Supporting Information for

Lithium and magnesium complexes from the employment of pyridyl-pendanted unsymmetrical β-diketiminates: syntheses and utilization as catalysts for the hydroboration of carbonyl compounds

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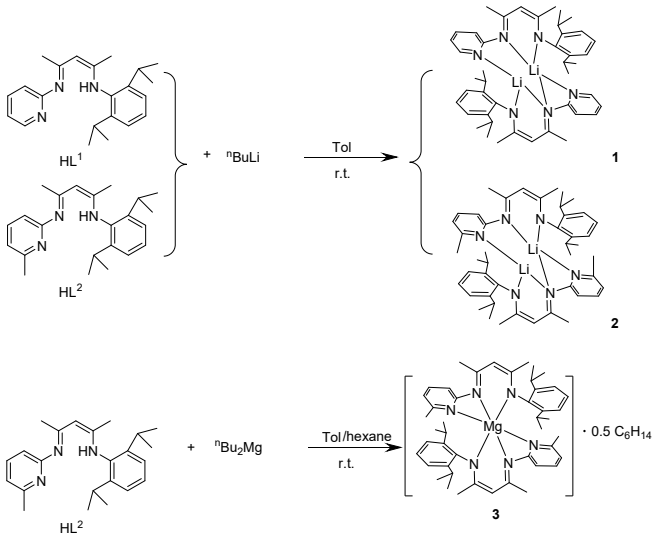
[†]*These two authors contribute equally to this paper.*

1. Synthesis of complexes 1-3



Scheme S1. Synthesis of complexes **1-3**

2. NMR spectra of complexes 1-3

Complex 1：^{1}H NMR (600 MHz, Chloroform-d) δ 7.23 – 7.20 (m, 2H), 7.06 (d, 2H), 7.00 (dd, 1H), 6.50 (d, 1H), 6.26 (m, 1H), 4.83 (s, 1H), 2.99 (m, 2H), 1.80 (s, 3H), 1.68 (s, 3H), 1.15 (d, 6H), 1.03 (d, 6H). ^{13}C NMR (151 MHz, Chloroform-d) δ 166.75, 166.59, 161.01, 147.62, 146.30, 145.64, 139.75, 136.68, 123.00, 122.89, 122.72, 117.66, 113.73, 100.46, 28.26, 27.90, 23.83, 23.58, 23.41, 23.31, 22.57, 22.54.

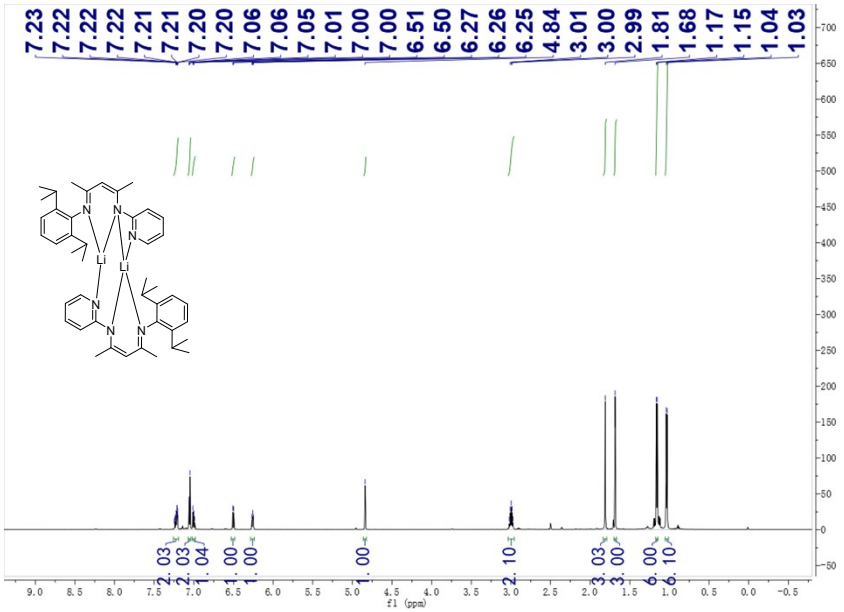


Fig. S1 ^{1}H NMR spectrum of complex **1**.

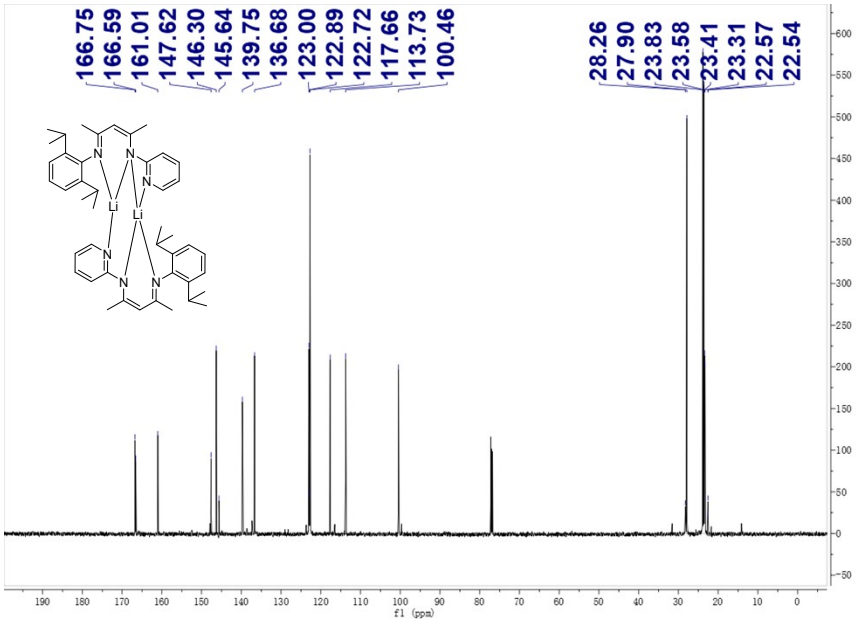


Fig. S2 ^{13}C NMR spectrum of complex **1**.

Complex 2: ^{1}H NMR (600 MHz, Chloroform-d) δ 7.16 (t, 1H), 7.09 – 6.96 (m, 3H), 6.36 (d, 1H), 6.17 (d, 1H), 4.78 (s, 1H), 3.02 (m, 2H), 1.77 (s, 6H), 1.68 (s, 3H), 1.20 – 1.12 (m, 6H), 1.10 (s, 3H), 0.92 (s, 3H). ^{13}C NMR (151 MHz, Chloroform-d) δ 167.25, 165.79, 160.91, 155.10, 147.81, 140.33, 139.51, 136.84, 123.00, 122.84, 114.14, 112.83, 100.74, 27.96, 27.58, 24.52, 24.06, 23.90, 23.75, 23.49, 23.16, 23.07, 22.57.

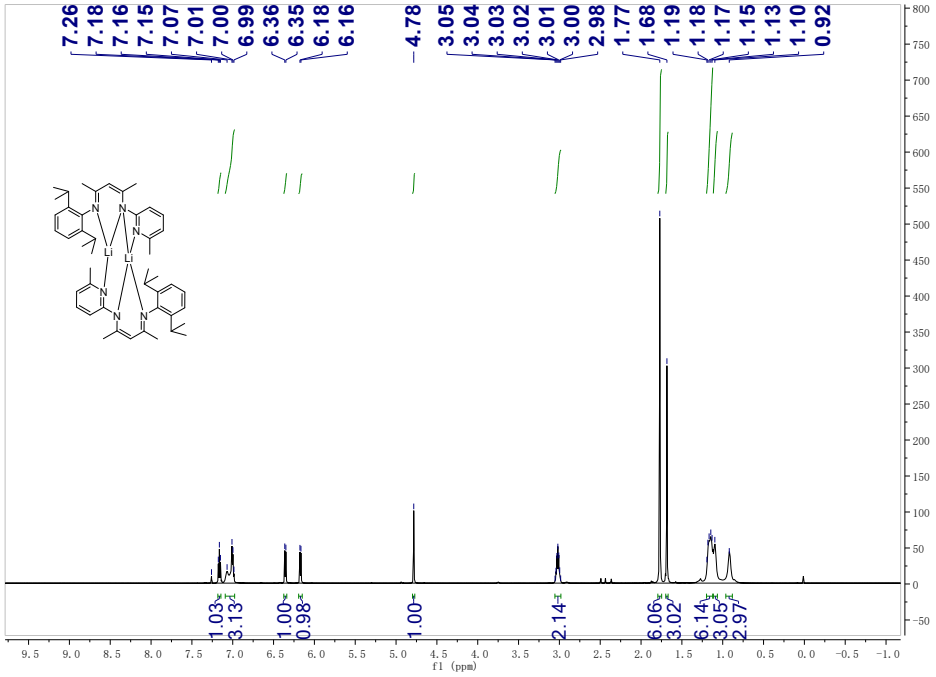


Fig. S3 ^{1}H NMR spectrum of complex **2**.

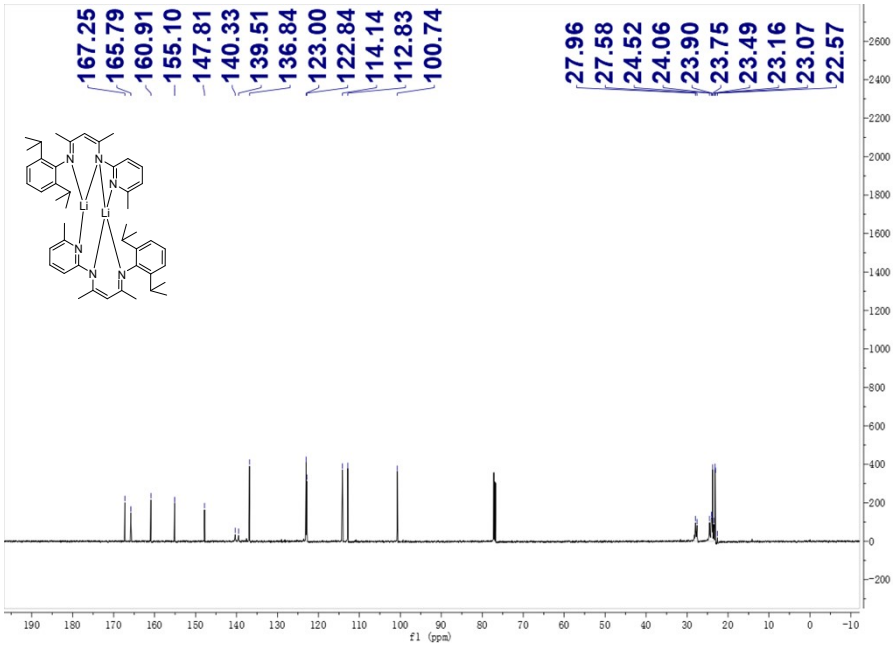


Fig. S4 ^{13}C NMR spectrum of complex **2**.

Complex 3：^{1}H NMR: (400 MHz, Benze-d_6) δ 7.22 (d, 1H), 7.06 (t, 1H), 6.95 (d, 1H), 6.88 (t, 1H), 6.27 (d, 1H), 6.06 (d, 1H), 4.76 (s, 1H), 3.52 (m, 1H), 3.11 (m, 1H), 1.80 (s, 3H), 1.76 (s, 3H), 1.64 (s, 3H), 1.56 (d, 3H), 1.30 (d, 3H), 1.04 (d, 3H), 0.61 (d, 3H). ^{13}C NMR (151MHz, Benze-d_6) δ 170.55, 161.76, 158.07, 156.42, 148.51, 142.20, 141.61, 137.77, 124.55, 123.77, 123.20, 28.97, 27.94, 27.26, 26.54, 25.53, 25.49, 24.28, 23.61, 22.10.

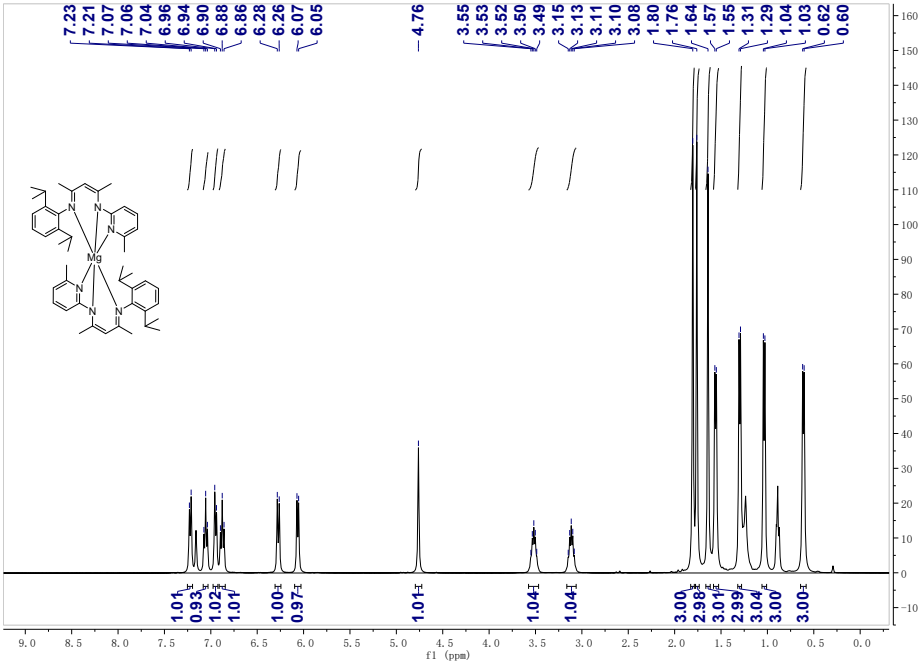


Fig. S5 ^{1}H NMR spectrum of complex **3**.

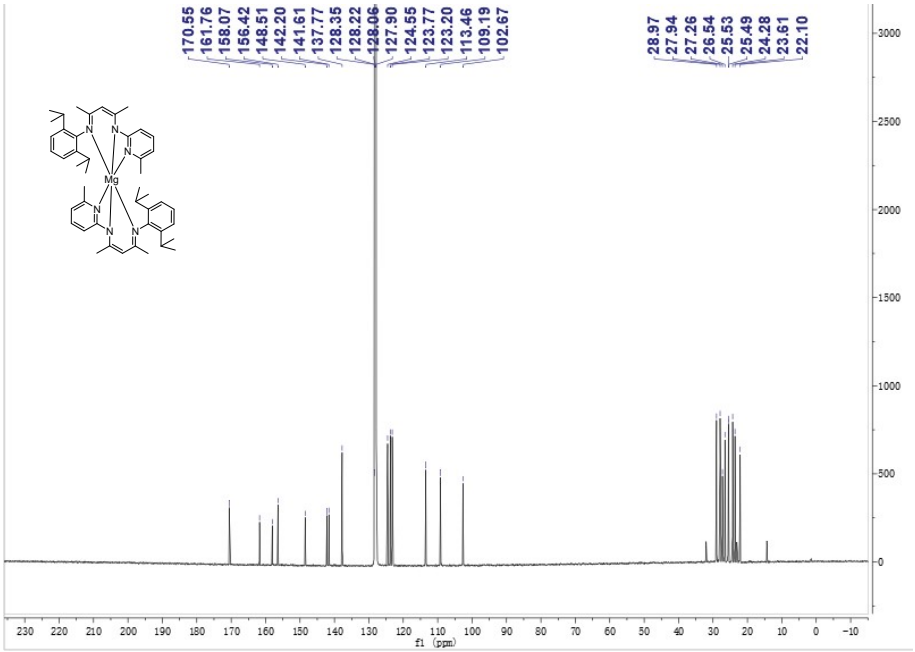
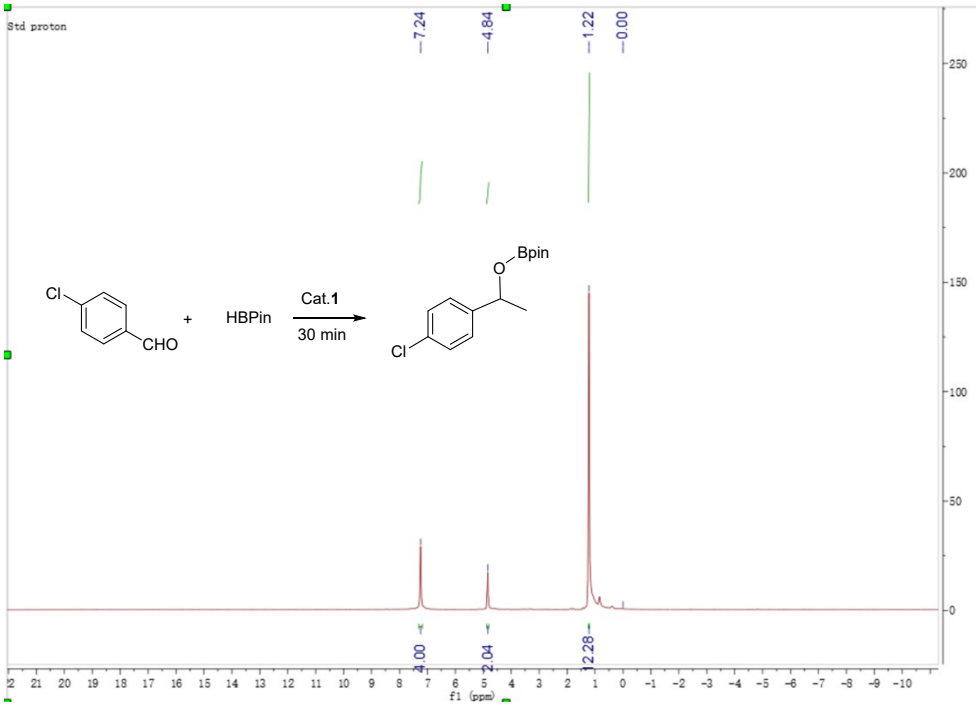


Fig. S6 ^{13}C NMR spectrum of complex **3**.

3. NMR spectra of the products of the hydroboration of aldehydes with HBpin

(a)



(b)

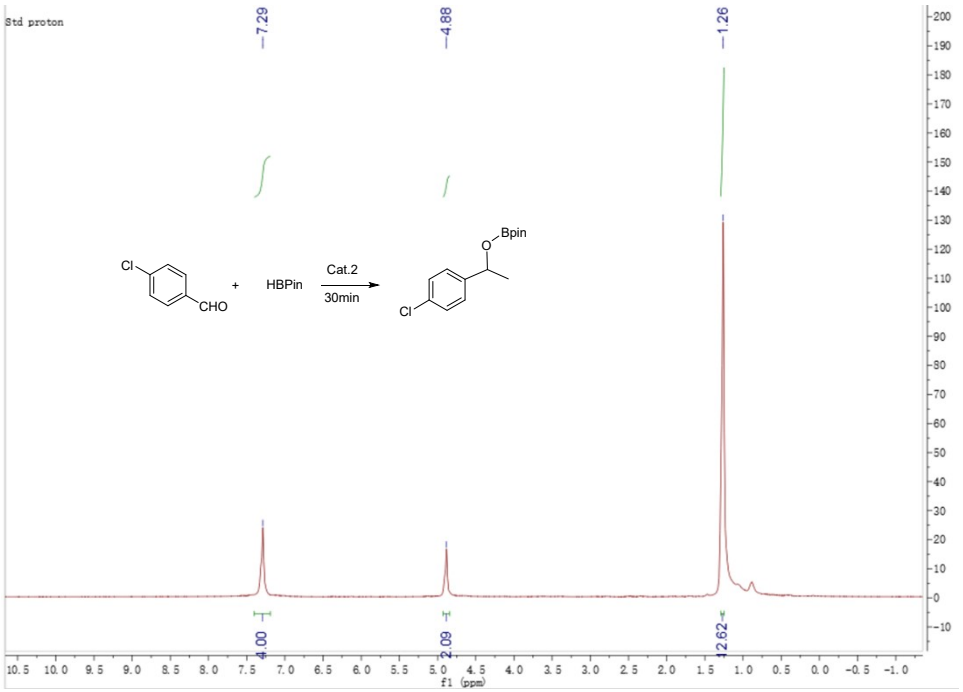


Fig. S7 ^{1}H NMR spectra of **5a** catalyzed by compounds **1** (a) and **2** (b).

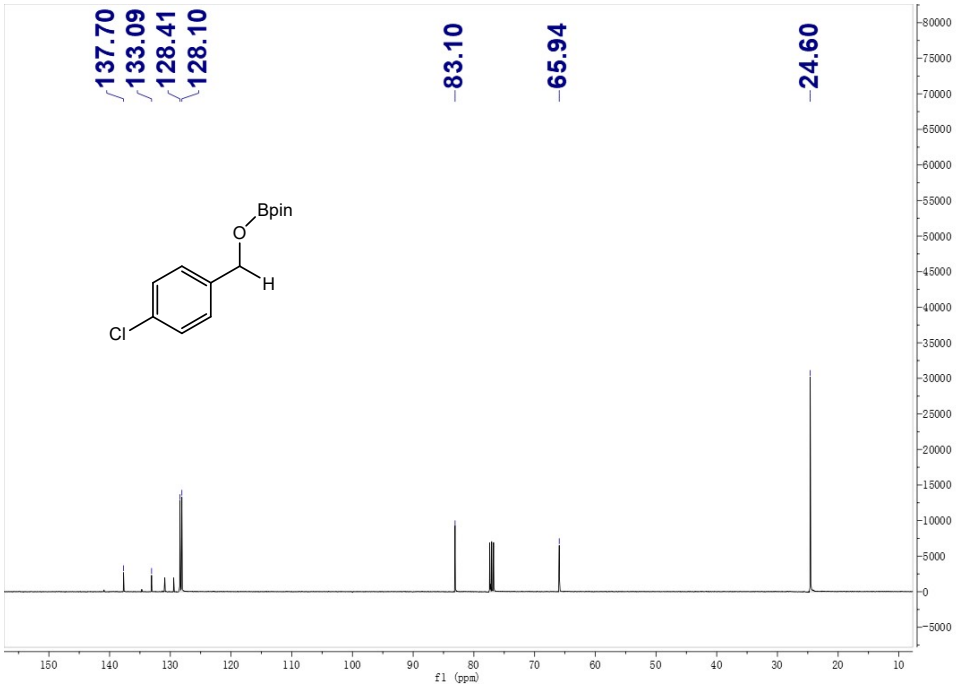
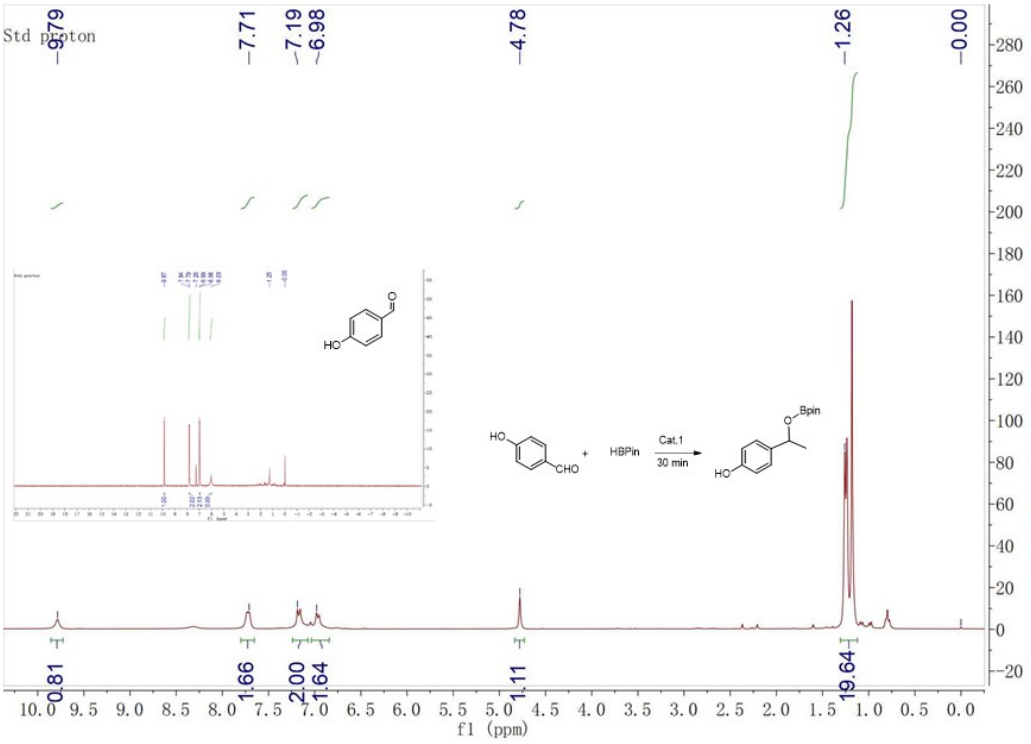


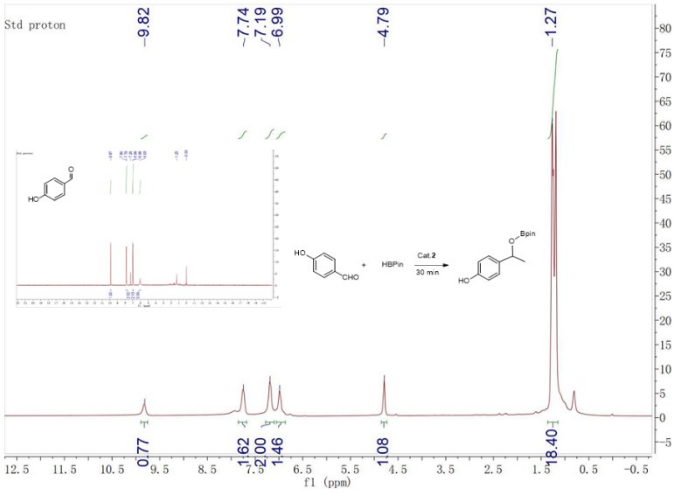
Fig. S8 ^{13}C NMR spectrum of **5a**.

5a: ^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.29 (d, 4H), 4.88 (s, 2H), 1.26 (s, 12H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 137.70, 133.09, 128.41, 128.10, 83.10, 65.94, 24.60.

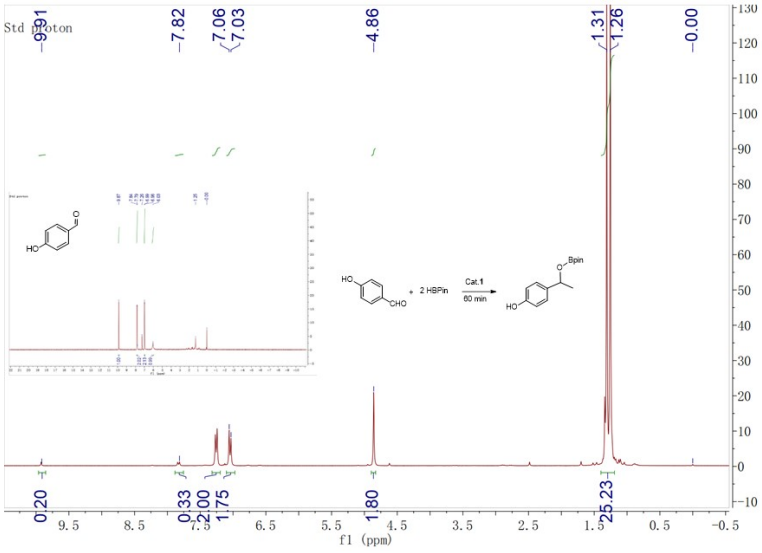
(a)



(b)



(c)



(d)

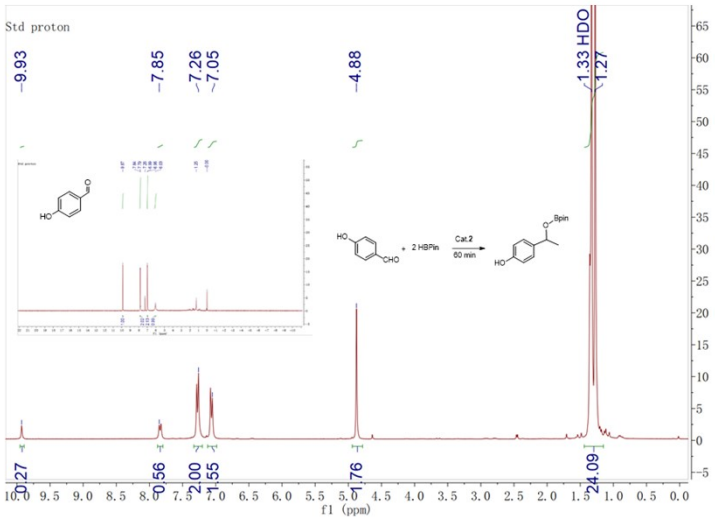


Fig. S9 ^{1}H NMR spectra of **5b** catalyzed by compound **1** after 30 min (a) and 60 min with 2 equiv of HBpin (c), and catalyzed by **2** after 30 min (b) and 60 min with 2 equiv of HBpin (d).

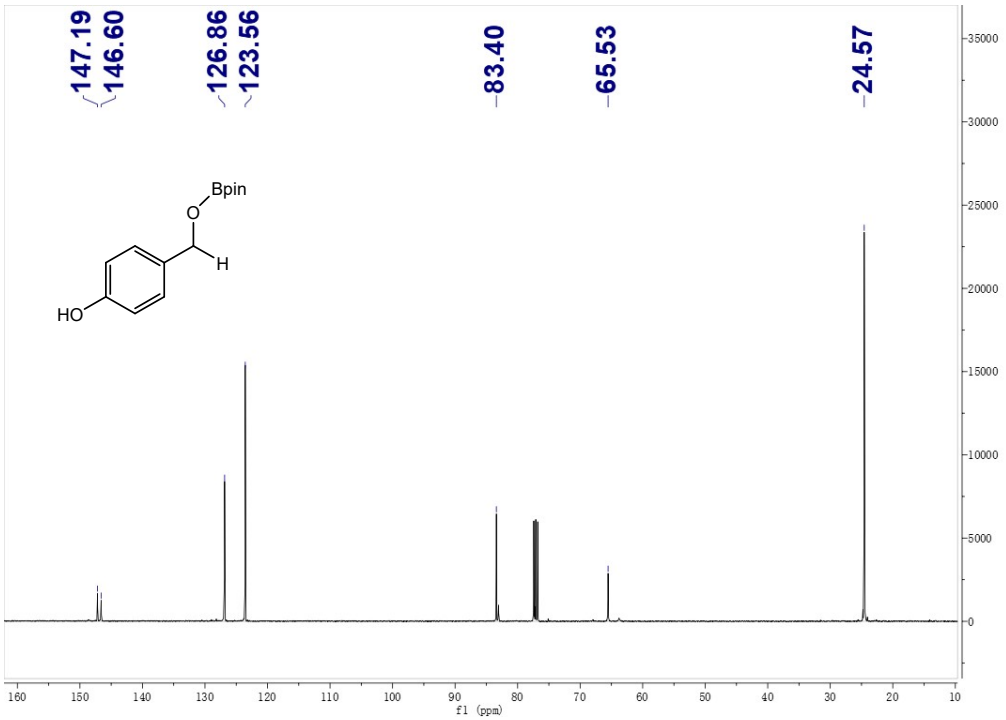


Fig. S10 ^{13}C NMR spectrum of **5b**.

5b: ^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.24 (d, 2H), 7.05(d, 2H), 4.88 (s, 2H), 1.26 (s, 12H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 147.19, 146.60, 126.86, 123.56, 83.40, 65.53, 24.57.

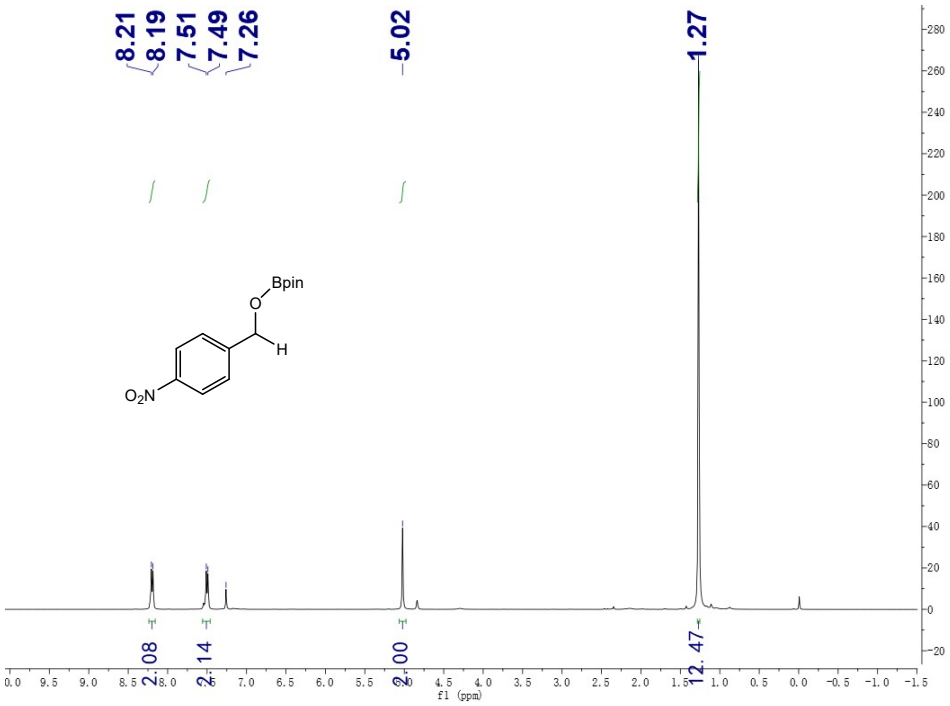


Fig. S11 ^{1}H NMR spectrum of **5c**.

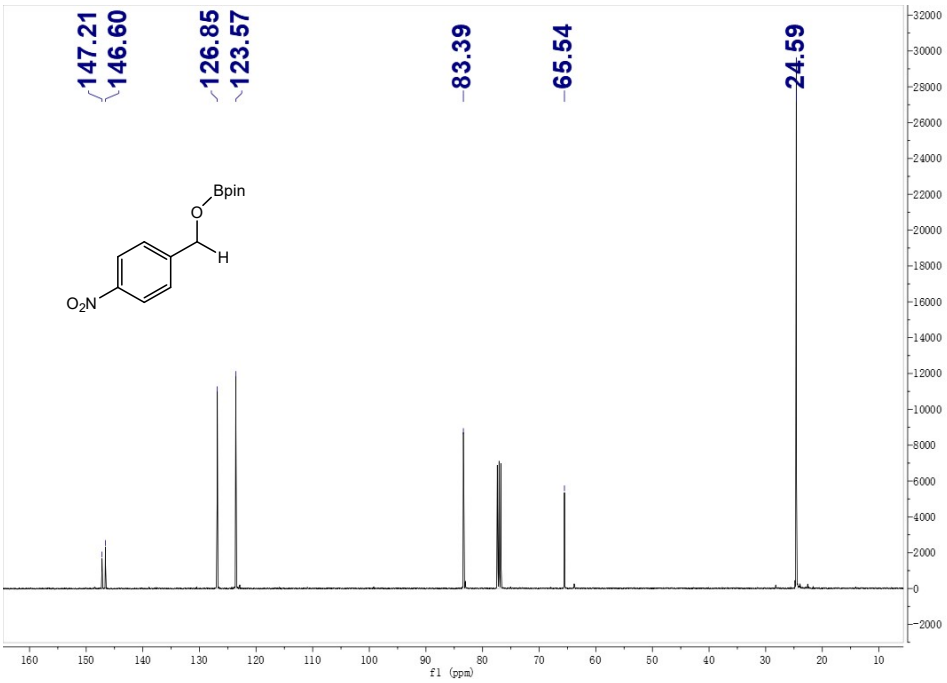


Fig. S12 ^{13}C NMR spectrum of product **5c**.

5c: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.20 (d, 2H), 7.50 (d, 2H), 5.02 (s, 2H), 1.27 (s, 12H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 147.21, 146.60, 126.85, 123.57, 83.39, 65.54, 24.59.

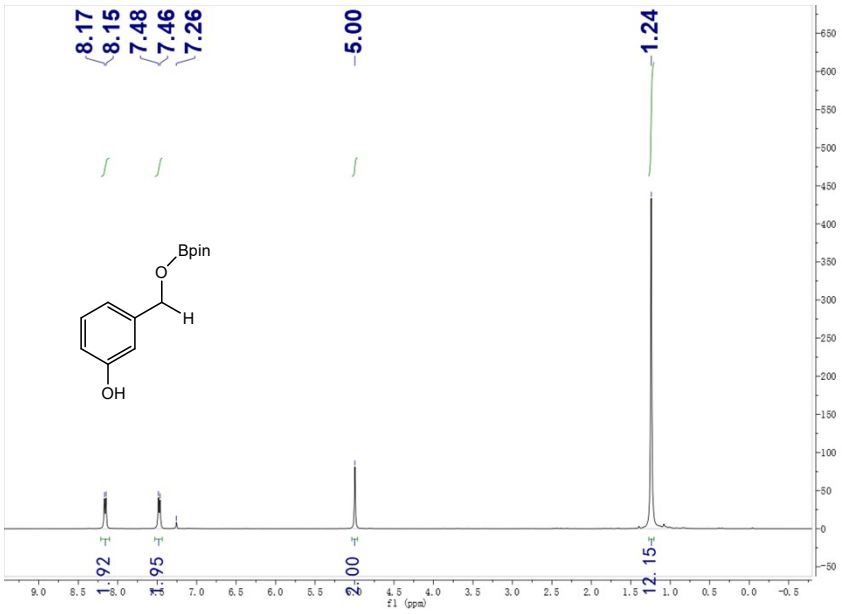


Fig. S13 ^{1}H NMR spectrum of **5d**.

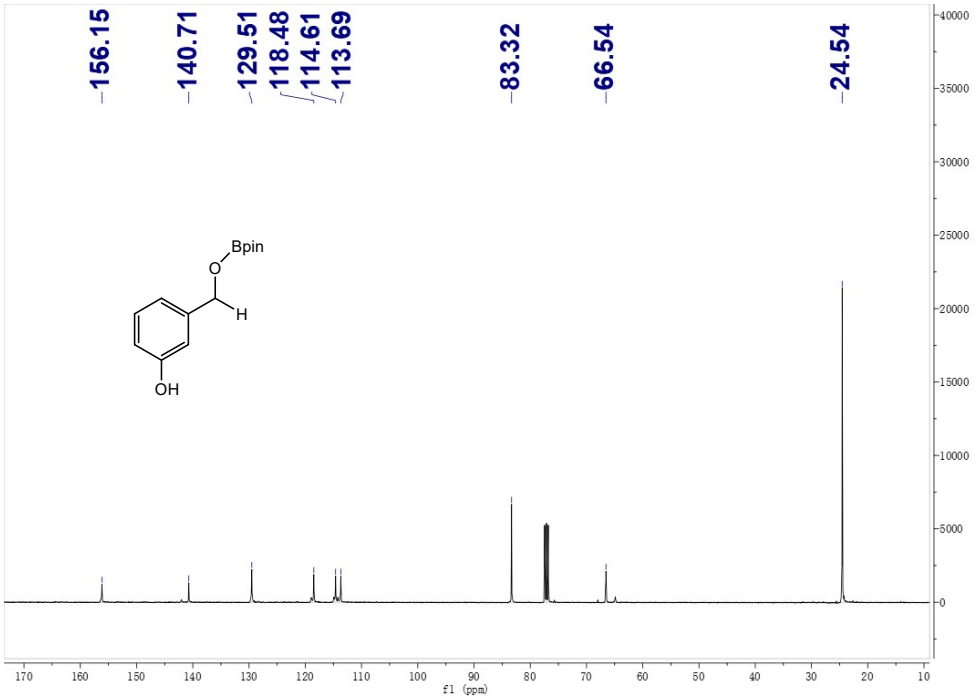


Fig. S14 ^{13}C NMR spectrum of **5d**.

5d: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.16 (d, 2H), 7.47 (d, 2H), 5.00 (s, 2H), 1.24 (s, 12H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 156.15, 140.71, 129.51, 118.48, 114.61, 113.69, 83.32, 66.54, 24.54.

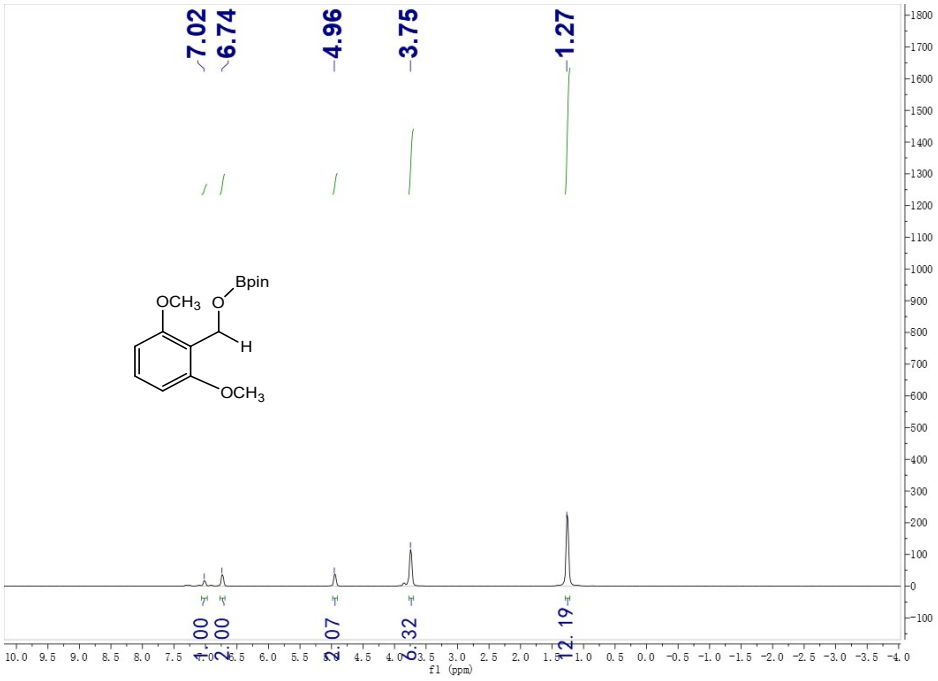


Fig. S15 ^{1}H NMR spectrum of **5e**.

5e: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.02 (s, 1H), 6.74 (s, 2H), 4.96 (s, 2H), 3.75 (s, 6H), 1.27 (s, 12H).

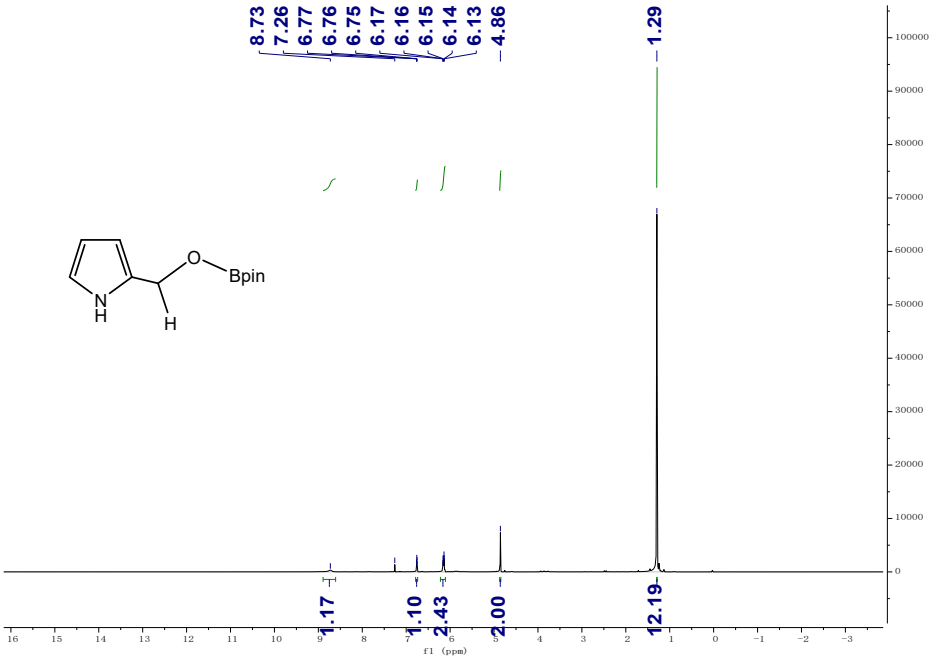


Fig. S16 ^{1}H NMR spectrum of **5f**

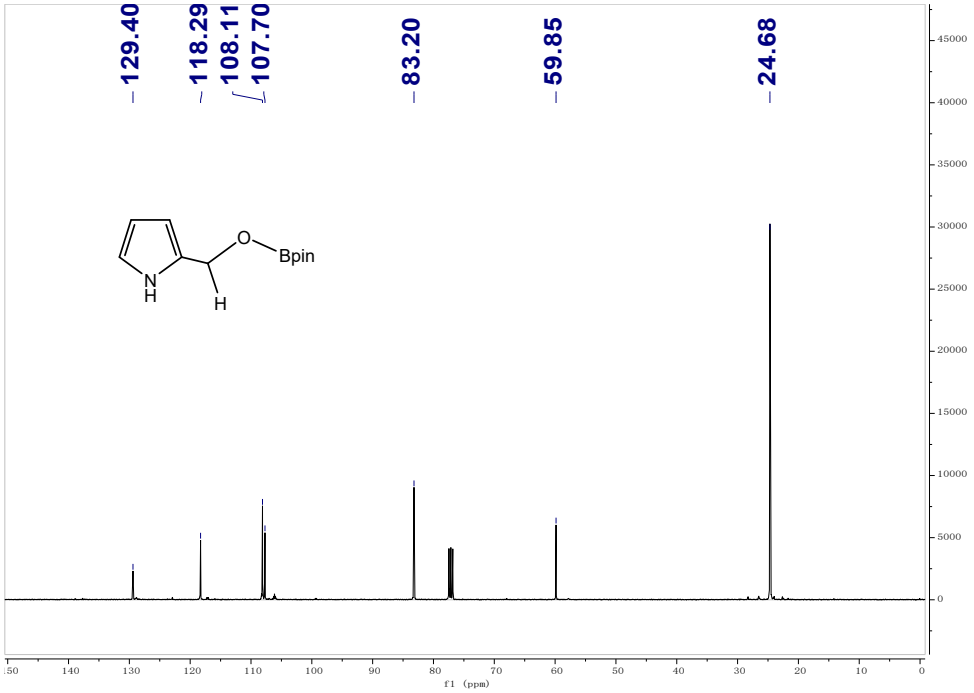


Fig. S17 ^{13}C NMR spectrum of **5f**.

5f: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.73 (s, 1H), 6.76 (t, 1H), 6.17 – 6.13 (m, 2H), 4.86 (s, 2H), 1.29 (s, 12H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 129.40, 118.29, 108.11, 107.70, 83.20, 59.85, 24.68.

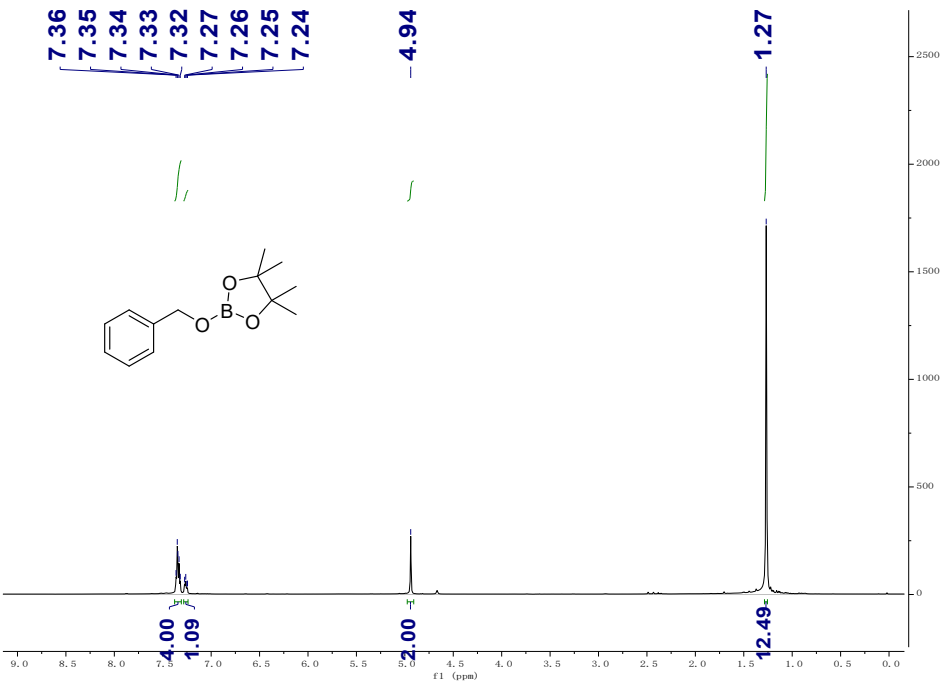


Fig. S18 ^{1}H NMR spectrum of **5g**.

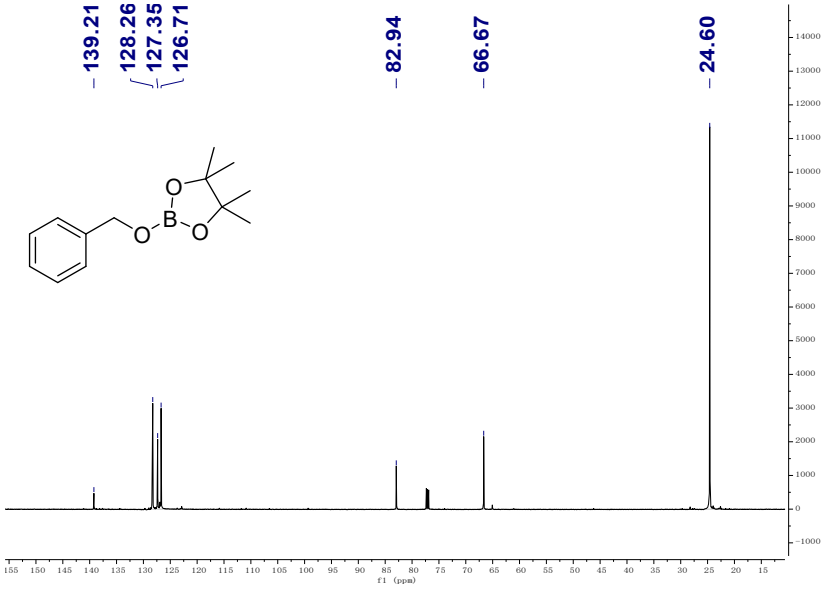


Fig. S19 ^{13}C NMR spectrum of **5g**.

5g: ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.37 – 7.31 (m, 4H), 7.27 – 7.24 (m, 1H), 4.94 (s, 2H), 1.27 (s, 12H).^{13}C NMR (151 MHz, Chloroform-*d*) δ 139.21, 128.26, 127.35, 126.71, 82.94, 66.67, 24.60.

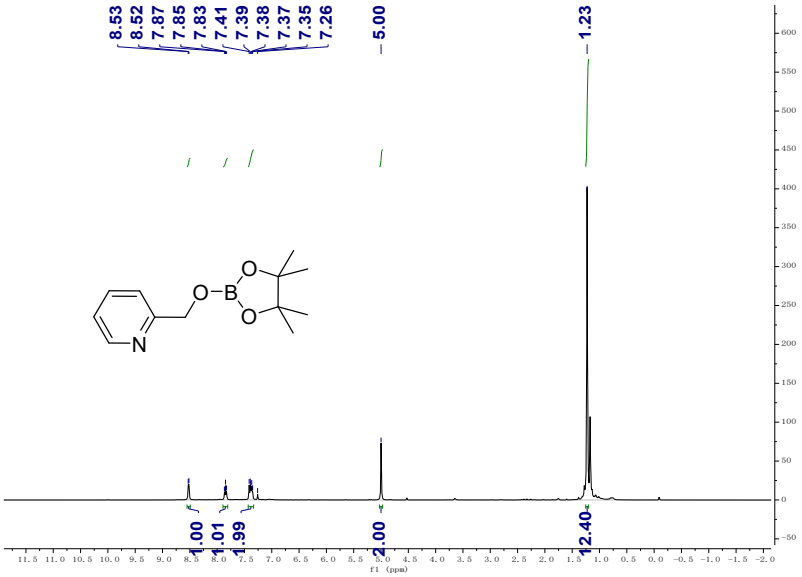


Fig. S20 ^{1}H NMR spectrum of **5h**

5h: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.52 (d, 1H), 7.85 (t, 1H), 7.43 – 7.33 (m, 2H), 5.00 (s, 2H), 1.23 (s, 12H).

4. NMR Spectra of the products of the hydroboration of ketones with HBpin

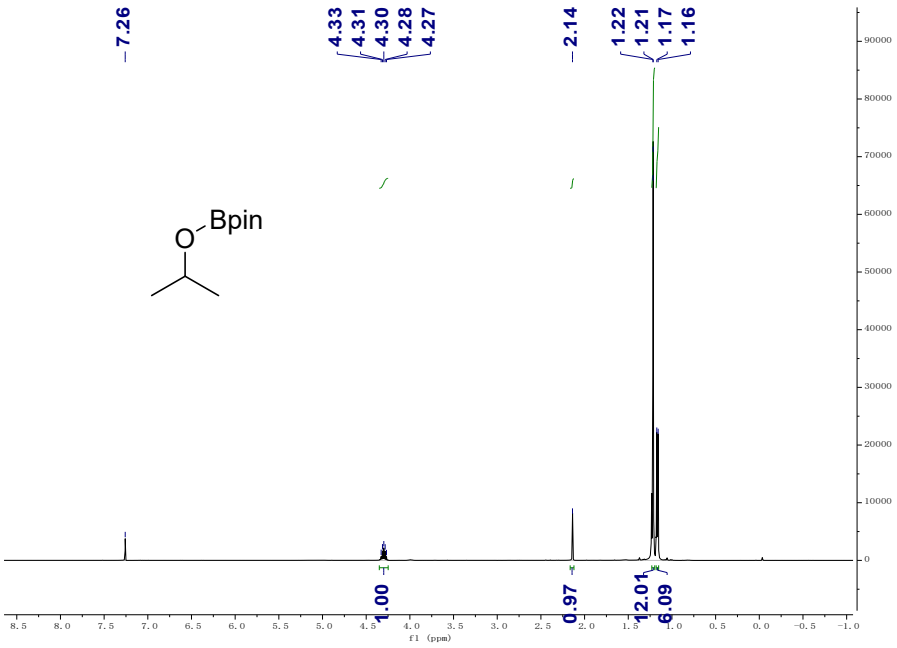


Fig. S21 ^{1}H NMR spectrum of **7a**.

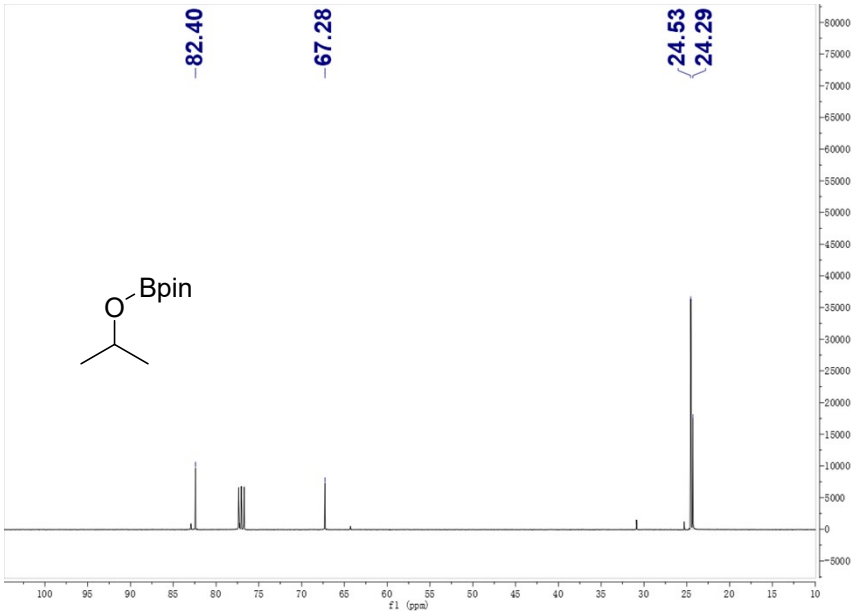


Fig. S22 ^{13}C NMR spectrum of **7a**.

7a: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 4.33 – 4.27 (m, 1H), 1.22 (d, 12H), 1.17 (d, 6H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 82.40, 67.28, 24.53, 24.29.

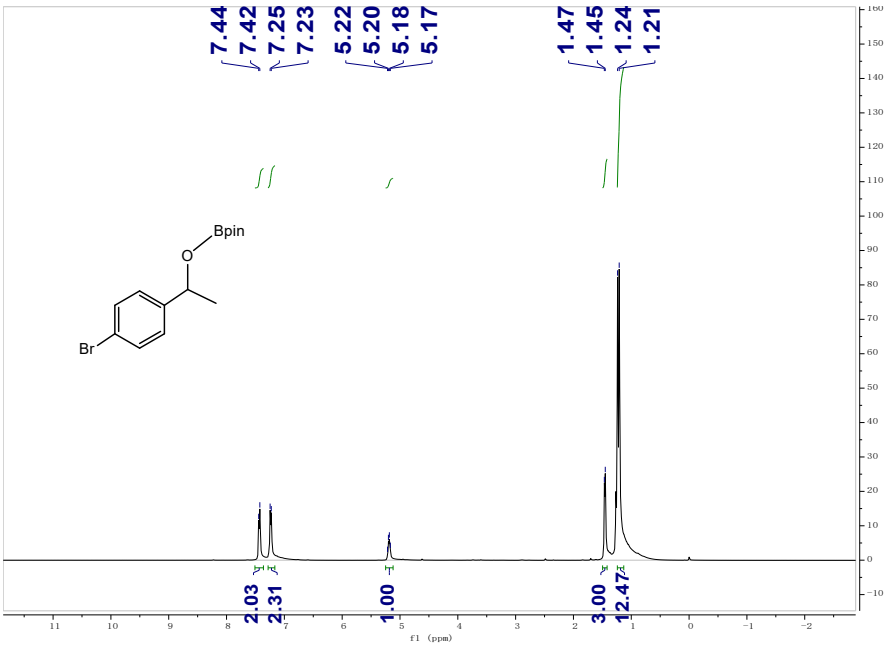


Fig. S23 [1]H NMR spectrum of **7b**.

7b:[1]H NMR (400 MHz, Chloroform-*d*) δ 7.43 (d, 2H), 7.24 (d, 2H), 5.19 (q, 1H), 1.46 (d, 3H), 1.22 (d, 12H).

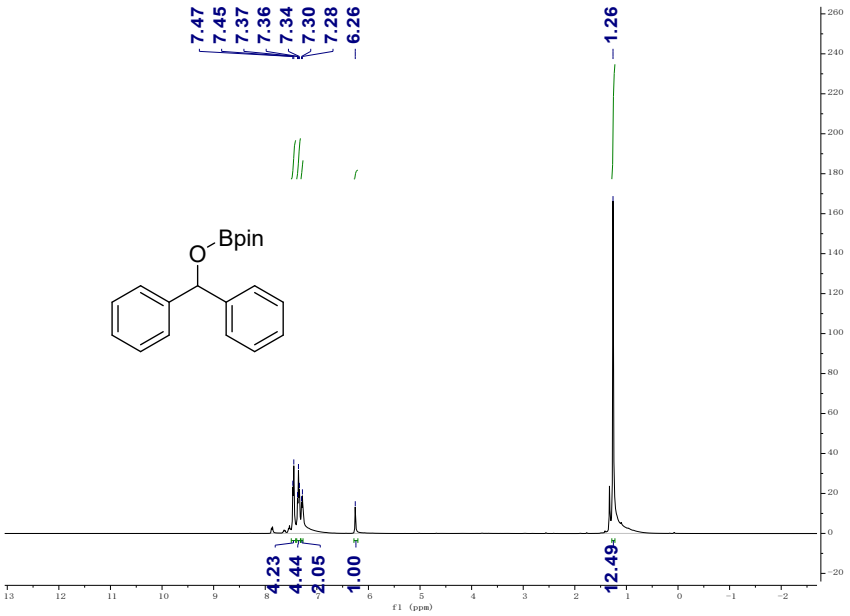


Fig. S24 [1]H NMR spectrum of **7c**.

7c: [1]H NMR (400 MHz, Chloroform-*d*) δ 7.46 (d, 4H), 7.36 (t, 4H), 7.29 (d, 2H), 6.26 (s, 1H), 1.26 (s, 12H).

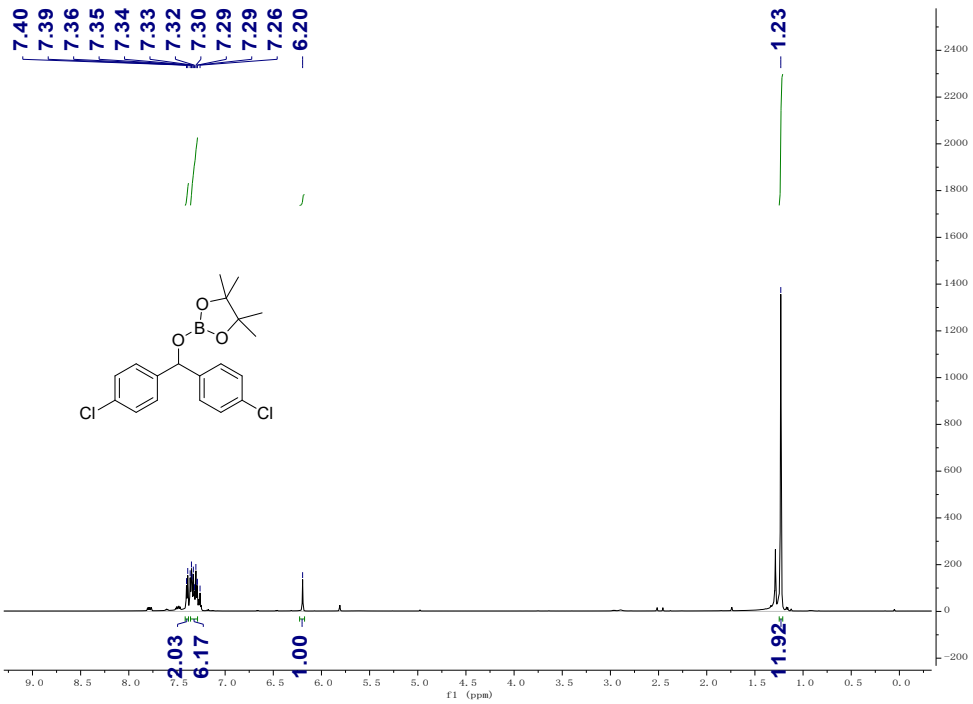


Fig. S25 [1]H NMR spectrum of **7d**.

7d: [1]H NMR (600 MHz, Chloroform-*d*) δ 7.39 (d, 2H), 7.32 (m, 6H), 6.20 (s, 1H), 1.23 (s, 12H).

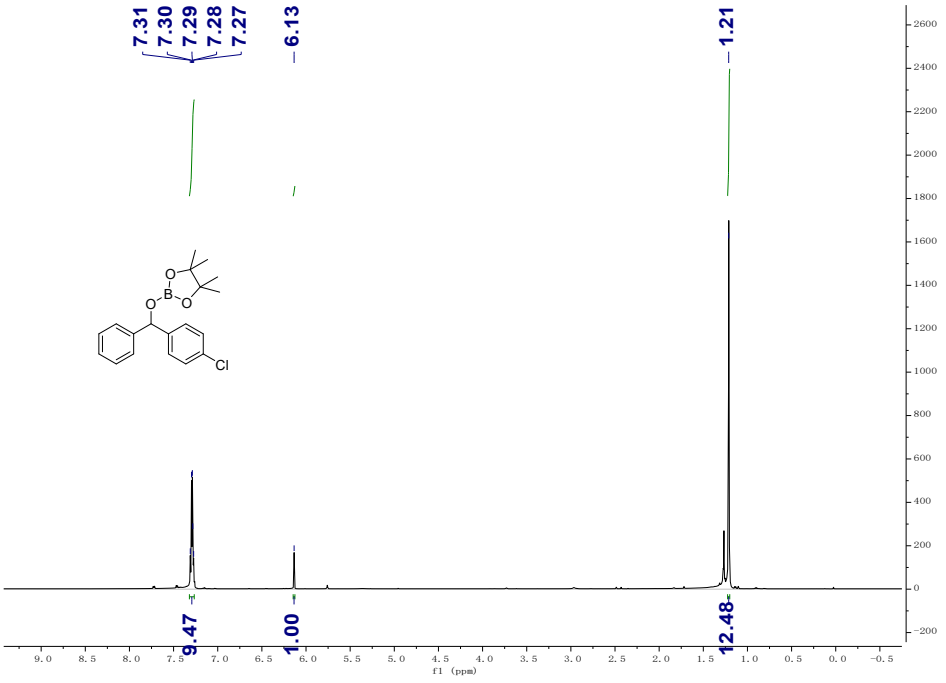


Fig. S26 [1]H NMR spectrum of **7e**.

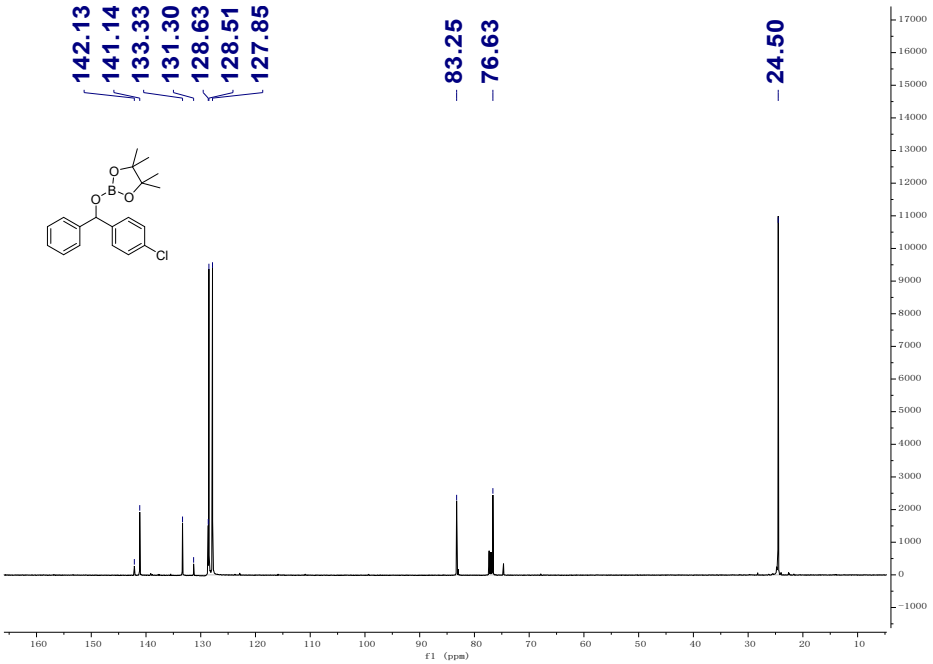


Fig. S27 ^{13}C NMR spectrum of **7e**.

7e: ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.32 – 7.27 (m, 9H), 6.13 (s, 1H), 1.21 (s, 12H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 142.13, 141.14, 133.33, 131.30, 128.63, 128.51, 127.85, 83.25, 76.63, 24.50.

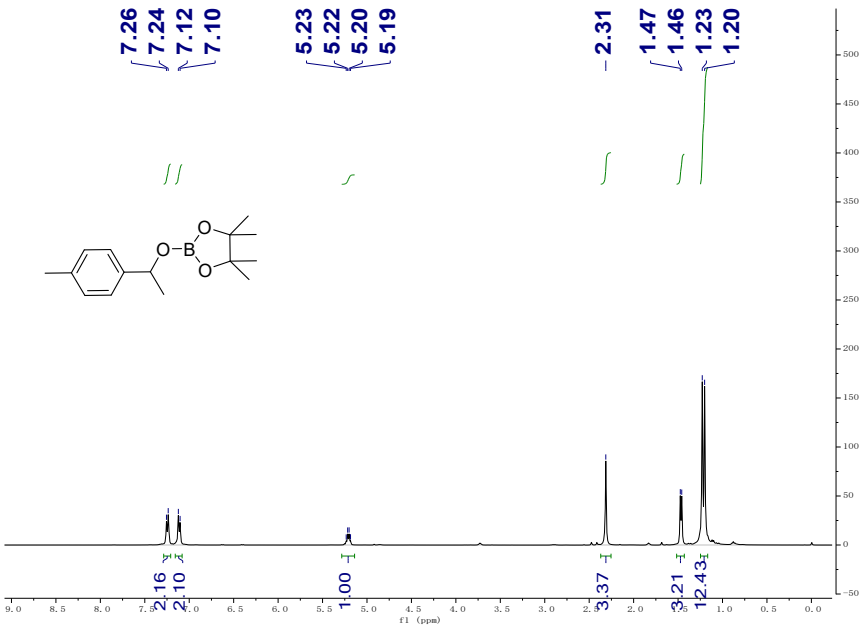


Fig. S28. ^{1}H NMR spectrum of **7f**.

7f: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.25 (d, 2H), 7.11 (d, 2H), 5.21 (q, 1H), 2.31 (s, 3H), 1.47 (d, 3H), 1.21 (d, 12H).

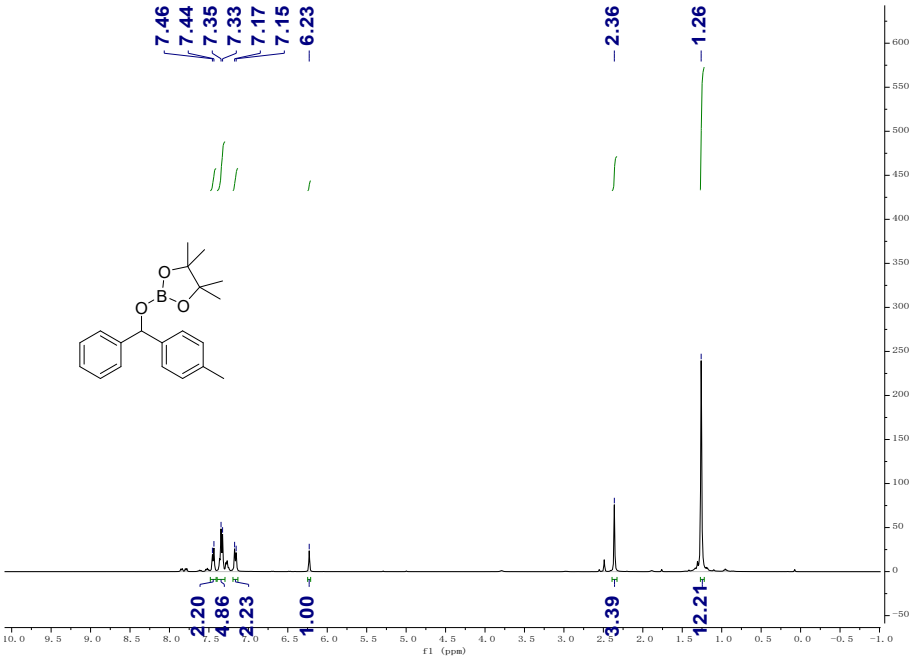


Fig. S29 ^{1}H NMR spectrum of **7g**.

7g: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.45 (d, 2H), 7.34 (d, 5H), 7.16 (d, *J* = 7.8 Hz, 2H), 6.23 (s, 1H), 2.36 (s, 3H), 1.26 (s, 12H).

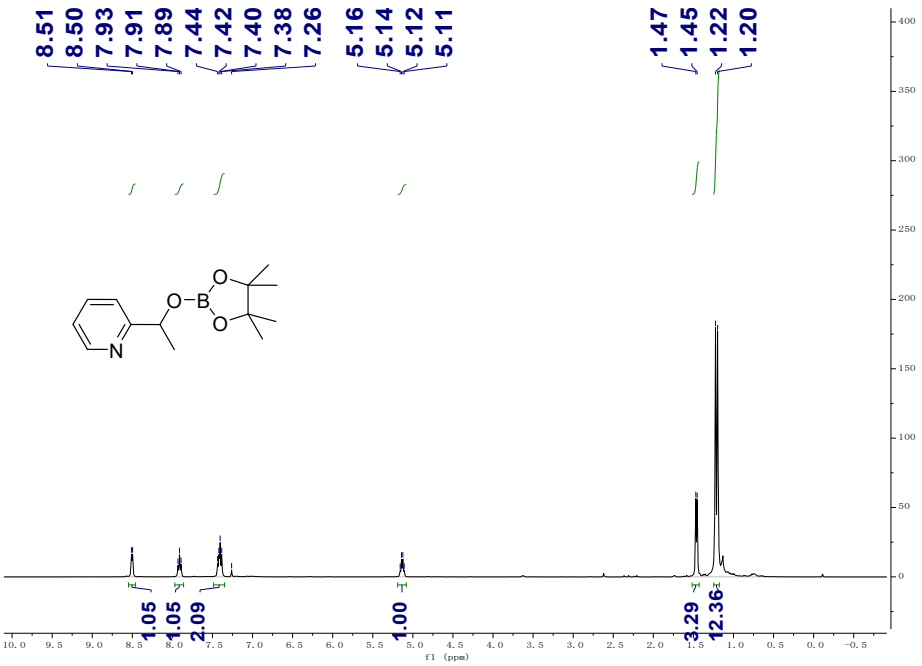


Fig. S30 ^{1}H NMR spectrum of **7h**.

7h: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.50 (d, 1H), 7.91 (t, 1H), 7.47 – 7.36 (m, 2H), 5.13 (m, 1H), 1.46 (d, 3H), 1.21 (d, 12H).

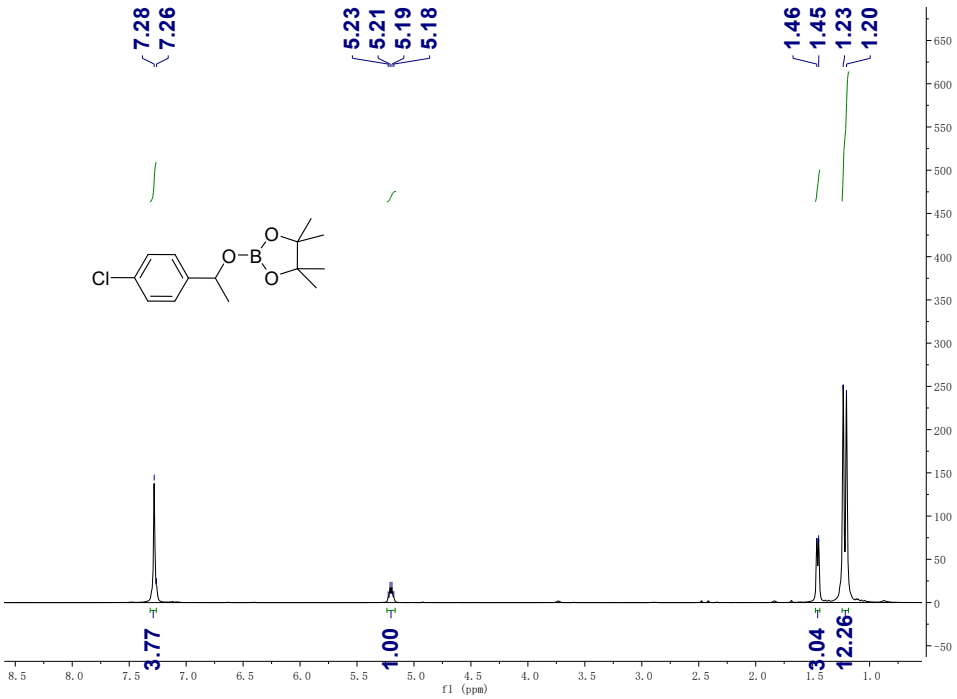


Fig. S31 ^{1}H NMR spectrum of **7i**.

7i: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.28 (s, 4H), 5.20 (q, 1H), 1.46 (d, 3H), 1.22 (d, 12H).

5. Chemoselective hydroboration of aldehydes catalyzed by 1

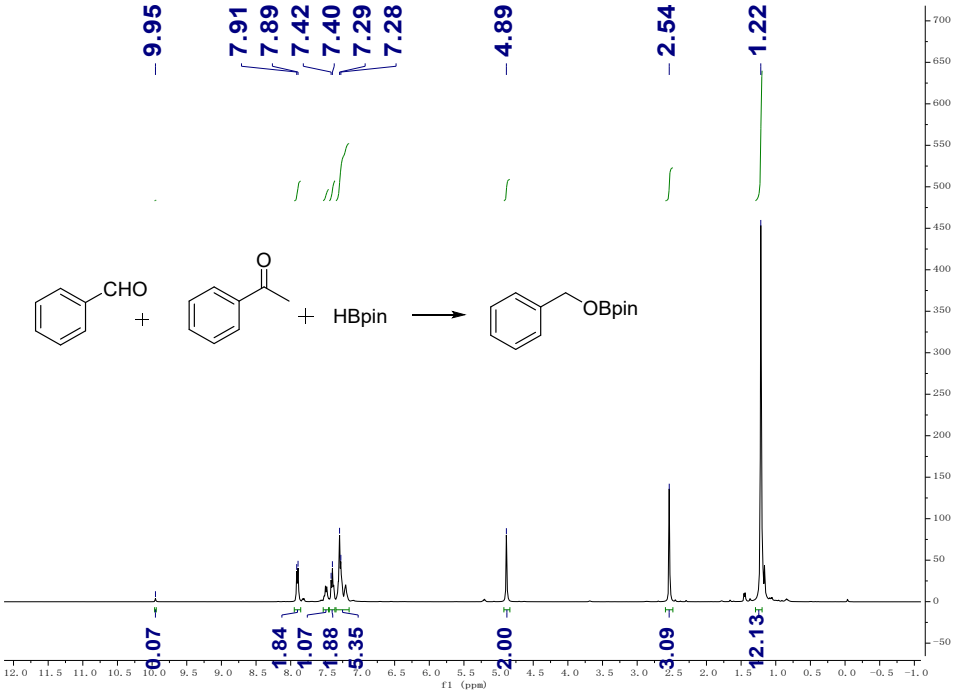


Fig. S32 ^{1}H NMR spectrum of the product of the reaction of benzaldehyde and acetophenone with HBpin in a 1:1:1 molar ratio.

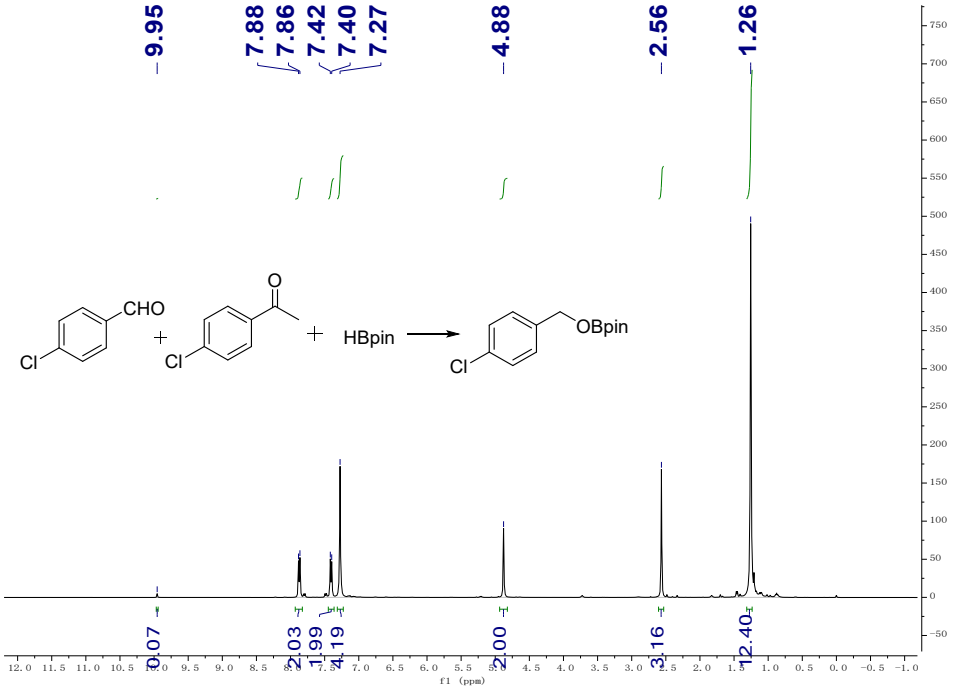


Fig. S33 ^{1}H NMR spectrum of the products of the reaction of 4-cholorobenzaldehyde and 1-(4-chlorophenyl)ethan-1-one with HBpin in a 1:1:1 molar ratio.

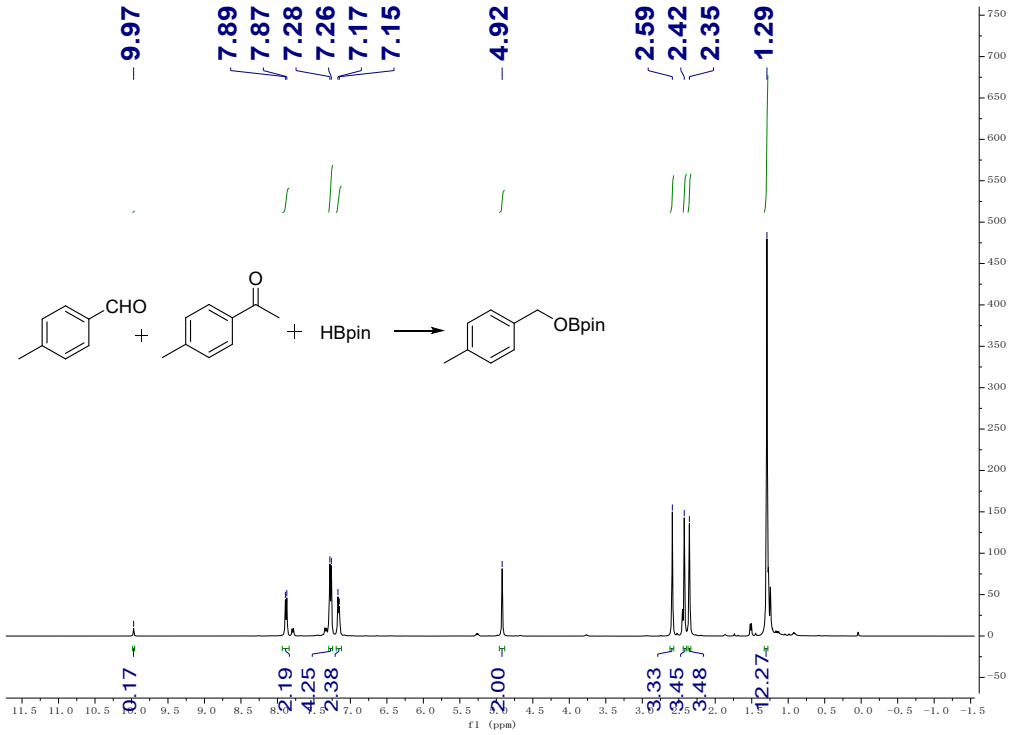
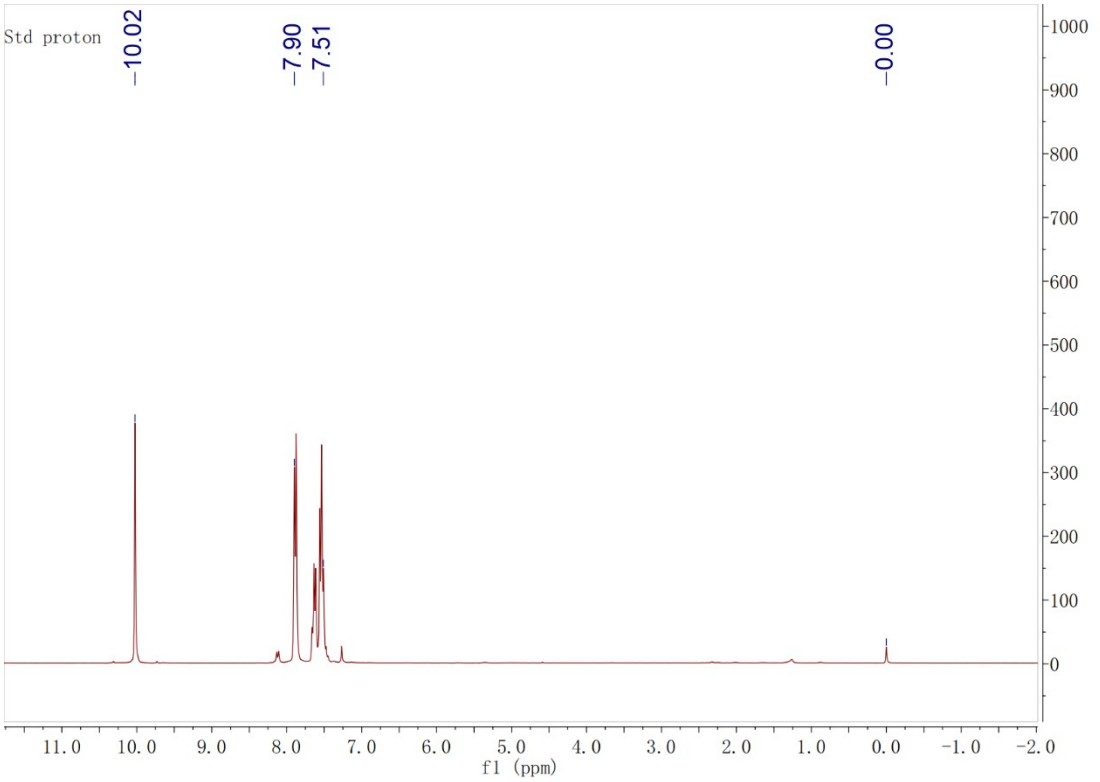


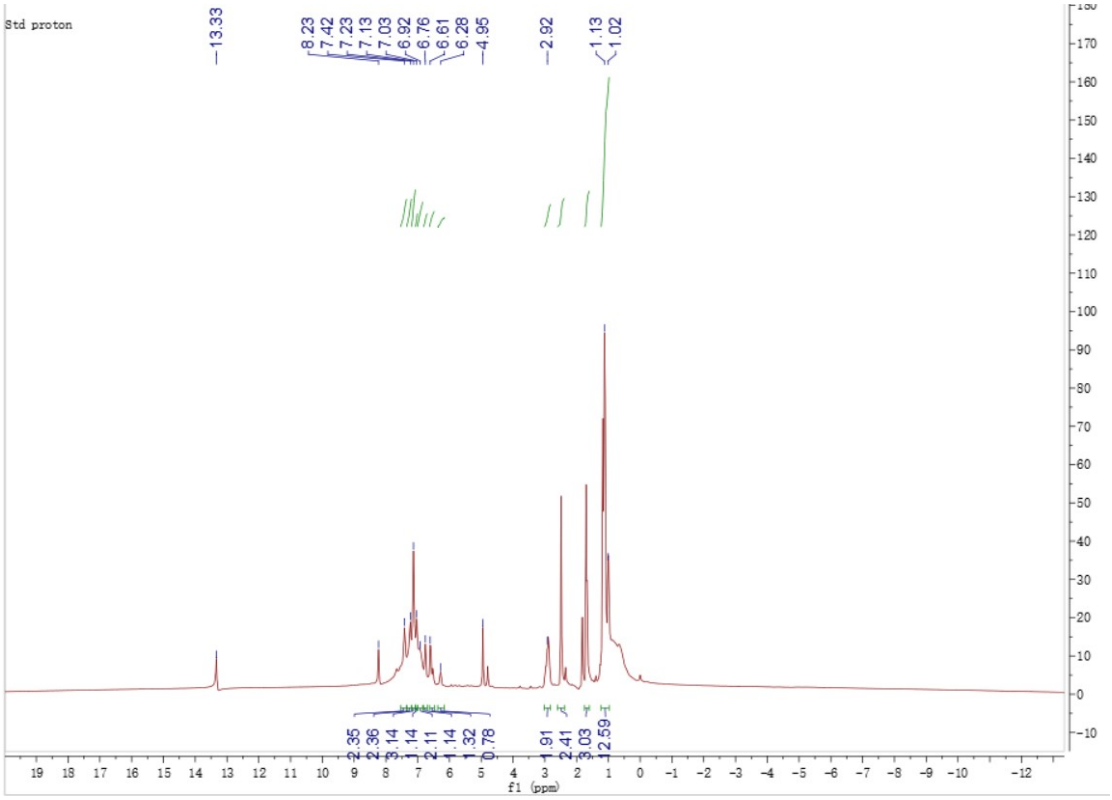
Fig. S34 ^{1}H NMR spectrum of the products of the reaction of 4-methylbenzaldehyde and 1-(p-tolyl)ethan-1-one with HBpin in a 1:1:1 molar ratio.

6. Stoichiometric reactions of complex 1 with benzaldehyde and HBpin

(a)



(b)



(c)

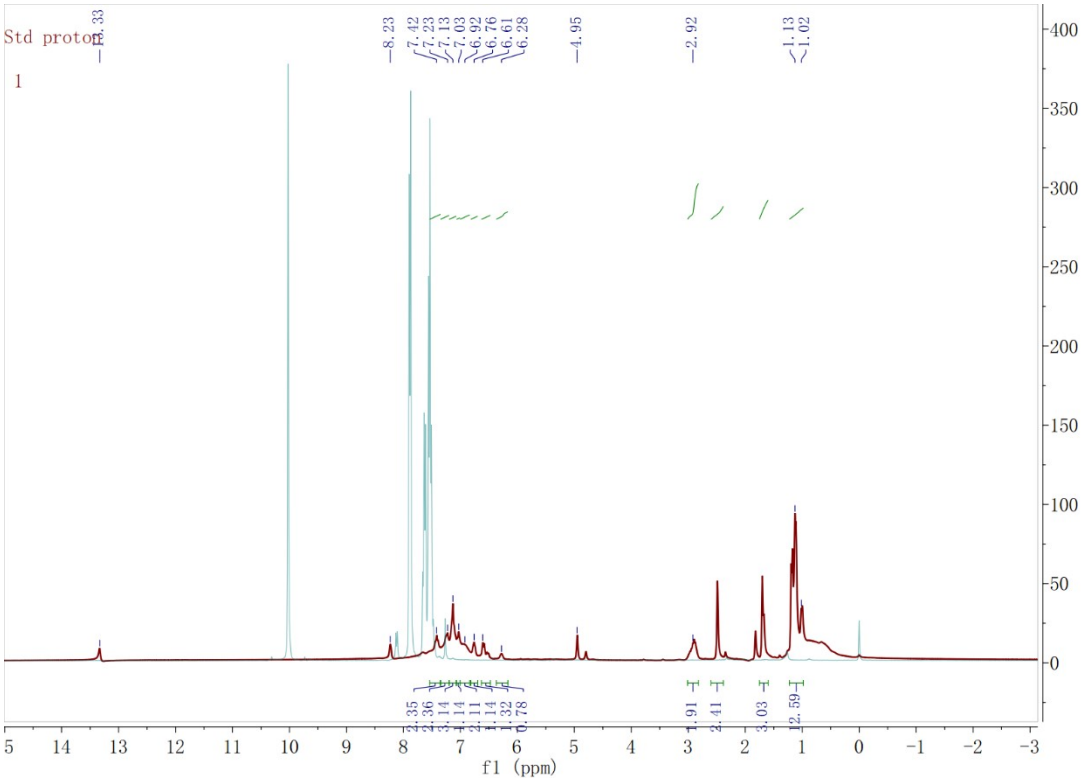
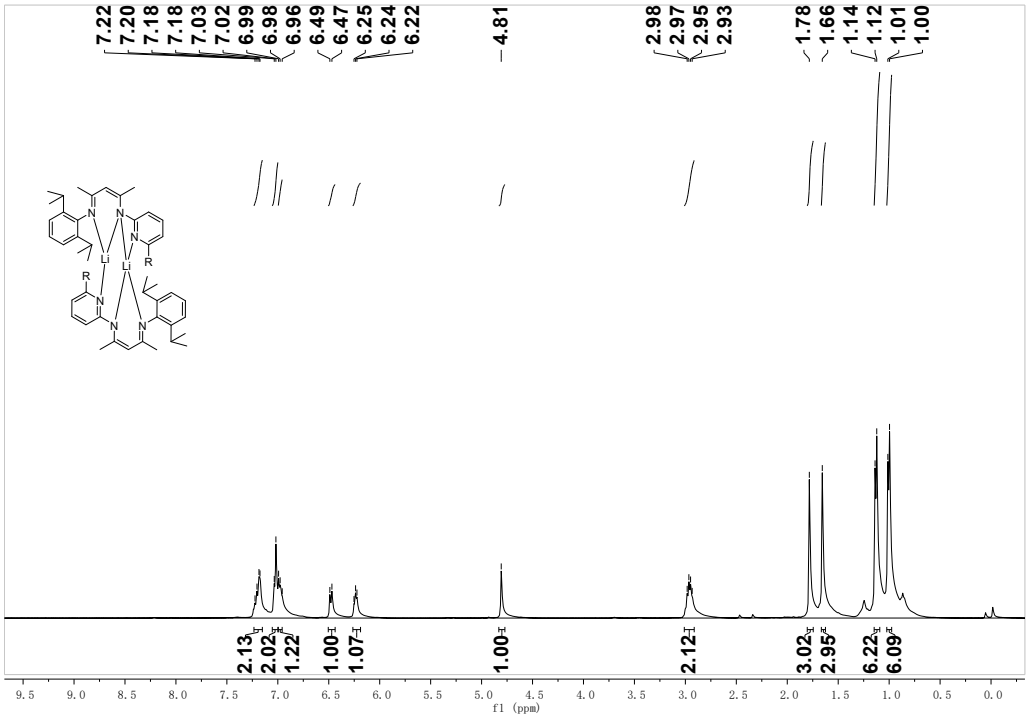
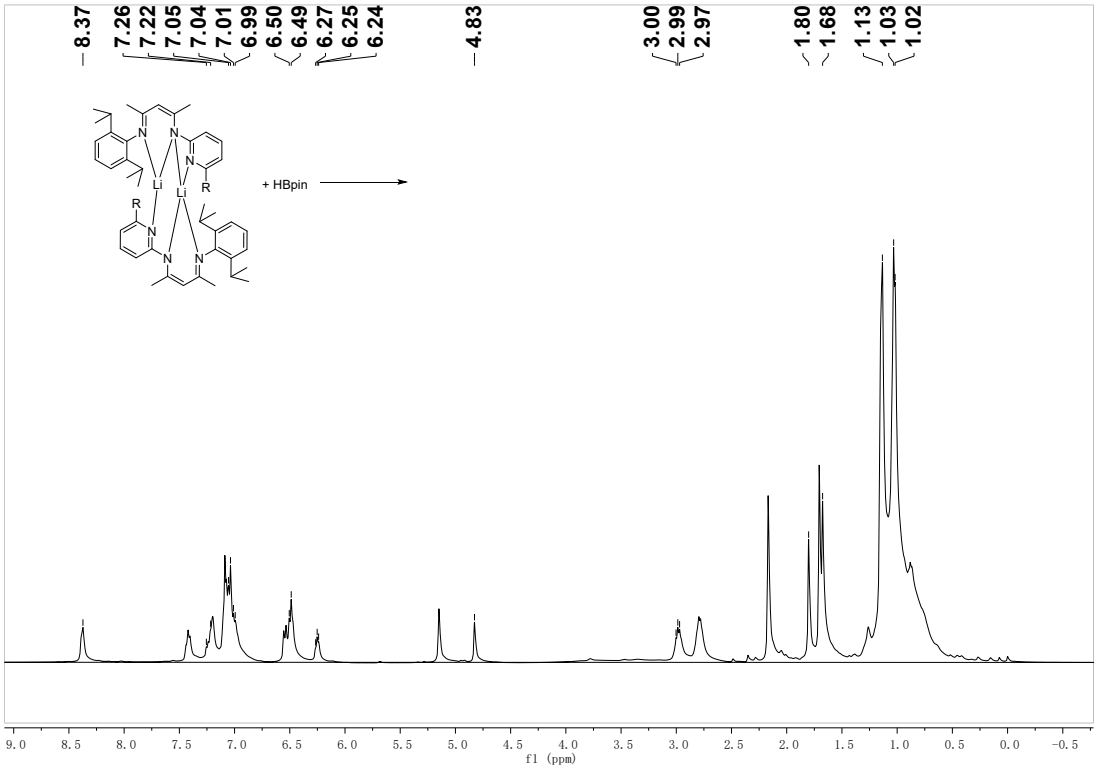


Fig. S35 ^{1}H NMR spectra for the stoichiometric reaction of complex **1** with benzaldehyde. (a) ^{1}H NMR spectrum of benzaldehyde. (b) ^{1}H NMR spectrum of the mixture of complex **1** and benzaldehyde after 60 minutes. (c) Superposition of (b) and (a).

(a)


7.22
7.20
7.18
7.18
7.03
7.02
6.99
6.98
6.96
6.49
6.47
6.25
6.24
6.22
4.81
2.98
2.97
2.95
2.93
1.78
1.66
1.14
1.12
1.01
1.00
2.13
2.02
1.22
1.00
1.07
1.00
2.12
3.02
2.95
6.22
6.09
f1 (ppm)

(b)


8.37
7.26
7.22
7.05
7.04
7.01
6.99
6.50
6.49
6.27
6.25
6.24
4.83
3.00
2.99
2.97
1.80
1.68
1.13
1.03
1.02
+ HBpin
f1 (ppm)

(c)

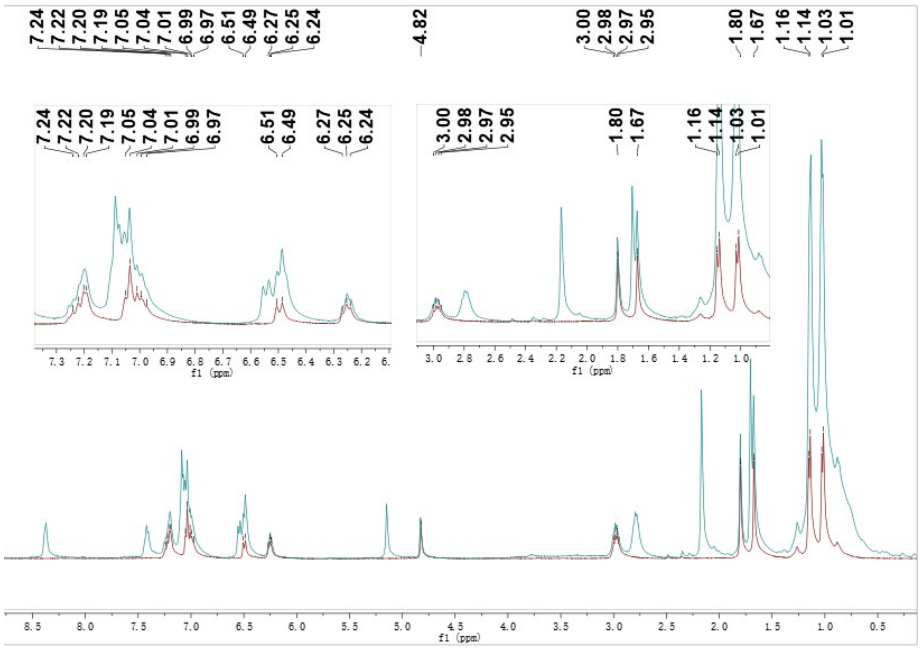


Fig. S36 ^{1}H NMR spectra for the stoichiometric reaction of complex **1** with HBpin. (a) ^{1}H NMR spectrum of complex **1**. (b) ^{1}H NMR spectrum of the mixture of complex **1** and HBPin. (c) Superposition of (b) and (a).

7. Gram-scale synthesis of 8f catalyzed by complex 2

Magnetic stir bar, 1-(*p*-tolyl)ethanone (**6f**) (2.0 g, 14.9 mmol, 1.0 equiv), and catalyst (**2**) (19.5 mg, 0.03 mmol, 0.2 mol%) were placed in a round-bottom flask and following flushing with argon gas. After cooling with ice bath, HBpin (1.91 g, 14.9 mmol, 1.0 equiv) was added dropwise through a syringe. After stirring for 30 min at room temperature, additional HBpin (573 mg, 4.47 mmol, 0.3 equiv) was added, and the reaction was stirred for 1 h and monitored with TLC. After 1-(*p*-tolyl)ethanone (**6f**) was consumed completely, NaOH (20 mL, 2M in water) and THF (20 mL) were added. The reaction was stirred for 1.5 h at room temperature. The solvent of THF was evaporated and the water phase was extracted with CH_2Cl_2 (30 mL x 3). The combined organic layers were washed with brine dried with anhydrous Na_2SO_4 and concentrated under vacuum. The crude product was purified by silicon gel column with ethyl acetate in petroleum ether (5% to 10%) to afford 1-(*p*-tolyl)ethanol (**8f**) (1.87 g, 13.7 mmol, 92% yield) as a colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.27 (d, J = 8.0 Hz, 2H), 7.16 (d, J = 7.9 Hz, 2H), 4.87 (q, J = 6.5 Hz, 1H), 2.34 (s, 3H), 1.78 (s, 1H), 1.48 (d, J = 6.5 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.9, 137.2, 129.2, 125.4, 70.3, 25.1, 21.1.

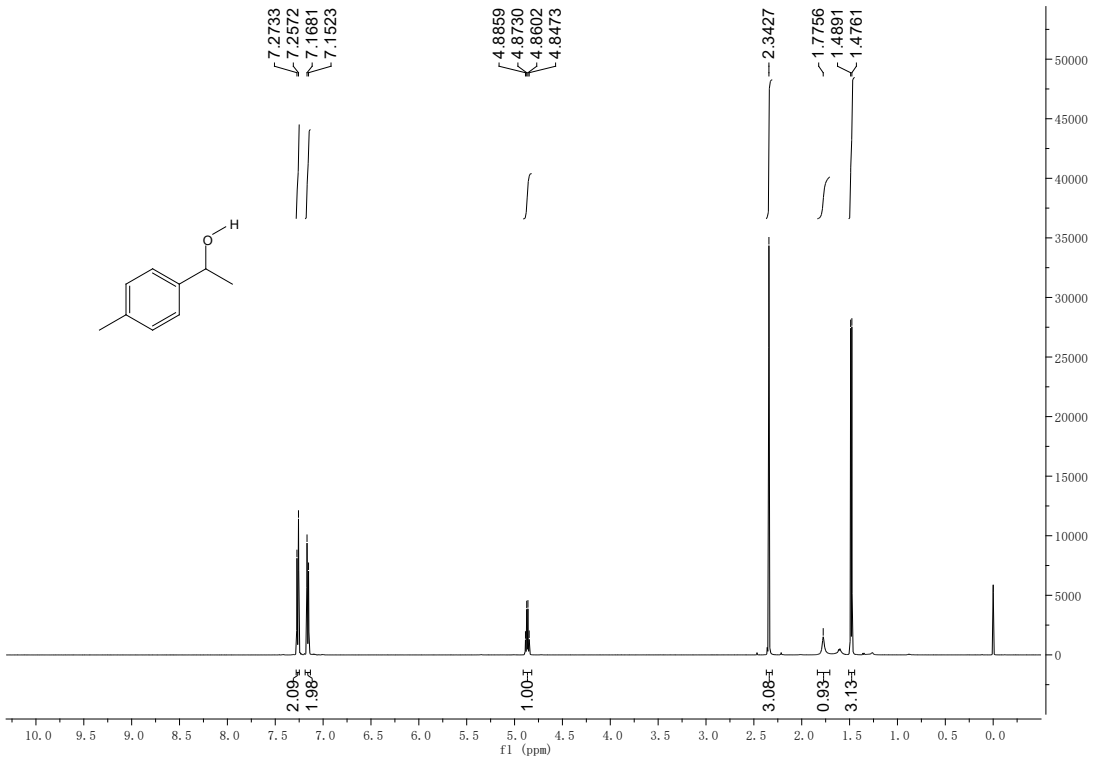


Fig. S37 ^{1}H NMR spectrum for **8f**.

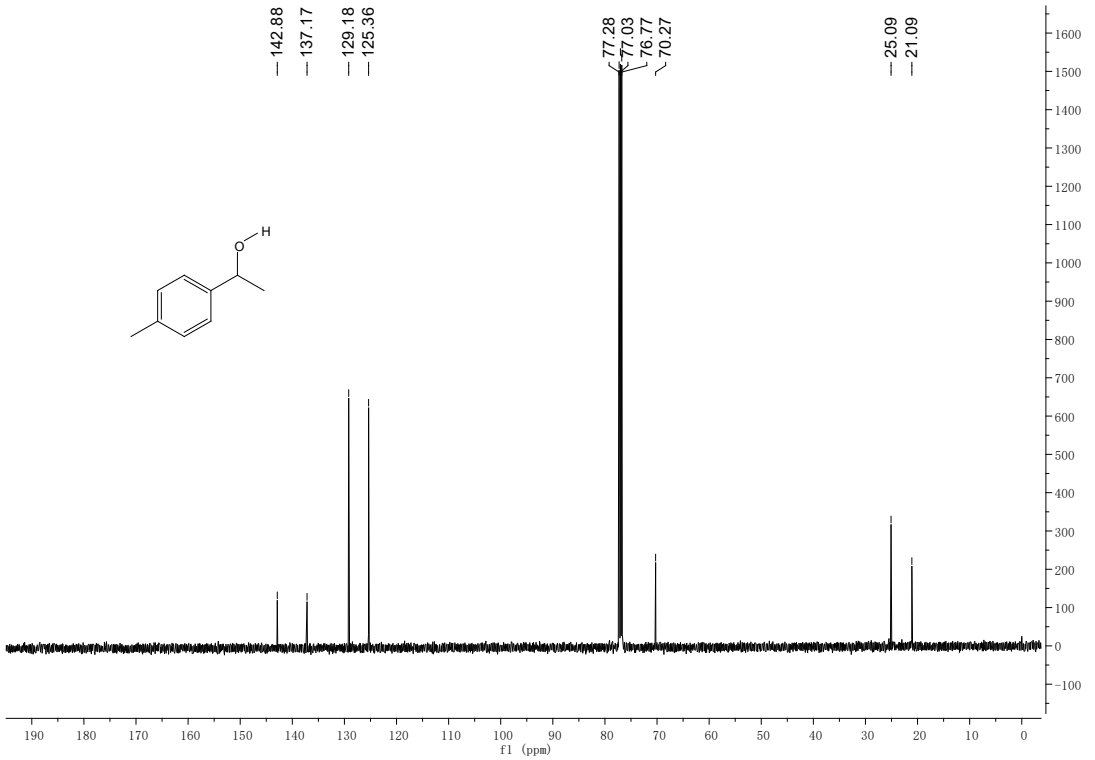


Fig. S38 ^{13}C NMR spectrum for **8f**.

8. Crystallographic data and structure refinements for complexes 1-3

Table S1 Crystallographic data and structure refinements for complexes **1-3**

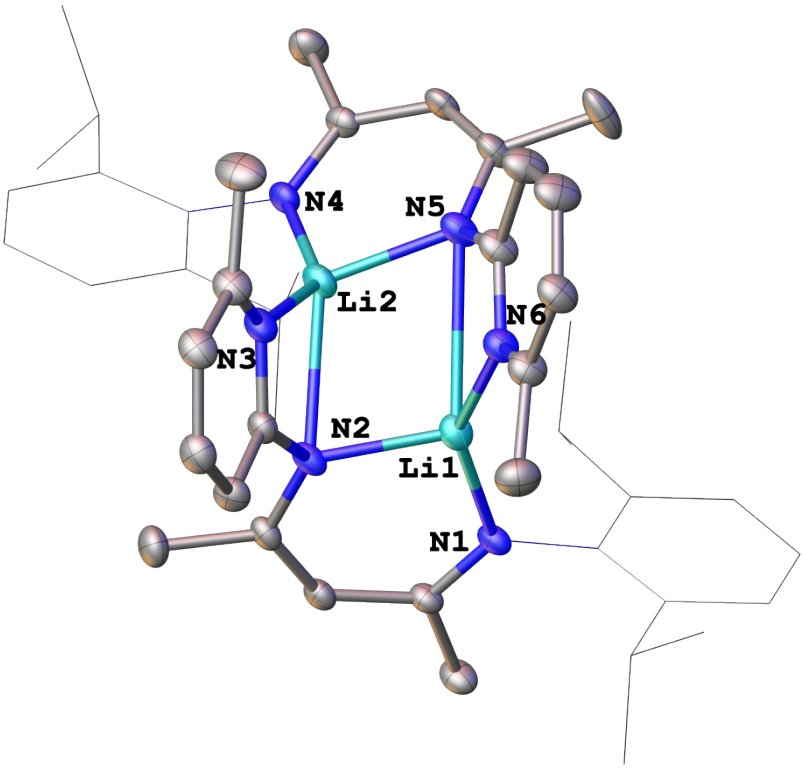
	1	**2**	**3**
Empirical formula	$C_{44}H_{56}Li_2N_6$	$C_{184}H_{240}Li_8N_{24}$	$C_{49}H_{67}MgN_6$
Formula weight	682.82	2843.51	764.39
Temperature [K]	189.0	120.02	296.15
Crystal system	monoclinic	triclinic	monoclinic
Space group	$P2_1/c$	P-1	C2/c
a/Å	11.2500(8)	19.401(3)	17.8797(11)
b/Å	17.6853(11)	19.525(3)	21.1458(13)
c/Å	21.0440(15)	25.019(3)	24.3580(15)
α/°	90	105.371(3)	90
β/°	93.665(2)	105.614(3)	96.658(2)
γ/°	90	97.599(4)	90
Volume/Å^3	4178.3(5)	8587.0(19)	9147.2(10)
Z	4	2	8
ρ_{calc}g/cm^3	1.085	1.100	1.110
μ/mm^{-1}	0.063	0.064	0.078
F(000)	1472.0	3072.0	3320.0
Crystal size/mm^3	0.18 × 0.04 × 0.02	0.25 × 0.2 × 0.1	0.16 × 0.03 × 0.02
Radiation	Mo-K$_\alpha$ (λ = 0.71073)	Mo-Kα (λ = 0.71073)	Mo-Kα (λ = 0.71073)
2Θ range for data collection/°	5.864 to 50	3.252 to 50	5.118 to 55.162
Index ranges	-13 ≤ h ≤ 13, -21 ≤ *k* ≤ 21, -25 ≤ *l* ≤ 25	-23 ≤ h ≤ 23, -23 ≤ k ≤ 23, -29 ≤ l ≤ 29	-23 ≤ h ≤ 23, -25 ≤ k ≤ 27, -31 ≤ l ≤ 29
Reflections collected	50327	158605	86204
Independent reflections	7330 [R_{int} = 0.1065]	30173 [R_{int} = 0.1245],	10512 [R_{int} = 0.0885]
Data/restraints/parameters	7330/0/481	30173/3520/2001	10512/47/520
Goodness-of-fit on F^2	1.098	1.036	0.993
Final *R* indexes [*I*>=2σ (*I*)]	R_1 = 0.0588, wR_2 = 0.1481	R_1 = 0.1733, wR_2 = 0.4196	R_1 = 0.0690, wR_2 = 0.1791
Final R indexes [all data]	R_1 = 0.1130, wR_2 = 0.1686	R_1 = 0.2238, wR_2 = 0.4358	R_1 = 0.1233, wR_2 = 0.2119
Largest diff. peak/hole/e Å^{-3}	0.29/-0.22	0.57/-0.47	1.17/-0.95

9. Selected bond lengths [Å] and angles [°] for complexes 1-3

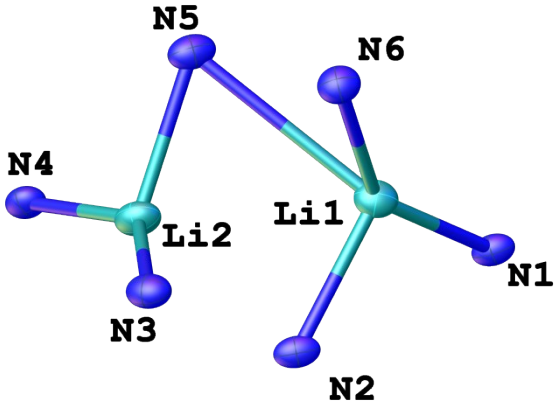
Table S2 Selected bond lengths [Å] and angles [°] for complexes **1-3**

Complex**1**			
N1–Li1	1.934(4)	N3–Li2	1.971(4)
N2–Li1	1.960(4)	N6–Li1	1.975(4)
N5–Li1	2.381(4)	N5–Li2	1.986(4)
N4–Li2	1.921(4)		
N1–Li1–N5	134.8(2)	Li2–N5–Li1	74.42(16)
N4–Li2–N5	99.23(18)	N4–Li2–N3	141.6(2)
N3–Li2–N5	111.3(2)	N6–Li1–N5	62.90(12)
N6–Li1–N2	107.49(18)	N1–Li1–N6	138.3(2)
N1–Li1–N2	99.80(17)	N2–Li1–N5	109.63(18)
Complex **2**			
N1–Li1	1.964(16)	N3–Li2	2.023(15)
N2–Li1	1.979(15)	N6–Li1	2.053(15)
N5–Li1	2.384(15)	N5–Li2	1.957(15)
N4–Li2	1.982(15)		
N1–Li1–N5	133.5(7)	Li2–N5–Li1	76.3(6)
N4–Li2–N5	97.6(6)	N4–Li2–N3	146.4(8)
N3–Li2–N5	112.0(7)	N6–Li1–N5	61.8(4)
N6–Li1–N2	107.3(7)	N1–Li1–N6	140.5(8)
N1–Li1–N2	99.3(6)	N2–Li1–N5	110.8(7)
Complex **3**			
Mg1–N1	2.232(2)	Mg1–N4	2.314(2)
Mg1–N2	2.056(2)	Mg1–N5	2.054(2)
Mg1–N3	2.324(2)	Mg1–N6	2.234(2)
N1–Mg1–N2	87.25(6)	N4–Mg1–N2	107.79(8)
N1–Mg1–N3	142.57(8)	N4–Mg1–N6	141.95(8)
N1–Mg1–N4	96.68(8)	N1–Mg1–N5	102.65(8)
N1–Mg1–N6	108.34(8)	N2–Mg1–N5	165.28(9)
N2–Mg1–N6	101.73(8)	N3–Mg1–N5	106.28(8)
N2–Mg1–N3	60.47(7)	N4–Mg1–N5	60.71(8)
N4–Mg1–N3	77.76(7)	N6–Mg1–N5	85.61(8)
N6–Mg1–N3	97.17(7)		

10. Molecular structure of complex 2



(a)



(b)

Fig. S39 (a) ORTEP drawing of **2** with thermal ellipsoids drawn at the 30% probability level. Hydrogen atoms are omitted for clarity. (b) Coordination polyhedron of lithium ions.

11. Computational details and results

All DFT calculations were carried out with the Gaussian 09 suite of computational programs.[1] The geometries of all stationary points were optimized using the B3LYP hybrid functional at the basis set level of 6-31G(d). Frequencies were analytically computed at the same level of theory to obtain the free energies and to confirm whether the structures are minima (no imaginary frequency) or transition states (only one imaginary frequency). The solvent effect of toluene was evaluated by using the SMD polarizable continuum model by carrying out single point calculations at the M06/6-311+G(d,p) level. All transition state structures were confirmed to connect the proposed reactants and products by intrinsic reaction coordinate (IRC) calculations. All the energies given in the text are relative free energies corrected with solvation effects.

[1] Gaussian 09, Revision A.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Table S3. Calculated Energies (in Hartree)

Species	G_{298}[a]	E[b]	E_{Sol}[c]
1	-2053.369038	-2054.194054	-2053.177088
1'	-1026.679443	-1027.078415	-1026.566717
4g	-345.493771	-345.5734477	-345.4220617
IN1	-1372.174265	-1372.672319	-1372.010389
HBpin	-411.712156	-411.8705623	-411.7159823
IN2	-1783.872176	-1784.552778	-1783.746669
TS1	-1783.8501	-1784.53417	-1783.727181
IN3	-1783.91899	-1784.609227	-1783.803014
5g	-757.241925	-757.5055264	-757.201211

[a] Sum of electronic and thermal free energies

[b] Electronic energies

[c] Single point energies in solution

Cartesian Coordinates for All Species

1

C	1.31255200	-0.66348500	0.52693000

C	2.38663500	0.22217400	0.67461800	C	8.62683800	1.72026700	4.03889700
C	3.04090900	0.70399400	-0.48903500	H	6.92131800	2.85973500	3.38883800
C	2.61463600	0.27863900	-1.77235900	C	9.64813900	0.43175000	2.31521300
C	1.52793700	-0.59956100	-1.86461700	C	9.62217700	0.81615600	3.64869800
C	0.87623600	-1.07282400	-0.72969200	H	8.55012200	2.04292600	5.07451500
H	0.80647400	-1.03707300	1.41408500	H	10.40620600	-0.26046800	1.95583400
H	1.18667000	-0.91988500	-2.84602000	H	10.34864000	0.42263700	4.35127400
H	0.03547900	-1.75525500	-0.82384300	N	8.78458800	0.87998500	1.38738600
C	3.29710000	0.76501100	-3.04885600	Li	5.99804700	0.73063000	-0.27704400
C	2.38290000	1.70190400	-3.86432700	C	13.89243800	-0.26135200	0.52513200
C	3.78194600	-0.40389800	-3.92685800	C	12.78963100	-0.31224100	-0.33600900
H	4.17816600	1.34224800	-2.75067200	C	12.07020300	0.88308400	-0.59726100
H	2.07346400	2.57428200	-3.27904300	C	12.45887200	2.09679800	0.02330500
H	2.90260200	2.06382000	-4.75995500	C	13.57761300	2.09536000	0.86502900
H	1.47428300	1.18216200	-4.19221300	C	14.29484600	0.93045900	1.12056400
H	4.44659000	-1.07223800	-3.36985400	H	14.44901700	-1.17314200	0.72880800
H	2.94422000	-1.00354200	-4.30235100	H	13.89204400	3.02621400	1.33034100
H	4.32712300	-0.02316000	-4.79923800	H	15.15932300	0.95113500	1.77913000
C	2.83184600	0.63017900	2.07825300	C	11.70360700	3.40099100	-0.22037000
C	3.41023900	-0.56578000	2.86013700	C	12.52352300	4.38094100	-1.08410000
C	1.69602000	1.29982500	2.87581200	C	11.27470700	4.07841400	1.09469700
H	3.63697500	1.36262500	1.97436000	H	10.79350300	3.15440500	-0.77686000
H	4.26665900	-1.00652000	2.33681000	H	12.78782000	3.94216800	-2.05199500
H	3.75200700	-0.24941000	3.85327400	H	11.95306900	5.29839200	-1.27446500
H	2.66232600	-1.35564600	3.00016000	H	13.45615600	4.66493300	-0.58129600
H	1.28397300	2.16068400	2.33777600	H	10.68008700	3.40165300	1.71707600
H	0.87075100	0.60394100	3.06791400	H	12.13895300	4.40267900	1.68661900
H	2.06442400	1.65035600	3.84761300	H	10.67271800	4.97060500	0.88337500
C	4.08607400	2.83465100	-0.22287200	C	12.38947100	-1.64991900	-0.95737700
C	5.18419000	3.69047500	0.10925400	C	11.90870900	-2.65108800	0.11118100
C	6.41106600	3.37241600	0.68753500	C	13.52808300	-2.26080800	-1.79783100
H	4.96589600	4.75210900	0.04444500	H	11.54633900	-1.46816500	-1.62934800
N	4.19460600	1.52989800	-0.35088700	H	11.05089700	-2.25697300	0.66847400
C	2.74713700	3.54594500	-0.36128100	H	11.60026400	-3.59521800	-0.35432000
H	2.88104000	4.52637100	-0.82884700	H	12.70093500	-2.87836500	0.83455200
H	2.02933800	2.96679200	-0.94482100	H	13.86758700	-1.56698800	-2.57479500
H	2.30761200	3.71883100	0.62953700	H	14.39736200	-2.51432300	-1.17921400
C	7.22421200	4.56503000	1.18730200	H	13.19162100	-3.18245000	-2.28811800
H	7.08232100	5.41390700	0.51144800	C	10.96313700	0.91121100	-2.71274500
H	6.90643700	4.89441600	2.18354200	C	9.84965500	0.67326900	-3.58017800
H	8.29145300	4.33709000	1.23642500	C	8.65369800	0.00603500	-3.32489300
N	6.90727200	2.11691500	0.77734600	H	10.03235300	0.91035000	-4.62397000
C	7.81743900	1.76515400	1.75012800	N	10.89422000	0.83138500	-1.40156100
C	7.72455200	2.19147000	3.10000500	C	12.27037200	1.21194100	-3.43368700

H	12.70463900	0.28504600	-3.82958700
H	12.09026100	1.87162200	-4.28861700
H	13.01032700	1.67268500	-2.77724200
C	7.82182500	-0.33594900	-4.55941100
H	7.93186700	0.45514500	-5.30729900
H	8.14814400	-1.26987700	-5.03180100
H	6.76122500	-0.43788000	-4.31748400
N	8.19932700	-0.29562800	-2.08661800
C	7.32824800	-1.34156800	-1.87090800
C	7.45562200	-2.60669800	-2.50001200
C	6.59261100	-3.63679800	-2.16609700
H	8.25485100	-2.76226100	-3.21573800
C	5.54280600	-2.16591100	-0.61382600
C	5.60206900	-3.42252000	-1.20016200
H	6.69591400	-4.60784300	-2.64450300
H	4.78719700	-1.94339900	0.13608400
H	4.90469900	-4.20068700	-0.90976600
N	6.36921100	-1.15182100	-0.92491300
Li	9.12005600	0.56073600	-0.58100600

1’

C	-2.69004100	1.10613600	0.57530500
C	-1.34252000	1.18096100	0.94603600
C	-0.64248800	2.39614100	0.73360400
C	-1.30621000	3.51045000	0.16072900
C	-2.65456300	3.38370700	-0.19328100
C	-3.34800800	2.19361300	0.00714300
H	-3.23624000	0.18019700	0.73697600
H	-3.17201900	4.23367500	-0.63134100
H	-4.39481500	2.11473200	-0.27448200
C	-0.59232300	4.84635700	-0.03310900
H	0.47486500	4.68065000	0.14123800
C	-1.06767700	5.88131200	1.00695500
H	-0.90771100	5.52176000	2.03118600
H	-0.52365900	6.82701100	0.89374100
H	-2.13842600	6.09144600	0.89670600
C	-0.74311000	5.40399100	-1.46063000
H	-0.14852300	6.31800500	-1.57696200
H	-0.40240000	4.68098300	-2.21037900
H	-1.78369100	5.65825900	-1.69408800
C	-0.66655300	-0.01732300	1.60894900
H	0.41048400	0.17334800	1.62066900
C	-1.11788600	-0.15996000	3.07691000
H	-2.19726200	-0.34297400	3.14320600
H	-0.60160800	-0.99546400	3.56535800
H	-0.90290200	0.74970100	3.65137100
C	-0.89021500	-1.33428100	0.84306400
H	-0.57819600	-1.24632400	-0.20382400
H	-0.31030500	-2.14372200	1.30232200
H	-1.94254700	-1.64161700	0.85139300
N	0.69075600	2.54061100	1.21928400
C	1.72886700	2.24997300	0.44830500
C	1.49591500	1.75779600	-0.97377900
H	0.88527100	0.84794100	-0.97751500
H	0.94470200	2.50367500	-1.55786700
H	2.43680400	1.54514100	-1.48597800
C	3.09859000	2.36296300	0.84254300
H	3.81720000	2.07731200	0.08231400
C	3.63587700	2.79053900	2.06288900
C	5.14770700	2.80598000	2.19479800
H	5.47900400	2.15670900	3.01449700
H	5.62656700	2.45953600	1.27564100
H	5.51586700	3.81724400	2.40738500
N	2.80852300	3.16039200	3.04273000
C	1.75287100	4.30264700	6.16950100
C	2.88641800	4.56527900	6.93574000
C	4.12911200	4.33414300	6.33995500
C	4.20639300	3.86140300	5.03625200
C	3.01149900	3.61581000	4.31419600
N	1.79714400	3.84909900	4.91671800
H	5.04533200	4.52343500	6.89455600
H	0.75727300	4.46380500	6.57998600
H	2.79686200	4.93396800	7.95186700
H	5.17191200	3.68616800	4.58348900
Li	0.92177800	3.19030600	3.04340200

4g

C	-1.37705900	-0.31516800	0.00000600
C	0.01698100	-0.29895600	0.00057400
C	0.70671600	0.92036800	0.00012200
C	-0.00776800	2.12836600	-0.00090500
C	-1.39830500	2.11139500	-0.00147300
C	-2.08303100	0.89008600	-0.00101600
H	-1.91211900	-1.26064600	0.00035900
H	0.57758900	-1.23167200	0.00137400
H	0.54948900	3.06025400	-0.00124000
H	-1.95429700	3.04489200	-0.00227200
H	-3.16981100	0.87966200	-0.00146200
C	2.18702600	0.92888500	0.00072700

H	2.65553300	-0.08104700	0.00165700
O	2.87526800	1.93167800	0.00028600

IN1

C	-2.75785600	2.05034100	1.33408400
C	-1.38138800	1.84964400	1.49748300
C	-0.47604100	2.80926300	0.96902200
C	-0.97597700	3.93917300	0.26731100
C	-2.36099100	4.09492500	0.13308300
C	-3.25451300	3.16607200	0.66281900
H	-3.45317800	1.31759500	1.73728500
H	-2.74799500	4.96087500	-0.39902400
H	-4.32620100	3.30242900	0.54037400
C	-0.03805600	4.99139700	-0.32264700
H	0.98383800	4.61706700	-0.21672200
C	-0.11302800	6.32111300	0.45386000
H	0.14947100	6.17959500	1.50723400
H	0.58210000	7.05562100	0.02882600
H	-1.12129400	6.75206500	0.41108800
C	-0.29411800	5.22784600	-1.82354700
H	0.45263300	5.91871700	-2.23299600
H	-0.23883800	4.29348500	-2.39340100
H	-1.28216000	5.66755200	-2.00537800
C	-0.88088100	0.61889700	2.25196700
H	0.20848900	0.59780200	2.15822300
C	-1.20537600	0.70514700	3.75682200
H	-2.28810900	0.74657000	3.92976600
H	-0.81474000	-0.17095000	4.28845500
H	-0.75856800	1.59706800	4.21169400
C	-1.42287700	-0.69404000	1.65557700
H	-1.18658100	-0.77596200	0.58866600
H	-0.98004300	-1.55676300	2.16767500
H	-2.51174200	-0.77253500	1.76119000
N	0.90521100	2.70889300	1.27514000
C	1.74852700	2.11468100	0.44411100
C	1.23760800	1.53013000	-0.86704800
H	0.44861900	0.79189200	-0.68278900
H	0.79451600	2.30871400	-1.49810100
H	2.03803400	1.04634200	-1.43140900
C	3.13872300	1.94514000	0.69263700
H	3.67990500	1.40850300	-0.07892900
C	3.89487900	2.32954700	1.81029300
C	5.35222700	1.89204500	1.81465500
H	5.64270100	1.48994300	2.79109700
H	5.52493400	1.12010100	1.06055400
H	6.02613900	2.72872200	1.59011400
N	3.32957600	2.99888900	2.81610700
C	3.27467400	4.11177500	6.13827800
C	4.58704900	4.39497500	6.51421200
C	5.57941100	4.21063600	5.54891400
C	5.24437000	3.73815600	4.28621900
C	3.89063300	3.43450300	3.99288900
N	2.92738600	3.65695300	4.93482500
H	6.61748600	4.44307500	5.77611900
H	2.45455400	4.26224400	6.83956700
H	4.81575400	4.75945300	7.51042400
H	6.01176800	3.63131100	3.53232800
Li	1.44489800	3.45554600	3.07361100
C	-4.14020300	6.82838300	4.80543900
C	-3.38307100	5.82176200	4.21024200
C	-1.99185900	5.78966900	4.39126100
C	-1.36025800	6.77234300	5.17250400
C	-2.11932900	7.77358600	5.76678000
C	-3.50768300	7.80124000	5.58350100
H	-5.21686900	6.85701800	4.66532900
H	-3.85823900	5.06050200	3.59595300
H	-0.28290400	6.72892300	5.29917200
H	-1.63720200	8.53499000	6.37329200
H	-4.09720400	8.58609800	6.04995200
C	-1.21987300	4.71632600	3.75248000
H	-1.80454000	3.96823000	3.19161000
O	0.00337500	4.61897200	3.81575900

HBpin

C	-1.65307200	1.07174000	0.65444300
C	-1.22463500	-0.37835700	0.87074600
H	-0.14993000	-0.44249500	1.07660400
H	-1.75917500	-0.79263500	1.73148600
H	-1.45148600	-1.00170800	0.00303400
C	-1.50769300	1.86403500	1.96029100
H	-0.47506400	1.85644200	2.32477800
H	-1.82381300	2.90410900	1.83319800
H	-2.14617000	1.40939700	2.72388600
C	-1.00439100	1.78941400	-0.59485600
C	-0.62883800	0.82646100	-1.72896200
H	-1.46240300	0.16422900	-1.98320700
H	-0.37840300	1.40944500	-2.62057100
H	0.23682000	0.20973000	-1.46540900

C	0.17091500	2.71274900	-0.27972700
H	0.51819100	3.18954200	-1.20181000
H	-0.11042000	3.50146700	0.42150300
H	1.00826800	2.14781300	0.14583200
O	-3.07438100	1.08446000	0.32125200
O	-2.10670300	2.60518700	-1.09575100
B	-3.26506400	2.06631000	-0.61020200
H	-4.34375000	2.42055300	-0.96643900

IN2

C	-3.70481800	3.47468100	1.95152200
C	-2.37774500	3.02869200	1.94442000
C	-1.34909200	3.94519700	1.59577900
C	-1.67874800	5.28412300	1.25971700
C	-3.02373500	5.67574600	1.27128700
C	-4.03670100	4.78567200	1.61923300
H	-4.49526900	2.77766700	2.22011300
H	-3.28177300	6.69603100	0.99805900
H	-5.07504200	5.10754600	1.62124800
C	-0.60486700	6.29107200	0.85543800
H	0.36646600	5.82552300	1.05041700
C	-0.67120100	7.58870000	1.68166300
H	-0.58995300	7.38337600	2.75493900
H	0.15156500	8.25868800	1.40650800
H	-1.60783000	8.13357700	1.51295600
C	-0.66986400	6.60660400	-0.65270300
H	0.13407900	7.29591800	-0.93878100
H	-0.56689800	5.69819200	-1.25595700
H	-1.62464100	7.07655700	-0.91908700
C	-2.07978600	1.57706200	2.31880200
H	-1.00192800	1.42174500	2.22608300
C	-2.45163000	1.27095100	3.78309200
H	-3.52308600	1.41858200	3.96641200
H	-2.21404900	0.22820900	4.02739800
H	-1.89705400	1.91375500	4.47336800
C	-2.77932500	0.58639100	1.36675300
H	-2.52023100	0.78222200	0.32056100
H	-2.48632900	-0.44386800	1.60287900
H	-3.87095500	0.64657200	1.45308200
N	0.01271700	3.55842800	1.70988000
C	0.61348800	2.86755000	0.76782100
C	-0.05012600	2.58368100	-0.57406700
H	-0.41997100	1.55112300	-0.60534800
H	-0.89384200	3.24895700	-0.76765600
H	0.67763500	2.68649800	-1.38576900
C	1.92342100	2.31111000	0.90994300
H	2.34476300	1.91458400	-0.00877800
C	2.69222100	2.09187200	2.05303400
C	4.01921400	1.37437400	1.79968700
H	3.91776400	0.28356500	1.84434800
H	4.38513300	1.62115900	0.79940600
H	4.78406600	1.66418100	2.52524600
N	2.35638500	2.53070400	3.28278300
C	3.90069000	2.63802100	6.52201300
C	4.27095800	1.33533200	6.78464000
C	3.94753500	0.36183100	5.82792600
C	3.31563900	0.74333900	4.66277100
C	2.99659100	2.10676400	4.40743700
N	3.27496100	3.02648200	5.38791700
H	4.17849700	-0.68583500	6.00399400
H	4.09754900	3.44127700	7.22261600
H	4.77512300	1.08710400	7.71177800
H	3.02198100	0.00683500	3.92521900
Li	1.01589400	4.04114800	3.42426400
C	-4.29668200	5.59560200	7.35644900
C	-3.56760500	5.52639500	6.17125900
C	-2.30056300	4.92443900	6.16055100
C	-1.76103100	4.39554100	7.34512900
C	-2.48944100	4.47167100	8.52699700
C	-3.75600200	5.06912600	8.53222900
H	-5.27973900	6.05749700	7.36685200
H	-3.97560400	5.92820700	5.24655300
H	-0.77351000	3.94541400	7.31474200
H	-2.07576100	4.06985400	9.44762200
H	-4.32178300	5.12550400	9.45850200
C	-1.55062500	4.86307800	4.89750000
H	-2.01348900	5.37687600	4.03600800
O	-0.47729500	4.28674900	4.76485300
C	4.11010200	6.53476900	5.13373200
C	5.60663400	6.85594700	5.09214500
H	5.81769000	7.69004000	4.41197200
H	5.94547400	7.14359600	6.09333100
H	6.19332600	5.98972700	4.77690800
C	3.34863900	7.71707700	5.76117600
H	3.52720200	8.65803900	5.22775900
H	2.27168900	7.52379300	5.77981400
H	3.68672000	7.83884200	6.79537100
C	3.49511900	6.08168500	3.75638000

C	4.47412300	5.24941000	2.91273800
H	4.92568700	4.44971600	3.50630200
H	3.93445400	4.79182900	2.07798400
H	5.27726700	5.87177700	2.50200700
C	2.92319100	7.21393400	2.90332100
H	2.51806000	6.80968600	1.96878700
H	2.11855400	7.74067700	3.42145400
H	3.70373700	7.93875000	2.64234200
O	3.91146400	5.38758300	5.96262300
O	2.40504100	5.23710100	4.19247600
B	2.76617100	4.65626100	5.48013700
H	1.81846900	4.55666800	6.23183900

TS1

C	-4.25863800	0.91724600	8.03804900
C	-3.81276100	2.31324900	8.47434800
H	-4.47452500	3.08253500	8.06007000
H	-3.85552600	2.38478300	9.56599700
H	-2.78810700	2.52721200	8.16193600
C	-5.61674000	0.58325000	8.67060000
H	-6.37468200	1.32879300	8.40669300
H	-5.97950900	-0.40238000	8.36855200
H	-5.50622700	0.57948200	9.75960500
C	-4.21443200	0.66613900	6.47854900
C	-3.09796500	1.44652600	5.77082500
H	-2.13938500	1.31977700	6.28330300
H	-2.98972300	1.06523700	4.75084200
H	-3.32508800	2.51672400	5.71820100
C	-5.54180900	0.87193600	5.75556700
H	-5.41975200	0.65686100	4.68916700
H	-6.31939100	0.21282900	6.14677900
H	-5.87902800	1.91048500	5.85280400
O	-3.28102600	-0.03412300	8.52883800
O	-3.85207100	-0.74324900	6.39815900
B	-3.24142700	-1.09298900	7.61270700
H	-4.11633700	-2.17334600	8.09869100
C	-6.16322500	-6.04130500	2.76382000
C	-4.99952100	-5.34089200	3.10144400
C	-4.98729200	-3.93382900	2.93752800
C	-6.14041200	-3.25344800	2.47793600
C	-7.27386900	-4.00331900	2.14258000
C	-7.29220400	-5.38801500	2.27874400
H	-6.18516300	-7.12109800	2.88793700
H	-8.15853400	-3.49289700	1.77023300
H	-8.18268900	-5.95320900	2.01593100
C	-6.16276200	-1.73507900	2.32132900
H	-5.26561900	-1.34234800	2.81248400
C	-7.38285400	-1.09564300	3.01004000
H	-7.43715300	-1.38215200	4.06580800
H	-7.32347700	-0.00170900	2.95420600
H	-8.32366800	-1.39471800	2.53356400
C	-6.09745000	-1.31591700	0.83880100
H	-6.08725200	-0.22290400	0.74299200
H	-5.19802300	-1.70621600	0.35025300
H	-6.96614600	-1.69325400	0.28549500
C	-3.80390400	-6.10427300	3.66744700
H	-2.97935300	-5.39583600	3.78775700
C	-4.12057100	-6.66333300	5.06912100
H	-4.94257800	-7.38912500	5.03064000
H	-3.24220100	-7.17745400	5.48105600
H	-4.40387400	-5.85380200	5.74914400
C	-3.31912300	-7.21871500	2.72044700
H	-3.07765500	-6.82784600	1.72500900
H	-2.41900600	-7.69736800	3.12522500
H	-4.07628500	-8.00153700	2.59286100
N	-3.83800300	-3.18404200	3.33438600
C	-2.81861700	-3.04493500	2.53345300
C	-2.81583700	-3.57776100	1.10784100
H	-2.35176000	-2.85289300	0.43049000
H	-2.21761400	-4.49635900	1.05280100
H	-3.82085300	-3.80850000	0.75192200
C	-1.58715500	-2.39140500	2.92088600
H	-0.91919600	-2.17756900	2.09145700
C	-1.08326300	-2.09046200	4.16948200
C	0.31004000	-1.46305200	4.19508600
H	1.10904900	-2.21298800	4.22848500
H	0.46752400	-0.86982300	3.29013200
H	0.43641800	-0.80644300	5.06112100
N	-1.79002800	-2.23631100	5.32569400
C	-1.40445100	-2.08046600	8.90171600
C	-0.22939800	-2.73575100	9.15265900
C	0.48219800	-3.25491300	8.04878800
C	-0.00386000	-3.07660600	6.77886500
C	-1.22749000	-2.37519600	6.52645800
N	-1.90405800	-1.88823100	7.64360800
H	1.40206400	-3.81274300	8.20350300
H	-2.00910100	-1.65623300	9.69403100
H	0.12011400	-2.85717300	10.17093600

H	0.50114100	-3.51512400	5.92810300
Li	-3.82291100	-2.54040900	5.25079800
C	-7.22548200	-3.09812400	10.64257100
C	-6.01217600	-3.19888600	9.96332300
C	-5.97839000	-3.21286200	8.56357900
C	-7.17848500	-3.13313200	7.85011800
C	-8.39497300	-3.03391400	8.52802400
C	-8.42191100	-3.01391200	9.92420600
H	-7.24121200	-3.09057400	11.72974200
H	-5.07994100	-3.26891800	10.52227000
H	-7.13408300	-3.17174000	6.76607300
H	-9.32454100	-2.97918100	7.96645800
H	-9.36961600	-2.93972600	10.45164200
C	-4.66166700	-3.33142600	7.81746200
H	-3.92937400	-3.92892000	8.40637200
O	-4.68775700	-3.52189100	6.53908000

IN3

C	-4.07445300	1.07886900	7.89530700
C	-3.72262500	2.29419800	8.75576500
H	-4.21778800	3.19913200	8.38412800
H	-4.05981700	2.12475100	9.78400700
H	-2.64465000	2.47203800	8.78068600
C	-5.57389800	0.76684600	8.03519600
H	-6.19925600	1.62056300	7.75098000
H	-5.85694900	-0.09512200	7.42480000
H	-5.78532800	0.52192700	9.08117500
C	-3.60430000	1.17252300	6.39113100
C	-2.27430900	1.92744300	6.22646900
H	-1.51859800	1.55892300	6.92642800
H	-1.90255300	1.76722600	5.20922000
H	-2.39451800	3.00520400	6.38280200
C	-4.64158900	1.74886500	5.42747200
H	-4.23610900	1.75713900	4.40970700
H	-5.55794800	1.15477800	5.42187400
H	-4.89618100	2.78102200	5.69618800
O	-3.33153900	-0.05310300	8.38506800
O	-3.37443600	-0.20964700	6.05609800
B	-3.07964700	-0.92892100	7.27916500
H	-3.98165200	-2.39278900	9.24326800
C	-6.57986000	-5.92505300	3.65167500
C	-5.31821500	-5.32197000	3.71619100
C	-5.22541800	-3.92189500	3.50915700
C	-6.39357700	-3.15612900	3.26487800
C	-7.62865600	-3.81126900	3.20041500
C	-7.72973200	-5.18642400	3.39086100
H	-6.66192200	-6.99724000	3.81122000
H	-8.52683800	-3.23560700	2.99258500
H	-8.69753100	-5.67835700	3.33679900
C	-6.32128200	-1.64982500	3.02629600
H	-5.32442600	-1.31387000	3.33205400
C	-7.34715800	-0.86360700	3.86253700
H	-7.24145300	-1.07986400	4.93179800
H	-7.20721600	0.21418100	3.71799800
H	-8.37877600	-1.09859200	3.57587500
C	-6.47310800	-1.31326700	1.52873100
H	-6.37687000	-0.23330000	1.36196700
H	-5.71034700	-1.81808800	0.92609400
H	-7.45504600	-1.62593700	1.15267000
C	-4.09873200	-6.18684100	4.03187200
H	-3.20981600	-5.55234200	3.97520900
C	-4.16218000	-6.74617600	5.46678200
H	-5.02838000	-7.40491400	5.60115200
H	-3.26019500	-7.33035800	5.68913000
H	-4.24265900	-5.94283300	6.20495600
C	-3.91785500	-7.33084900	3.01476400
H	-3.86894100	-6.95569200	1.98666200
H	-2.99198400	-7.88173400	3.22058400
H	-4.74444600	-8.04966200	3.06460900
N	-3.97480300	-3.25151100	3.65051400
C	-3.07260900	-3.27597600	2.69938000
C	-3.34169000	-3.91610900	1.34446100
H	-2.93569300	-3.28953200	0.54344400
H	-2.83752200	-4.88810200	1.27723700
H	-4.40665400	-4.07503900	1.16688500
C	-1.75781100	-2.70624100	2.82765000
H	-1.20558900	-2.66160400	1.89384000
C	-1.05274500	-2.27256900	3.94268600
C	0.35396000	-1.74907000	3.65740700
H	1.10894000	-2.54428400	3.68168000
H	0.38642500	-1.30896200	2.65715400
H	0.65457800	-0.98370400	4.37826200
N	-1.58744700	-2.22774900	5.18673300
C	-0.85213100	-1.21141100	8.54223800
C	0.42815800	-1.66021600	8.78500600
C	1.07366300	-2.37325600	7.76176900
C	0.43433500	-2.57042700	6.55687000
C	-0.87360500	-2.05643200	6.31837300

N	-1.49748000	-1.40211300	7.36728900
H	2.06838600	-2.78279100	7.91886200
H	-1.42934200	-0.66651200	9.27915500
H	0.89738000	-1.47756500	9.74479500
H	0.90361400	-3.15556500	5.77755000
Li	-3.57480300	-2.19195600	5.27939600
C	-6.11159900	-6.01684100	9.12494700
C	-5.03848000	-5.12684600	9.11004700
C	-5.06370000	-3.98606700	8.29587800
C	-6.18527200	-3.75736200	7.49307500
C	-7.25583800	-4.65464700	7.49605000
C	-7.22509100	-5.78418800	8.31378400
H	-6.07420100	-6.89719700	9.76173000
H	-4.16842700	-5.32142700	9.73487800
H	-6.21203100	-2.88001600	6.85565000
H	-8.10844500	-4.47165500	6.84794500
H	-8.05807800	-6.48238100	8.31565800
C	-3.89912100	-3.01829200	8.34203400
H	-2.96004700	-3.58768900	8.43035400
O	-3.86308500	-2.17335600	7.20828200

5g

C	-1.67924700	0.62739100	-0.22839500
C	-0.37473400	0.48975100	-0.70002100
C	0.62072700	1.40085300	-0.32381900
C	0.28771600	2.45622300	0.52920200
C	-1.02045400	2.59730400	0.99835500
C	-2.00700000	1.68489700	0.62407400
H	-2.44129900	-0.08636000	-0.53092100
H	-0.12789500	-0.33248800	-1.36952800
H	1.05630900	3.16562900	0.81580900
H	-1.26713100	3.42478200	1.65889300
H	-3.02434500	1.79666100	0.98988900
C	2.03476300	1.19482300	-0.82460500
H	2.02962100	0.96376500	-1.89642300
O	2.83778200	2.34451900	-0.56857700
C	5.52095000	3.92241200	-2.30494000
C	6.90312000	4.39849200	-1.86302800
H	7.57455600	4.50355600	-2.72299100
H	6.81583800	5.37713800	-1.38028700
H	7.35684700	3.71022700	-1.14638700
C	4.83262600	5.00566800	-3.14647700
H	5.42356800	5.27392200	-4.02869000
H	3.84129600	4.68138300	-3.47918800
H	4.70469900	5.90171100	-2.53156800
C	5.48689000	2.49395100	-2.98111700
C	6.56192300	1.54178400	-2.44013500
H	6.56397500	1.52523100	-1.34551800
H	6.34878400	0.52822500	-2.79386600
H	7.56284000	1.82265600	-2.78398000
C	5.50378100	2.49376600	-4.50829800
H	5.44960100	1.46390300	-4.87600500
H	4.65498200	3.04352300	-4.92114200
H	6.42922500	2.94056600	-4.88917200
O	4.70219900	3.72565800	-1.12076600
O	4.20278900	1.97315200	-2.53561300
B	3.87477800	2.65998900	-1.38498700
H	2.48808900	0.33369600	-0.31224700