04008200188501
C	-0.60432533752063	2.35778664623954	0.80380128559249
C	-2.57263821581256	1.89484350910574	1.96868576175759
N	-1.36547381107614	2.58817509019659	1.96227747140823
N	-2.52300692623883	1.21992367704633	0.74974978761505
C	-3.42451874711557	0.21800978228910	0.24891696374989
C	-4.14545328654281	0.44883203549352	-0.94617661923228
C	-3.41486634338370	-1.05895149268172	0.86026172340008
C	-4.86092396472083	-0.62655990639814	-1.51167443817793

C	-4.14832006521179	-2.09890518907229	0.26037940774734
C	-4.87846934826398	-1.90698614313895	-0.92859846206544
H	-5.42209211295216	-0.45265697467177	-2.44166928358286
H	-4.13680849713882	-3.09173006734758	0.73372698171505
C	-0.76812073625678	3.20504988612902	3.11357978683142
C	-0.93176201081159	4.58171349448042	3.36501393337528
C	0.09363669379761	2.40717255078199	3.90559136475374
C	-0.25300275914768	5.14407926505957	4.46297971073054
C	0.72268661467980	3.00243619305279	5.01320805835946
C	0.55771792247747	4.37019777753332	5.31373274957987
H	-0.36427499552134	6.22182011165559	4.65419013299811
H	1.37586273814508	2.38440257458065	5.64733290115803
C	0.37587287554614	0.97401586062695	3.52616263368024
H	-0.54527792229462	0.43332200940884	3.24476258112594
H	1.05392809831950	0.92243815294047	2.64914483019930
H	0.86803492010987	0.43192977001854	4.35409614950640
C	-1.80551575515590	5.43098567192651	2.48249493044494
H	-1.69190591636399	5.16817278309860	1.41282284340308
H	-2.86950574846959	5.26993194069805	2.73710447482625
H	-1.58770654851441	6.50709688723290	2.61164302364316
C	1.23085589888777	4.97969063011670	6.52299293743186
H	1.23664976117533	6.08472345675620	6.47191748079058
H	0.70430555868985	4.69197425847621	7.45620979274544
H	2.27676188404266	4.63130879619682	6.62664438587226
C	-2.61080421507822	-1.30720838575824	2.10668481463173
H	-1.52286507912989	-1.21523321698290	1.90780406689349
H	-2.85348946714397	-0.56662123112559	2.88977034380761
H	-2.79970160198850	-2.31492670160612	2.51728238243971
C	-4.19560293093986	1.79111314029388	-1.63862969963112
H	-3.41669870242169	2.48775032642289	-1.28404912843666
H	-4.08135427731878	1.67539848590672	-2.73356768574512
H	-5.17736069383936	2.27220682977715	-1.45622338975225
C	-5.69645900720583	-3.02752730036669	-1.52966963793057
H	-6.72356804340071	-3.03516152725180	-1.10838281470412
H	-5.79584060646056	-2.92012979666324	-2.62672831695744
H	-5.25180700315258	-4.01759805150122	-1.31360787208744
C	0.71411354797954	3.01852215728156	0.56832959356664
H	0.62192175177888	4.12347428064480	0.58272998596599
H	1.46294810502888	2.74802802743137	1.33905345130852
H	1.11962717403572	2.72578546933914	-0.41642759181815
C	-0.97075019765670	0.79118664474040	-1.23964395137468
H	-1.03056049551669	-0.30999999562096	-1.13136377456211
H	-1.63631593410575	1.06863965001757	-2.07997049854321
H	0.06276407291503	1.04929454683863	-1.53144830014744
Ni	-3.82292911674660	2.18370640143172	3.35142311327479
N	-5.33323181944361	3.36213155215351	2.39471978624416
C	-4.86254120396763	3.92899518611487	1.11290229014066
H	-5.71076668695061	4.34955278840193	0.52847992809584
H	-4.13774256994150	4.73573335371985	1.30719347036226

H	-4.37093125009397	3.14733894731814	0.52272423224957
C	-5.86558473224947	4.44005236665909	3.25374891907315
H	-6.67480124384018	4.99578943441459	2.72899508212205
H	-6.25527982585834	4.02531799752490	4.19111899688925
H	-5.05804175028634	5.14994593238804	3.50243582628140
C	-5.52632404736719	1.61467879430098	5.59967279316455
C	-5.64224670540688	0.24704495417458	5.69606080161131
C	-4.48293802449630	-0.60554474858064	5.57317040254589
C	-3.20239161941762	-0.00238410874889	5.31044826212068
C	-3.11570419694381	1.43588101163146	5.04622283793716
C	-4.26947262478286	2.28170245019570	5.33608275799552
H	-5.54472584949907	-2.46637194153227	5.93428915666911
H	-6.40985403285825	2.24351065916546	5.76883613103985
H	-6.61497959164298	-0.21755546120488	5.91314107522609
C	-4.55845799720301	-2.01178005677807	5.75609350202861
C	-2.05139302992664	-0.82656846614568	5.37350025568699
H	-2.12039100203533	1.88380378602257	5.18956097115484
C	-2.14203868223609	-2.21061365271174	5.57448296132846
C	-3.40993226073854	-2.81346923193098	5.74171760452545
H	-1.06749329994876	-0.36006531272204	5.24719404963959
H	-1.22930933576214	-2.82265620737408	5.59997379778889
H	-3.49299965487816	-3.90000271811113	5.88826100271511
C	-7.16143319813433	0.48506670596347	0.81833175638501
C	-7.53786497466482	-0.22971181609047	2.12646774247150
C	-8.06016622497559	0.84806916079658	3.09390859092400
H	-8.06948435769221	0.90948200483323	0.33900181627470
H	-6.69515493518419	-0.22102769943907	0.10812982033005
H	-9.06098102333666	1.20019361548622	2.76641841206605
H	-8.15915471783126	0.43382972722257	4.11594294115635
C	-6.31140244492698	-0.94910221404204	2.71305838157419
H	-6.56485766491663	-1.43203797457760	3.67363970831099
H	-5.94878604335870	-1.72470243105669	2.01408745690303
H	-5.46653734970845	-0.26046033017933	2.90551148433177
C	-8.65924953833904	-1.24435017467148	1.84473672230270
H	-8.31248539087918	-2.01847730336887	1.13186885170844
H	-8.96612039502362	-1.75783761068538	2.77755155575533
H	-9.55602710709053	-0.75812475958334	1.41154316670359
O	-6.22005119444776	1.54265519002127	1.02788386365916
O	-7.19935880576122	1.98836999298258	3.18315871265477
B	-6.24878991554201	2.21948203959752	2.22115110031623
C	-2.55613847104551	5.28266523396443	7.01967380486051
C	-3.63348720885441	6.35677137764933	6.78910364667402
C	-4.99615590884011	5.68010003333383	7.02889411649991
H	-2.53352664492720	4.99484059152223	8.09286378796327
H	-1.55752764481711	5.67788376864665	6.75761077705683
H	-5.12979594659761	5.47990216149935	8.11379664453395
H	-5.82120844266720	6.34816570762293	6.70877160188850
C	-3.53691191111227	6.90110548478497	5.35329189882858
H	-4.35701281258981	7.61503171577604	5.14204188894466

H	-2.57406090084531	7.42697372340061	5.19884188180641
H	-3.59055582881373	6.08577305890588	4.61050776398349
C	-3.44751613982024	7.49611808708967	7.80360435292152
H	-2.45954125018711	7.98197993895820	7.67314663808330
H	-4.22380682699623	8.27588698353597	7.66971129571675
H	-3.50976177031811	7.12651850214582	8.84653387910921
O	-2.76623996325333	4.11030840886408	6.23408453836206
O	-5.14556754572016	4.44592203494556	6.32196032554150
B	-4.04967620853762	3.68632736926478	5.95185002529497

Reaction complex: (IMes^{Me})Ni{Me₂NB(nep)}+ (nep)B-2-C₁₀H₇:

C	1.11896697720950	1.58903365248398	-0.41043265584922
C	0.17889954650056	1.97295509851950	0.52137749694721
C	0.15031592080200	-0.34082483141774	0.43440914251516
N	-0.39385993042349	0.78397039034870	1.01810990727275
N	1.08107315705299	0.18702550064980	-0.44298315384261
C	1.83794096599446	-0.66527480155122	-1.31093614537210
C	1.31187094282357	-0.96903441976231	-2.58766410820053
C	3.06468526362183	-1.19903368369521	-0.85834773985348
C	2.05592521831110	-1.81669358950826	-3.42693319324623
C	3.77602507992096	-2.04423816408732	-1.73172480868221
C	3.29203606984559	-2.36028676101248	-3.01782488109014
H	1.65741594390318	-2.07041262951573	-4.41823044746145
H	4.73279760147489	-2.47021667688023	-1.39638259407829
C	-1.45166100080604	0.75404300091046	1.97900618709173
C	-2.77969744929598	0.90777545636722	1.52609644828632
C	-1.14038988562036	0.60614562530541	3.34810931551089
C	-3.80686597586922	0.96640772767710	2.48773527908429
C	-2.19750389562780	0.66856631525920	4.27549872466830
C	-3.53336264573838	0.86919933564376	3.86775964543188
H	-4.84698579292067	1.08291822696080	2.14968894782085
H	-1.97332963231320	0.54865728294525	5.34578793688879
C	0.28302628035582	0.34035907624042	3.76986413135434
H	0.65103773957531	-0.58180591046009	3.27194183815543
H	0.96441530953493	1.15819697962408	3.45960459197198
H	0.36263919591355	0.21666648825986	4.86551724611505
C	-3.06213577254894	0.97387256189439	0.04567331003476
H	-2.61308008280303	1.87075663327379	-0.42629028424967
H	-2.61939068493461	0.09593238860812	-0.46767351126265
H	-4.14853798347221	0.99409432848041	-0.15335959449764
C	-4.64180224240670	0.97922813777153	4.89073529796444
H	-5.62775162185864	0.73857903664466	4.45160450544710
H	-4.47088257821288	0.30190967772435	5.74847313542050
H	-4.70601789083049	2.00983999560761	5.29662838286960
C	3.55102052655851	-0.90153038475038	0.53862545092805
H	3.68613385154565	0.18496266526134	0.70834491338950
H	2.79777107638202	-1.24715983300769	1.27818042887816
H	4.51137180444423	-1.40778196088260	0.74559645252461

C	-0.04727722358639	-0.44703391799636	-2.97861511714766
H	-0.82136316528846	-0.97183086115648	-2.38002173892149
H	-0.16306062768909	0.63216916449345	-2.75983392130868
H	-0.25779579651995	-0.61887238531832	-4.04697767668817
C	4.06223500498295	-3.28269283729220	-3.93499948025800
H	3.59257419673660	-4.28544379953366	-3.97363493680355
H	4.07348704327530	-2.90356963954839	-4.97466822829387
H	5.10792646167928	-3.41299611624402	-3.59913446535258
C	-0.23212677157942	3.31953737526225	1.01869255449461
H	-1.31202712983989	3.50947623227164	0.85176886214211
H	-0.05281077081911	3.42633570542785	2.10803113163752
H	0.33575819771293	4.11269408226029	0.50134379716329
C	2.05180669609795	2.37798976181768	-1.26842541912814
H	3.11157210142216	2.11647673337267	-1.06883182270075
H	1.87176654352602	2.19264568928192	-2.34756894984080
H	1.92995554935949	3.46175613594250	-1.08523269868624
Ni	-0.00869775973131	-2.11926087538030	0.61720801739876
N	-0.07993882935545	-4.04133866587543	0.77959595493653
C	1.03715110850611	-4.60767660243060	1.55369023286543
H	0.88832980155552	-5.69951574490132	1.71275329261442
H	1.99078754865447	-4.45518796242947	1.01130534133548
H	1.09687590788171	-4.10948667251614	2.53442833335918
C	-0.21549228950816	-4.66451887309769	-0.54886639777161
H	-0.43708212292974	-5.75207599902941	-0.45334638855609
H	-1.02644750842704	-4.17316016653519	-1.11044960145419
H	0.72815243720257	-4.54141421592407	-1.11551230796806
C	-3.61723406992834	-2.98609833667564	1.44383593325746
C	-3.72569415656164	-3.37877355063336	2.93072375541764
C	-2.38051861470711	-2.98097500484002	3.57243620334731
H	-3.50580163509633	-1.88099788745470	1.36549092665373
H	-4.53512675741730	-3.27968661264606	0.89431243496916
H	-2.27917015071708	-1.87442918746814	3.55144465172364
H	-2.34269106135291	-3.30963168660658	4.63070677606804
C	-3.97048966665070	-4.89232240702104	3.07048535053592
H	-4.03479406218431	-5.18295821096742	4.13811506992694
H	-4.92183127469648	-5.18220720361257	2.58028299862112
H	-3.15640554725828	-5.47817586522639	2.60450244288316
C	-4.86417357226461	-2.58443512050802	3.58650629226956
H	-5.84029793131622	-2.84746474707237	3.13086829047547
H	-4.93031653509427	-2.80418315941039	4.67120730822317
H	-4.70862154053531	-1.49657714771576	3.46684898640736
O	-2.51251278345012	-3.61993623504037	0.80995550229082
O	-1.26368890973803	-3.56765915820223	2.90264008152356
B	-1.28804441488633	-3.55768393722274	1.49732272290729
C	-3.83065858405102	-1.12743220031043	-3.79801288544433
C	-4.58639377041763	-2.14994870140271	-2.92908793877372
C	-3.53642203186025	-2.85386877641819	-2.05469172416449
H	-3.40057663952212	-0.32354137607761	-3.16328092090560
H	-4.51002270027933	-0.65198688569452	-4.53175035286298

H	-3.09336606663896	-2.15943018188641	-1.31171822699889
H	-3.98956018054697	-3.68686258595022	-1.48747559183268
C	-5.32109452659903	-3.17149125004716	-3.82147427183706
H	-5.83179895663335	-3.93296345349931	-3.20007967849656
H	-6.08582932259213	-2.66468655404544	-4.44217044939914
H	-4.63110676483109	-3.70244727822730	-4.50494134171519
C	-5.59280147409993	-1.42445014008139	-2.02253508316158
H	-6.35437045910999	-0.88944995220504	-2.62362782691316
H	-6.12503628157416	-2.14855942267154	-1.37341690073065
H	-5.09622984399934	-0.68572106740251	-1.36460442794429
O	-2.76080494487157	-1.73392518092045	-4.54124633177747
O	-2.46789691279265	-3.40844993767641	-2.83468787699479
B	-2.10209583223292	-2.82030164984266	-4.01743638187515
C	-0.43399582391872	-2.85057950642901	-6.02239252759116
C	0.67325233380766	-3.35772437098277	-6.68813807275468
C	1.39265925547520	-4.47490982874190	-6.16203050317352
C	0.94515554355398	-5.05990800705931	-4.91945182450018
C	-0.19342228366218	-4.50286942431867	-4.26941116380358
C	-0.88645156954402	-3.41906963194596	-4.79356053605592
H	2.87276813169021	-4.58736658335354	-7.76025426206801
H	-0.97436441546631	-1.98780101454146	-6.43492637235718
H	1.01242197398207	-2.90810522534520	-7.63161140011851
C	2.53231326786566	-5.03395431429945	-6.81590089079124
C	1.65570652552478	-6.17675193173009	-4.38244394956934
H	-0.52626889834009	-4.94343695647152	-3.32151241069209
C	2.75927850020179	-6.70179935695528	-5.04454685762957
C	3.20021916479711	-6.12518814700309	-6.27122292006800
H	1.31187124487268	-6.61291750052993	-3.43446805164212
H	3.29747296021007	-7.56134291867677	-4.62331362797324
H	4.07553052605089	-6.54555891978466	-6.78432481083829

(IMes^{Me})Ni{Me₂NB(nep)}:

C	1.17530375596064	1.45901321825205	-0.79972724606854
C	0.20009066410961	1.85111760042521	0.09086393704416
C	0.30102501609293	-0.46285961003115	0.16319246139290
N	-0.31430754540348	0.66847955392622	0.65979563396120
N	1.21532701436363	0.05746399396306	-0.73770369008956
C	2.09060209396820	-0.79161648174683	-1.48778157549289
C	1.65111178947129	-1.30526116920651	-2.72877456125294
C	3.36241792631450	-1.10191254612318	-0.95571328558902
C	2.52822975646381	-2.13945289446915	-3.44673728563912
C	4.20754493571973	-1.93775488426899	-1.70957436367217
C	3.80913276666415	-2.46693837346198	-2.95505876420731
H	2.19979849461555	-2.54908456956056	-4.41267311428646
H	5.20097968890635	-2.18891428658683	-1.30986744337838
C	-1.34722369967425	0.65516955152967	1.64888594985410
C	-2.69368312368560	0.69902063431273	1.23031055048669
C	-0.98738831770699	0.65585195212964	3.01581851283369

C	-3.69238282066150	0.78904491029040	2.22079472194006
C	-2.01669925028421	0.74441976208934	3.97060147711876
C	-3.37438306614732	0.82779185224568	3.59338719817513
H	-4.74665261105161	0.82881610926249	1.90942800013760
H	-1.75209938390090	0.74095928017029	5.03876762167257
C	0.46026291084933	0.51539699951294	3.41265307351422
H	0.84274481676457	-0.46993024380383	3.07427109459437
H	1.09800709852791	1.27908490057772	2.92585676225070
H	0.58855125885258	0.59461134750321	4.50773972347451
C	-3.03001169568002	0.61166121765366	-0.23804039023900
H	-2.58552910206825	1.44783503804128	-0.81444292875116
H	-2.61541306967216	-0.32243608125059	-0.66862131714873
H	-4.12317789983809	0.62206840810173	-0.40023414886187
C	-4.45582151607481	0.93262262806382	4.64521752846680
H	-5.46465985498377	0.93633786115601	4.19305693201387
H	-4.40689253067511	0.08660429293282	5.35932874387109
H	-4.34853565482456	1.86250619824899	5.23992423953183
C	3.75833990213267	-0.58322872109809	0.40543831640846
H	3.73696246261470	0.52369528431317	0.45152494104894
H	3.03767398970571	-0.94129282825962	1.16935125935903
H	4.77112980699679	-0.92424773467984	0.68530474153944
C	0.26237466113821	-0.99055386894009	-3.22673589270341
H	0.11805246003056	0.09596974943977	-3.38948351203582
H	0.04814358146636	-1.51424822614309	-4.17606107449619
H	-0.48701291765258	-1.30112279273349	-2.46914755542932
C	4.72113863049220	-3.39453302829403	-3.72781724744424
H	4.55691383380198	-4.45199119872438	-3.43097514250895
H	4.53890174203274	-3.33069006572713	-4.81814093834362
H	5.78801759634882	-3.16684617330272	-3.53914205445804
C	-0.30063053435828	3.20327997039646	0.47949503766039
H	-1.38251418812945	3.32069129809721	0.26491884922932
H	-0.16693273991359	3.39366770307520	1.56383495020459
H	0.24171368107639	3.99012329644447	-0.07360485720990
C	2.07101699854239	2.24160760012010	-1.70223807019950
H	3.14223110770602	2.07365113976948	-1.46703452163251
H	1.92717615760767	1.96117596747313	-2.76604452083219
H	1.86939789146970	3.32471431373370	-1.60811601117854
Ni	0.13743763412393	-2.22641569489790	0.46237569692503
N	-0.08720248320955	-4.11906975583239	0.75264070100714
C	0.93471538429285	-4.69961651023353	1.64165854484962
H	0.64075941393577	-5.72453653307864	1.96297443668643
H	1.90676306619173	-4.75787646542832	1.11450036199974
H	1.04992467739007	-4.06507930026262	2.53520763060075
C	-0.24594197253556	-4.89383062743936	-0.49059645947111
H	-0.57216972632098	-5.93430842449053	-0.26587235166232
H	-1.00234232638490	-4.41252983745921	-1.13126150460958
H	0.71447631633984	-4.93293299402501	-1.03904195947027
C	-3.66552872225103	-3.00931832119548	1.22411386005227
C	-3.78174467359789	-3.35508605652268	2.72200546273320

C	-2.48474655712699	-2.83985031918374	3.37767522411967
H	-3.65481182924849	-1.90362934295517	1.10647325712549
H	-4.53621401484698	-3.40652220934733	0.66403912764759
H	-2.44258838464277	-1.73212566240200	3.30427380172070
H	-2.46063648830305	-3.11259700429045	4.45280862164588
C	-3.91934961489440	-4.87673621372939	2.91639057750748
H	-3.98024981807502	-5.13077917000606	3.99347972184216
H	-4.83715514501251	-5.25475265410466	2.42323990294643
H	-3.05680085173617	-5.41967064456985	2.48730546060601
C	-4.99051285266660	-2.62345576711314	3.32451909285559
H	-5.93499936311759	-2.97663281506502	2.86377509128490
H	-5.06030470757067	-2.80520716983485	4.41626412196652
H	-4.91675394100599	-1.53126821417565	3.16531437694353
O	-2.49103263619945	-3.56092009263475	0.63528002509933
O	-1.31944280393572	-3.39872854758261	2.77141650158956
B	-1.29592022801298	-3.49690711697909	1.37192684082321

Cyclooctadiene(cod):

C	-4.60803508740991	0.56022220657848	-0.25794373878996
H	-4.50061715974540	1.02003195233380	0.74020755772919
H	-5.69844498817501	0.50309148671659	-0.44368711597158
C	-4.05104979343478	-0.84382451818707	-0.28173307017064
H	-4.64431814234191	-1.56809882885084	-0.85662371739857
C	-2.92377598029061	-1.31206816556097	0.27426269604999
H	-2.71880985744255	-2.38104608751203	0.12209715968026
C	-1.87202720916657	-0.60739220217020	1.08908167371602
H	-0.88399589030189	-0.98753906401576	0.75233554163112
H	-1.95580958493661	-0.94081963198064	2.14784711621379
C	-1.84545692553458	0.93755508900254	1.05261511729312
H	-2.76254809060875	1.34643973344832	1.51002698728535
H	-1.01375579556446	1.27100548704000	1.70359923808712
C	-1.62092002587892	1.50394189494175	-0.32931613751859
H	-0.57623532737971	1.74636676543191	-0.56665077365138
C	-4.00021949191708	1.48164588349996	-1.34020764329359
H	-4.52300654298198	2.46357779875655	-1.31292095735286
H	-4.24399617735417	1.06234463990266	-2.33985147881968
C	-2.51443030081228	1.72276594398602	-1.30539965119808
H	-2.11657960872285	2.14915022663895	-2.23652005352103

B₂nep:

C	-3.40002447002152	0.90112510329007	-0.74573785143448
C	-2.54322047446227	1.33501206533121	0.45766176983729
C	-1.49968478932550	2.33054321900547	-0.08094729138287
H	-4.00444182295641	1.75590329042169	-1.11424818216948
H	-4.09769139308244	0.09056964761704	-0.45820427998186
H	-1.99562813279649	3.26374826350907	-0.41951811426563
H	-0.77181954674334	2.59909417494320	0.70865240661780

C	-1.84672615874219	0.11503598929705	1.09493456812188
H	-1.21223250641532	0.42983104973214	1.94647969770669
H	-2.59771612678020	-0.60711147094988	1.47070184505218
H	-1.19821269957089	-0.41748892440169	0.37309795782064
C	-3.43509944237081	2.03951674395041	1.49261574536004
H	-4.21397114441948	1.35075237843704	1.87627648997896
H	-2.83598987887953	2.38443436416166	2.35813614491460
H	-3.94332618264724	2.92211217603231	1.05685659962053
O	-2.60212259865074	0.40732865171857	-1.83624987958316
O	-0.74979811673467	1.79011190064094	-1.18318203869163
B	-1.31217389233218	0.84980060784056	-2.01507540466024
C	1.77383383339573	-0.00580634527219	-4.42744997558883
C	1.28479695661917	-1.39214033580508	-4.88572153301826
C	-0.20110027888506	-1.23468998360745	-5.25608105689376
H	1.78190877299958	0.70080463014807	-5.28330420892019
H	2.80496320390529	-0.06560373685486	-4.02844875067320
H	-0.30729155233508	-0.59171737408254	-6.15406416595722
H	-0.65405227094377	-2.21823954739420	-5.48651412506676
C	1.45287736002126	-2.42786214348369	-3.75520140835561
H	1.08784206144371	-3.42138908838638	-4.08137445940119
H	2.51933556777812	-2.52948773516285	-3.47465348728983
H	0.89065876393063	-2.14789821325541	-2.84385556341199
C	2.07934211474542	-1.82662351807214	-6.12857813933902
H	3.15721994032517	-1.92403229772874	-5.89164229946695
H	1.72539715882627	-2.80948794918803	-6.49683031089377
H	1.97514239188909	-1.09518953047251	-6.95507492758587
O	0.94855429068289	0.55038406956735	-3.38886055005048
O	-0.97047363807133	-0.65318036130859	-4.18845381247508
B	-0.37933664939587	0.20619876978237	-3.29199525847327

N,N-dimethyl-2-naphthylamine:

C	-4.44415160617571	-0.74913566974478	0.73567589266285
C	-3.06257621963886	-0.61237116709417	0.81493856318195
C	-2.40205127719640	0.53342172853404	0.26547169876301
C	-3.21072924034797	1.54607444250574	-0.37256798164407
C	-4.62550112981311	1.37870683252722	-0.43822206556233
C	-5.23754051959851	0.25238327994395	0.10376244033919
H	-0.41099949996047	-0.08754571553257	0.83560513736756
H	-4.93022570678319	-1.63770335091247	1.16251824499509
H	-2.45612773674408	-1.38990270069204	1.30218509046453
C	-0.99082918165986	0.69725670585493	0.33739905989006
C	-2.54052059007452	2.68679140605267	-0.90805499195431
H	-5.22686644032044	2.15937276050535	-0.92685053038288
H	-6.32825217593155	0.13190992107979	0.04619058698296
C	-1.16524222299067	2.82510941266244	-0.83050243071215
C	-0.34817823041935	1.81871550615459	-0.21043066236324
H	-3.13578917858774	3.47637293359787	-1.38937687345979
H	-0.69825425451564	3.72136283671139	-1.25204267365480

N	1.02855273051853	1.96206239045539	-0.17673154682270
C	1.62964134769563	3.25828374785933	-0.48240903414493
H	1.28963621776207	4.06109012436124	0.20899736240376
H	2.72590821005199	3.16943858905448	-0.39821970632738
H	1.40035025956096	3.57202381978162	-1.51884091525555
C	1.81038529745915	1.02085477100802	0.61632336683998
H	1.65346960394146	-0.01716227354447	0.26264540153945
H	2.88183378365282	1.25730846604001	0.50363922059665
H	1.55066228011544	1.05739282283041	1.69884107625711

(nep)B-2-C₁₀H₇:

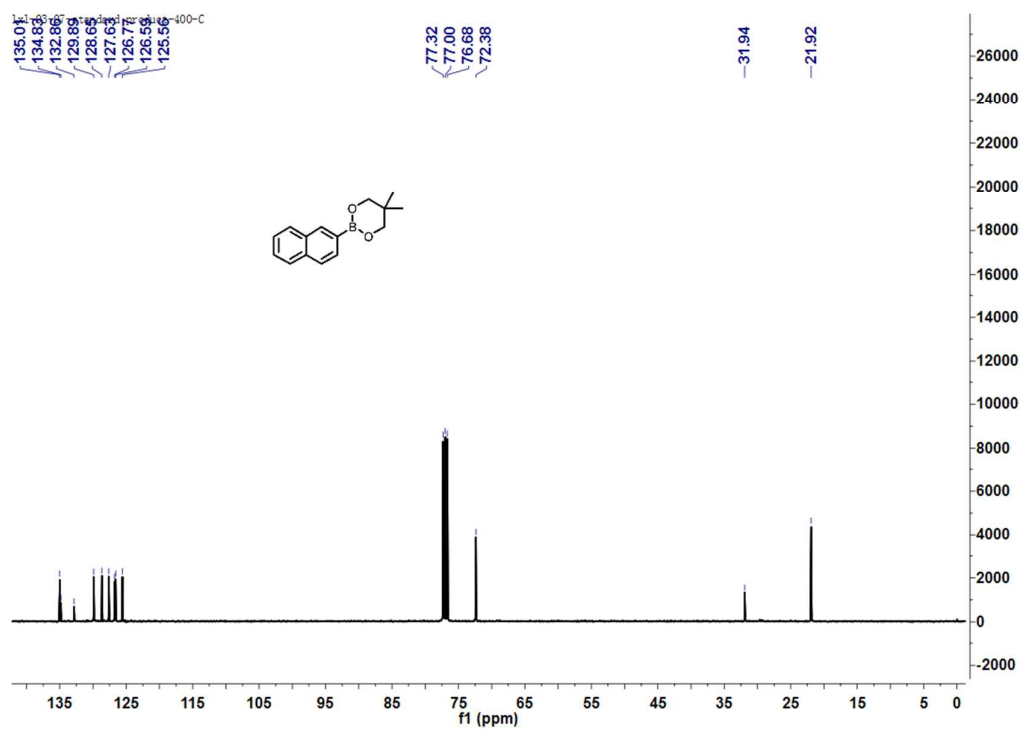
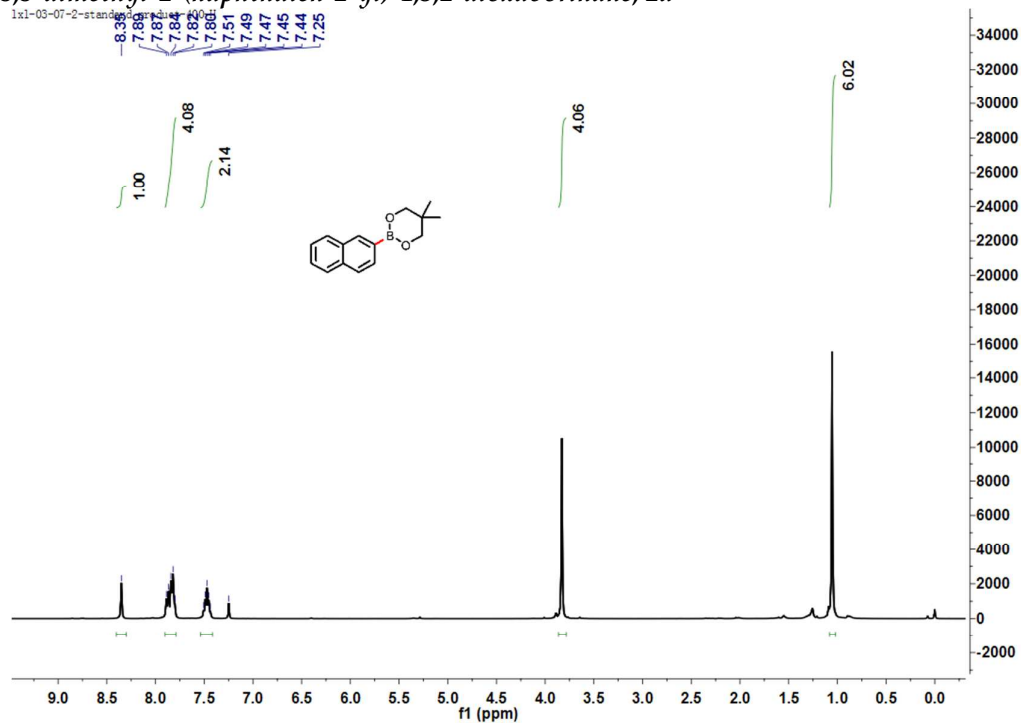
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C	-2.46803764923622	1.34561462746357	0.41404047243684
C	-1.44905134842292	2.32704966506383	-0.19482925041138
H	-3.98704378012891	1.70879220377935	-1.11715437908646
H	-4.05411665513468	0.06804287943013	-0.39919731046587
H	-1.96139399494366	3.24686453848426	-0.54568789426960
H	-0.69486661981704	2.62392101316458	0.55882697112113
C	-1.74261169859775	0.14994620716524	1.06446119463190
H	-1.07492631624169	0.49506408462194	1.87799127083943
H	-2.47503805761034	-0.55949072463642	1.49713444820393
H	-1.12228278411529	-0.40860268397861	0.33734874542287
C	-3.32486928994832	2.08085894233785	1.45723009349724
H	-4.08801843415867	1.40226169024257	1.88757090446857
H	-2.69664767496815	2.45188884997669	2.29056003254794
H	-3.84999268121886	2.94913267842087	1.01304891044699
O	-2.60944923873073	0.33514993867391	-1.83774775870784
O	-0.73762650229728	1.75274604192144	-1.30315173707759
B	-1.33370372239873	0.78408457659992	-2.07133676419973
C	-1.11416763069299	-0.84435916187617	-4.08821151562963
C	-0.41043862010641	-1.41539101763292	-5.13833230006672
C	0.93479292354499	-1.02127629281990	-5.41549308147599
C	1.54578523731332	-0.01437029805848	-4.57830152391983
C	0.78396101989054	0.54692206807399	-3.51139867236285
C	-0.52496902256259	0.15298336528535	-3.25255660481376
H	1.22645469346145	-2.35006409126862	-7.12056570471072
H	-2.14653413329555	-1.15773528706848	-3.88519957201952
H	-0.87904307155437	-2.18163844862348	-5.77279710742726
C	1.69450034238978	-1.58452113770408	-6.48531678924134
C	2.89102059573270	0.38585196949465	-4.84764809917595
H	1.25348064475350	1.31345207138142	-2.87792389236611
C	3.60523722705776	-0.18016877762164	-5.89717925828744
C	3.00171153429567	-1.17388493809667	-6.72207971432126
H	3.35193912884875	1.15276330793807	-4.20871461545199
H	4.63760850508868	0.13704503765237	-6.09570562991751
H	3.57504594511201	-1.61461563480629	-7.54900607002889

Me₂NB(nep):

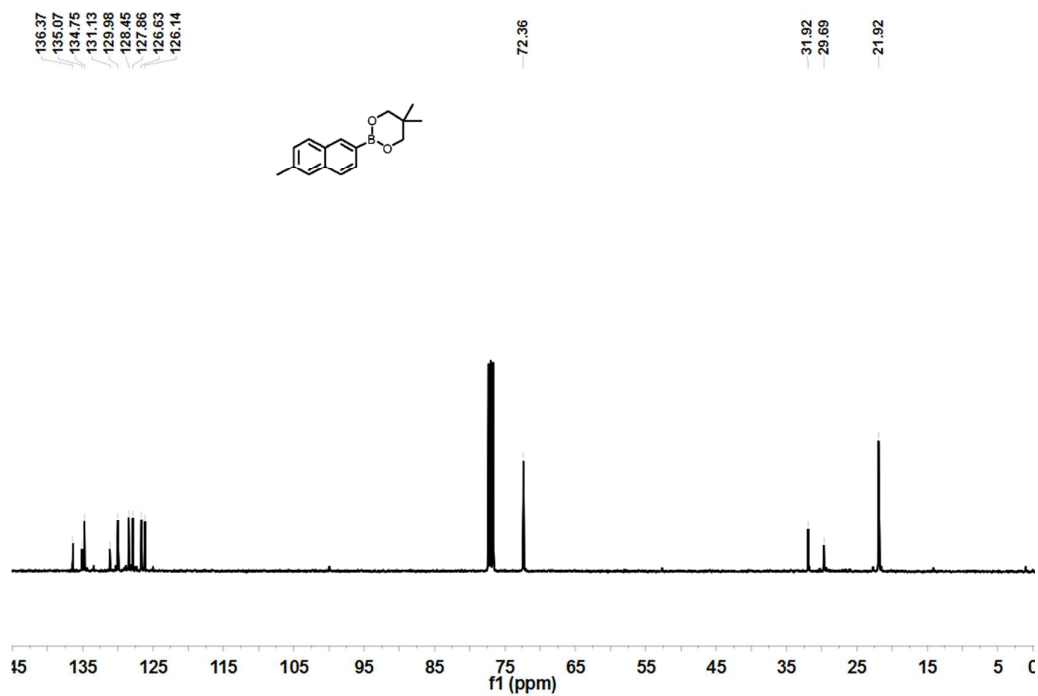
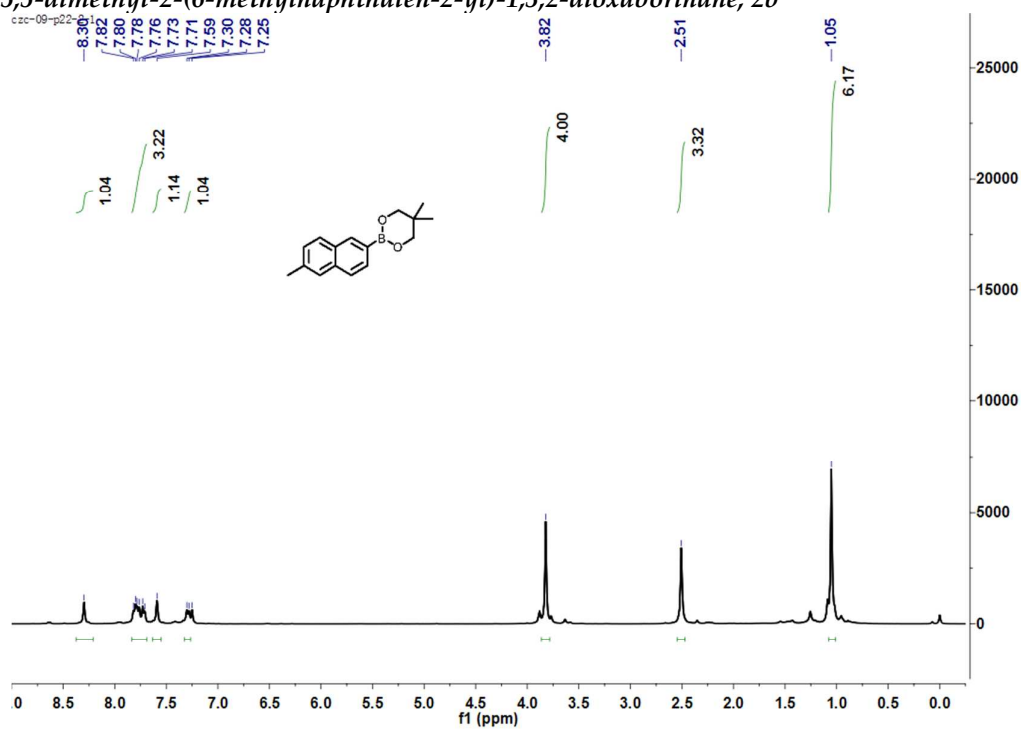
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C	-1.79551710801927	2.46505683689902	-0.27067431547191
H	-4.29048927291354	1.42984463072324	-0.82952788443530
H	-3.99736362107544	-0.18659626030418	-0.11484156907082
H	-2.51023612090451	3.27284307425474	-0.53806743803368
H	-1.01475160295946	2.90806131071662	0.37959732394275
C	-1.54101907379200	0.28995005085929	1.00118361806197
H	-0.83534053537947	0.75258489912289	1.71951016319754
H	-2.07329466000192	-0.52965534427890	1.52301603291665
H	-0.94283320046089	-0.16298154808417	0.18763622617560
C	-3.35273243666882	1.93636470255174	1.62917542939346
H	-3.93154643817098	1.14837029398774	2.15092161758077
H	-2.68473187039790	2.41063084092523	2.37515295933686
H	-4.06724889534957	2.70558225058479	1.27416615359597
O	-2.82588968244881	0.26975153838967	-1.73869532236971
O	-1.14854852784659	2.00281696696047	-1.45958591384002
B	-1.68403525425538	0.93301896231980	-2.15944036612731
N	-1.03179492577331	0.49221320318086	-3.34315630958827
C	-1.49681068880580	-0.64573877712848	-4.12145427665748
H	-1.71494347119989	-0.35172870700649	-5.17162940842962
H	-0.73066110450840	-1.45301646910914	-4.15378114010337
H	-2.41767328582508	-1.05584510901772	-3.67482160093854
C	0.18058946839894	1.11649251688478	-3.85178205637369
H	0.45247468680787	1.98008818831892	-3.22178854914542
H	1.03271932275897	0.40026651378226	-3.85698553414694
H	0.03878563956497	1.47258154455109	-4.89571792453005

(VII) Spectral data for compounds

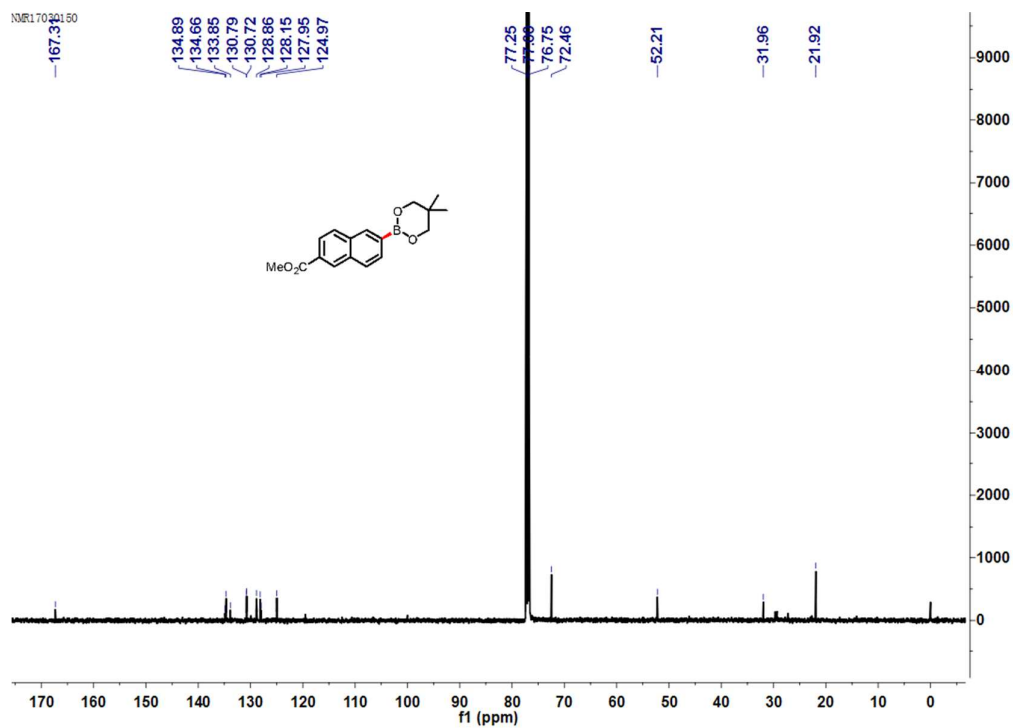
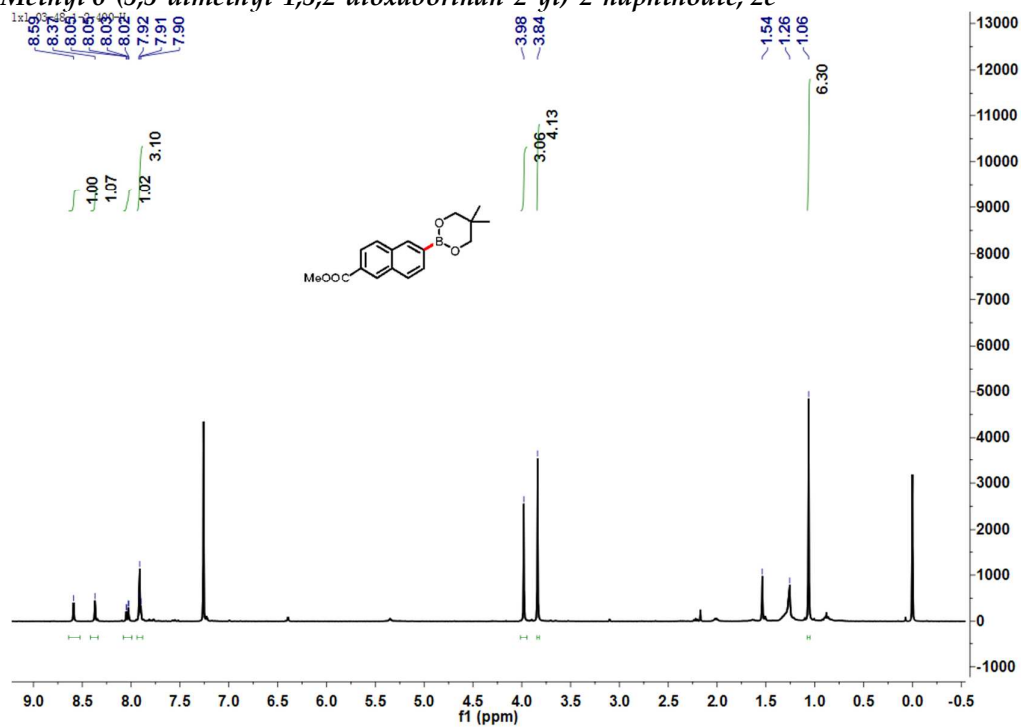
5,5-dimethyl-2-(naphthalen-2-yl)-1,3,2-dioxaborinane, 2a



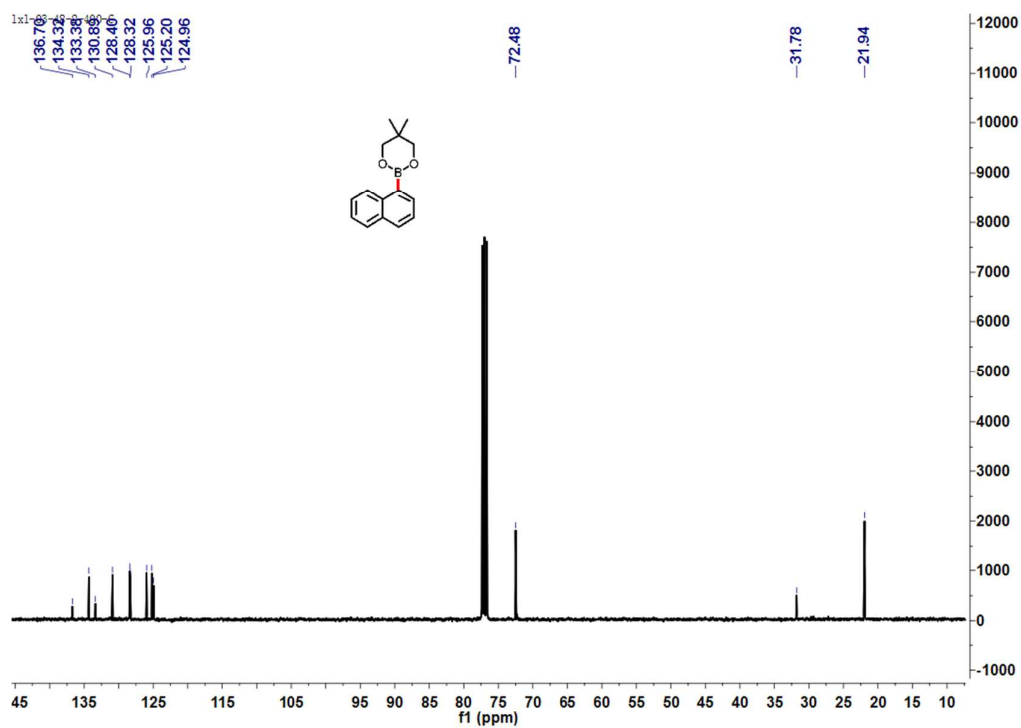
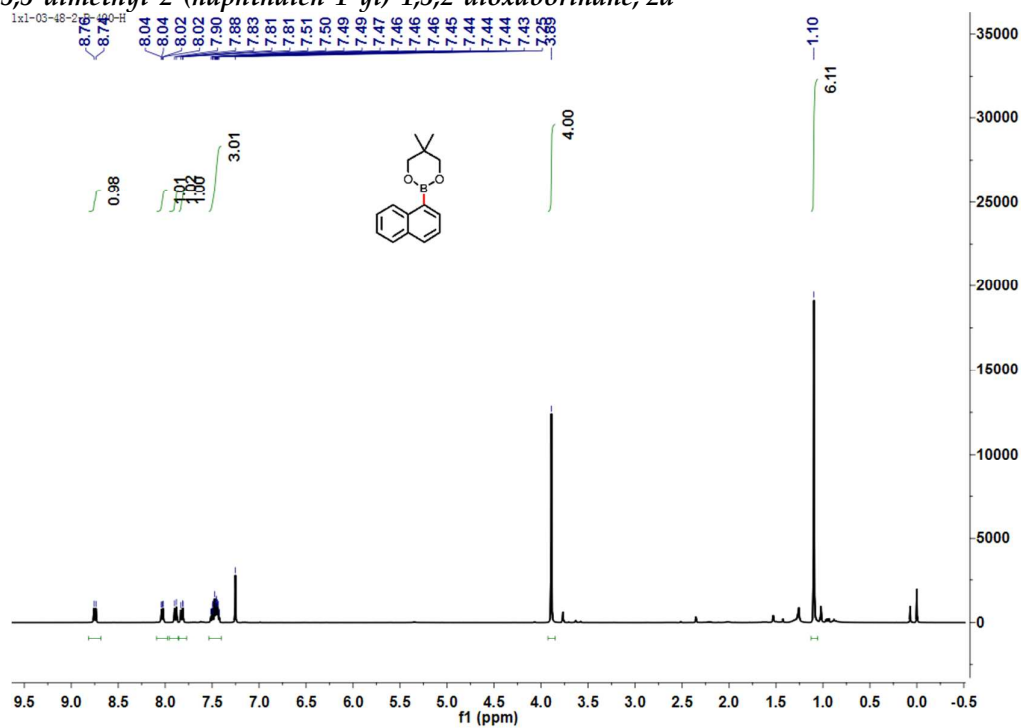
5,5-dimethyl-2-(6-methylnaphthalen-2-yl)-1,3,2-dioxaborinane, 2b



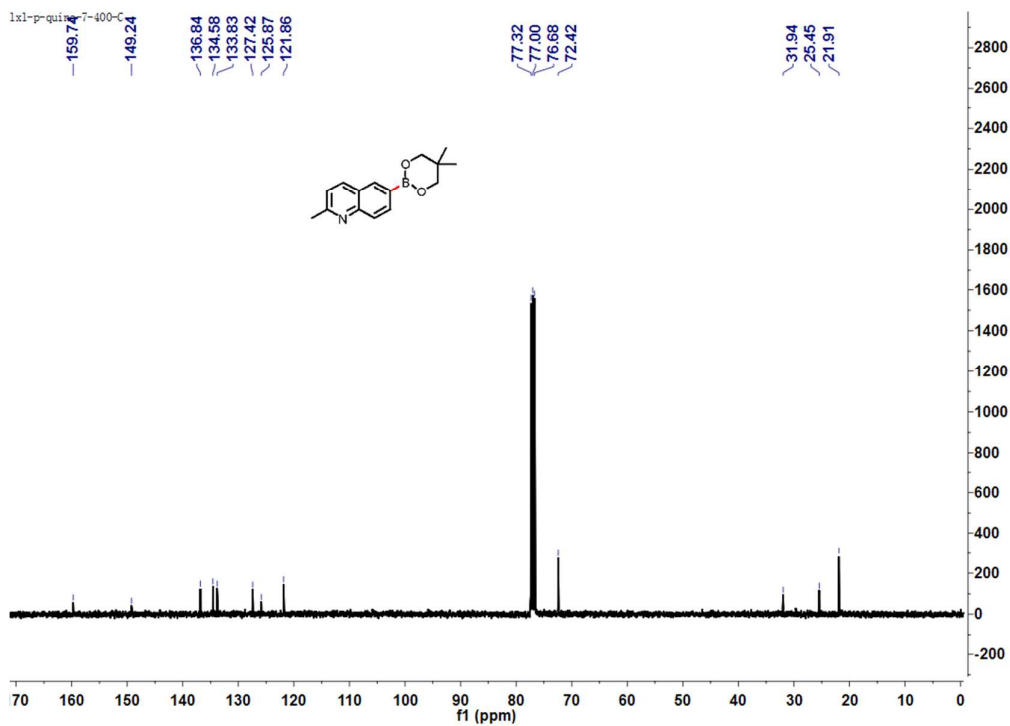
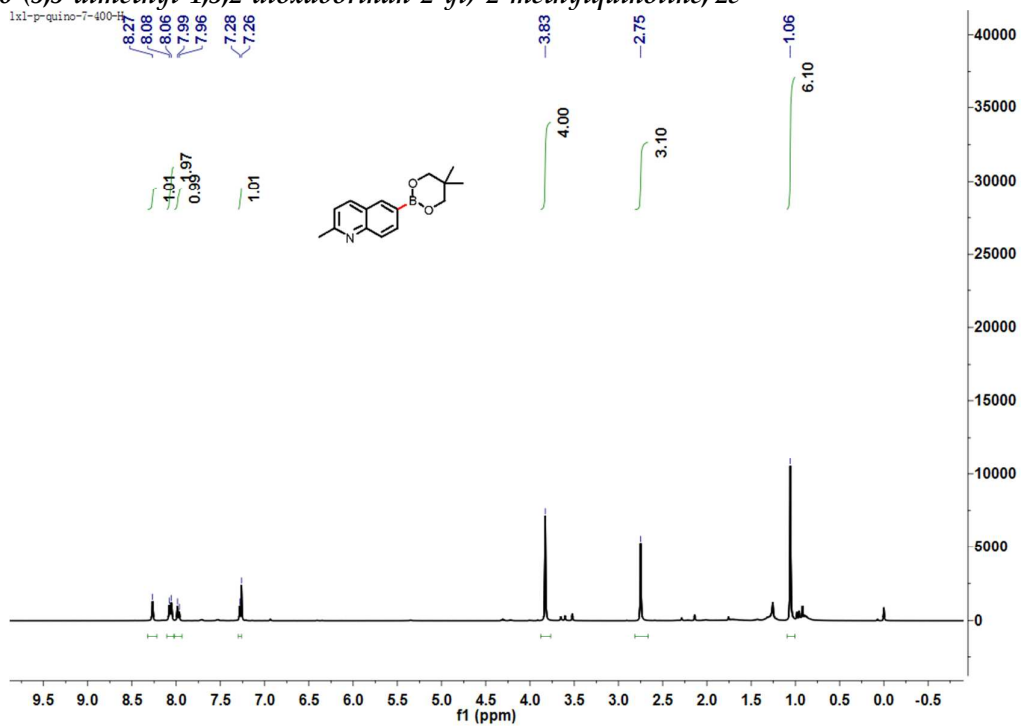
Methyl 6-(5,5-dimethyl-1,3,2-dioxaborinan-2-yl)-2-naphthoate, 2c



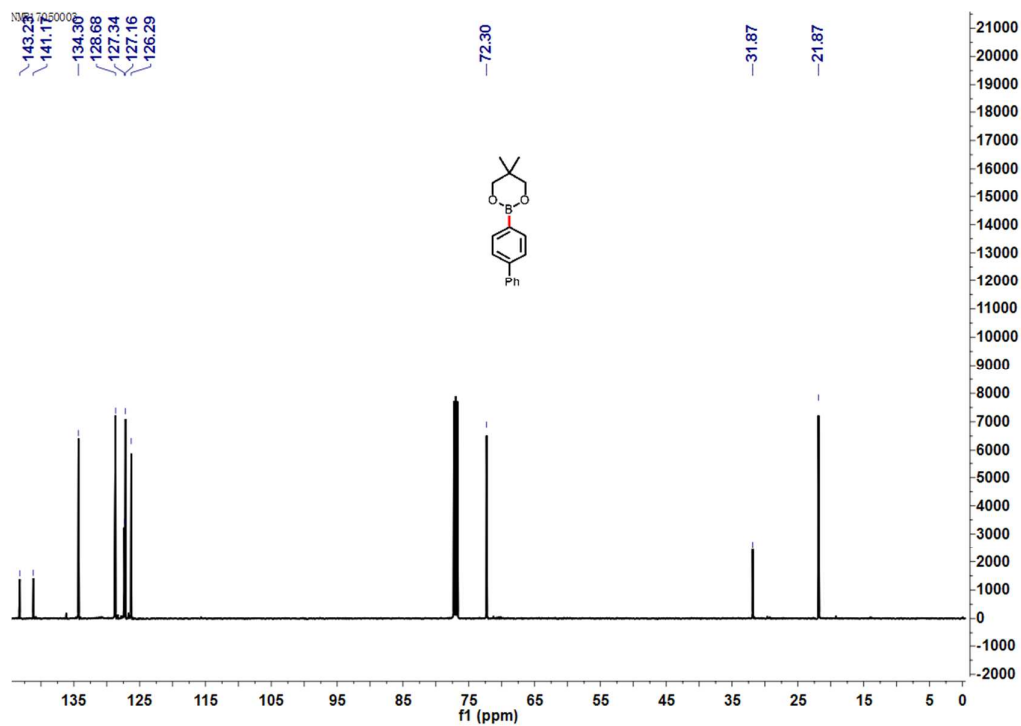
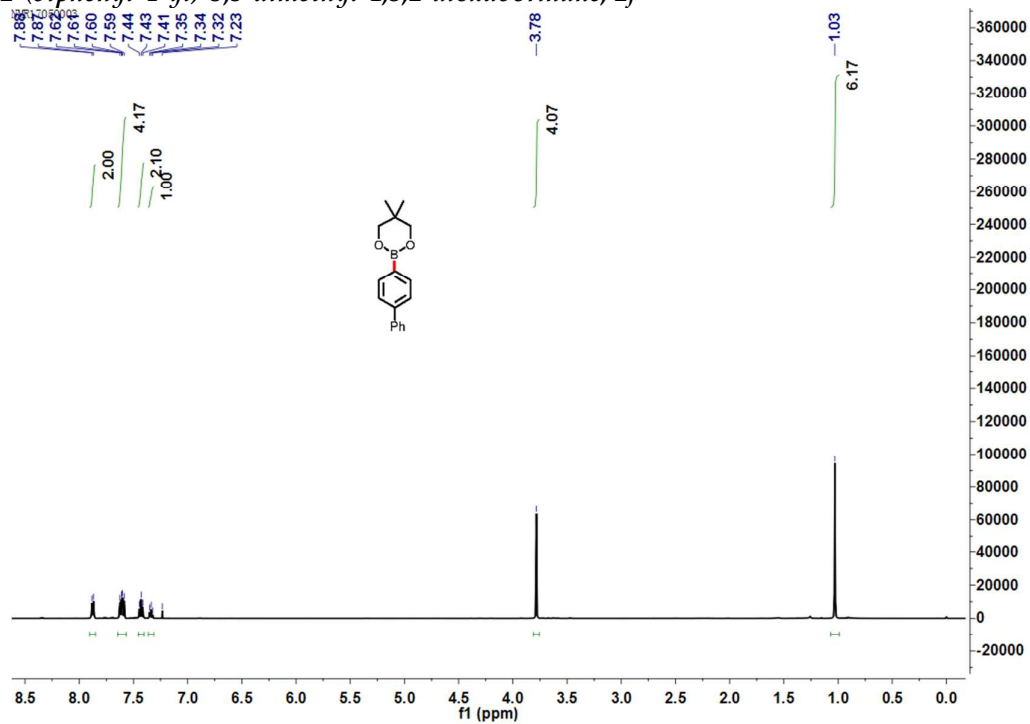
5,5-dimethyl-2-(naphthalen-1-yl)-1,3,2-dioxaborinane, 2d



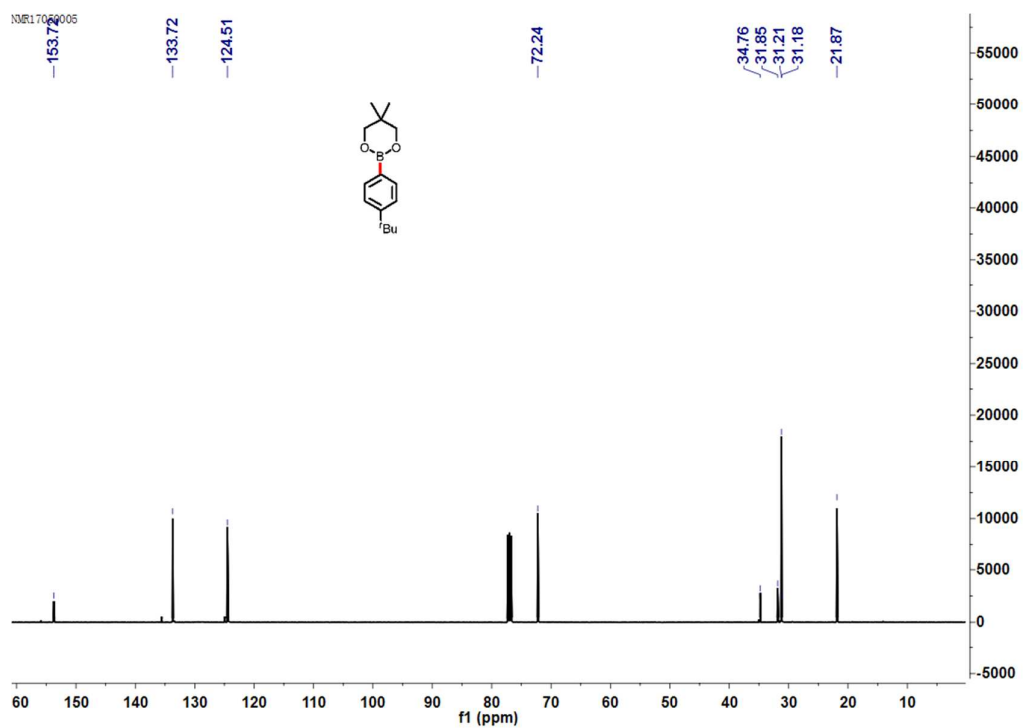
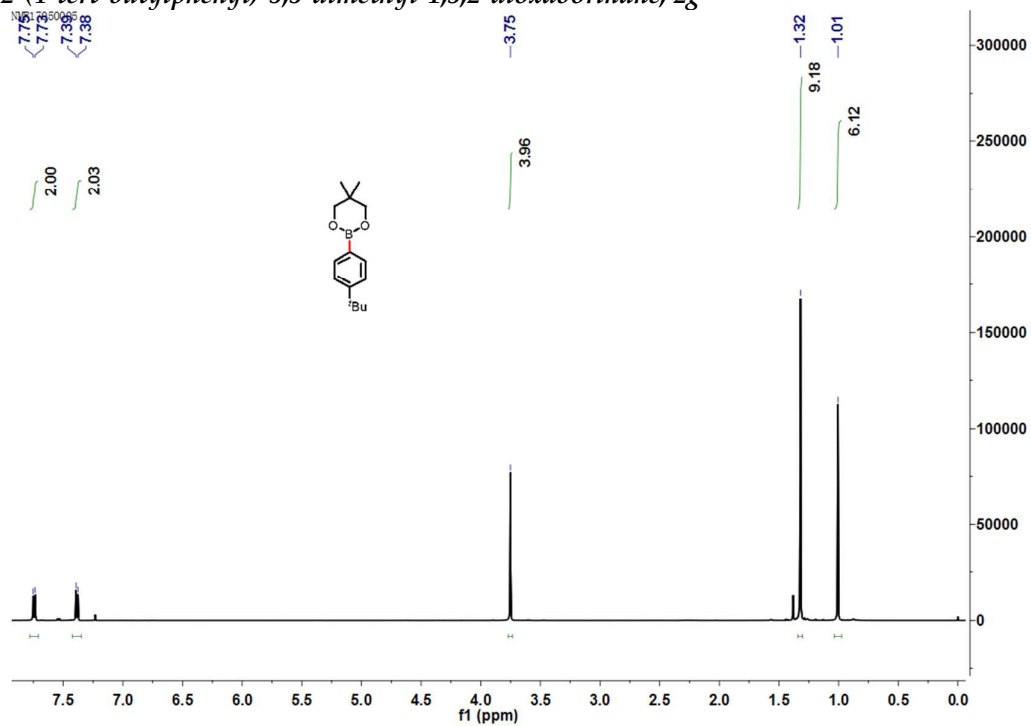
6-(5,5-dimethyl-1,3,2-dioxaborinan-2-yl)-2-methylquinoline, 2e



2-(biphenyl-4-yl)-5,5-dimethyl-1,3,2-dioxaborinane, 2f

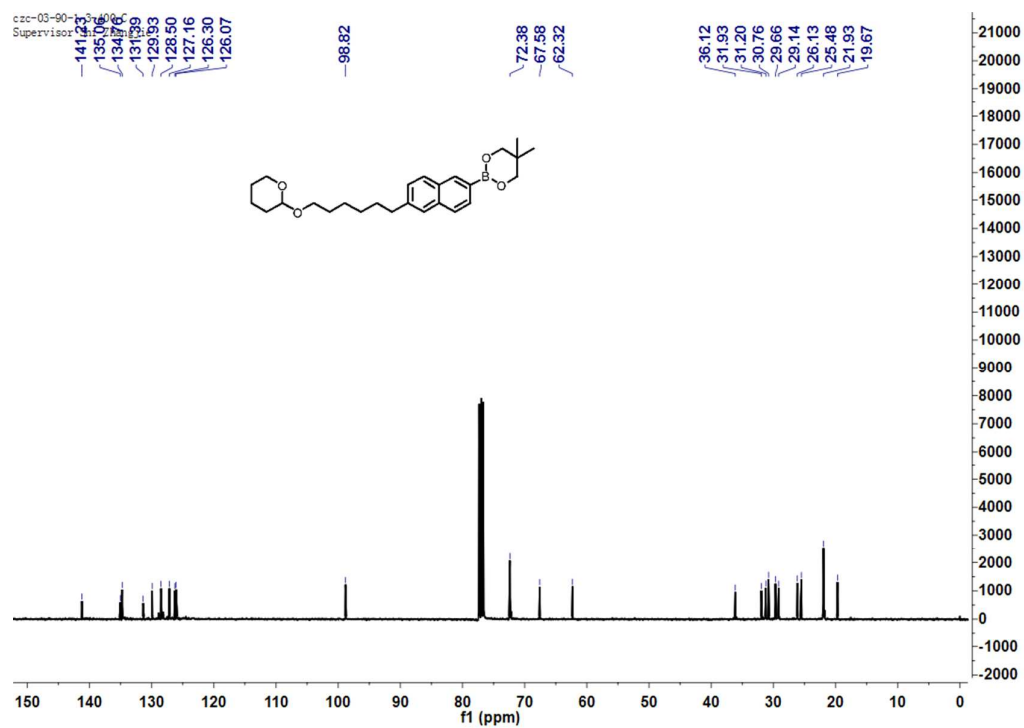
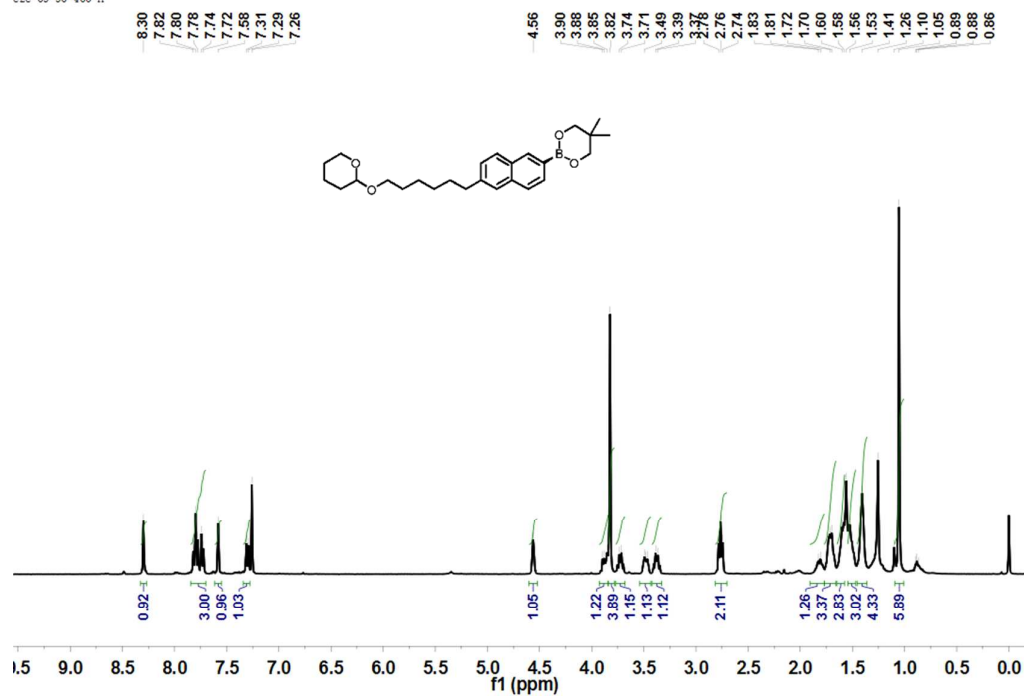


2-(4-*tert*-butylphenyl)-5,5-dimethyl-1,3,2-dioxaborinane, 2g

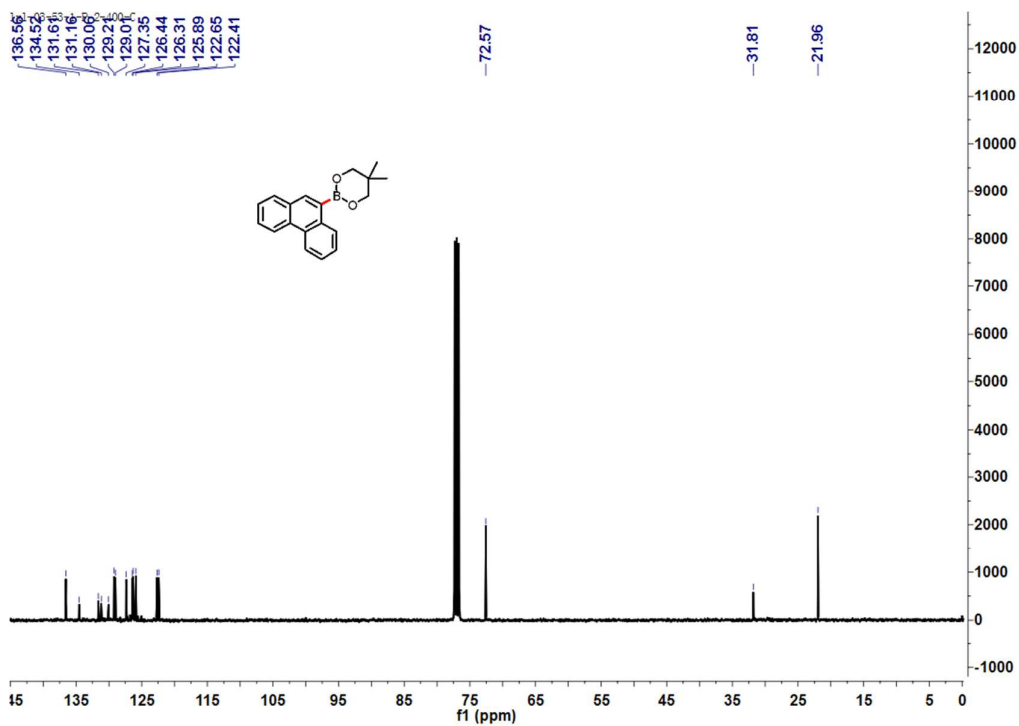
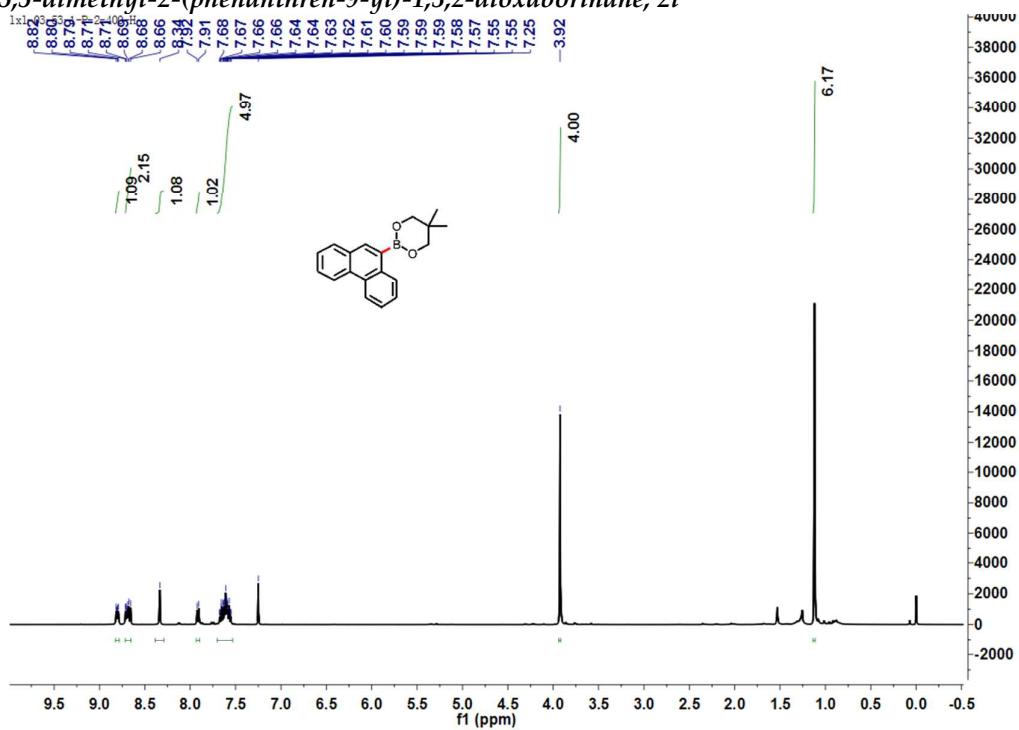


5,5-dimethyl-2-(6-(6-(tetrahydro-2H-pyran-2-yloxy)hexyl)naphthalen-2-yl)-1,3,2-dioxaborinane, 2h

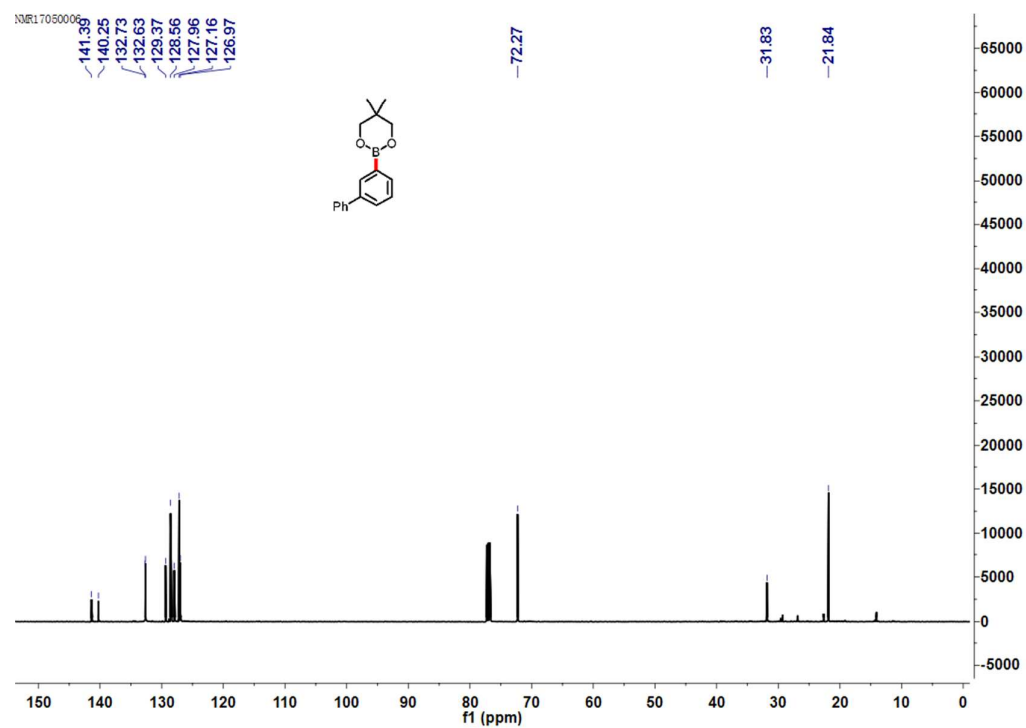
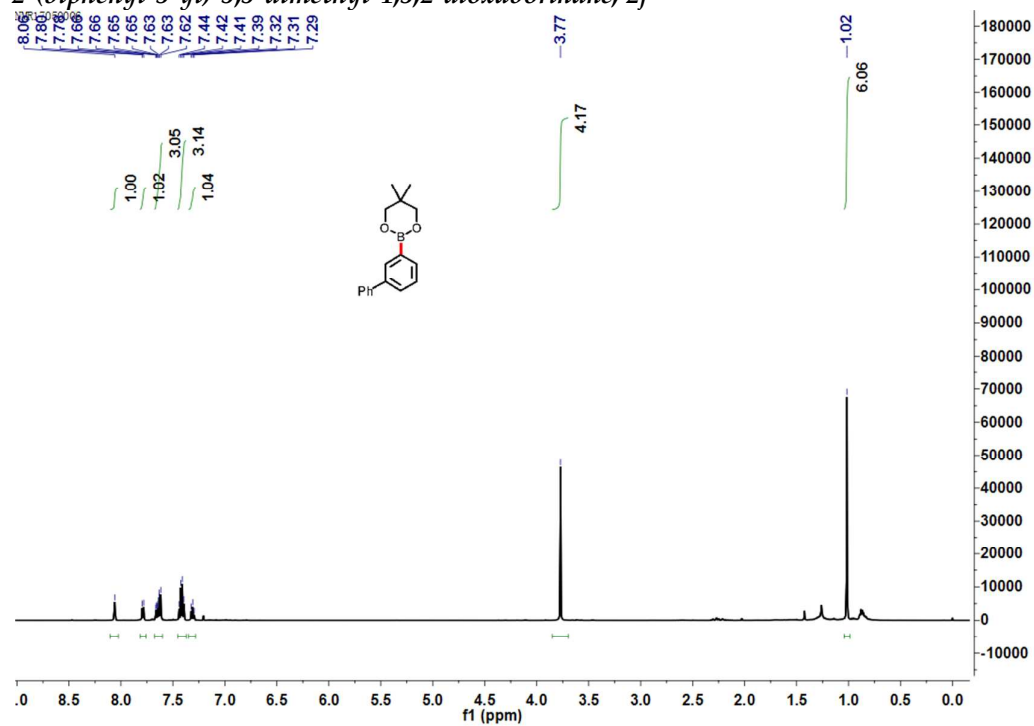
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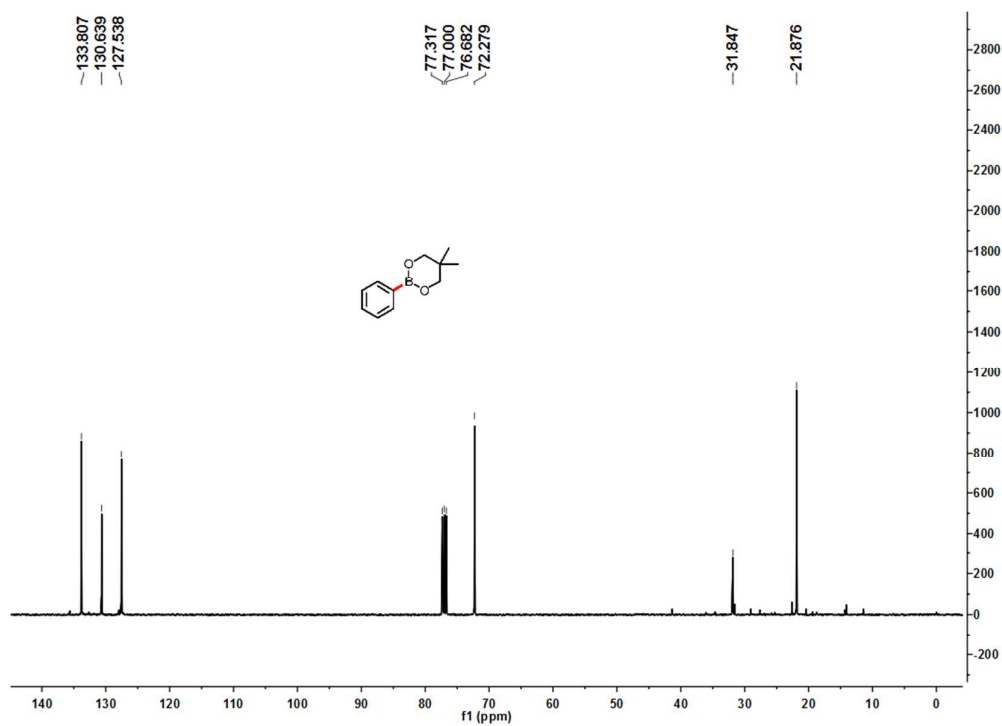
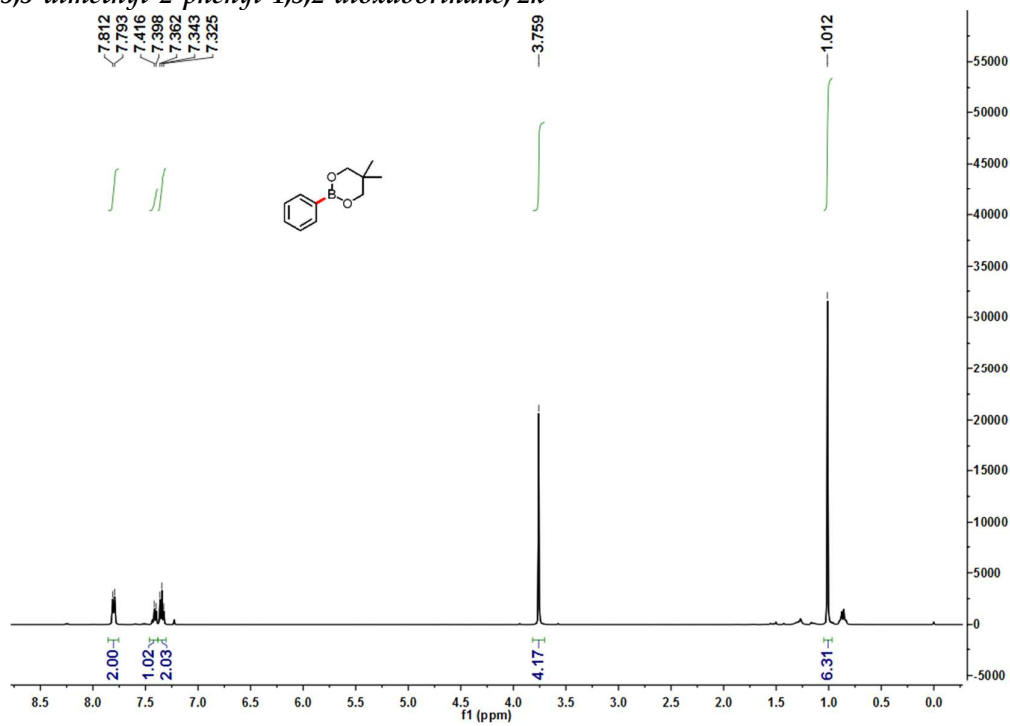
5,5-dimethyl-2-(phenanthren-9-yl)-1,3,2-dioxaborinane, 2i



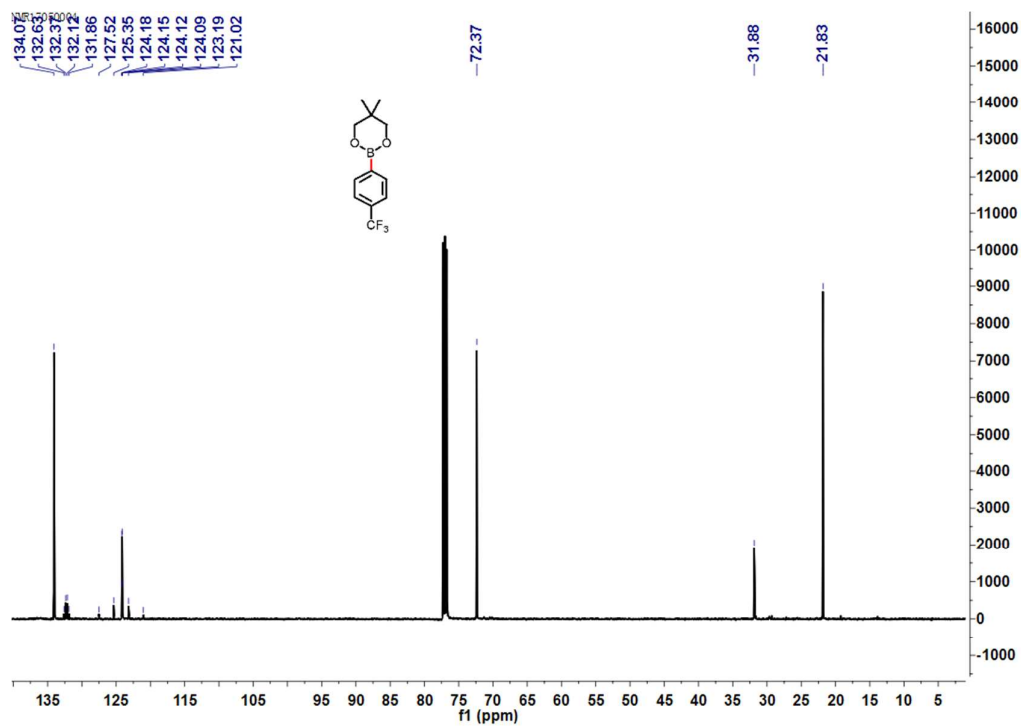
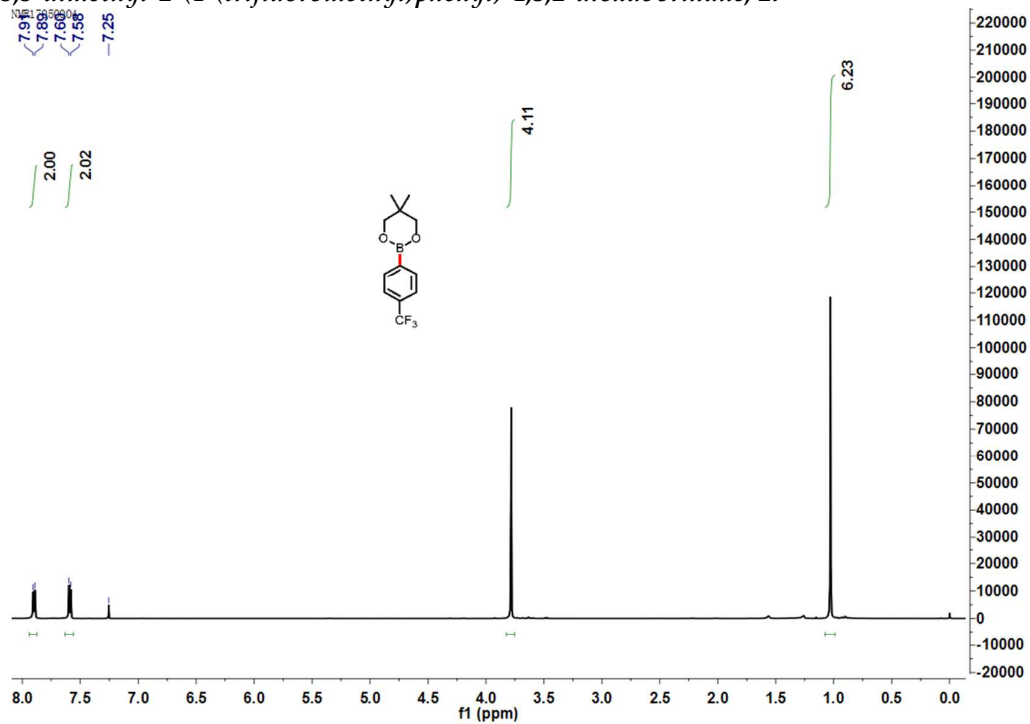
2-(biphenyl-3-yl)-5,5-dimethyl-1,3,2-dioxaborinane, 2j



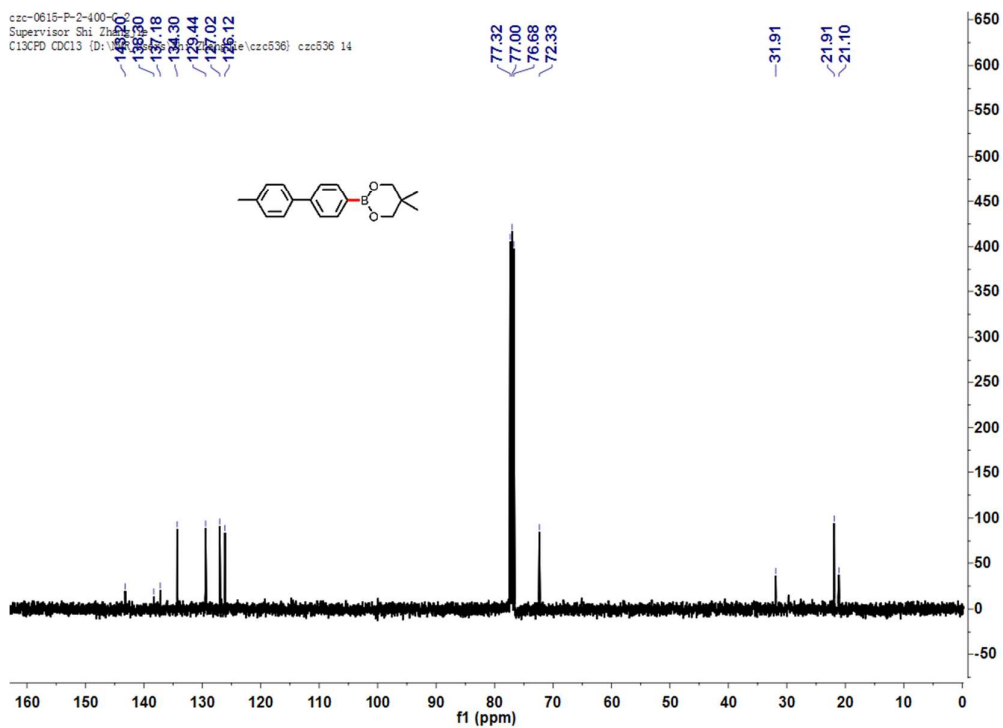
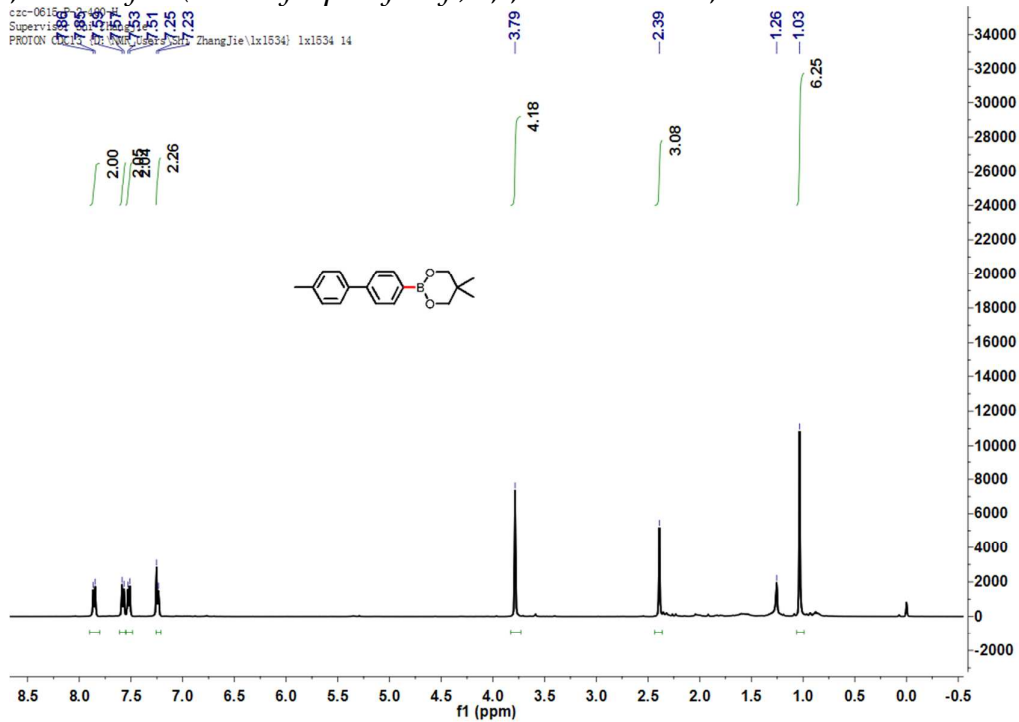
5,5-dimethyl-2-phenyl-1,3,2-dioxaborinane, 2k



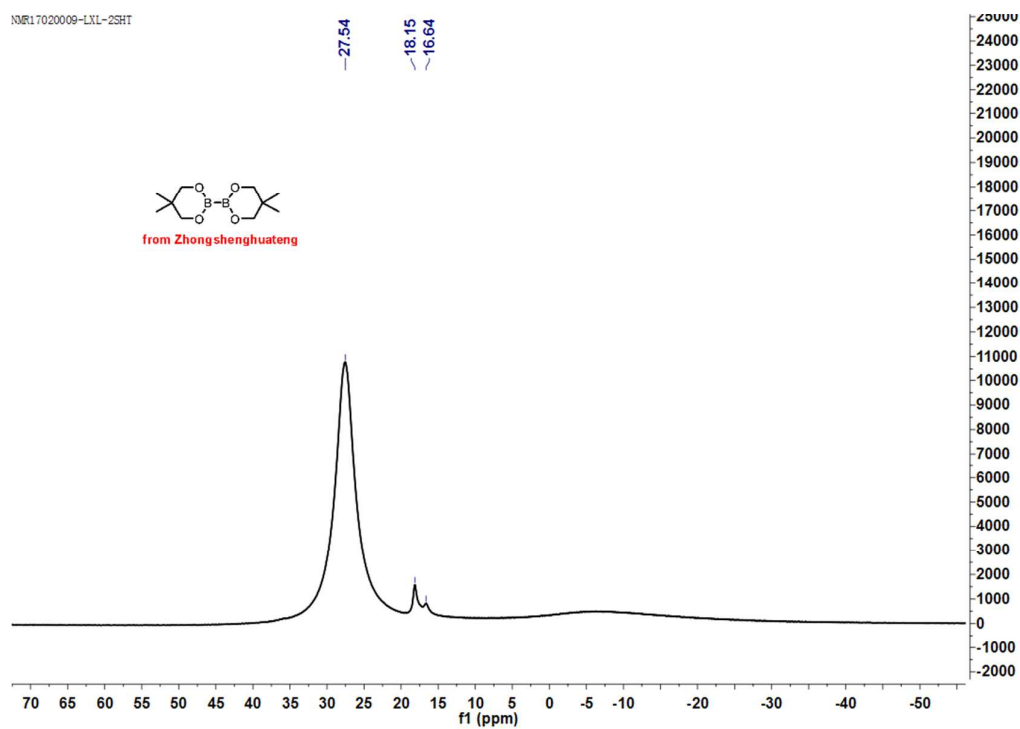
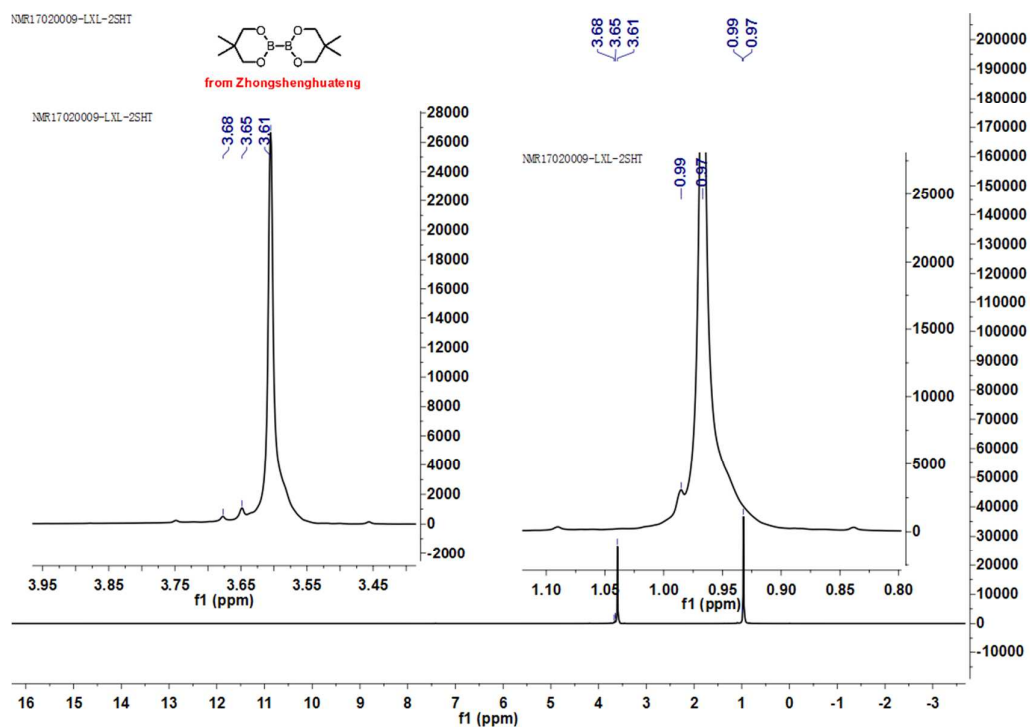
5,5-dimethyl-2-(4-(trifluoromethyl)phenyl)-1,3,2-dioxaborinane, 2l

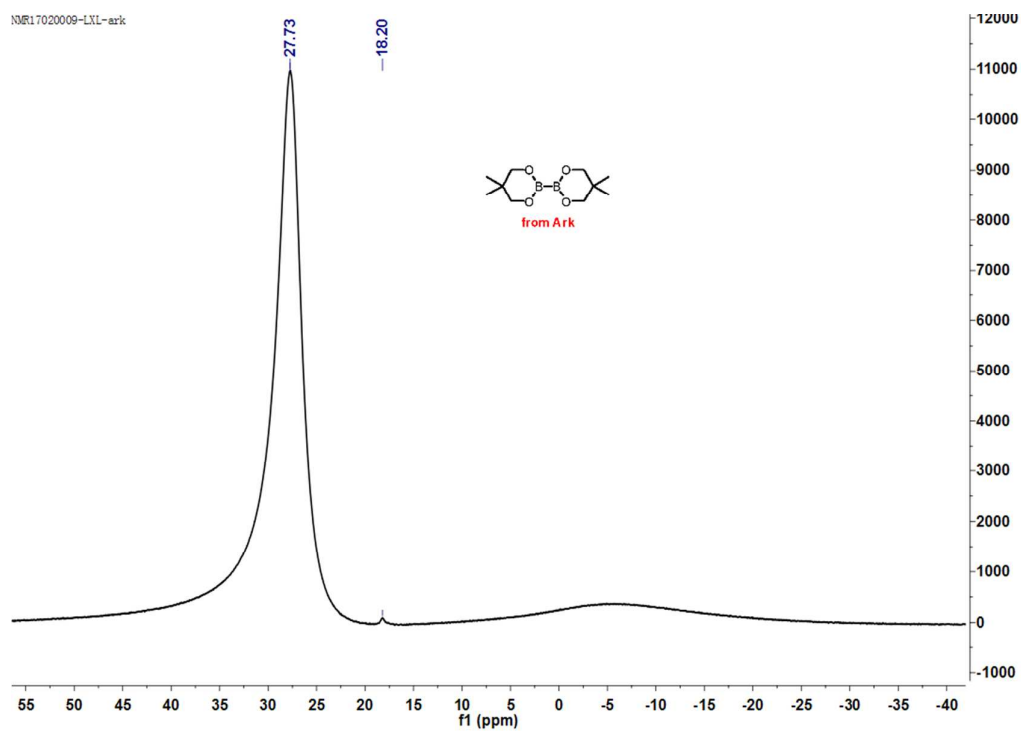
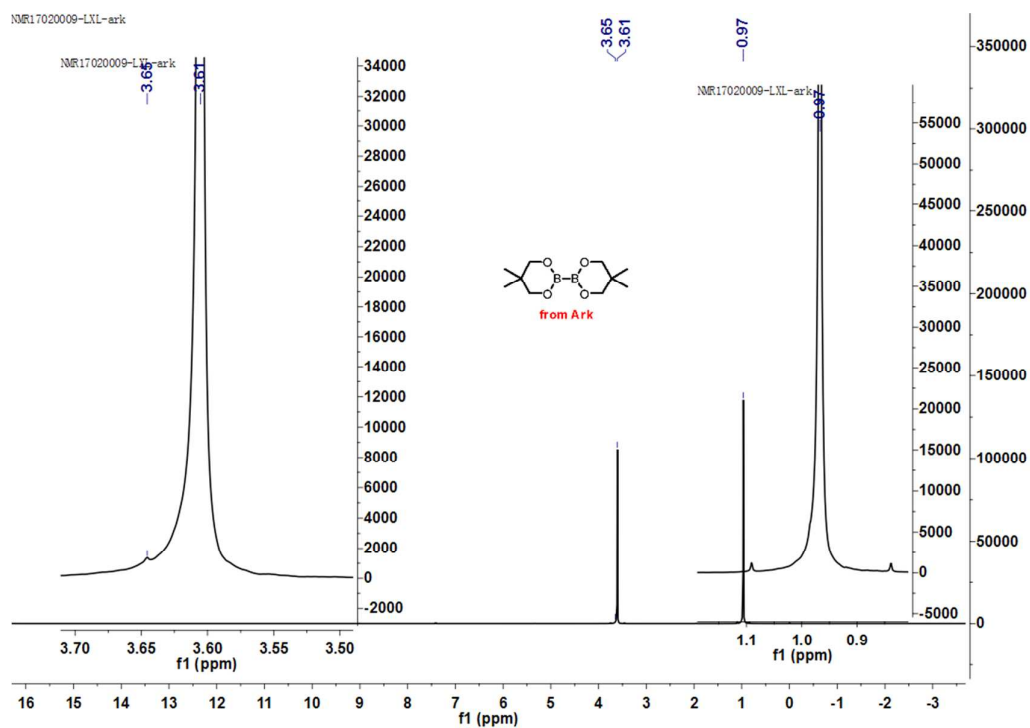


5,5-dimethyl-2-(4'-methylbiphenyl-4-yl)-1,3,2-dioxaborinane, 2m



NMR spectroscopy of B₂nep₂ (different sources) in CDCl₃





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