Supporting Information

Synthesis of a BC_6 Polymer via Cyclotrimerization of Alkynylborane and Its Application as a Heterogeneous Lewis Acid Catalyst

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1. Materials

Acetonitrile super dehydrated, benzene super dehydrated, boric acid, 1-butanol, copper(II) chloride, hexane, methanol, nickel(II) chloride, pyridine dehydrated, toluene super dehydrated and trimethylammonium Chloride were purchased from WAKO PURE CHEMICAL INDUSTRIES Ltd., 2-aminoethyl diphenylborinate, boron trifluoride ethyl ether complex and pyridine hydrochloride were purchased from TOKYO CHEMICAL INDUSTRY Co., Ltd., dicobalt octacarbonyl and ethylene glycol dimethyl ether dehydrated were purchased from KANTO CHEMICAL Co., Inc., ethynylmagnesium bromide in THF and sodium acetylide slurry in xylene were purchased from SIGMA-ALDRICH Co. LLC., palladium(II) chloride was purchased from TANAKA PRECIOUS METAL TECHNOLOGIES Co., Ltd., tetraphenylborate sodium salt was purchased from DOJINDO LABORATORIES Co., Ltd., Nitric acid was purchased from NACALAI TESQUE, INC.

2. General information

^{1}H (600 MHz, 400 MHz), ^{11}B (192 MHz, 128 MHz) and ^{13}C (151 MHz, 101 MHz) NMR spectra were recorded on JEOL JNM-ECZ600R and JEOL JNM-ECZL400S spectrometers. Proton and carbon chemical shifts are relative to solvent peaks [$CDCl_3$: 7.24 (^{1}H), 77.16 (^{13}C), DMSO-d_6: 2.49 (^{1}H), 39.52 (^{13}C)]. Boron chemical shifts are relative to $BF_3 \cdot Et_2O$ [$CDCl_3$: 0.0 (^{11}B)] or $NaBPh_4$ [DMSO-d_6: -7.8(^{11}B)] as an external standard. ^{11}B ss MAS NMR spectra and ^{13}C ss MAS NMR spectra were recorded on an Agilent DD2 500 MHz NMR spectrometer. Boron chemical shifts are relative to BPO_4 [-3.60 (^{11}B)] as an external standard. Carbon signals were accumulated using adamantane as an external reference (38.52 adamantane vs. 0 ppm TMS). NMR data were multiplied with an exponential window function with a line broadening factor of 40 Hz, prior to

Fourier transformation. FT-IR (ATR) spectra were measured with SHIMADZU IR Tracer-100 with a diamond. GC was carried out with SHIMADZU GC-2014 with FID detector. X-ray photoelectron spectroscopy (XPS) measurements were performed on a JEOL JPS-9030. ICP-OES was carried out with Agilent 5800 VDV. N_2 adsorption isotherm was measured with BELSORP MINI X, SEM and STEM observations were carried out with HITACHI SU9000.

3. Computation method

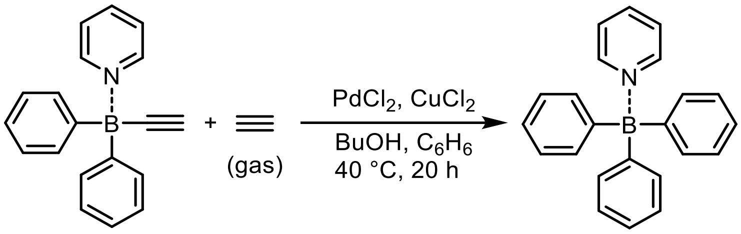
All calculations were conducted using Gaussian 09. The geometries for triphenylborane (BPh_3) and 1,3,5-tris(diphenylboranyl)benzene (TDBB) were optimized at the B3LYP/6-31+G(d) level of theory.

Table S1. GEI values of BPh_3 and TDBB at B3LYP/6-31+G(d)

	E_{LUMO} (eV)	E_{HOMO} (eV)	GEI (eV)
BPh_3 (optimized)	-2.014	-6.833	2.03
TDBB (optimized)	-2.039	-6.718	2.05
BPh_3 (planar, constrained)	-2.260	-6.806	2.26
TDBB (planar, constrained)	-2.393	-6.822	2.40

4. Catalyst screening using ethynyldiphenylborane·pyridine complex

4.1. Palladium catalysts



Ethynyldiphenylborane·pyridine complex (27 mg, 0.1 mmol), $PdCl_2$ (27 mg, 0.1 mmol), $CuCl_2$ (323 mg, 2.4 mmol), n-BuOH (720 μL, 7.86 mmol), and benzene (12 mL) were placed in a Schlenk tube under an argon atmosphere. An acetylene filled balloon was attached to the Schlenk tube. The mixture was stirred at 40 °C for 20 h. All solvents were removed under reduced pressure, and the product was dried under vacuum. The product was monitored by ^{11}B NMR spectroscopy.

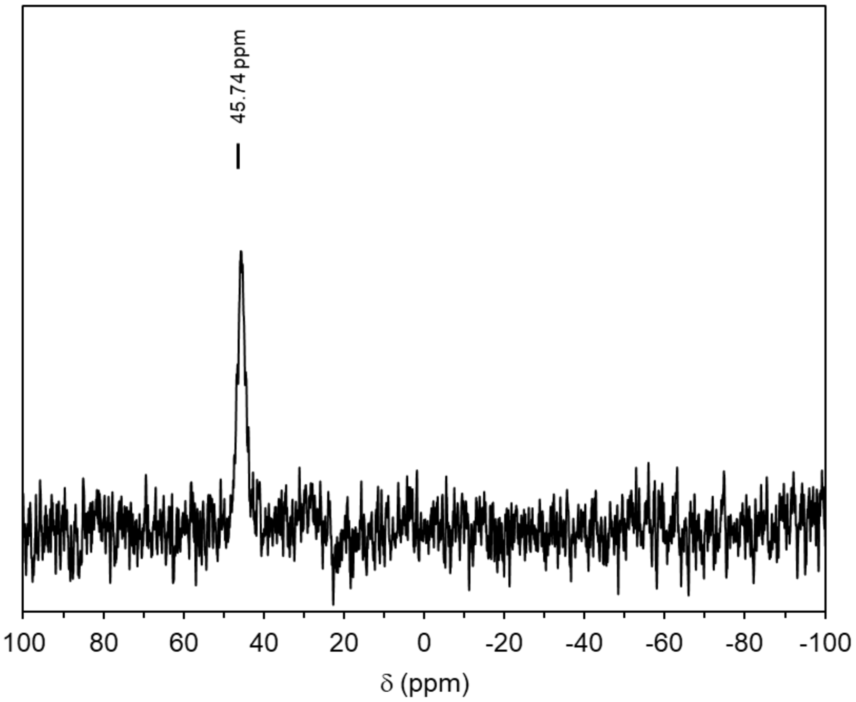
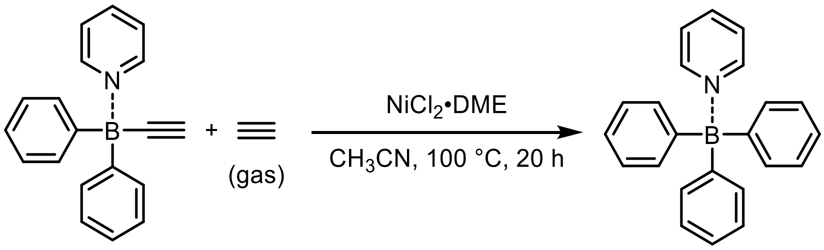


Fig. S1. ^{1}H NMR spectrum of the crude reaction mixture of the Pd-catalyzed model reaction.

4.2. Nickel catalysts



Ethynyldiphenylborane·pyridine complex (27 mg, 0.1 mmol), $NiCl_2$•DME (220 mg, 0.12 mmol) and CH_3CN (10 mL) were placed in a Schlenk tube under an argon atmosphere. An acetylene filled balloon was attached to the Schlenk tube. The mixture was stirred at 100 °C for 20 h. All solvents were removed under reduced pressure and dried under vacuum. The product was monitored by ^{11}B NMR spectroscopy.

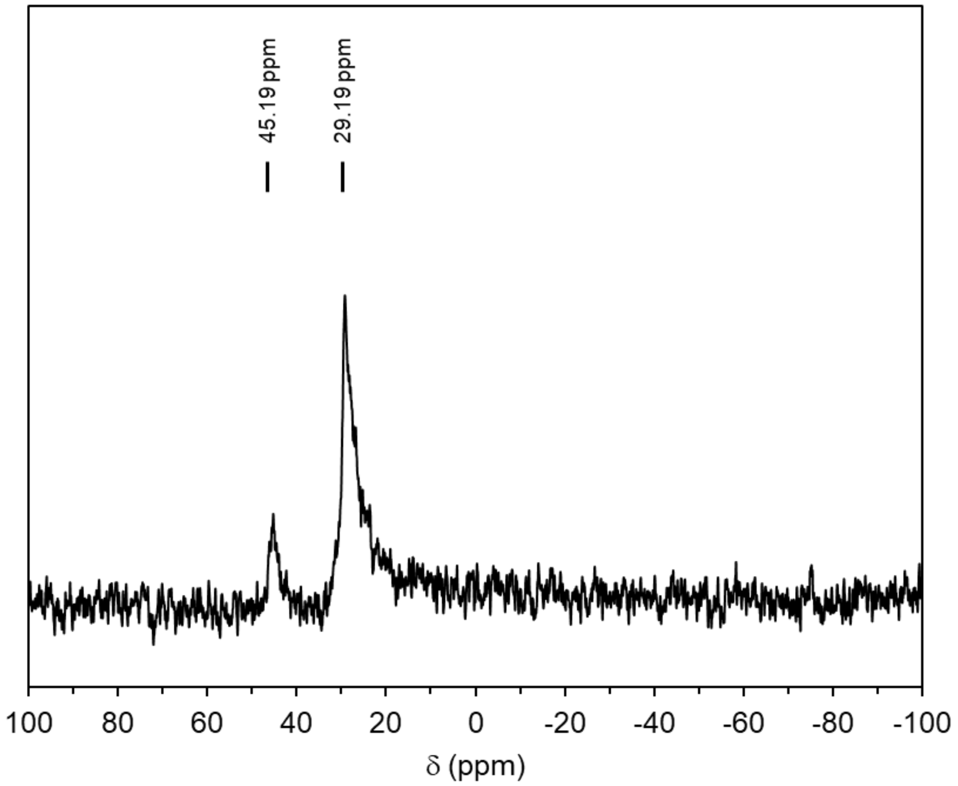
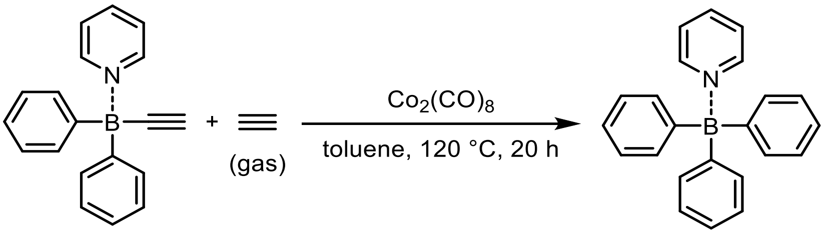


Fig. S2. ^{1}H NMR spectrum of the crude reaction mixture of the Ni-catalyzed model reaction.

4.3. Cobalt catalysts



Ethynyldiphenylborane·pyridine complex (27 mg, 0.1 mmol), $Co_2(CO)_8$ (41 mg, 0.12 mmol) were dissolved in toluene (12 mL) in a Schlenk tube under an argon atmosphere. An acetylene filled balloon was attached to the Schlenk tube. The mixture was stirred at 120 °C for 20 h. All solvents were removed under reduced pressure and dried under vacuum. The product was monitored by ^{11}B NMR spectroscopy.

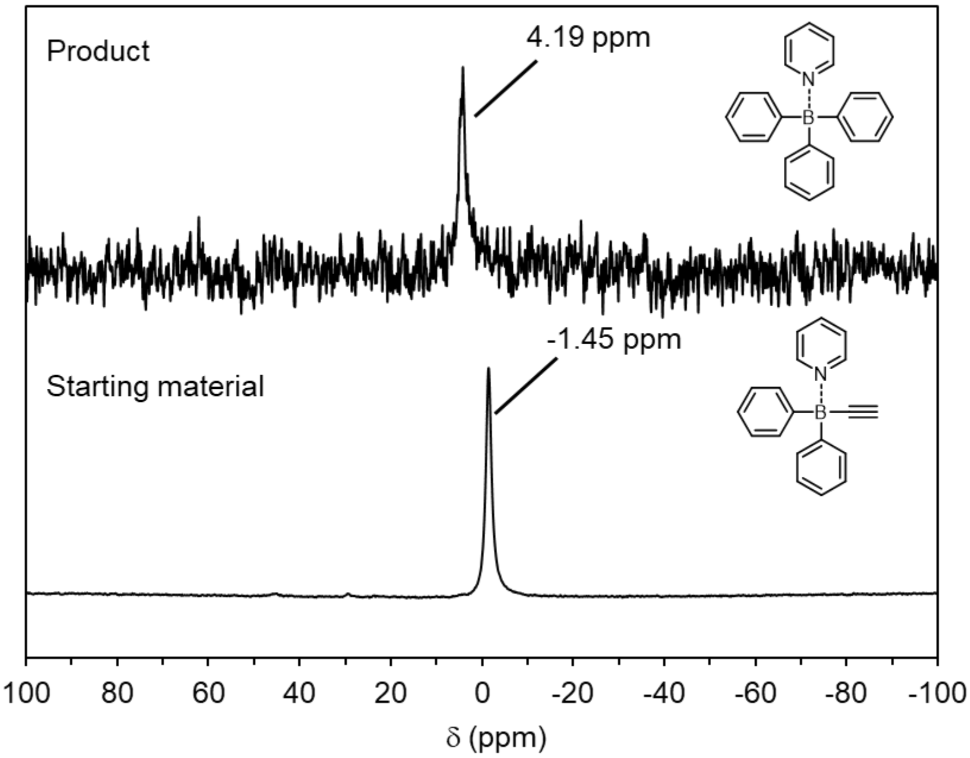
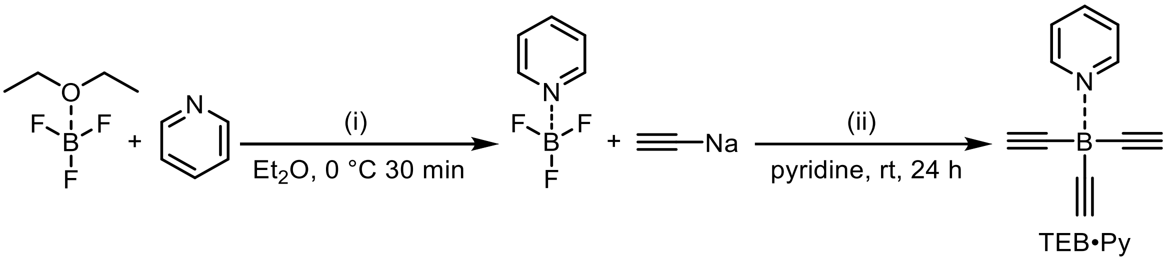


Fig. S3. ^1H NMR spectrum of the crude reaction mixture of the Co-catalyzed model reaction (top) and the starting material (bottom).

5. Synthesis

Preparation of triethynylborane pyridine



This compound was prepared following literature procedure.[1,2]

(i) Preparation of BF_3·pyridine

$BF_3 \cdot Et_2O$ (3.39 mL, 27 mmol) was dissolved in Et_2O (20 mL). Pyridine (2.17 mL, 27 mmol) was added to the solution. The reaction mixture was stirred for 30 minutes at 0 °C. A white crystal was filtrated under an argon atmosphere using a cannula technique.

(ii) Synthesis of triethynylborane·pyridine (TEB·Py)

BF_3·pyridine (27 mmol) was dissolved in pyridine (72 mL) at 0 °C. A slurry of sodium acetylide (24.5 mL, 81 mmol) was added to the solution. The reaction mixture was stirred for 24 h at room temperature. After completion of the reaction, the solvents were removed under reduced pressure. The crude product was purified by column chromatography on silica gel using chloroform as eluent to afford TEB·Py (34% yield)

^{1}H NMR (400 MHz, $CDCl_3$): $\delta = 9.22$ (dd, J = 6.5, 1.4 Hz, 2H), 8.13 (tt, J = 7.7, 1.5 Hz, 1H), 7.71 (dd, J = 7.7, 6.8 Hz, 2H), 2.36 (s, 3H). ^{11}B NMR (128 MHz, $CDCl_3$): $\delta = -17.2$ (s). ^{13}C NMR (101 MHz, $CDCl_3$): $\delta = 146.1, 142.0, 126.1, 85.2$

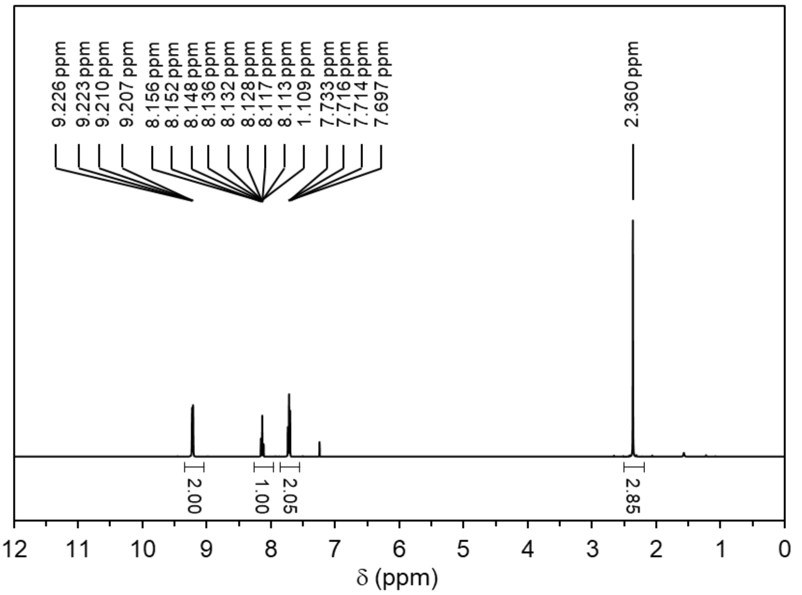


Fig. S4. ^{1}H NMR spectrum of TEB·Py

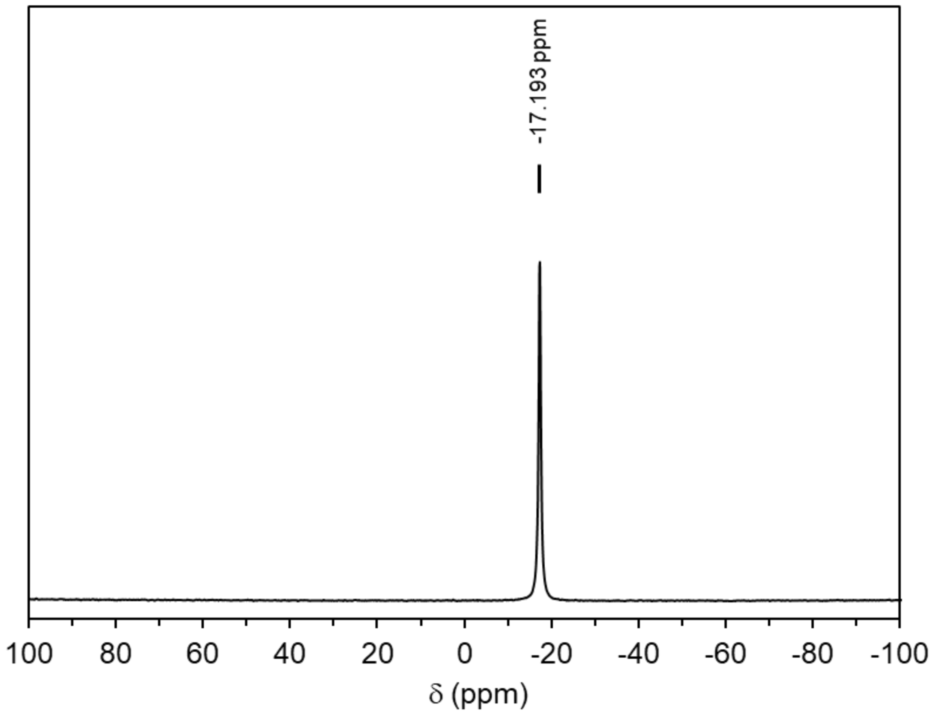


Fig. S5. ^{11}B NMR spectrum of TEB·Py

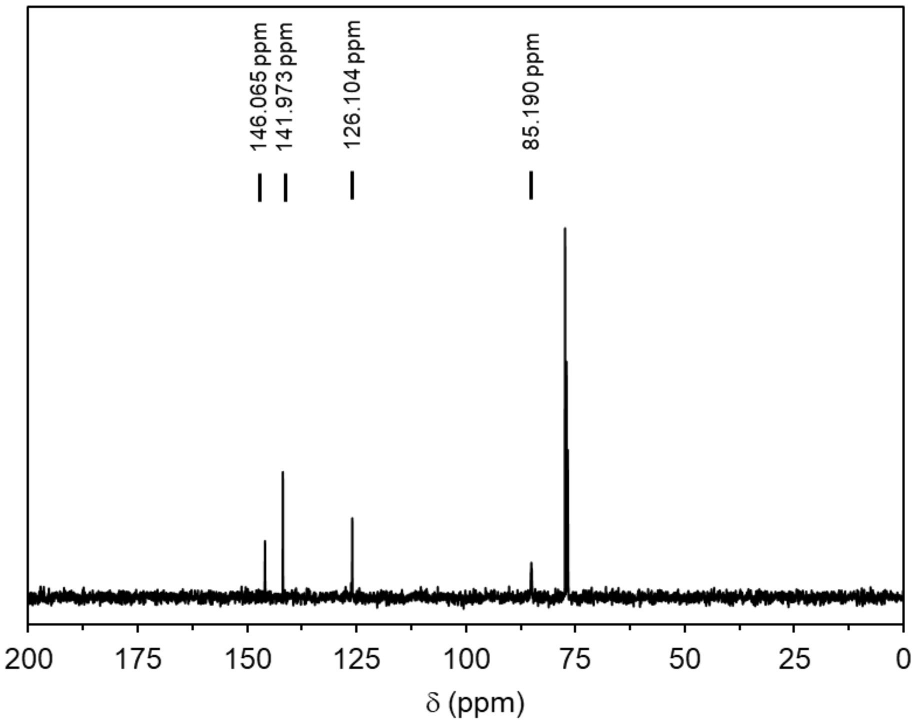
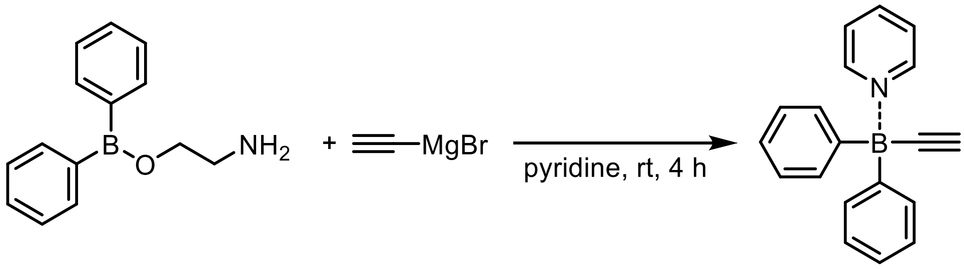


Fig. S6. ^{13}C NMR spectrum of TEB·Py

Preparation of ethynyldiphenylborane·pyridine



This compound was prepared following literature procedure.[3]

2-aminoethoxydiphenylborane (675 mg, 3.0 mmol) was dissolved in pyridine (20 mL). A THF solution of ethynyl magnesium bromide (4.95 mmol, 9.9 mL) was added to the solution. The reaction mixture was stirred at room temperature for 4 h. The reaction was quenched by the addition of methanol. The solvents were removed under reduced pressure. The crude product was purified by column chromatography using chloroform/ethyl acetate (6:4) as the eluent to afford ethynyldiphenylborane·pyridine (62% yield) .

^{1}H NMR (400 MHz, DMSO-d$_6$): δ = 8.65 (d, J = 5.4 Hz, 2H), 8.30 (t, J = 7.6 Hz, 1H), 7.84 (t, J = 6.8 Hz, 2H), 7.18-7.08 (m, 10H), 2.96 (s, 1H). ^{11}B NMR (128 MHz, DMSO-d$_6$): δ = -2.9 (s). ^{13}C NMR (101 MHz, DMSO-d$_6$): δ = 146.2, 142.2, 133.2, 127.1, 126.4, 125.6, 88.6.

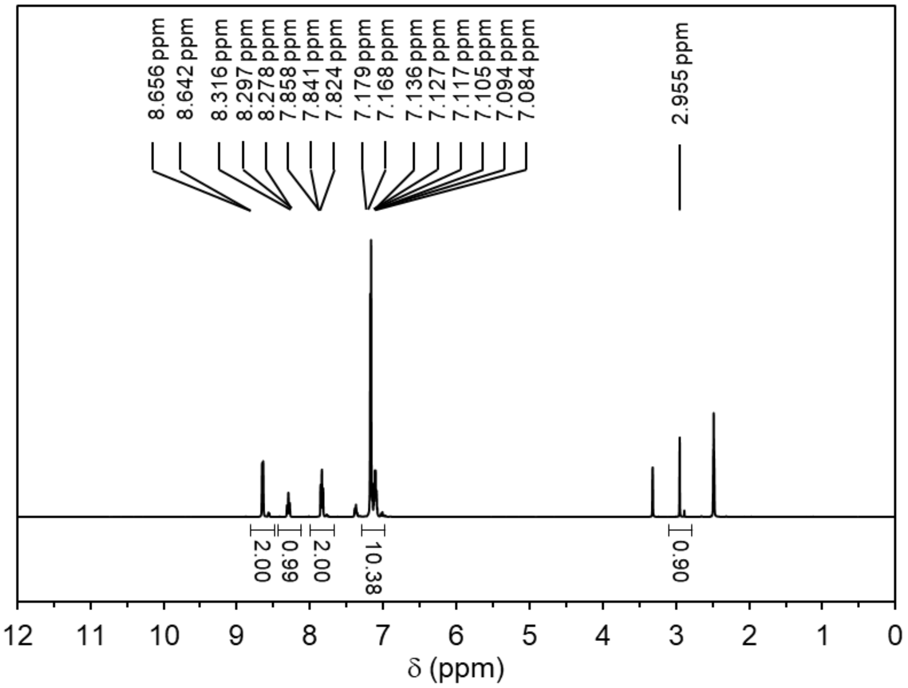


Fig. S7. ^{1}H NMR spectrum of ethynyldiphenylborane·pyridine

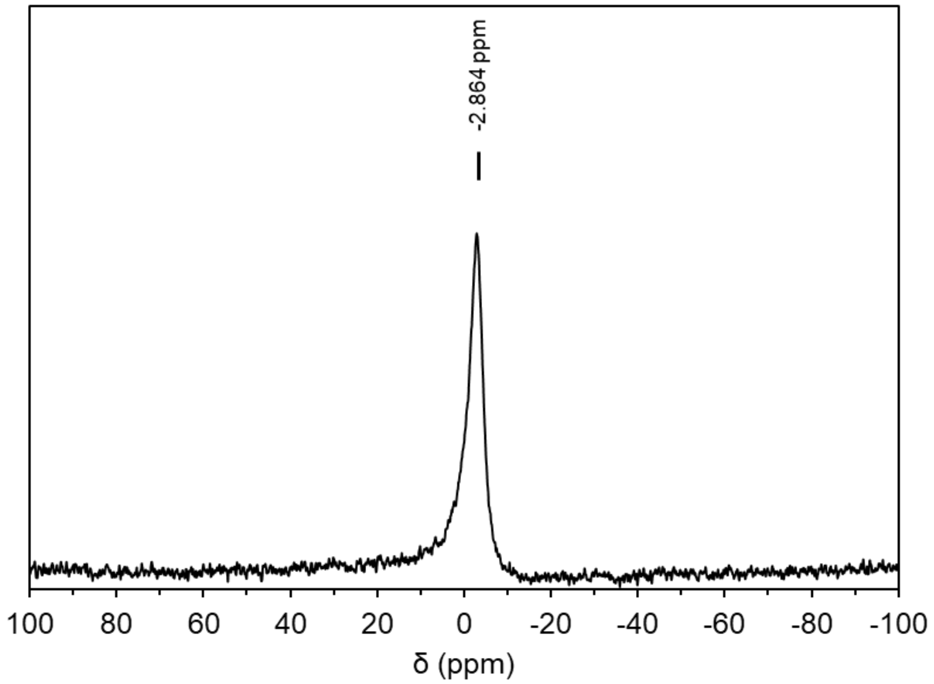


Fig. S8. ^{11}B NMR spectrum of ethynyldiphenylborane·pyridine

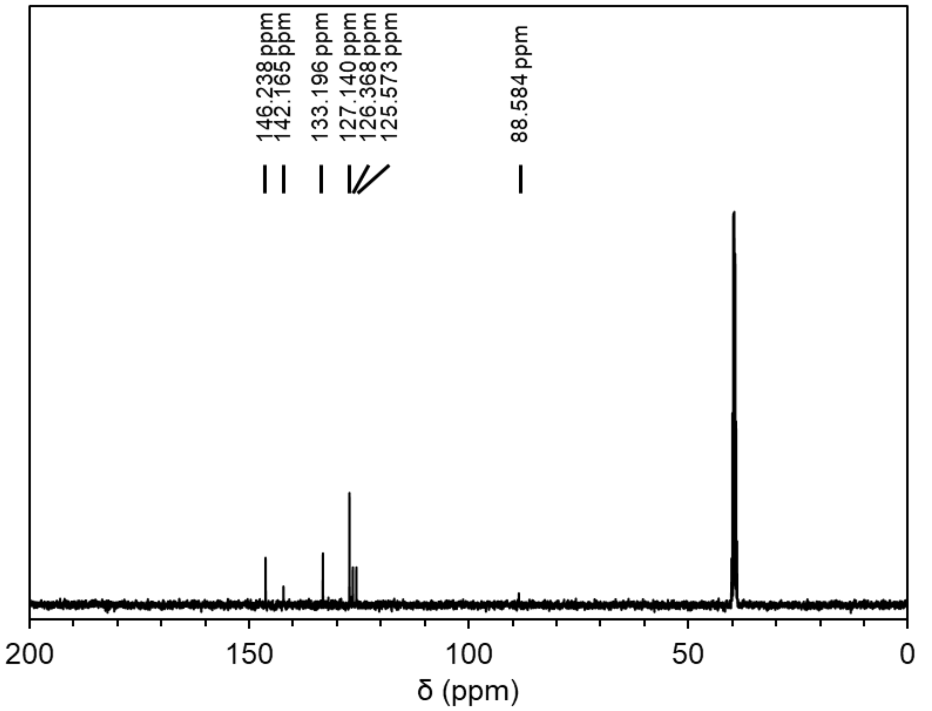
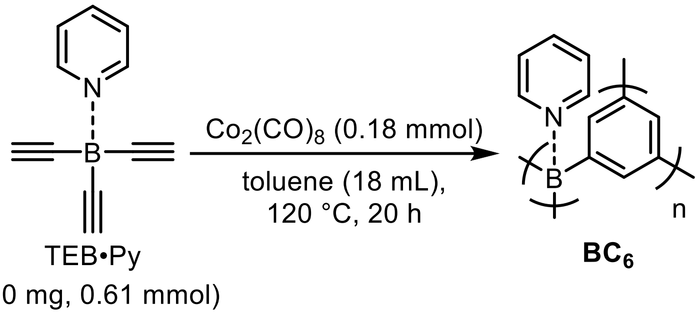


Fig. S9. ^{13}C NMR spectrum of ethynyldiphenylborane·pyridine

Synthesis of BC_6



TEB·Py (100 mg, 0.61 mmol) and $Co_2(CO)_8$ (62 mg, 1.82 mmol) were dissolved in toluene (18 mL) in a Schlenk tube under an argon atmosphere. The mixture was stirred at 120 °C for 20 h. All volatiles were removed under reduced pressure. The product was purified by washing with hexane, water, and methanol to afford a brown solid (120 mg). The polymer was used in the catalytic reaction without purification.

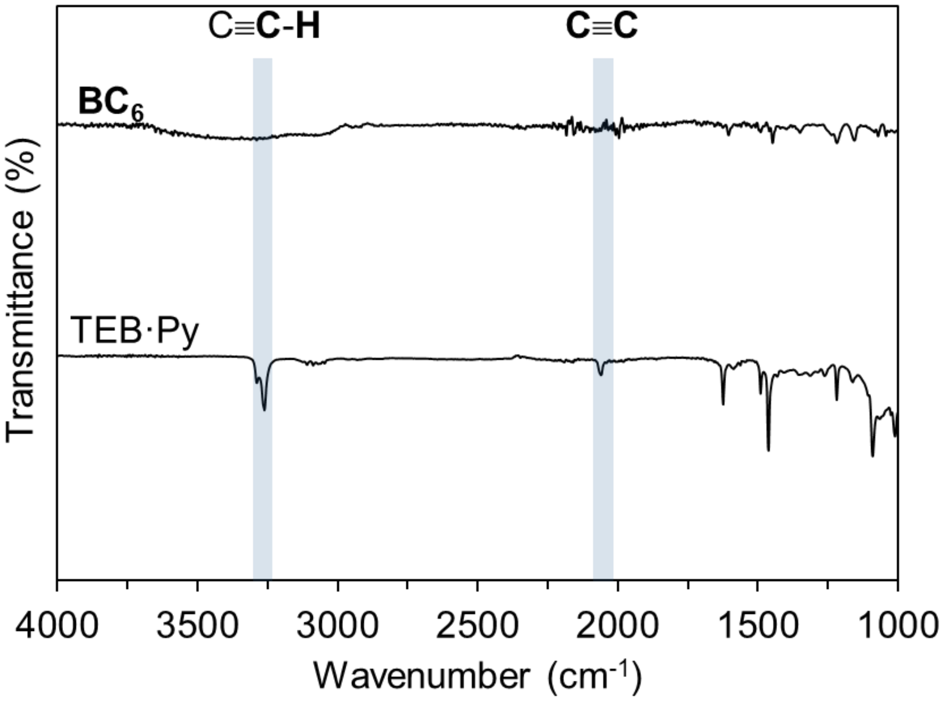


Fig. S10. IR spectra of **BC_6** and TEB·Py

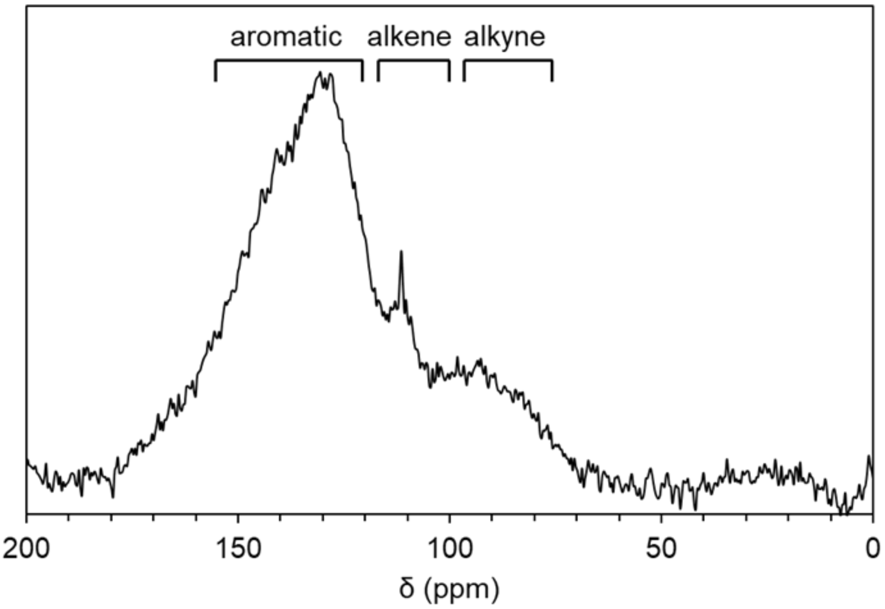


Fig. S11. ^{13}C ss MAS NMR spectrum of **BC$_6$**

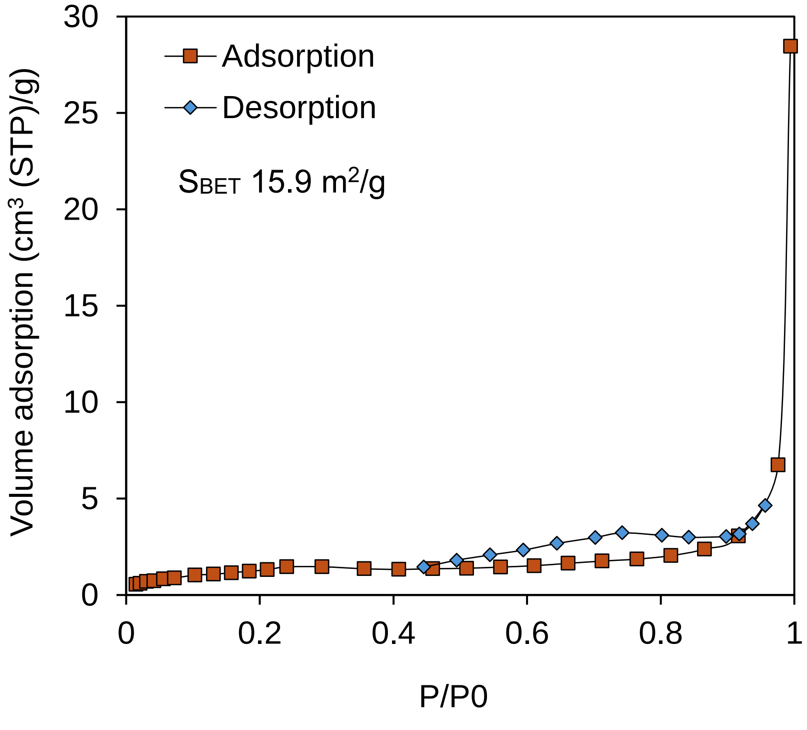


Fig. S12. N_2 adsorption-desorption isotherms of **BC$_6$**

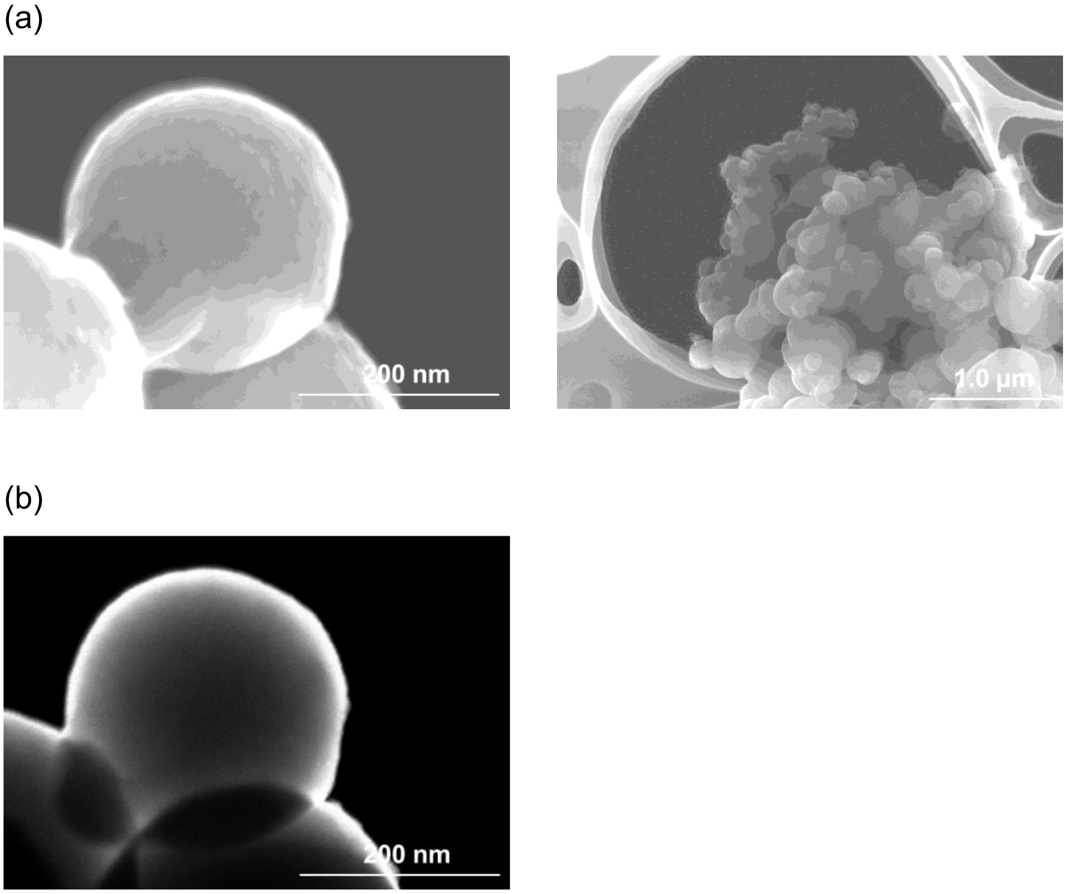


Fig. S13. (a) Scanning electron microscopy (SEM) and (b) scanning transmission electron microscopy (STEM) of **BC_6**

Table S2. Elemental analysis of **BC_6** by XPS

Elements	C (atomic%)	B (atomic%)	N (atomic%)	O (atomic%)	Co (atomic%)
Exp.	70.2	4.4	1.4	21.7	2.4
Calcd. (complexed)	84.6	7.7	7.7		
Calcd. (uncomplexed)	85.7	14.3			

Analysis of Reaction Filtrate

The filtrate was analyzed by ^{1}H and ^{11}B NMR spectroscopy using 1,1,2,2-tetrachloroethane (0.61 mmol) as an internal standard.

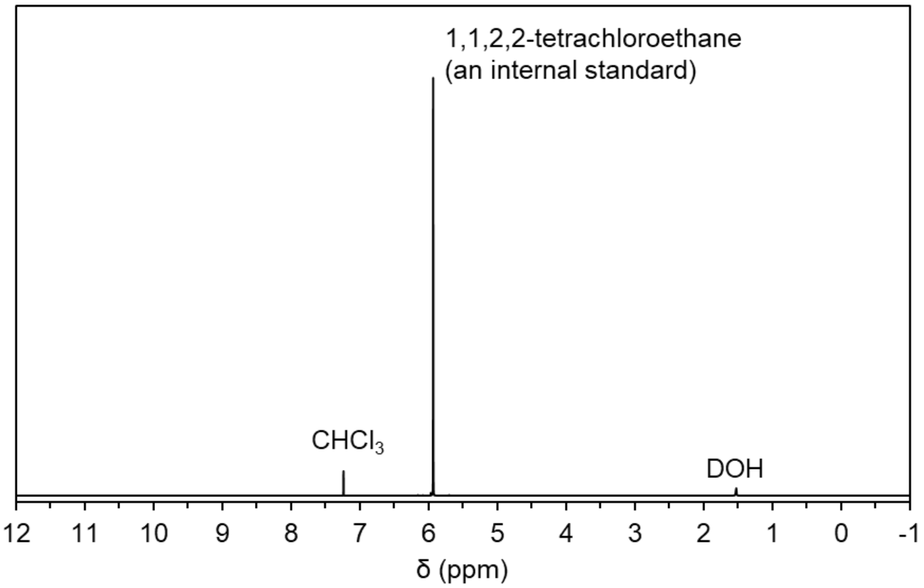


Fig. S14. ^{1}H NMR spectrum of the filtrate

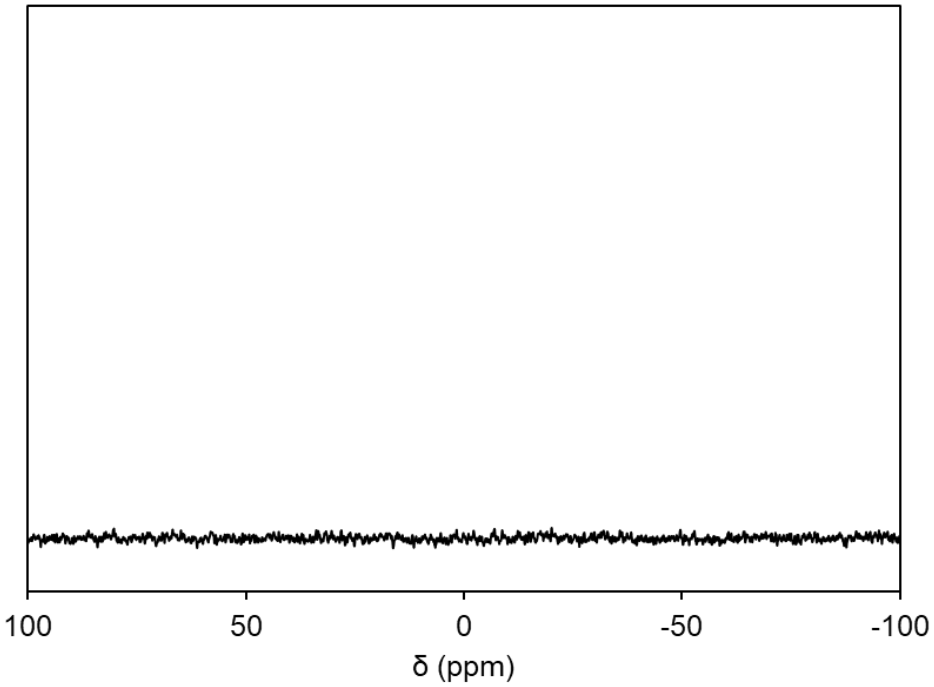
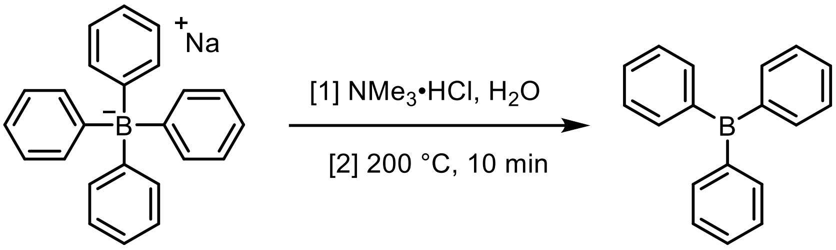


Fig. S15. ^{11}B NMR spectrum of the filtrate

Synthesis of triphenylborane (BPh_3)



BPh_3 was prepared following the literature.[4] Sodium tetraphenylborate (3422 mg, 10.0 mmol) was dissolved in H_2O (50 mL). A solution of trimethylamine hydrochloride (998 mg, 10.5 mmol) in H_2O (10 mL) was added to the solution. The resulting white suspension was washed with H_2O and MeOH. The residue was dried under reduced pressure. The obtained solid was then transferred to a Schlenk tube and heated at 200 °C for 10 minutes under an argon atmosphere. The resulting white solid was washed with hexane under inert condition and dried under reduced pressure to yield BPh_3 as a white powder (68% yield).

^{1}H NMR (600 MHz, $CDCl_3$): $\delta = 7.62$ (d, 6H), 7.56-7.53 (m, 3H), 7.46 (t, 6H). ^{11}B NMR (128 MHz, $CDCl_3$): $\delta = 67.07$ (s). ^{13}C NMR (151 MHz, $CDCl_3$): $\delta = 143.2$, 138.8, 131.4, 127.5.

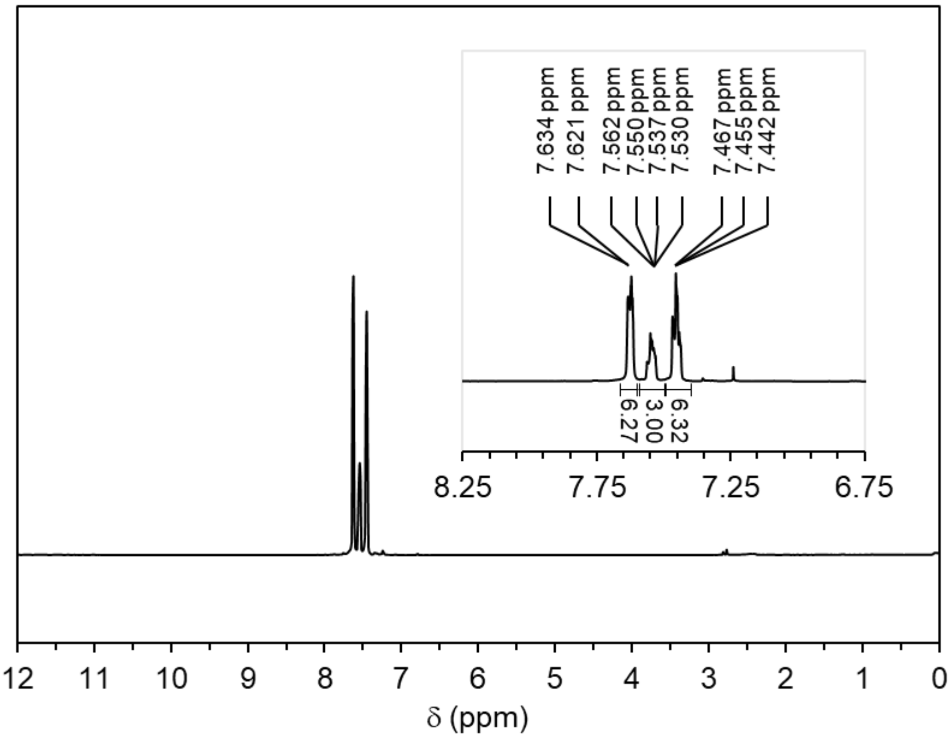


Fig. S16. ^{1}H NMR spectrum of BPh_3

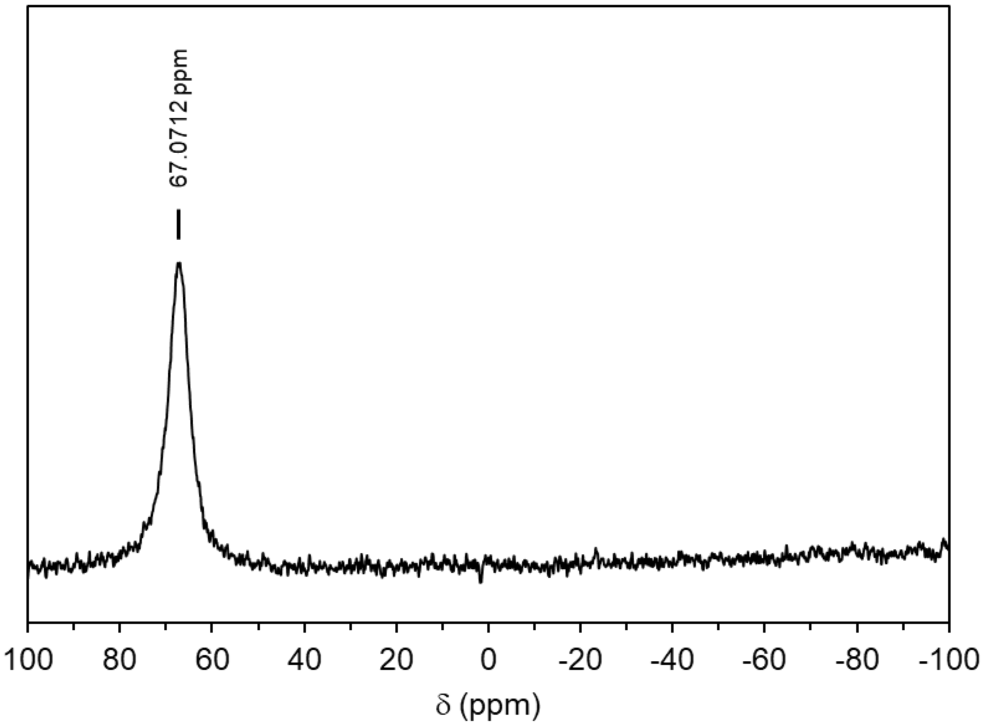


Fig. S17. ^{11}B NMR spectrum of BPh_3

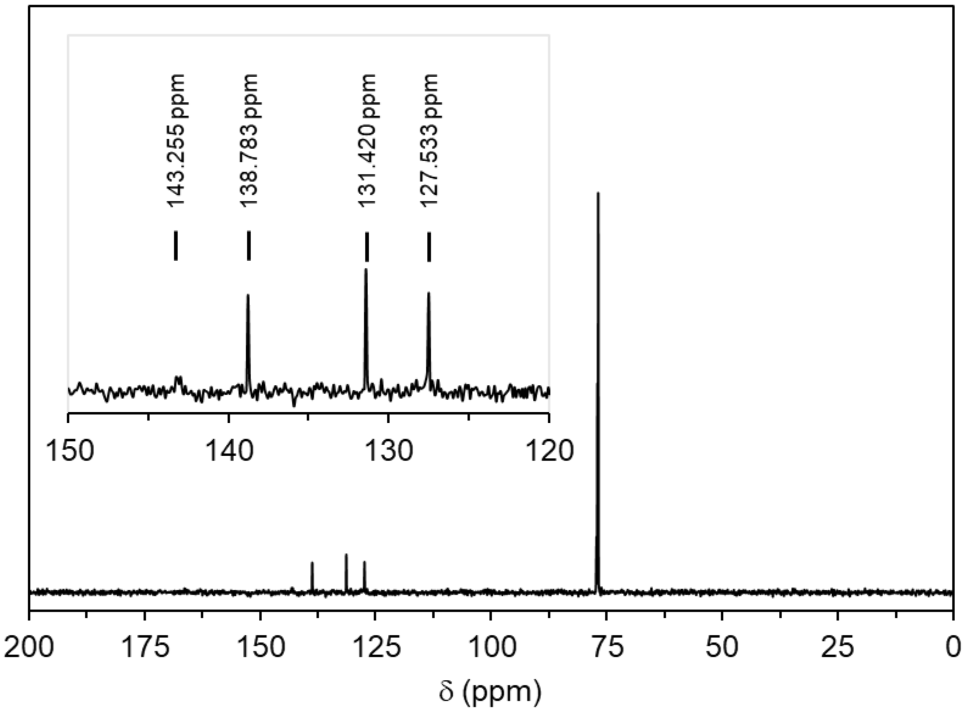
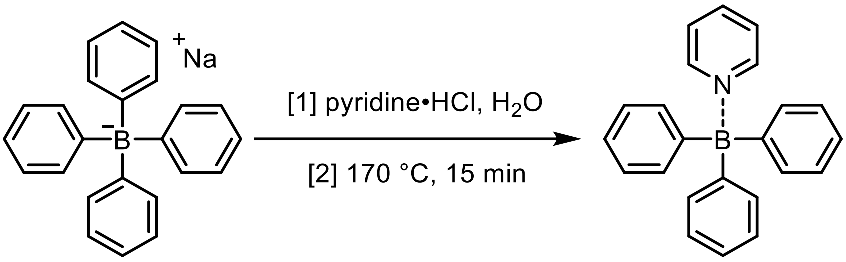


Fig. S18. ^{13}C NMR spectrum of BPh_3

Synthesis of triphenylborane·pyridine complex (BPh_3·Py)



The synthesis of BPh_3·Py was adapted from similar syntheses of aryl boranes reported in the literatures.[5] Sodium tetraphenylborate (1711 mg, 5.0 mmol) and pyridinium chloride (578 mg, 5.0 mmol) were dissolved separately in 20 mL and 5 mL of water, respectively. The two solutions were combined and stirred, and an additional 10 mL of water was used to ensure complete mixing. The resulting precipitate was collected by filtration and washed with water. The residue was dried under reduced pressure. The obtained solid was then heated at 170 °C for 15 minutes The obtained solid was then transferred to a Schlenk tube and heated at 200 °C for 10 minutes under an argon atmosphere. The resulting products were washed with Et_2O and dried under reduced pressure to yield BPh_3·Py complex as a white powder (83% yield).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.58 (d, 2H), 8.02 (t, 1H), 7.53 (t, 2H), 7.23-7.20 (m, 12H), 7.17-7.14 (m, 3H). ^{11}B NMR (193 MHz, $CDCl_3$): δ = 4.4. ^{13}C NMR (151 MHz, $CDCl_3$): δ = 152.2, 148.2, 140.4, 134.9, 127.2, 125.4, 125.1. [6]

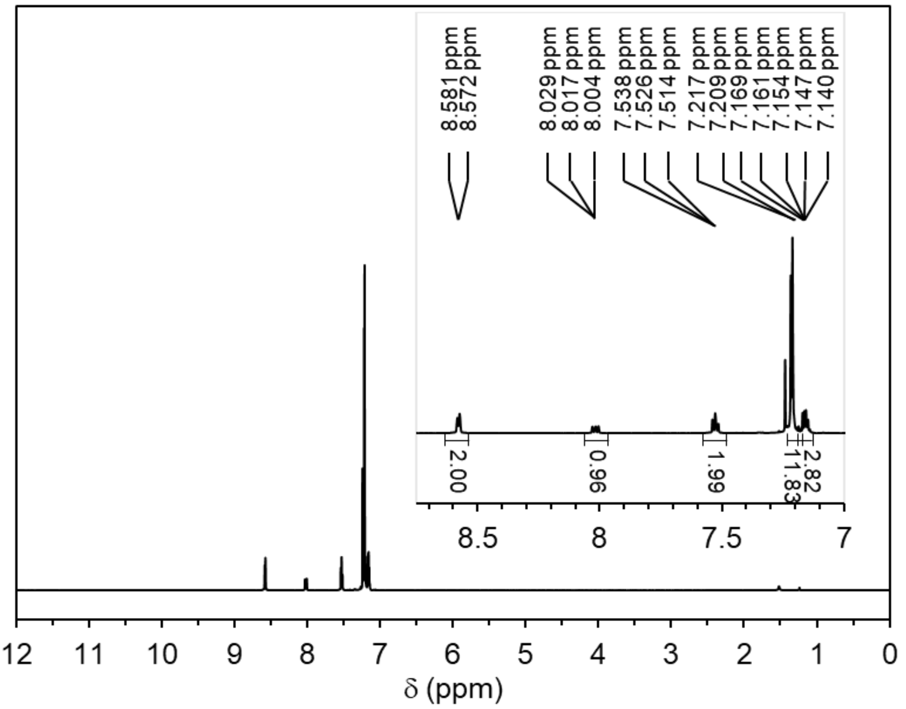


Fig. S19. ^{1}H NMR spectrum of $BPh_3 \cdot Py$

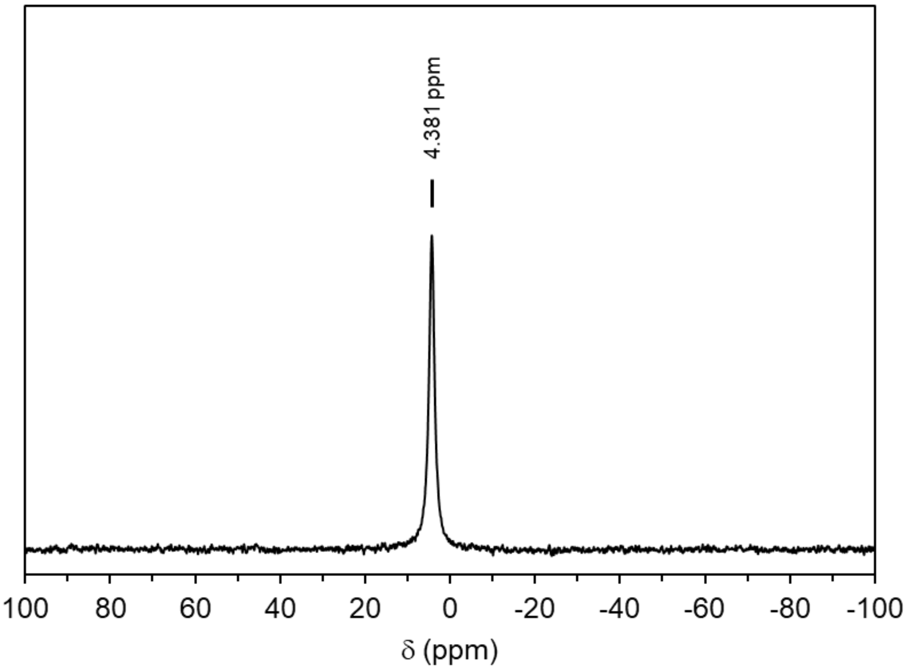


Fig. S20. ^{11}B NMR spectrum of $BPh_3 \cdot Py$

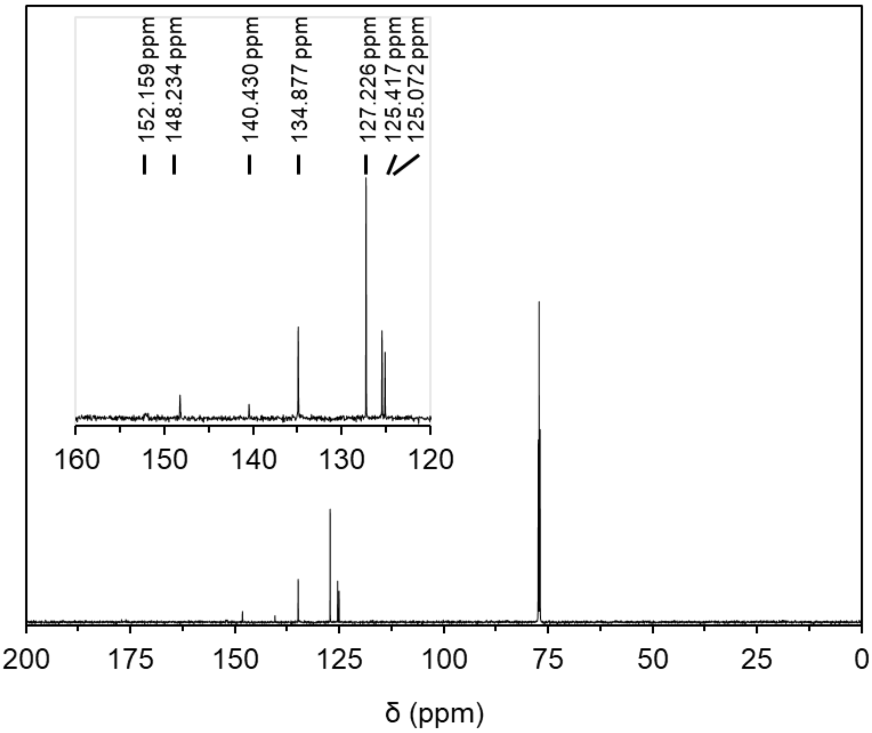


Fig. S21. ^{13}C NMR spectrum of $BPh_3 \cdot Py$

6. Typical procedure for the catalytic esterification of methyl benzoate

Methyl benzoate (63 μL, 0.5 mmol), 1-octanol (392 μL, 2.5 mmol), and the catalyst (10 mg) were placed in a Schlenk tube under an argon atmosphere. The reaction mixture was stirred at 180 °C for 1 h. The yield was calculated by GC-FID using dodecane as an internal standard.

For catalyst recycling, hexane (10 mL × 2) was added, and the solution was removed by decantation. The recovered catalyst was then dried under vacuum. Fresh substrates were subsequently added for the next run.

7. Controlled experiments for transesterification of methyl benzoate

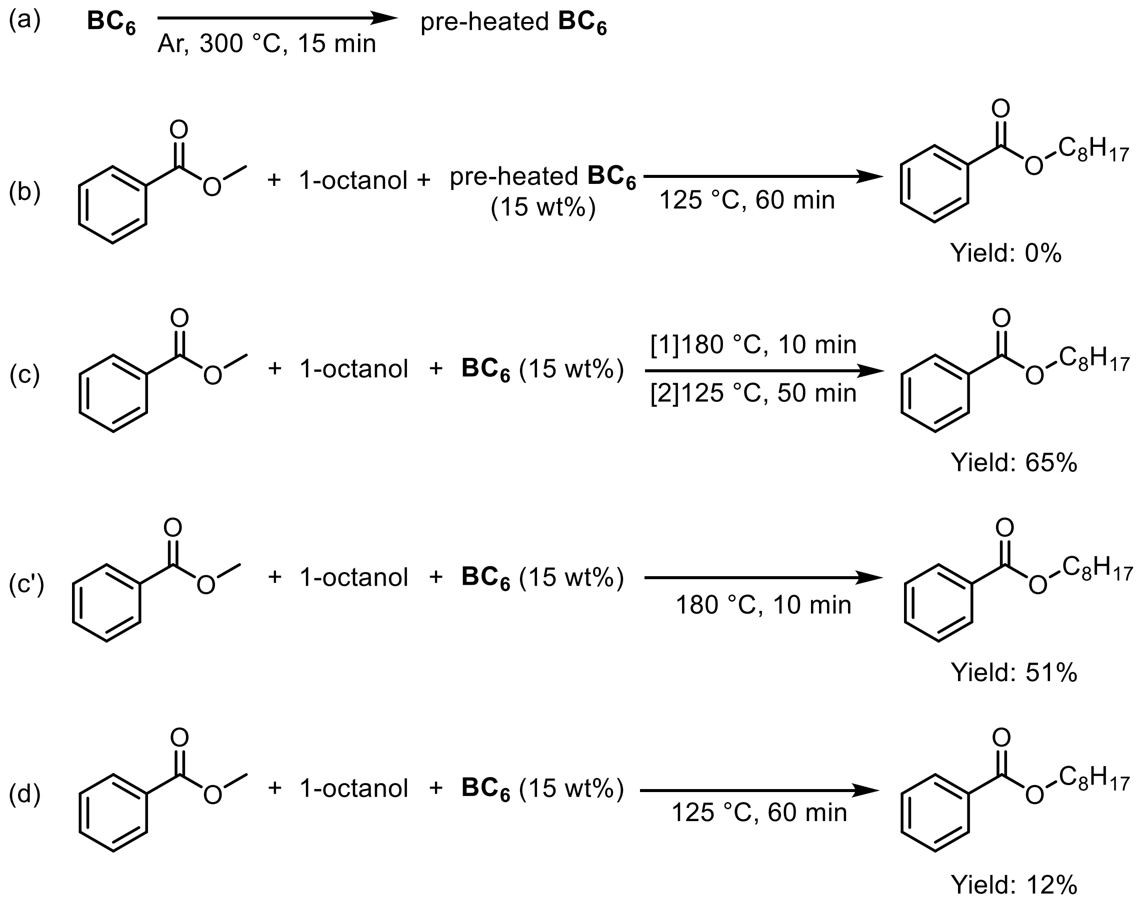


Fig. S22. Controlled experiments (a)-(d)

The reaction rate constant k was calculated using the following equation.

$$k = \frac{1}{t} ln \frac{[PhCOOMe]_0}{[PhCOOMe]_t}$$

The reaction rate constants at 125 °C (experiment c[2] and d) were calculated

$k_{c[2]} = 6.72\times10\text{-}3\ [s^{-1}]$

$k_d = 2.13\times10\text{-}3\ [s^{-1}]$

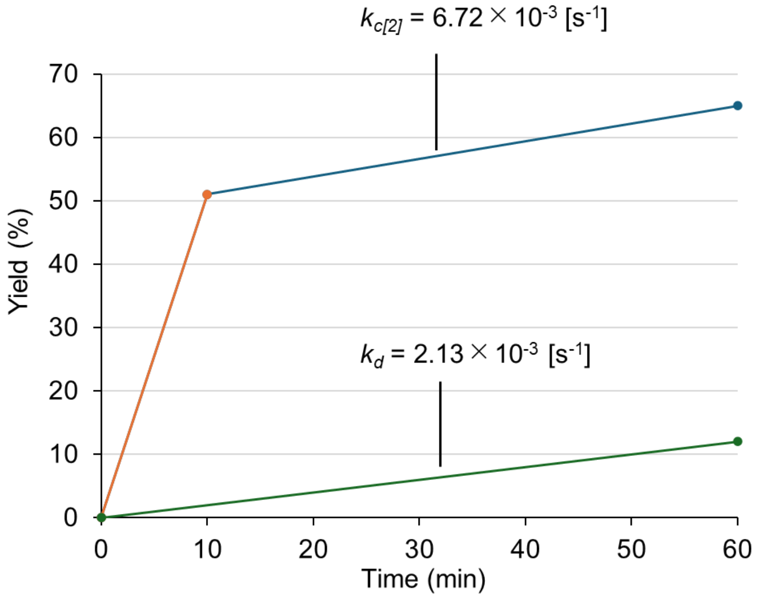


Fig. S23. Product yield for experiments Figure S22 (c) and (d)

8. Determination of boron leaching by ICP-OES

After the catalyst recycling test, the collected solution was dried under reduced pressure. The remaining solids were dissolved by 50 mL of 1% HNO_3. Standard samples (0, 0.1, 0.5, 1.0, 2.0 and 5.0 ppm) were prepared from boric acid in 1% HNO_3. The boron concentration was determined by ICP-OES at 182.577 nm.

9. Cartesian coordinates of the model structure

BPh_3 (optimized)

B	-0.00027500	-0.00086900	0.00025500
C	1.07347400	-1.14708700	-0.00044000
C	-1.53007200	-0.35694200	0.00017200
C	0.45541800	1.50221100	0.00147300
C	-2.02457000	-1.49548200	-0.67524900

C	0.84757300	-2.37183900	0.66780900
C	1.80648100	-3.38655500	0.68402600
C	3.01433300	-3.21693100	-0.00000100
C	-3.38586800	-1.80561100	-0.69086600
C	-4.29406000	-0.99813600	0.00099200
C	-3.83389500	0.12686600	0.69242800
C	1.62551200	1.91960300	0.67516500
C	2.02652800	3.25691500	0.68937500
C	1.28105300	4.21680000	-0.00222900
C	-2.47513800	0.44784900	0.67579000
C	0.12659900	3.83288700	-0.69174200
C	-0.28506100	2.49886700	-0.67369600
C	3.26131200	-2.02269900	-0.68428300
C	2.31025100	-1.00063100	-0.66845300
H	-1.33038200	-2.13921500	-1.20986000
H	-0.09038500	-2.52362600	1.19622500
H	1.61010800	-4.31111800	1.22200500
H	3.75821700	-4.01031800	0.00009000
H	-3.73782400	-2.67908300	-1.23488000
H	-5.35349400	-1.24394800	0.00123400
H	-4.53425200	0.75635200	1.23651600
H	2.22205100	1.18407300	1.20918800
H	2.92261200	3.54969000	1.23168900
H	1.59757300	5.25729800	-0.00374500
H	-2.13514800	1.33210700	1.20924800
H	-0.45512300	4.57375200	-1.23535200
H	-1.19049100	2.21846200	-1.20622200
H	4.19663600	-1.88616500	-1.22214700
H	2.52205300	-0.07440900	-1.19689100

TDBB (optimized)

C	0.00052000	-1.37961500	0.00001700
C	1.21114600	-0.70787700	0.27107000
C	1.18367100	0.70204900	0.21367700
C	-0.00057700	1.43906800	-0.00001700
C	-1.18425000	0.70111700	-0.21373000

C	-1.21063400	-0.70883600	-0.27108200
B	-2.52512600	-1.49833400	-0.61492600
B	2.52626900	-1.49633500	0.61487800
B	-0.00119200	3.01073800	-0.00000900
C	3.91955500	-0.96432100	0.12389100
C	2.44314800	-2.82139000	1.45350100
C	-2.44090800	-2.82345600	-1.45333900
C	-3.91887600	-0.96730000	-0.12421100
C	-1.20571100	3.79594700	0.63038400
C	1.20273300	3.79692200	-0.63030900
C	4.05965600	-0.30638700	-1.11830000
C	5.29930600	0.14623900	-1.57361000
C	6.43731300	-0.01756200	-0.77822400
C	6.32860900	-0.64869000	0.46494500
C	5.09069100	-1.12747400	0.89790500
C	1.45585900	-3.00597400	2.44769000
C	1.38703400	-4.17603700	3.20600000
C	2.29099000	-5.21601900	2.96836200
C	3.27012000	-5.07082300	1.98062600
C	3.35112800	-3.88494400	1.24828400
C	-1.64004300	5.03504900	0.10774500
C	-2.71411600	5.73039500	0.66643200
C	-3.36701600	5.21929700	1.79243000
C	-2.95112500	4.00276900	2.34180800
C	-1.89844600	3.29732700	1.75604500
C	1.63587600	5.03645500	-0.10770100
C	2.70940600	5.73271800	-0.66628200
C	3.36295200	5.22210400	-1.79212400
C	2.94825900	4.00514400	-2.34145200
C	1.89610100	3.29882000	-1.75581000
C	-1.45348900	-3.00739000	-2.44751300
C	-1.38364300	-4.17757100	-3.20554700
C	-2.28666000	-5.21830700	-2.96762600
C	-3.26590800	-5.07373700	-1.97991500
C	-3.34795900	-3.88775200	-1.24786000
C	-4.05965900	-0.30923000	1.11782500

C	-5.29971300	0.14259000	1.57283700
C	-6.43746500	-0.02220300	0.77729300
C	-6.32810400	-0.65352100	-0.46572400
C	-5.08976600	-1.13149600	-0.89838000
H	0.00093800	-2.46702100	0.00006400
H	2.11095200	1.24662900	0.37698700
H	-2.11193500	1.24499600	-0.37707700
H	3.18194900	-0.16056600	-1.74312900
H	5.37775000	0.63445600	-2.54214400
H	7.40217500	0.34620500	-1.12375700
H	7.20874800	-0.77370200	1.09138000
H	5.02531200	-1.62592700	1.86188400
H	0.73913900	-2.21102100	2.63805300
H	0.62521200	-4.28125500	3.97492600
H	2.23216900	-6.13393400	3.54862500
H	3.97267200	-5.87806100	1.78697700
H	4.12381300	-3.78502200	0.49014100
H	-1.13568800	5.45125500	-0.76068200
H	-3.03699800	6.67283600	0.23028700
H	-4.19568700	5.76484900	2.23783100
H	-3.45269100	3.60204800	3.21961300
H	-1.59368600	2.34732800	2.18815200
H	1.13102000	5.45228100	0.76061600
H	3.03136800	6.67549000	-0.23017200
H	4.19120200	5.76836700	-2.23743900
H	3.45033600	3.60479100	-3.21913100
H	1.59224600	2.34851100	-2.18787300
H	-0.73747800	-2.21184100	-2.63805500
H	-0.62174700	-4.28229300	-3.97446600
H	-2.22703400	-6.13630800	-3.54767000
H	-3.96774800	-5.88154500	-1.78606800
H	-4.12072900	-3.78831600	-0.48973700
H	-3.18215400	-0.16264200	1.74275300
H	-5.37867500	0.63095400	2.54125500
H	-7.40264700	0.34094000	1.12259000
H	-7.20805100	-0.77930600	-1.09227400

H	-5.02385200	-1.63012000	-1.86223400

BPh_3 (planar, constrained)

C	1.21364800	2.35070000	0.00000000
C	0.00000000	1.65000000	0.00000000
C	-1.21364800	2.35070000	0.00000000
C	0.00000000	4.45280000	0.00000000
H	2.14029500	1.81570000	0.00000000
H	-2.14029500	1.81570000	0.00000000
H	0.00000000	5.52280000	0.00000000
B	0.00000000	0.00000000	0.00000000
C	-1.42894200	-0.82500000	0.00000000
C	-1.42894200	-2.22640000	0.00000000
C	-2.64259000	-0.12430000	0.00000000
C	-2.64259000	-2.92710000	0.00000000
H	-0.50229500	-2.76140000	0.00000000
C	-3.85623800	-0.82500000	0.00000000
H	-2.64259000	0.94570000	0.00000000
C	-3.85623800	-2.22640000	0.00000000
H	-2.64259000	-3.99710000	0.00000000
H	-4.78288500	-0.29000000	0.00000000
H	-4.78288500	-2.76140000	0.00000000
C	1.42894200	-0.82500000	0.00000000
C	1.42894200	-2.22640000	0.00000000
C	2.64259000	-0.12430000	0.00000000
C	2.64259000	-2.92710000	0.00000000
H	0.50229500	-2.76140000	0.00000000
C	3.85623800	-0.82500000	0.00000000
H	2.64259000	0.94570000	0.00000000
C	3.85623800	-2.22640000	0.00000000
H	2.64259000	-3.99710000	0.00000000
H	4.78288500	-0.29000000	0.00000000
H	4.78288500	-2.76140000	0.00000000
C	1.21364800	3.75210000	0.00000000
H	2.14029500	4.28710000	0.00000000
C	-1.21364800	3.75210000	0.00000000

H	-2.14029500	4.28710000	0.00000000

TDBB (planar, constrained)

C	1.20807400	0.69748200	0.00000000
C	0.00000000	1.39490100	0.00000000
C	-1.20807400	0.69748200	0.00000000
C	-1.20802000	-0.69745100	0.00000000
C	0.00000000	-1.39496400	0.00000000
C	1.20802000	-0.69745100	0.00000000
H	2.16036400	1.24728700	0.00000000
H	-2.16036400	1.24728700	0.00000000
H	0.00000000	-2.49457400	0.00000000
B	-2.63713500	-1.52255000	0.00000000
B	0.00000000	3.04510100	0.00000000
B	2.63713500	-1.52255000	0.00000000
C	4.06646900	-0.69739100	0.00000000
C	4.06673000	0.69776900	0.00000000
C	5.27431500	-1.39499900	0.00000000
C	5.27461200	1.39508100	0.00000000
H	3.11432000	1.24745500	0.00000000
C	6.48265200	-0.69762400	0.00000000
H	5.27429200	-2.49460200	0.00000000
C	6.48299100	0.69720100	0.00000000
H	5.27489700	2.49476100	0.00000000
H	7.43483000	-1.24792400	0.00000000
H	7.43523600	1.24722300	0.00000000
C	2.63719200	-3.17297000	0.00000000
C	3.84526200	-3.87019100	0.00000000
C	1.42907900	-3.87077600	0.00000000
C	3.84548600	-5.26532900	0.00000000
H	4.79753500	-3.32037000	0.00000000
C	1.42913000	-5.26548800	0.00000000
H	0.47683200	-3.32080800	0.00000000
C	2.63770100	-5.96303500	0.00000000
H	4.79814900	-5.81479000	0.00000000
H	0.47692200	-5.81557600	0.00000000

H	2.63749200	-7.06271500	0.00000000
C	-1.42927700	3.87036100	0.00000000
C	-1.42905300	5.26519000	0.00000000
C	-2.63765100	3.17300700	0.00000000
C	-2.63716600	5.96295300	0.00000000
H	-0.47675700	5.81497200	0.00000000
C	-3.84548200	3.87040700	0.00000000
H	-2.63748800	2.07335200	0.00000000
C	-3.84528900	5.26583400	0.00000000
H	-2.63668100	7.06271300	0.00000000
H	-4.79797500	3.32081500	0.00000000
H	-4.79774500	5.81549200	0.00000000
C	1.42927700	3.87036100	0.00000000
C	1.42905300	5.26519000	0.00000000
C	2.63765100	3.17300700	0.00000000
C	2.63716600	5.96295300	0.00000000
H	0.47675700	5.81497200	0.00000000
C	3.84548200	3.87040700	0.00000000
H	2.63748800	2.07335200	0.00000000
C	3.84528900	5.26583400	0.00000000
H	2.63668100	7.06271300	0.00000000
H	4.79797500	3.32081500	0.00000000
H	4.79774500	5.81549200	0.00000000
C	-4.06646900	-0.69739100	0.00000000
C	-5.27431500	-1.39499900	0.00000000
C	-4.06673000	0.69776900	0.00000000
C	-6.48265200	-0.69762400	0.00000000
H	-5.27429200	-2.49460200	0.00000000
C	-5.27461200	1.39508100	0.00000000
H	-3.11432000	1.24745500	0.00000000
C	-6.48299100	0.69720100	0.00000000
H	-7.43483000	-1.24792400	0.00000000
H	-5.27489700	2.49476100	0.00000000
H	-7.43523600	1.24722300	0.00000000
C	-2.63719200	-3.17297000	0.00000000
C	-1.42907900	-3.87077600	0.00000000

C	-3.84526200	-3.87019100	0.00000000
C	-1.42913000	-5.26548800	0.00000000
H	-0.47683200	-3.32080800	0.00000000
C	-3.84548600	-5.26532900	0.00000000
H	-4.79753500	-3.32037000	0.00000000
C	-2.63770100	-5.96303500	0.00000000
H	-0.47692200	-5.81557600	0.00000000
H	-4.79814900	-5.81479000	0.00000000
H	-2.63749200	-7.06271500	0.00000000

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