

Supporting Information

I. Experimental Section

General: Solvents were dried by reflux under N₂ over sodium or CaH₂ and freshly distilled prior to use. Air-sensitive compounds were handled under a N₂ atmosphere using standard Schlenk and glovebox techniques. NMR spectra were recorded on Bruker SPECT NMR (400 MHz for ¹H, 376 MHz for ¹⁹F, 100 MHz for ¹³C) and Bruker DMX500 NMR (160 MHz for ¹¹B) spectrometers. Chemical shifts δ are given in ppm and are referenced against residual solvent (¹H and ¹³C) or externally (¹¹B : BF₃OEt₂; ¹⁹F : CFCl₃). HRMS analyses were performed at Bruker micrOTOF II. The crystallographic measurements were performed using a CCD-Bruker SMART APEX Duo system. All the determinations of the unit cell and intensity data were performed with graphite-monochromated MoK α radiation (λ = 0.71073 Å). The structure was solved by direct methods, using Fourier techniques, and refined on F^2 by a full-matrix least-squares method. All calculations were carried out with the SHELXTL program.

Crystallographic data for the structure reported in this paper have been deposited with the Cambridge Crystallographic Data Center: CCDC 1015217 (2) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre at www.ccdc.cam.ac.uk/data_request/cif

Synthesis of **1**

To a solution of B₂pin₂ (2.358 g, 9.28 mmol) in Et₂O (15 mL) was added a solution of PhLi (prepared from C₆H₅Br and BuLi, 11.2 mmol) in Et₂O/hexane (1:1, 14 mL) at -78 °C. After stirring for 0.5 hour, the reaction mixture was allowed to warm up to room temperature and stirred for 12 hours. A white precipitate was observed. The precipitate was collected by filtration, then washed with Et₂O (5 mL x 2) and dried under vacuum, affording **1** as a white solid (2.290 g, 75% yield).

¹H NMR (400 MHz, [D₈]THF, 25 °C): δ = 7.37 (d, ³J_{HH} = 6.7 Hz, 2H, *ortho*-C₆H₅), 6.92 (t, ³J_{HH} = 7.4 Hz, 2H, *meta*-C₆H₅), 6.76 (t, ³J_{HH} = 7.2 Hz, 1H, *para*-C₆H₅), 1.19 (s, 3H, CH₃(B₂pin₂)), 1.13 (s, 12H, CH₃(sp²Bpin)), 1.04 (s, 6H, CH₃(sp³Bpin)), 0.93 ppm (s, 6H, CH₃(sp³Bpin)).

¹³C NMR (100 MHz, [D₈]THF, 25 °C): δ = 132.1 (*ortho*-C₆H₅), 126.1 (*meta*-C₆H₅), 123.3 (*para*-C₆H₅), 81.8 (OC(CH₃)₂), 77.9 (OC(CH₃)₂), 26.3 (CH₃), 25.6 (CH₃), 25.1 ppm (CH₃).

¹¹B NMR (160 MHz, [D₈]THF, 25 °C): δ = 39.2 (br s, Bpin), 30.5 (s, B₂pin₂), 4.0 ppm (s, BC₆H₅).

HRMS: [pinBB(Ph)pin]⁺ calc. for C₁₈H₂₉B₂O₄: 331.2252. Found: 331.2256

Activation of H₂

The degassed mixture of **1** (223 mg, 0.602 mmol) and B(C₆F₅)₃ (337 mg, 0.660 mmol) in bromobenzene (2 mL) was subjected to 4 bar H₂ and stirred at room temperature for 12 hours. The solution was condensed to around 0.5 mL and 15 mL hexane was added. Resulting white precipitate was filtered, rinsed with hexane (5 mL), and dried und vacuum, affording Li[HB(C₆F₅)₃] as a white solid (223 mg, 71% yield). The filtrate was subjected to aqueous workup, extrated with diethyl ether, then subjected to chromatography, affording PhBpin as a colorless oil (90 mg, 73% yield) and B₂pin₂ as a white solid (50 mg, 52% yield).

Charaterization of Li[HB(C₆F₅)₃]

¹H NMR (400 MHz, [D₆]benzene, 25 °C): δ = 2.67 (br q, ¹J_{BH} = 80.1 Hz, 1 H, BH).

¹¹B NMR (160 MHz, [D₆]benzene, 25 °C): δ = -23.7 (d, ¹J_{HB} = 77.9 Hz).

¹⁹F NMR (376 MHz, [D₆]benzene, 25 °C): δ = -137.3 (s, 6 F, *ortho*-C₆F₅), -159.3 (t, ³J_{FF} = 18 Hz, 3 F, *para*-C₆F₅), -163.8 (s, 6 F, *meta*-C₆F₅).

HRMS: [HB(C₆F₅)₃]⁺ calc. for C₁₈HB₁₅F₁₅: 512.9932. Found: 512.9928.

Characterization of **PhBpin**

¹H NMR (400 MHz, CDCl₃, 25 °C): δ = 1.36 (s, 12 H, CH₃), 7.37 (t, ³J_{HH} = 6.5 Hz, 2 H, *meta*-C₆H₅), 7.47 (t, ³J_{HH} = 7.4 Hz, 1 H, *para*-C₆H₅), 7.82 (d, ³J_{HH} = 6.7 Hz, 2 H, *ortho*-C₆H₅).

¹³C NMR (100 MHz, CDCl₃, 25 °C): δ = 24.8 (s, CH₃), 83.7 (s, CH₃CCH₃), 127.7 (s, *meta*-C₆H₅), 131.2 (s, *para*-C₆H₅), 134.7 (s, *ortho*-C₆H₅).

¹¹B NMR (160 MHz, CDCl₃, 25 °C): δ = 31.0 (s).

Characterization of **B₂pin₂**

¹H NMR (400 MHz, CDCl₃, 25 °C): δ = 1.23 (s, 12 H, CH₃).

¹³C NMR (100 MHz, CDCl₃, 25 °C): δ = 24.9 (s, CH₃), 83.4 (s, C(CH₃)₂).

¹¹B NMR (160 MHz, CDCl₃, 25 °C): δ = 30.5 (s).

Activation of **HBpin**

The mixture of HBpin (0.123 g, 0.960 mmol), **1** (357 mg, 0.966 mmol) and B(C₆F₅)₃ (545 mg, 1.06 mmol) in bromobenzene (2 mL) was stirred at room temperature for 12 hours. The solution was condensed to around 0.5 mL and 15 mL hexane was added. Resulting white precipitate was filtered, rinsed with hexane (5 mL), and dried under vacuum, affording Li[HB(C₆F₅)₃] as a white solid (364 mg, 73% yield). The filtrate was subjected to aqueous workup, extracted with diethyl ether, then subjected to chromatography, affording PhBpin as a colorless oil (0.157 g, 80% yield) and B₂pin₂ as a white solid (0.113 g, 41% yield).

Activation of **C₂H₄**

The mixture of **1** (90 mg, 0.243 mmol) and B(C₆F₅)₃ (151 mg, 0.295 mmol) in bromobenzene (3 mL) was subjected to 60 bar C₂H₄ and stirred at room temperature for 12 hours. Then hexane (8 mL) was added to the reaction mixture, resulting in formation of a white precipitate. The precipitate was collected by filtration and recrystallized from DME/hexane, affording **2** as a white solid (133 mg, 64% yield).

¹H NMR (500 MHz, CD₂Cl₂, 25 °C): δ = 3.67 (s, 8H, OCH₂), 3.48 (s, 12H, OCH₃), 1.21 (s, 12H, CCH₃), 1.13 (br t, ³J_{HH} = 8.3 Hz, 2H, pinBCH₂), 0.23 ppm (br t, ³J_{HH} = 8.3 Hz, 2H, (C₆F₅)₃BCH₂).

¹³C NMR (125 MHz, CD₂Cl₂, 25 °C): δ = 148.9 (dm, ¹J_{CF} = 230 Hz, *ortho*-C₆F₅), 138.0 (dm, ¹J_{CF} = 245 Hz, *para*-C₆F₅), 136.9 (dm, ¹J_{CF} = 235 Hz, *meta*-C₆F₅), 83.0 (CCH₃), 71.0 (OCH₃), 59.9 (OCH₂), 25.0 (s, CH₃), 16.1 (br s, pinBCH₂), 8.6 ppm (br s, (C₆F₅)₃BCH₂).

¹¹B NMR (160 MHz, CD₂Cl₂, 25 °C): δ = 35.0 (br s, pinB), -12.4 ppm (s, BC₆F₅).

¹⁹F NMR (376 MHz, CD₂Cl₂, 25 °C): δ = -133.0 (d, ³J_{FF} = 18 Hz, 6F, *ortho*-C₆F₅), -165.0 (t, ³J_{FF} = 20 Hz, 3F, *para*-C₆F₅), -167.7 ppm (t, ³J_{FF} = 20 Hz, 6F, *meta*-C₆F₅).

HRMS: [pinBC₂H₄B(C₆F₅)₃]⁺ calc. for C₂₆H₁₆B₂F₁₅O₂: 667.1097. Found: 667.1100

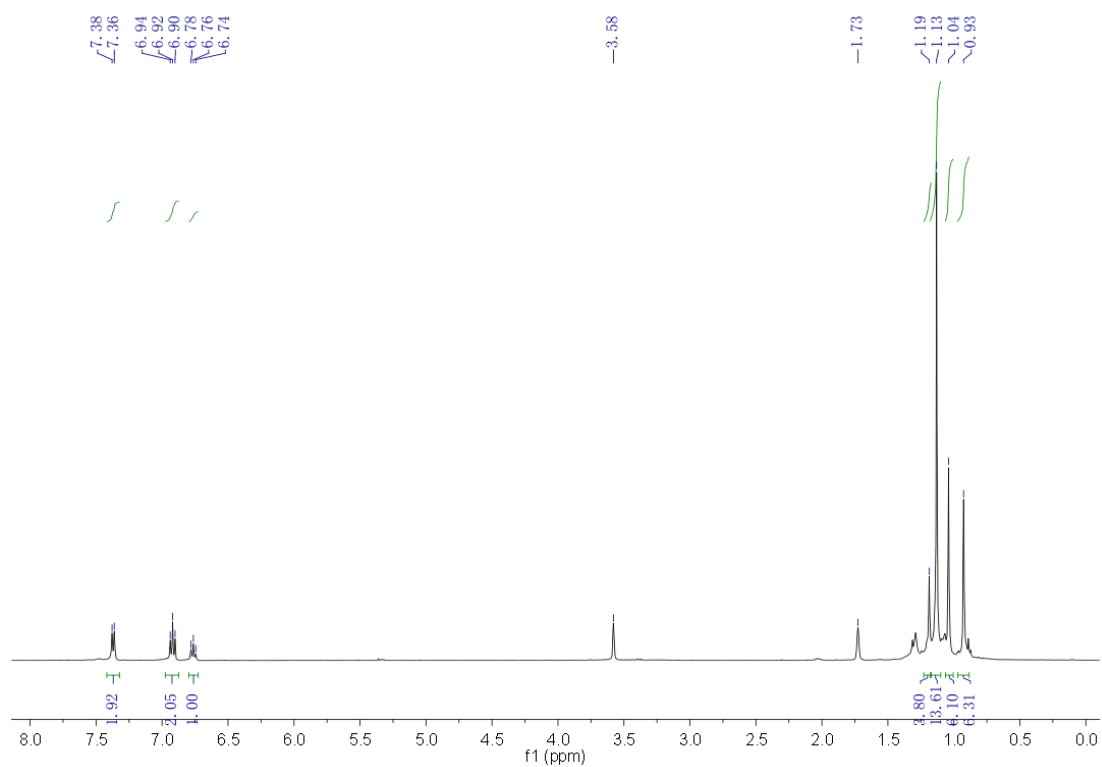


Figure S1: ¹H NMR spectrum of **1** in D₈-THF

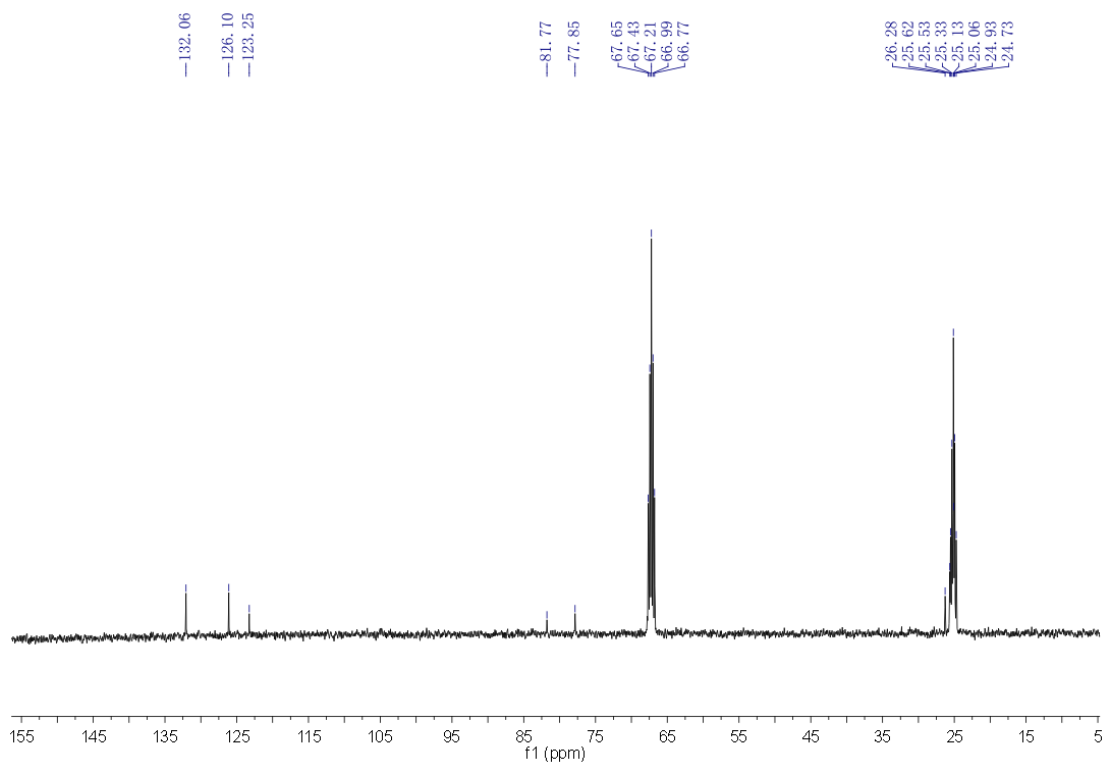


Figure S2: ¹³C NMR spectrum of **1** in D₈-THF

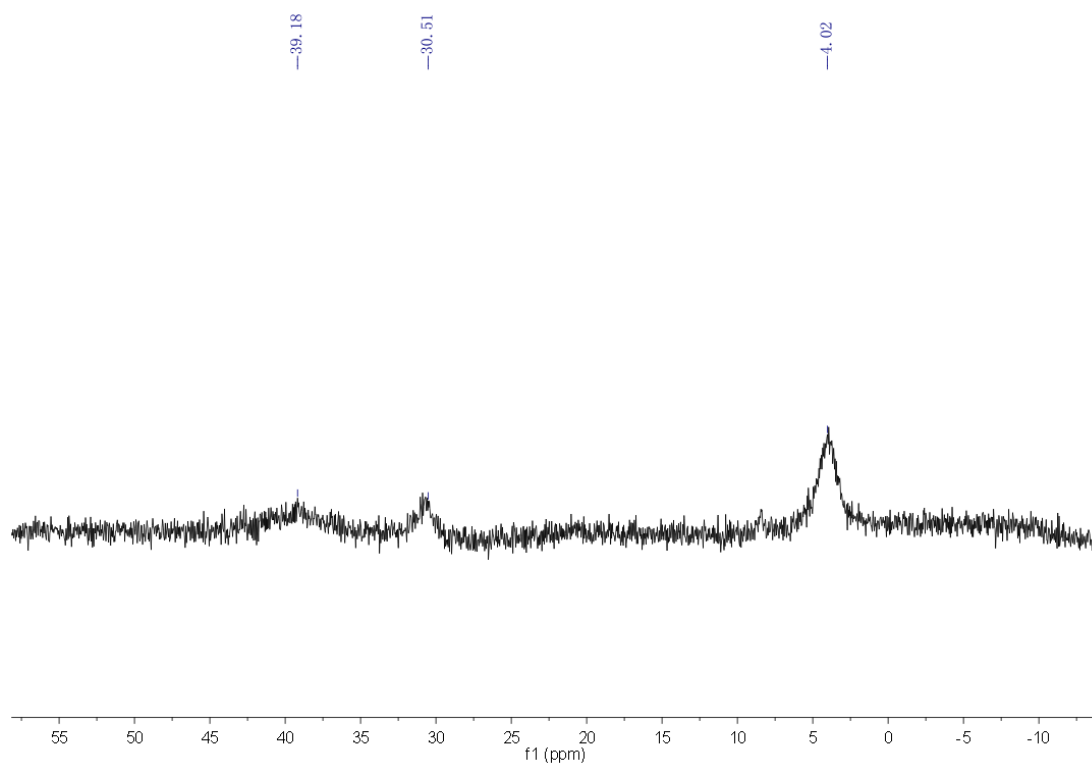


Figure S3: ¹¹B NMR spectrum of **1** in D₈-THF

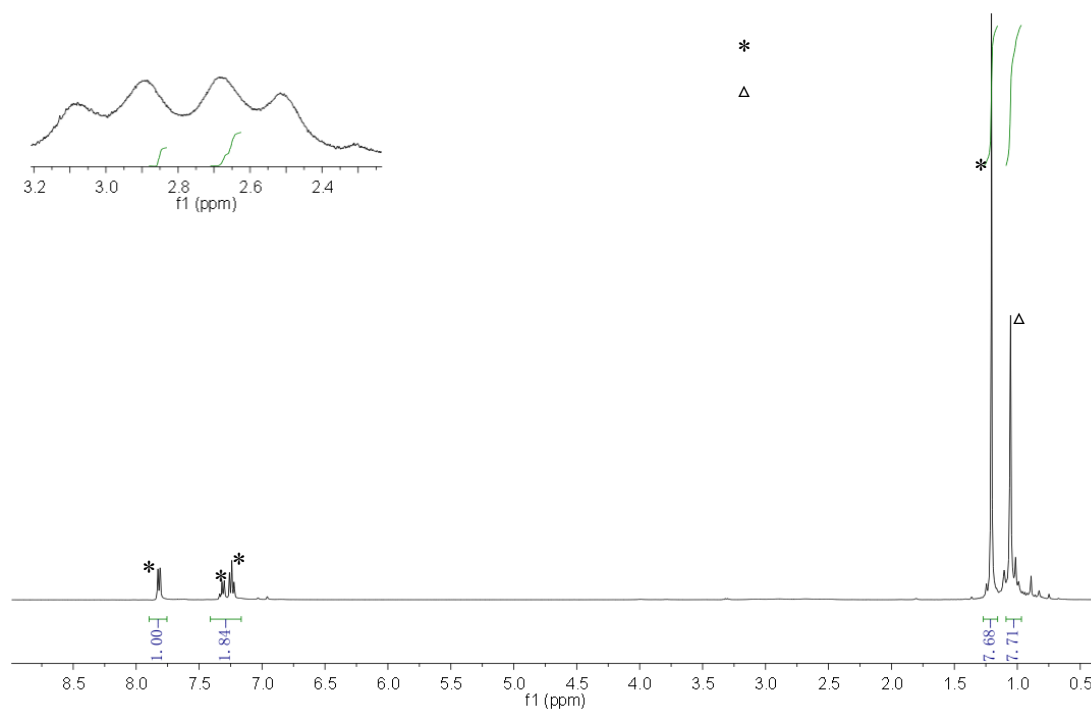


Figure S4: ¹H NMR spectrum of the C₆D₅Br solution of **1** and B(C₆F₅)₃ after stirring under H₂ for 12 h

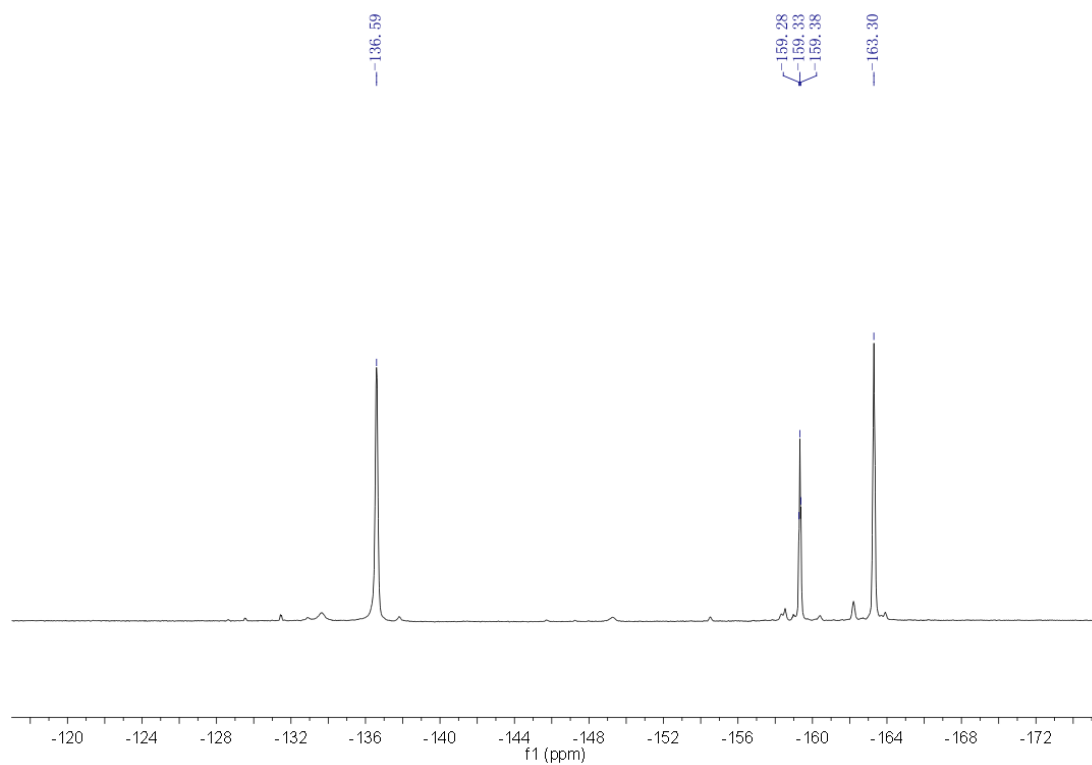


Figure S5: ^{19}F NMR spectrum of the $\text{C}_6\text{D}_5\text{Br}$ solution of **1** and $\text{B}(\text{C}_6\text{F}_5)_3$ after stirring under H_2 for 12 h

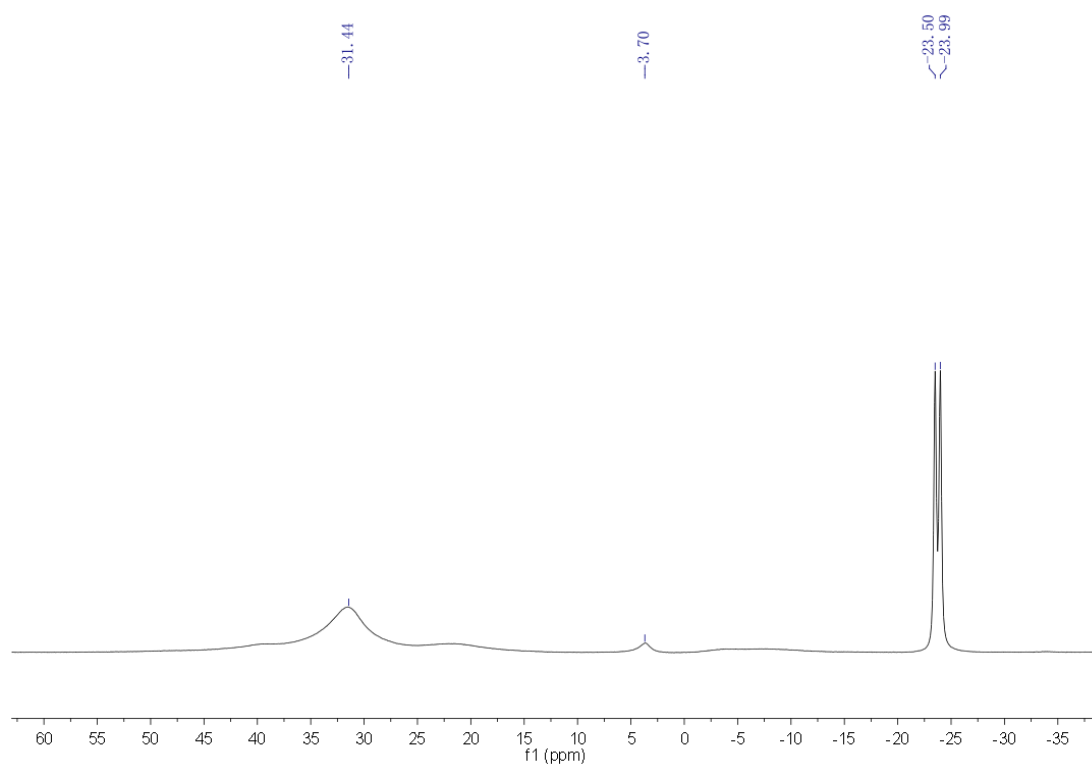


Figure S6: ^{11}B NMR spectrum of the $\text{C}_6\text{D}_5\text{Br}$ solution of **1** and $\text{B}(\text{C}_6\text{F}_5)_3$ after stirring under H_2 for 12 h

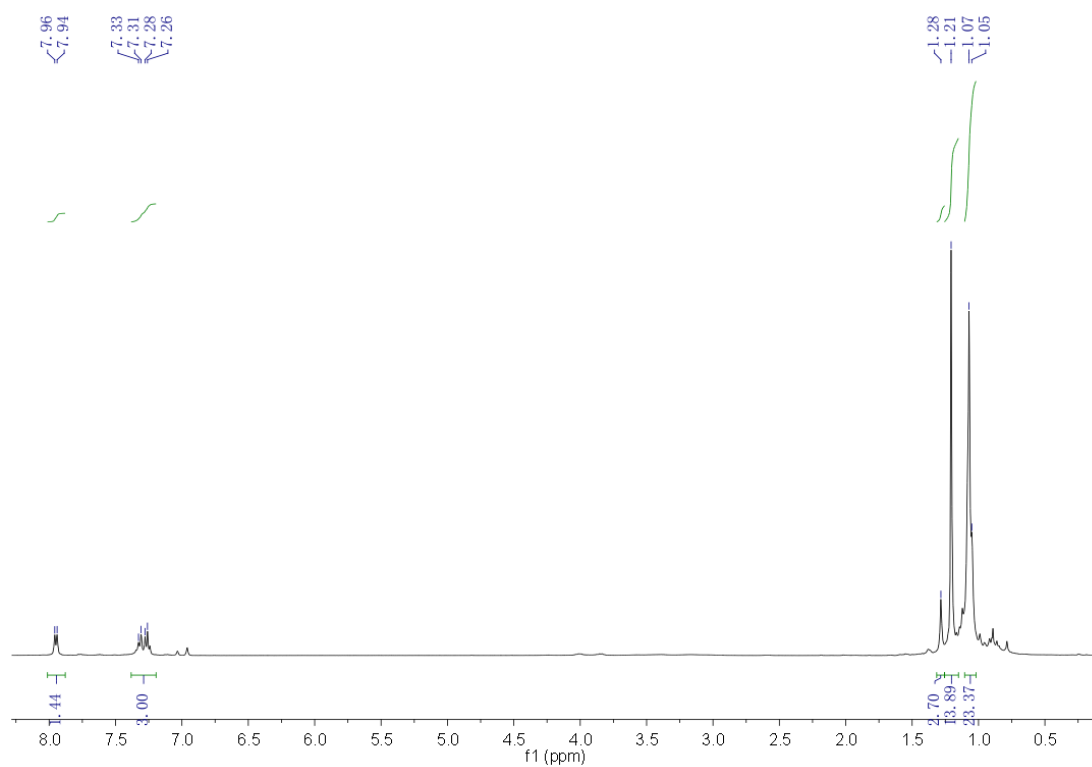


Figure S7: ¹H NMR spectrum of the C₆D₅Br solution of HBpin, **1** and B(C₆F₅)₃ after stirring for 12 h

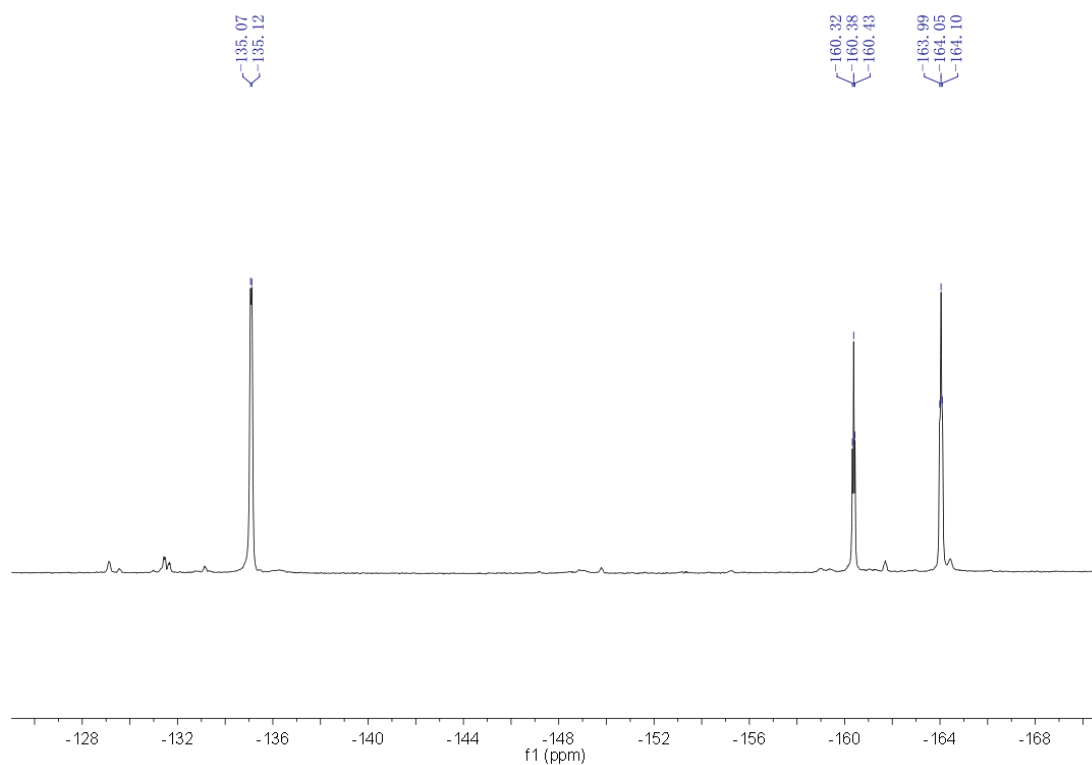


Figure S8: ¹⁹F NMR spectrum of the C₆D₅Br solution of HBpin, **1** and B(C₆F₅)₃ after stirring for 12 h

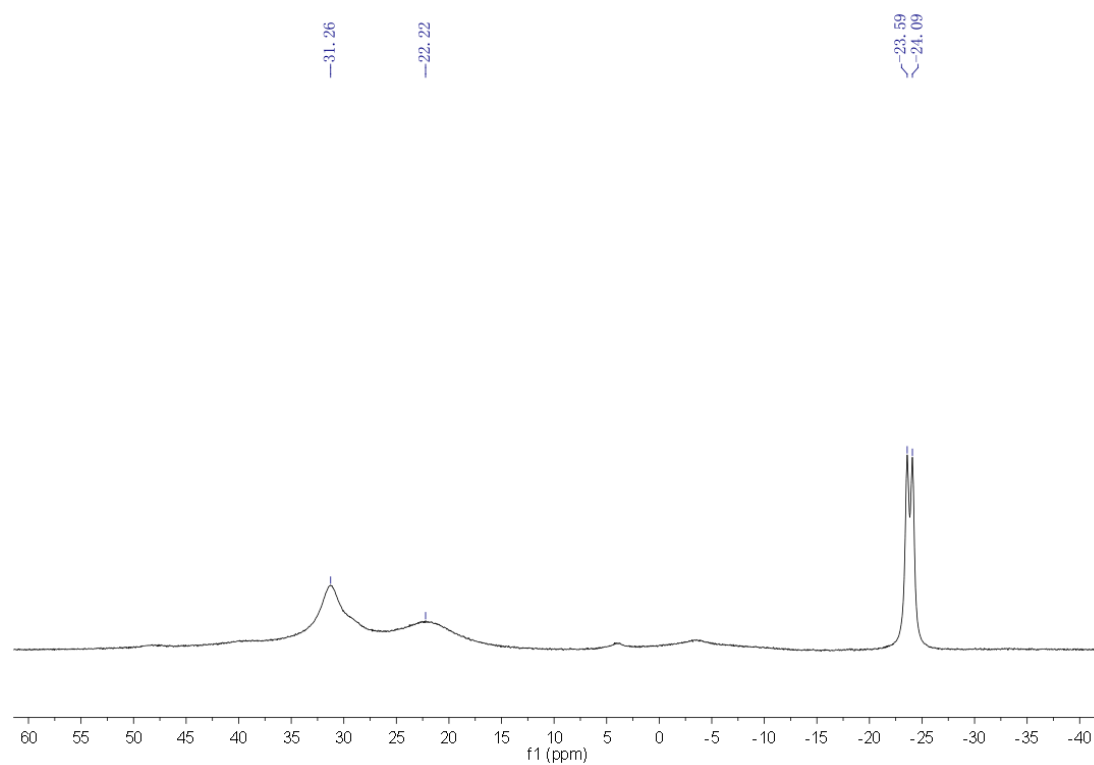


Figure S9: ^{11}B NMR spectrum of the $\text{C}_6\text{D}_5\text{Br}$ solution of HBpin, **1** and $\text{B}(\text{C}_6\text{F}_5)_3$ after stirring for 12 h

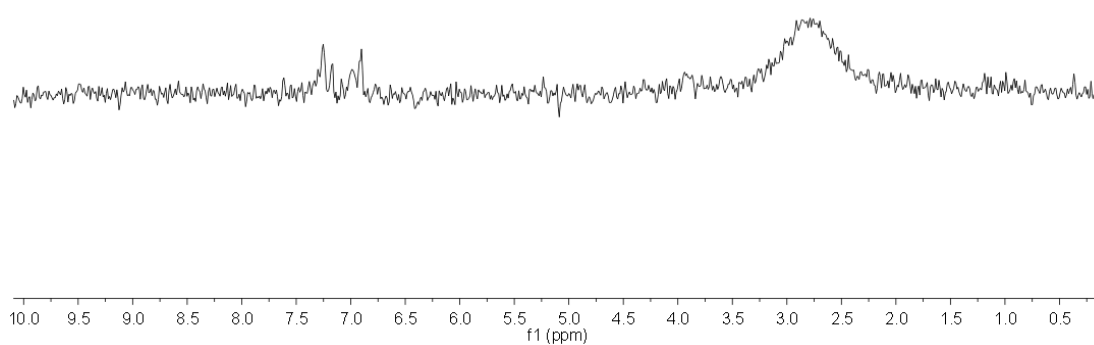


Figure S10: ^2H NMR spectrum of the $\text{C}_6\text{H}_5\text{Br}$ solution of **1** and $\text{B}(\text{C}_6\text{F}_5)_3$ after stirring under D_2 for 12 h

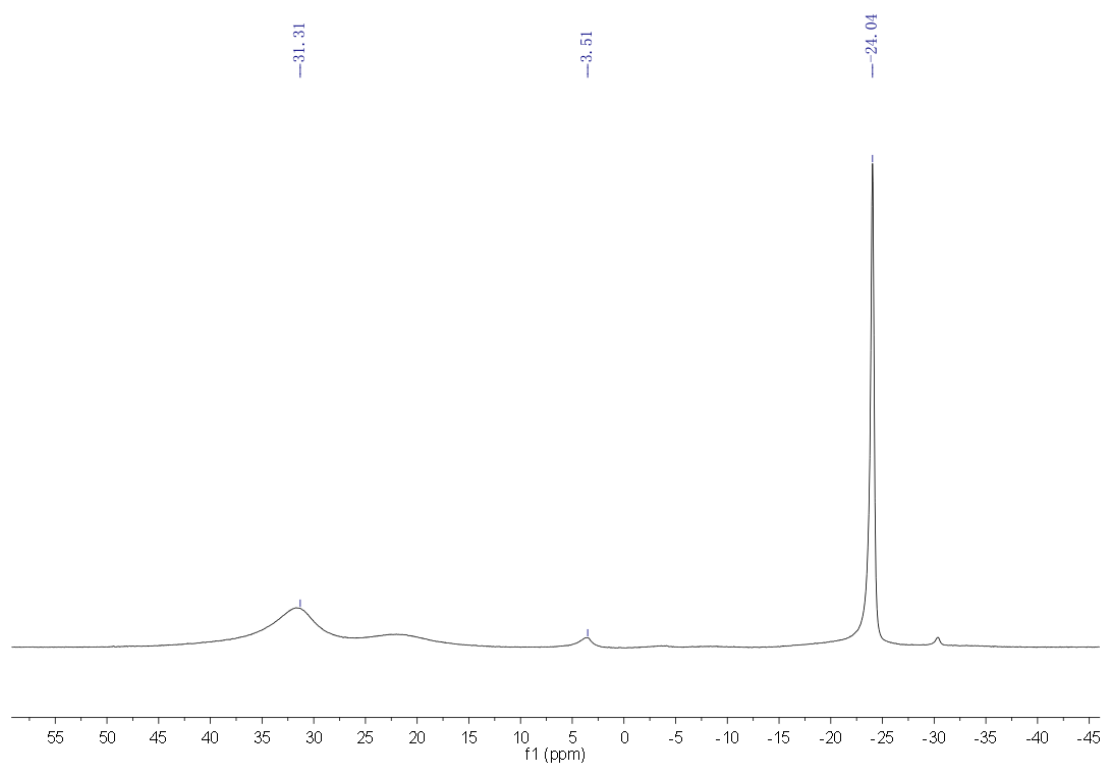


Figure S11: ^{11}B NMR spectrum of the $\text{C}_6\text{H}_5\text{Br}$ solution of **1** and $\text{B}(\text{C}_6\text{F}_5)_3$ after stirring under D_2 for 12 h

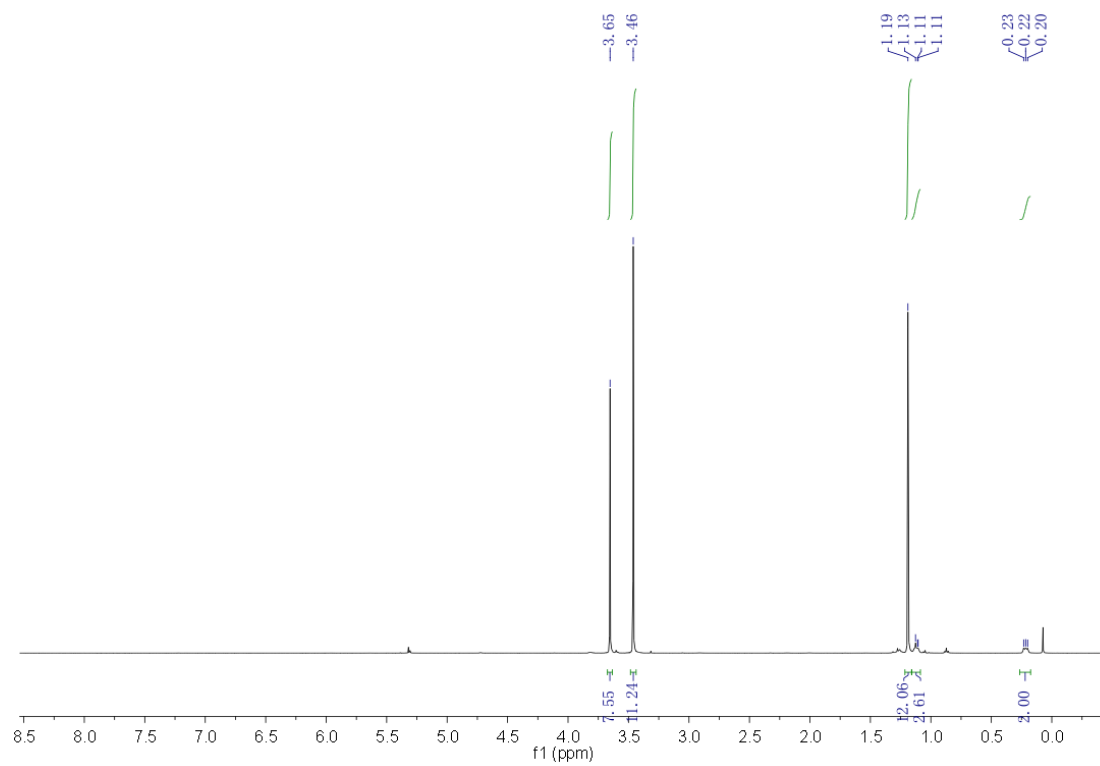


Figure S12: ^1H NMR spectrum of **2** in CD_2Cl_2

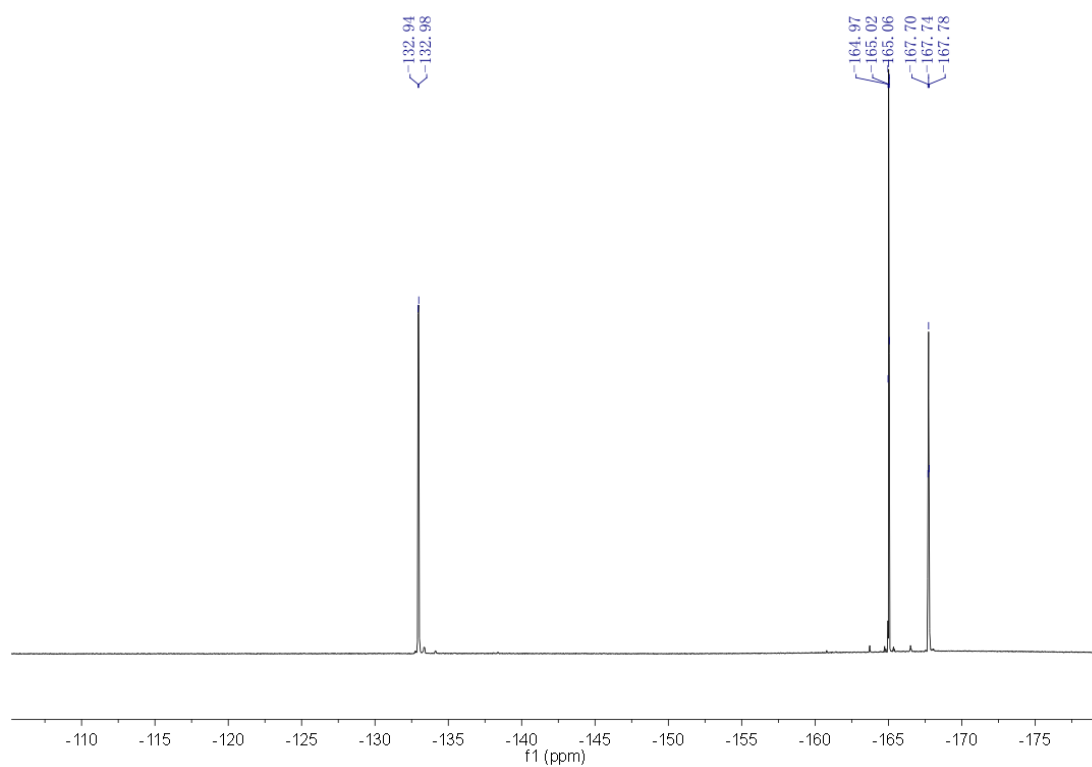


Figure S13: ¹⁹F NMR spectrum of **2** in CD₂Cl₂

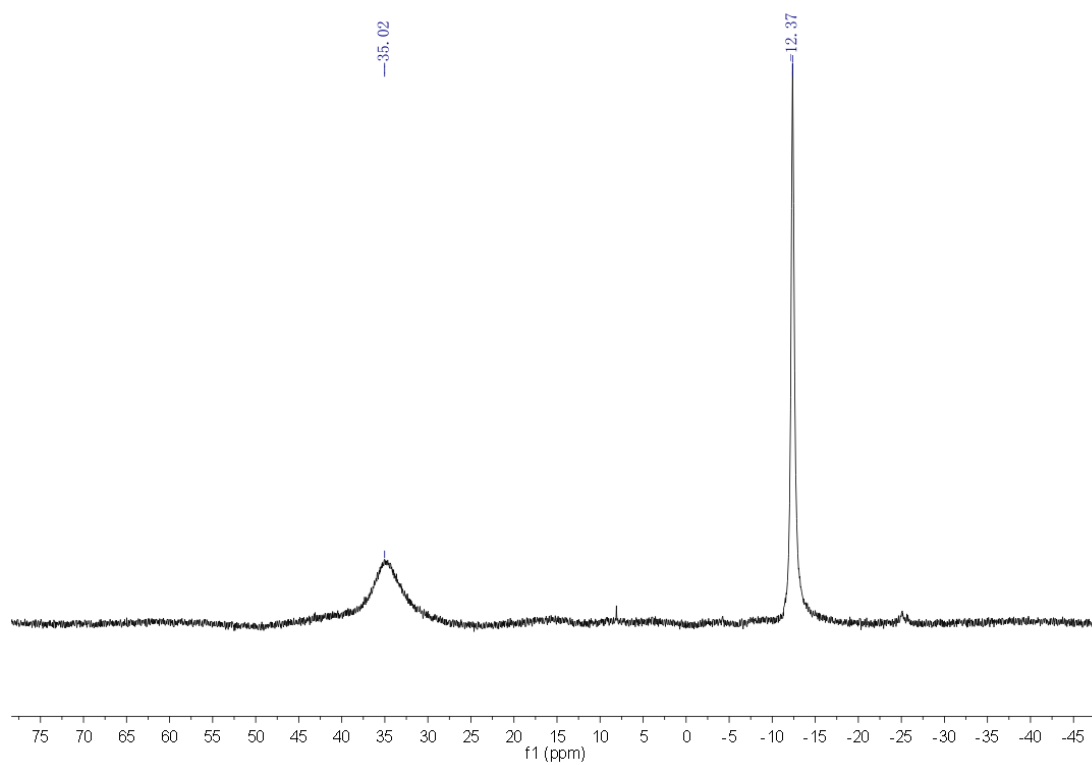


Figure S14: ¹¹B NMR spectrum of **2** in CD₂Cl₂

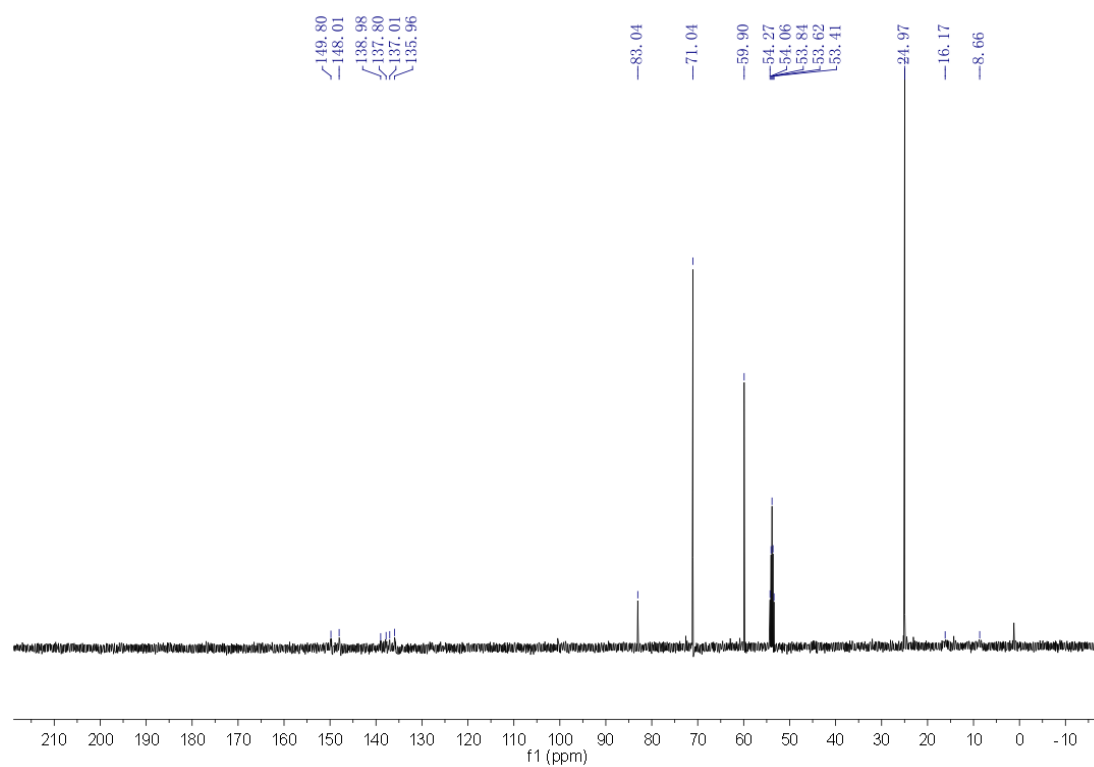


Figure S15: ¹³C NMR spectrum of **2** in CD₂Cl₂

II. Computation details

Quantum chemical calculations were all performed at the density functional theory level using the hybrid meta-GGA functional M06-2x,¹ which has been proven to give reliable results to the structural and energetic properties of the non-covalent systems and reaction energy barriers.² To reduce computational costs, a combined basis set was used: The 6-31+G(d,p) basis set³ was employed for the atoms involved directly in the reaction which are O, B, the H atoms of the hydrogen molecule, the C atom bonding to B(Bpin) of the phenyl group, C and H of ethylene; The 6-31G basis set was used for the rest of atoms. Full geometry optimization were carried out in the bromobenzene solution which was modelled by the polarizable continuum solvation model (IEFPCM)⁴ with radii and non-electrostatic terms for Truhlar and coworkers' SMD solvation model.⁵ The dielectric constant used is 5.3954. The convergence criteria used for the geometry optimization are 4.50×10^{-4} au. for gradients, and 1.80×10^{-3} au. for displacements. Harmonic vibrational analyses were carried out to verify if the optimized structure is a local minima or a first order transition state and to provide zero-point vibrational energy corrections and thermal corrections to various thermodynamic properties. Transition states were further confirmed by IRC calculations. All the calculations were performed by using the Gaussian 09 program.⁷

For the reactions of activation of H₂ and HBpin, the reaction pathway with sp² boryl of **1** functioning as the Lewis base site was also explored. For H₂ activation, we were able to locate a transition state TS_{H₂(B)} with a free Gibbs energy barrier of 27.9 kcal mol⁻¹, less favorable than the stepwise pathway. For HBpin activation, extensive efforts to employing sp² boron as the nucleophilic site failed to locate any transition state, which could be due to steric repulsion between these nucleophilic site and (C₆F₅)₃B···H-Bpin fragment.

For the activation of C₂H₄, we also explored the stepwise pathway which involves the oxygen atom from sp³ Bpin moiety of **1** as the Lewis base site. An intermediate **IM**_{C₂H₄} can be generated, which is -10.5 kcal mol⁻¹ in free Gibbs energy. However, no suitable transition state can be located from **IM**_{C₂H₄} to the final products Li[pinBC₂H₄B(C₆F₅)₃] and PhBpin. Considering the fact that proton is better electrophilic reagent than the sp³ carbon center in **IM**_{C₂H₄}, the rearrangement from **IM**_{C₂H₄} to final products would need overcome energy barrier higher than 27.2 kcal mol⁻¹ which is the energy requirement for the proton transfer. Therefore, we believe that for the activation of C₂H₄, the one step reaction pathway is more favored.

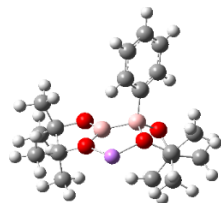
References:

1. (a) Zhao, Y.; Truhlar, D. G. *J. Chem. Phys.* 2006, *125*, 194101; (b) Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. A* 2006, *110*, 5121.
2. Zhao, Y.; Truhlar, D. G. *Theo. Chem. Acc.* 2008, *120*, 215.
3. (a) McLean, A. D.; Chandler, G. S. *J. Chem. Phys.* 1980, *72*, 5639-5648. (b) Krishnan, R.; Binkley, J. S.; Seeger, R.; Pople, J. A. *J. Chem. Phys.* 1980, *72*, 650-654.
4. Scalmani, G.; Frisch, M. J.; Map, V. *J. Chem. Phys.* 2010, *132*, 114110.
5. Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* 2009, *113*, 6378.
6. Hratchian, H. P.; Schlegel, H. B. *J. Chem. Phys.* 2004, *120*, 9918-24. (b) Hratchian, H. P.; Schlegel, H. B. *J. Chem. Theory and Comput.* 2005, *1*, 61-69.

7. Gaussian 09, Revision A.02, 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, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Geometries and Cartesian coordinates of the important intermediates and transition states involved in the reaction

1:

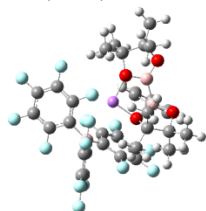


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1/B(C₆F₅)₃



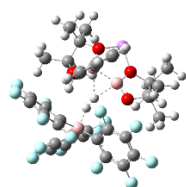
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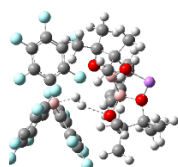
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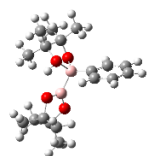
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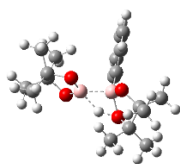


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H,0,-4.2536782864,1.4555036999,1.7600443394
H,0,-4.0478417435,1.8465587414,0.0473607101
H,0,-3.0923445953,-0.4510327799,2.7782010739
H,0,-4.1488554183,-1.5143446986,1.8208987696
H,0,-2.3817311338,-1.7308085893,1.7793659582
H,0,0.3465230683,-1.4464725826,-1.3525589739
C,0,1.2640931722,1.5821137996,-0.875871127
C,0,1.9904889222,2.6122054776,-0.259294029
C,0,0.8628330387,1.7796860846,-2.2078660172
C,0,2.3179307907,3.7847583222,-0.9458195525
H,0,2.3046833233,2.484231271,0.7734999844
C,0,1.1903238599,2.9442103999,-2.9059324993
H,0,0.2889005967,1.004020636,-2.7138093019
C,0,1.9217068066,3.9522846412,-2.2741138251
H,0,2.8821305779,4.566134397,-0.4470832962
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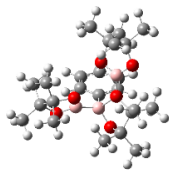


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O,0,1.7292479349,-0.1343554782,-1.2740820606
B,0,-0.6787160592,-0.7988434262,-0.1991561087
O,0,-1.1916618676,-1.2980322348,0.9676119443
O,0,-1.6165798089,-0.6794048916,-1.1964854183
C,0,2.9128187192,-0.8871974157,-0.8333982877
C,0,3.0856887311,-0.3776367869,0.6308046958
C,0,3.8636565693,-1.3297786144,1.5284159531
H,0,4.8671387788,-1.5103902853,1.1281478433
H,0,3.962817863,-0.887145103,2.5229653513

H,0,3.3392061122,-2.2814110636,1.6312377694
C,0,3.6873688368,1.0312369887,0.6803341196
H,0,3.5653590314,1.4208980919,1.6945112377
H,0,4.7532889365,1.019710525,0.4324074769
H,0,3.1679682536,1.7057984121,-0.0078267392
C,0,4.0535116845,-0.5375889542,-1.7762814197
H,0,4.9919090075,-0.9649642304,-1.4072112308
H,0,3.8537610321,-0.94781237,-2.7698182731
H,0,4.1667604287,0.5438406684,-1.8664735006
C,0,2.5796016541,-2.3790847326,-0.8917891187
H,0,2.2217869688,-2.6286410291,-1.8954222283
H,0,3.4667075128,-2.9836922026,-0.6843515701
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C,0,-2.5879508664,-1.6649475679,0.7062169862
C,0,-2.9279914787,-0.7939470901,-0.546445087
C,0,-3.4105763787,-1.3468044061,1.9453898771
C,0,-2.5971830242,-3.1653189927,0.4133555103
C,0,-3.9061546276,-1.4287521673,-1.5218236898
C,0,-3.3545642584,0.6307873091,-0.1875181093
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H,0,-4.8687268423,-1.611922403,-1.0324456535
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C,0,-0.0084567355,2.180449077,1.3884673944
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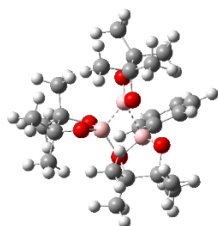


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B,0,-1.1183738266,1.0226883978,0.5887868434
O,0,-2.0257369221,2.0347880435,0.7410623805
O,0,0.0004818281,1.1267020862,1.3580248682
C,0,-0.1732008759,-1.9917062786,1.2784547449
C,0,1.0654536373,-2.3097883007,1.8551677193
C,0,-1.3083336162,-2.1364478443,2.0923508681
C,0,1.17000034,-2.753968742,3.1763295319
C,0,-1.220031582,-2.5674643599,3.4158125147
C,0,0.0261457846,-2.8806041347,3.9637611734
B,0,1.1565994671,-0.8894914491,-0.9550458289
O,0,2.316620806,-1.6241507159,-1.1375279094
O,0,1.3341761465,0.4235549553,-1.3635462691
C,0,-1.9470321977,-1.5183136572,-1.9805520221
C,0,-2.4442153043,-0.250089963,-1.1948457175
C,0,-2.6023709093,0.9914241412,-2.0628370521
H,0,-3.2469989923,0.7513728453,-2.9147137205
H,0,-3.0669186196,1.8013396927,-1.4966872403
H,0,-1.6380180507,1.3369632826,-2.4437445709
C,0,-3.6965409979,-0.5131757139,-0.3676493445
H,0,-3.8398658142,0.2959115853,0.3546918325
H,0,-4.5735323957,-0.543757546,-1.0208421927
H,0,-3.6278869111,-1.4635844185,0.1647674709
C,0,-3.1036899474,-2.3688183475,-2.497603211
H,0,-3.769746297,-1.7813364584,-3.1382579116
H,0,-2.6978049525,-3.1942731664,-3.0899734982
H,0,-3.6811284886,-2.7918348598,-1.6733634668
C,0,-1.0265664911,-1.1560091667,-3.1547838045
H,0,-0.4981630841,-2.0641519905,-3.4627118292
H,0,-1.607837041,-0.7901088853,-4.0070482313
H,0,-0.2925371037,-0.3936056489,-2.8913948266
C,0,-1.3359541691,3.0591501252,1.5464449758
C,0,-0.2777752241,2.2000596709,2.3199837231
C,0,-2.3573403556,3.7555785973,2.4281899976

C,0,-0.7009727068,4.0332941612,0.5570602516
C,0,1.0214746477,2.9228439165,2.6307370214
C,0,-0.8470997913,1.5306843863,3.5690681373
H,0,-1.8571034134,4.4508419888,3.1101636943
H,0,-3.0521380241,4.3273887326,1.8062281727
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H,0,-2.2875971638,-1.8993373304,1.6827690068
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H,0,3.9042692377,-1.733034099,-3.2598318147
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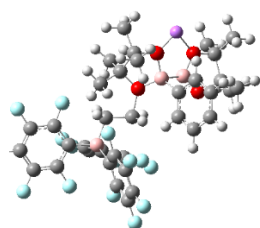


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O,0,0.2471083306,2.0751604231,0.3125013812
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C,0,-1.7206372064,-0.3716353885,2.5503925581
C,0,-3.1342727668,0.7862883239,0.9878055581
C,0,-2.5004978555,0.1045880847,3.6051829787
C,0,-3.9067396032,1.2814559611,2.037827458
C,0,-3.5897834477,0.9398533277,3.3534589164
B,0,0.780177965,-0.6353271949,0.2460859764
O,0,1.9866345925,-0.7577015529,-0.4877582502
O,0,1.0738900917,-0.5562627628,1.6305432705
C,0,-0.5630940821,-2.6242292697,-1.1529005737
C,0,-1.9961759885,-2.1446503709,-1.5458460433
C,0,-2.3304596877,-2.3047433043,-3.0206047947
H,0,-2.2486250711,-3.3533021788,-3.3251952293
H,0,-3.3605409639,-1.9783841878,-3.1907964272
H,0,-1.6705225485,-1.6978837473,-3.642691238
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H,0,-3.237171156,-3.8334965515,-0.9489447676
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C,0,-0.473190108,-4.0701404568,-0.697167739
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C,0,1.0563821542,4.3361080971,-0.0480830211
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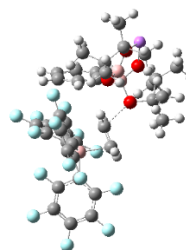
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O,0,4.5022908585,-0.604191923,1.5564747724
O,0,2.6108726196,0.6244147568,1.917155242
C,0,3.633383401,1.5509228315,-1.3212597562
Li,0,5.5513168769,-1.3185089949,0.1933098984
C,0,-3.4164104348,-3.1433249465,1.5639740982
C,0,-4.6746043602,-2.6142549735,1.7809395735
C,0,-4.9018918814,-1.2859538352,1.4709569899
C,0,-3.871488988,-0.5276109106,0.9406158838
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C,0,-2.7755100133,1.8665164599,-1.4537936756
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C,0,3.3883520528,0.6654048334,3.1721176885
C,0,5.6752459706,-0.4385159735,3.6897294706
C,0,3.6321269555,-1.8839078182,3.3990833129
C,0,2.4581774288,0.5835173842,4.3700833659
C,0,4.1434133116,1.9937366792,3.1592951854
H,0,5.5492055349,-0.2823801548,4.7659611152
H,0,6.2549968992,-1.356355956,3.5505004181
H,0,6.2418633153,0.4004520465,3.2801720232
H,0,4.2474192278,-2.7246030544,3.0635043408
H,0,3.5095350739,-1.9630172079,4.4826344731
H,0,2.6457712393,-1.9629428803,2.9301779453
H,0,3.0330219508,0.3524372581,5.2738329763
H,0,1.9682997732,1.5450639231,4.5335540038
H,0,1.6952685098,-0.1870566748,4.2348649752
H,0,3.4167074922,2.8057952783,3.0568799403
H,0,4.6975012672,2.1434848186,4.0905877642
H,0,4.8412912552,2.0501026148,2.3171751511
C,0,2.951008121,2.6370916486,-0.7423111865
C,0,4.5709940303,1.8528681157,-2.3254815524
C,0,3.1411672607,3.9510121104,-1.1796123035

H,0,2.2652010697,2.4509346133,0.0805878421
C,0,4.7820148517,3.1642351447,-2.7641313953
H,0,5.1538247711,1.049476831,-2.7645433681
C,0,4.0580711203,4.2174010894,-2.19892194
H,0,2.5845723264,4.7590348928,-0.7180212579
H,0,5.5114634403,3.3647759182,-3.5424556682
H,0,4.2152509935,5.2346251725,-2.5409088811

TS_{C₂H₄(O)}:



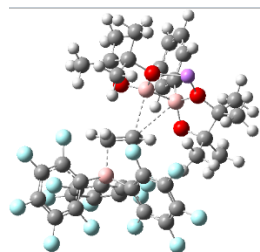
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B,0,1.9503959467,0.1174034294,-0.333392051
C,0,0.7796359365,-0.0047150447,-1.9359013946
C,0,-0.1877252951,0.0200111531,-0.9839822103
H,0,1.0850626398,0.9040360387,-2.4475355274
H,0,1.0362355886,-0.9506057998,-2.39207712
H,0,-0.6046114196,-0.9000067175,-0.5978532736
H,0,-0.6127833188,0.9445160848,-0.6024205306
B,0,-3.3603421438,-1.0136538238,-0.4028154309
O,0,-4.7331713795,-1.5635581369,-0.8607133068
O,0,-2.4659926104,-1.4893771708,-1.4839789889
B,0,-3.5655715483,0.7178000032,-0.2688059142
O,0,-4.8829309031,1.2382577468,-0.2280816481
O,0,-2.6687828605,1.7537936184,-0.1207357946
C,0,-2.9334102475,-1.6102145359,1.0554219641
Li,0,-5.9471032408,-0.2681392072,-0.503444019
C,0,5.050249941,-1.048869667,-2.6466516035
C,0,6.032277411,-1.169915569,-1.6833419997
C,0,5.7161694985,-0.8690094431,-0.3719639153
C,0,4.4271122493,-0.4757184639,-0.0589425786
C,0,3.3822385497,-0.3636073672,-0.9828345169
C,0,3.769896898,-0.6442482939,-2.2938429301
C,0,1.5736419012,-0.9507210746,0.8409032817
C,0,1.184374268,-2.2489063258,0.5129565341
C,0,1.6796719466,-0.7152985399,2.2103792072
C,0,0.8584821704,-3.2236701093,1.4386842756
C,0,1.3762866545,-1.6689701653,3.169156317
C,0,0.9536860713,-2.9279457278,2.7856304126
F,0,2.1090753718,0.502742957,2.6876920144

F,0,1.4428663782,-1.3551886703,4.5013120753
F,0,0.6090790928,-3.8572019943,3.7255819188
F,0,0.4234325585,-4.4570834232,1.0331157675
F,0,1.0859148398,-2.6077481103,-0.8213481302
F,0,4.205693693,-0.1320841743,1.2601884482
F,0,2.9130734645,-0.4911287734,-3.3672930537
F,0,5.3480914554,-1.3120563026,-3.9568990255
F,0,7.2958573093,-1.562832892,-2.0225811193
F,0,6.6757591648,-0.9478107403,0.6005867621
C,0,1.9223991426,1.6935259242,0.0385579949
C,0,0.9980874095,2.2567689259,0.9222035916
C,0,2.7706875281,2.6244376249,-0.5623417727
C,0,0.9386291299,3.6047196486,1.2238136778
C,0,2.7423025413,3.9841138038,-0.2865962567
C,0,1.8204772524,4.4806725579,0.6146729124
F,0,0.0529619179,1.4569136479,1.5322715176
F,0,3.6872289069,2.2330981386,-1.5172691294
F,0,3.6059048176,4.8370529123,-0.9189482765
F,0,1.7685675509,5.8173708878,0.8901517407
F,0,-0.0033570927,4.0841126198,2.096942586
C,0,-3.2461002859,-1.6496812265,-2.6732799421
C,0,-4.5690548729,-2.2708085429,-2.1158916106
C,0,-5.7997973883,-2.0309015041,-2.9858906802
H,0,-5.6647309335,-2.4680127375,-3.9812714746
H,0,-6.6766172761,-2.5053728266,-2.5306223909
H,0,-6.0045293611,-0.9622624968,-3.1134108097
C,0,-4.4172122027,-3.7638019176,-1.822581561
H,0,-5.2666441951,-4.0990940249,-1.2182127936
H,0,-4.4009899824,-4.3491367716,-2.7476897984
H,0,-3.4943153858,-3.9560037343,-1.2688712758
C,0,-2.4819533723,-2.5546611069,-3.6331475244
H,0,-3.0959650401,-2.8253701369,-4.4993206433
H,0,-1.5911243916,-2.0299752901,-3.9950664689
H,0,-2.1554564958,-3.4662166187,-3.1281284984
C,0,-3.4841506618,-0.2811086077,-3.3306577047
H,0,-2.5192715299,0.2288284624,-3.4290470667
H,0,-3.9271311419,-0.3847388039,-4.3270227691
H,0,-4.1459845713,0.3505770789,-2.7284121758
C,0,-4.8178238384,2.710744855,-0.2496422994
C,0,-3.3906585296,2.9503703372,0.3314370295
C,0,-5.9547277161,3.2686700478,0.5895591905
C,0,-4.9467171998,3.1381123874,-1.7098605011
C,0,-2.6872945383,4.1845892895,-0.2094800275
C,0,-3.3545313205,2.9300773304,1.859186834

H,0,-5.8562095576,4.3548429324,0.6858007322
H,0,-6.9133050305,3.0595451404,0.1041083042
H,0,-5.9673556995,2.8293491608,1.5890097063
H,0,-5.8842871749,2.7489291537,-2.1196559098
H,0,-4.9618588553,4.2282186179,-1.797854988
H,0,-4.1173753658,2.7506813464,-2.3099480181
H,0,-3.2790875224,5.0834345701,-0.0063941488
H,0,-1.721793961,4.3005963923,0.2911874128
H,0,-2.5177173038,4.1093007443,-1.2857786121
H,0,-2.3112712109,2.8914400706,2.1836756629
H,0,-3.8140639812,3.8304393925,2.2781486258
H,0,-3.8718993651,2.0506214461,2.2566780223
C,0,-2.1292945198,-0.8641085709,1.9399493191
C,0,-3.3776550541,-2.8632329249,1.5176811411
C,0,-1.7838892576,-1.3365744164,3.2120771264
H,0,-1.777106977,0.1190834325,1.6354002363
C,0,-3.0299059672,-3.3542461386,2.7812575089
H,0,-4.0215900312,-3.46064058,0.878199626
C,0,-2.2320103104,-2.5893526872,3.6378377576
H,0,-1.1695155156,-0.7277295923,3.8702546912
H,0,-3.3870013775,-4.3280130593,3.1025835172
H,0,-1.9634676222,-2.9635796571,4.6198400373

TS_{C₂H₄}:



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B,0,-1.8976951847,-0.0949448189,0.1413051024
C,0,-0.4363935689,-1.1751847705,-0.0693499598
C,0,0.5431408887,-0.2088162677,0.0908278104
H,0,-0.5418534798,-1.9135414405,0.7221383733
H,0,-0.587987077,-1.5413855744,-1.0757660741
H,0,0.8098906684,0.4646208461,-0.7135693526
H,0,0.9517916309,0.0601428261,1.0588327668
B,0,3.4371422108,0.3631998276,-0.0058036873
O,0,4.0382823769,0.9178169941,-1.2729231925
O,0,2.7061905856,1.4822960232,0.5635051404
B,0,2.7760123531,-1.2531399407,-0.4949671507
O,0,3.2497266186,-1.6493219091,-1.7676442637
O,0,2.3303052065,-2.3515663821,0.1905456598

C,0,4.5602038238,-0.2651911437,0.9975948357
Li,0,4.0790828022,-0.2381881036,-2.6436062893
C,0,-4.377903724,-2.9183000792,-1.2920030366
C,0,-5.5768476172,-2.2330061993,-1.2761948313
C,0,-5.5943225428,-0.9287838243,-0.8151966107
C,0,-4.4132240649,-0.3453009368,-0.3938586366
C,0,-3.1698034396,-0.9816586773,-0.3975883724
C,0,-3.2151755203,-2.2967522451,-0.8562039201
C,0,-1.8035961654,1.237316783,-0.8092135262
C,0,-1.3090916331,1.1686314579,-2.1104035489
C,0,-2.2384063695,2.511811032,-0.4405120302
C,0,-1.1936081257,2.2534292187,-2.9629238524
C,0,-2.1471643867,3.6231120011,-1.2648793582
C,0,-1.6152950497,3.4980256572,-2.5358940335
F,0,-2.777136492,2.742130041,0.8049128913
F,0,-2.5745330137,4.8481959262,-0.8275466681
F,0,-1.4964025716,4.589274545,-3.3508254972
F,0,-0.6270422611,2.1045129053,-4.2027818476
F,0,-0.8388285073,-0.0368717595,-2.6155650053
F,0,-4.5065953924,0.9435182341,0.0939900857
F,0,-2.0915407942,-3.1051644933,-0.8782666169
F,0,-4.3419760912,-4.2157288953,-1.7307306705
F,0,-6.7278654786,-2.8356683998,-1.7012967174
F,0,-6.7730061498,-0.233821285,-0.7709876
C,0,-1.9499867369,0.1833357186,1.74055509
C,0,-1.1707836913,1.168465301,2.3482611862
C,0,-2.6641005355,-0.6076918347,2.6381994765
C,0,-1.1074795825,1.3793082063,3.7128008362
C,0,-2.63441914,-0.4278368684,4.0140837177
C,0,-1.8532917191,0.5744228463,4.5575637623
F,0,-0.3797306562,1.9893328631,1.5637849916
F,0,-3.4310101344,-1.6674511314,2.1915556259
F,0,-3.3601262541,-1.2481081773,4.8363465599
F,0,-1.8061756494,0.7605167229,5.9109606215
F,0,-0.3091313533,2.3634500597,4.232457489
C,0,2.8407958869,2.6507160917,-0.2737775944
C,0,4.1397266191,2.3564309348,-1.0926263348
C,0,4.1998718351,3.0181925577,-2.4633952253
H,0,4.1430703547,4.107610437,-2.3679117051
H,0,5.1503468258,2.7757660799,-2.9516693086
H,0,3.3806703283,2.6872718954,-3.1076261982
C,0,5.412146005,2.6714823342,-0.3022841686
H,0,6.2721909817,2.2304474466,-0.8166025074
H,0,5.5675702943,3.752873667,-0.2364542989

H,0,5.3674609931,2.2601596126,0.7089592165
C,0,2.9309338705,3.8817297676,0.6210669778
H,0,3.1436282424,4.7808405074,0.0320055513
H,0,1.9752905711,4.0255047214,1.1351305724
H,0,3.708494092,3.7592991047,1.3779236395
C,0,1.6149825096,2.7712344959,-1.1887763245
H,0,0.7094634073,2.750833126,-0.5721430917
H,0,1.6300700417,3.7123952562,-1.7492246041
H,0,1.574675227,1.9456993442,-1.9103349734
C,0,2.9285268761,-3.0744975108,-1.9848160088
C,0,2.7272843226,-3.5744476678,-0.5156623956
C,0,4.0859895322,-3.7237839795,-2.7273580374
C,0,1.6545223886,-3.1065632804,-2.8237991769
C,0,1.6187641977,-4.6022681942,-0.3496730488
C,0,4.0190179927,-4.0538109339,0.1428373203
H,0,3.924841945,-4.8034623243,-2.8096327204
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H,0,5.0361066678,-3.5525595271,-2.2166878409
H,0,1.8321664949,-2.5865635237,-3.7703366463
H,0,1.3553982082,-4.1345378656,-3.0462212446
H,0,0.8287557412,-2.6077169021,-2.3085352
H,0,1.8356167032,-5.5013842015,-0.9358761232
H,0,1.5476911125,-4.8895038037,0.7031988734
H,0,0.6511769927,-4.2024335056,-0.6620827221
H,0,3.829847078,-4.2128713017,1.2083172344
H,0,4.3633881362,-4.9956313276,-0.2947414276
H,0,4.8123463131,-3.3057615617,0.0504839019
C,0,4.295631214,-0.3813205771,2.3737179651
C,0,5.7852626769,-0.7712197272,0.5335024185
C,0,5.216125772,-0.9630355723,3.2497103191
H,0,3.3551535237,0.0019458298,2.7646882399
C,0,6.7176546617,-1.353542518,1.4001812053
H,0,6.0223188174,-0.7000585822,-0.5274074789
C,0,6.4328198437,-1.4544176113,2.7639175141
H,0,4.9890574429,-1.0330423598,4.3089154573
H,0,7.6609379274,-1.7280304325,1.014268681
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