Electronic Supplementary Material (ESI) for Dalton Transactions.

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1. Figures S1-S24

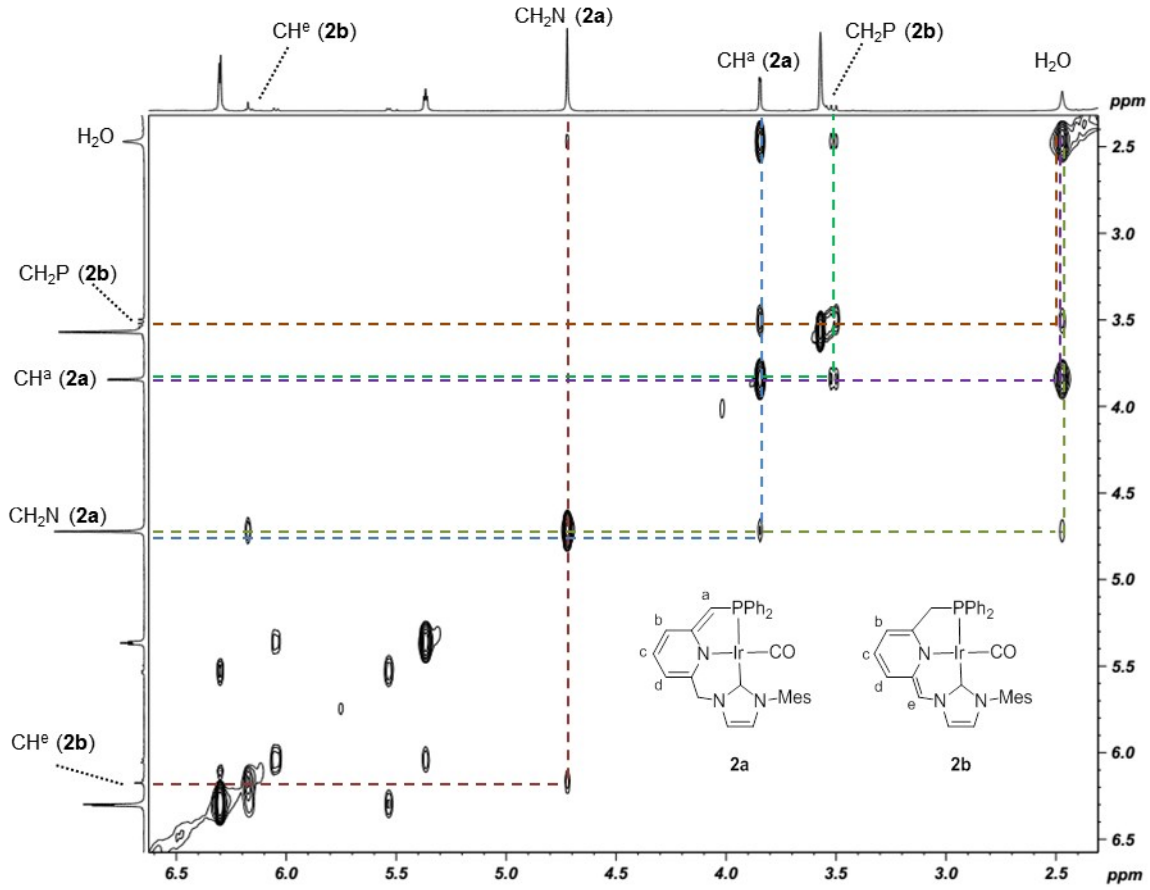


Figure S1. Region of the ^{1}H-^{1}H EXSY spectrum of a mixture of **2a** and **2b** in wet THF-d_8 (mixing time = 0.8 s) (500 MHz, 25 ^{o}C).

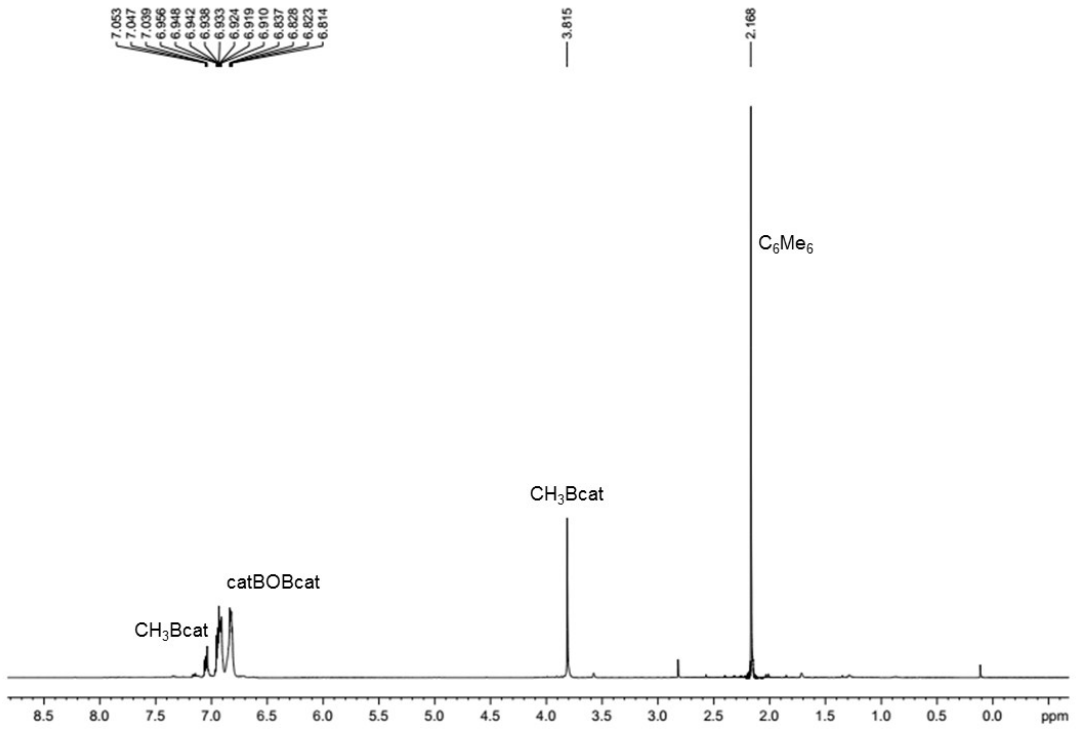


Figure S2. $^{1}H\{^{11}B\}$ NMR spectrum (400 MHz, THF-d_8) of the hydroboration of CO_2 with HBcat catalyzed by **2a**/**2b** (Table 1, entry 2).

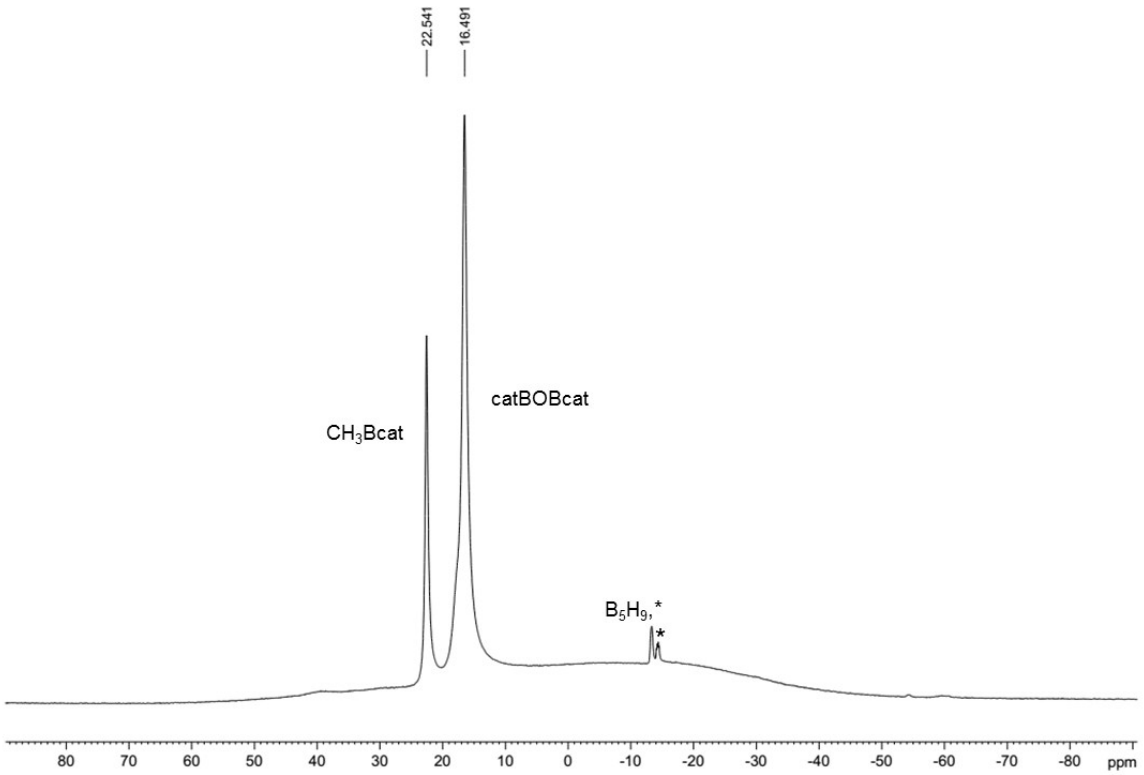


Figure S3. ^{11}B NMR spectrum (128 MHz, THF-d_8) of the hydroboration of CO_2 with HBcat catalyzed by **2a**/**2b** (Table 1, entry 2) (*, B_5H_9 and other boron species from commercial HBcat).

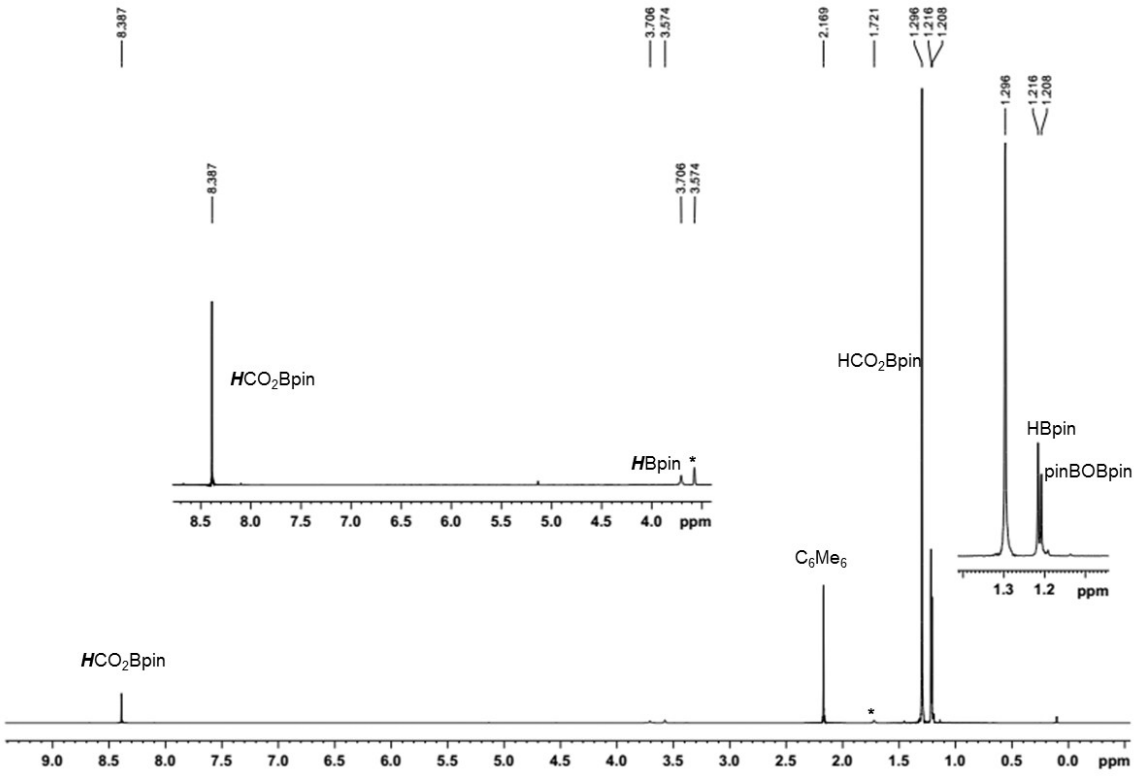


Figure S4. $^{1}H\{^{11}B\}$ NMR spectrum (400 MHz, THF-d_8) of the hydroboration of CO_2 with HBpin catalyzed by **2a**/**2b** (Table 2, entry 3) (reaction time: 10 min). (*, denotes solvent residual signals)

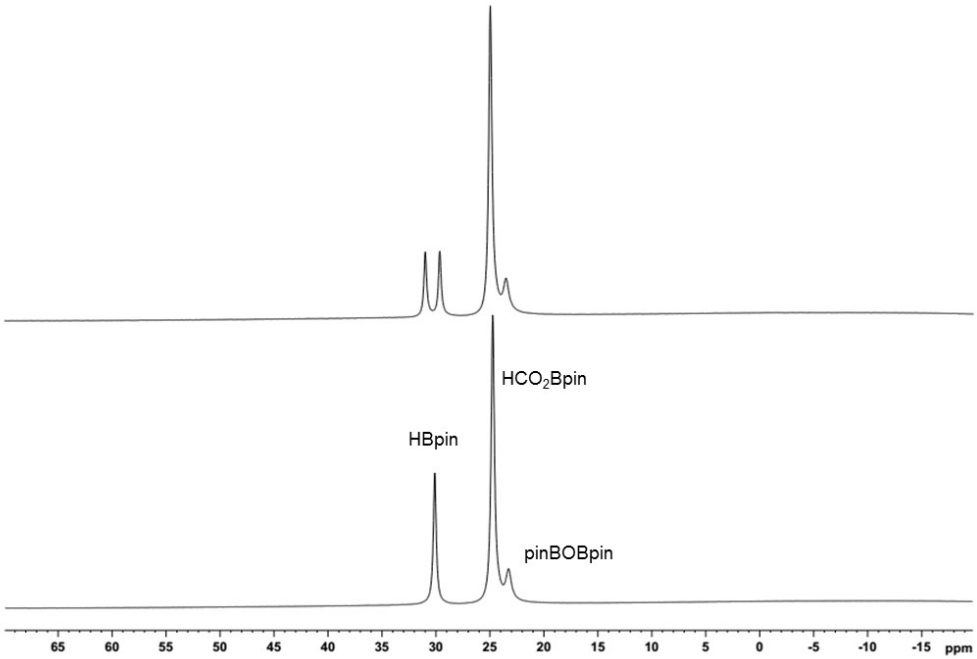


Figure S5. ^{11}B (top) and $^{11}B\{^{1}H\}$ (down) NMR spectra (128 MHz, THF-d_8) of the hydroboration of CO_2 with HBpin catalyzed by **2a**/**2b** (Table 2, entry 3) (reaction time: 10 min).

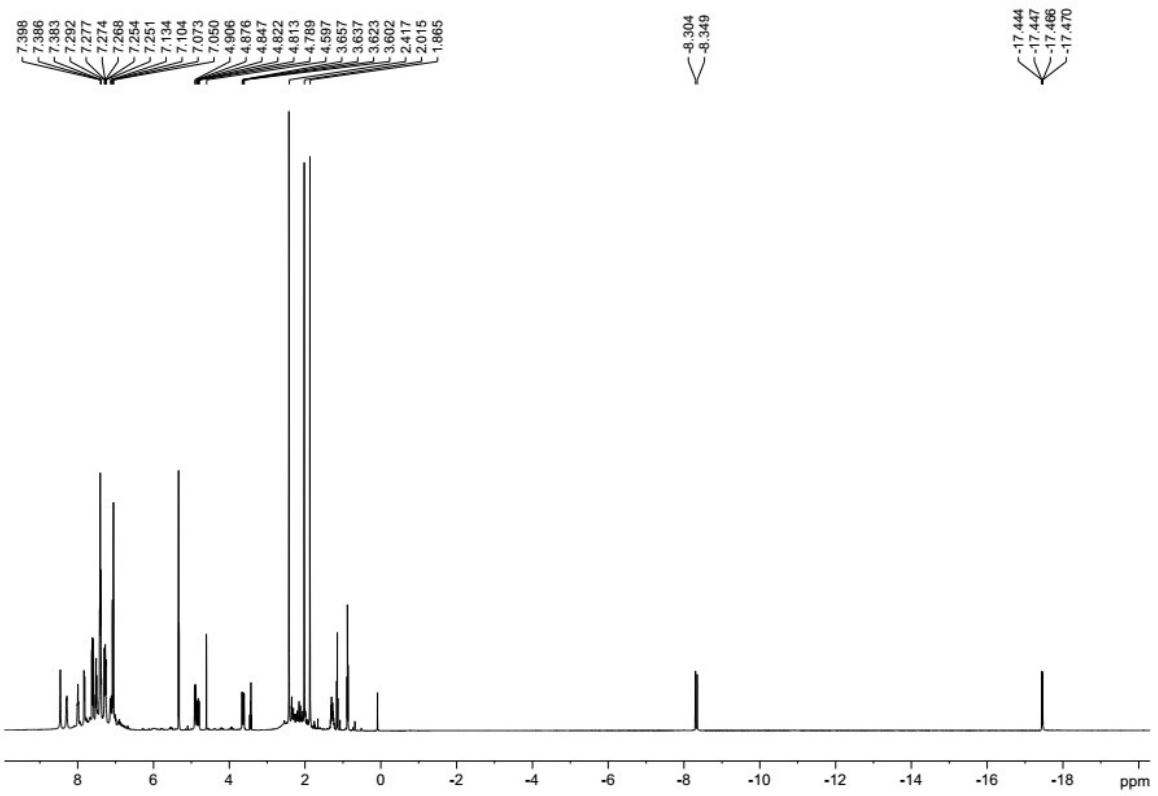


Figure S6. ^{1}H NMR spectrum (500 MHz, CD_2Cl_2) of complex **3(Cl)**.

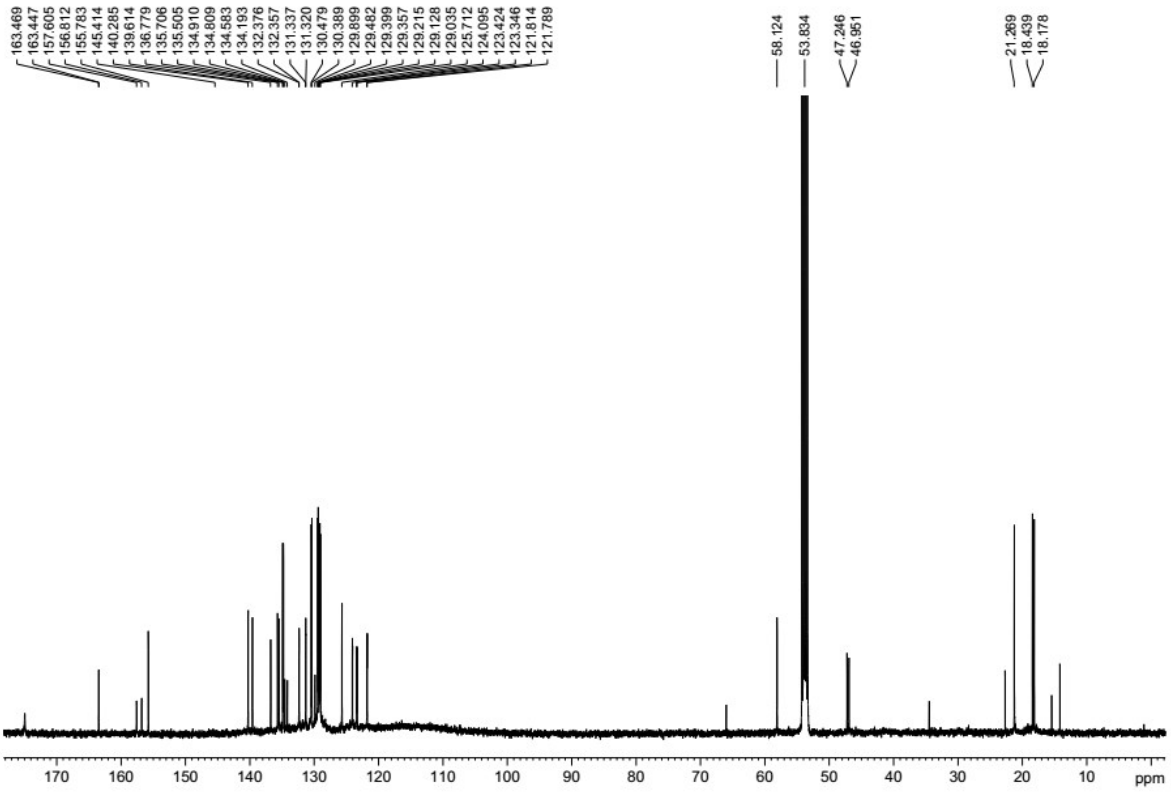


Figure S7. $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, CD_2Cl_2) of complex **3(Cl)**.

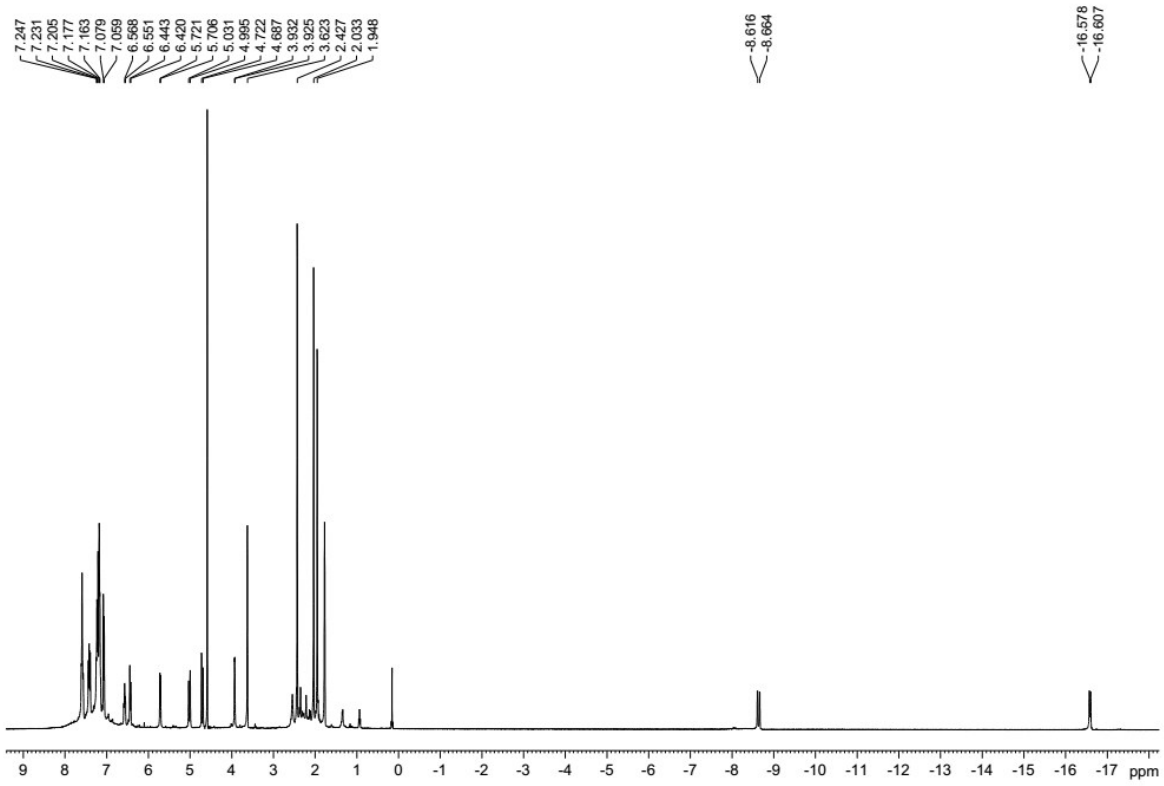


Figure S8. ^{1}H NMR spectrum (400 MHz, THF-d_8) of complex **4**.

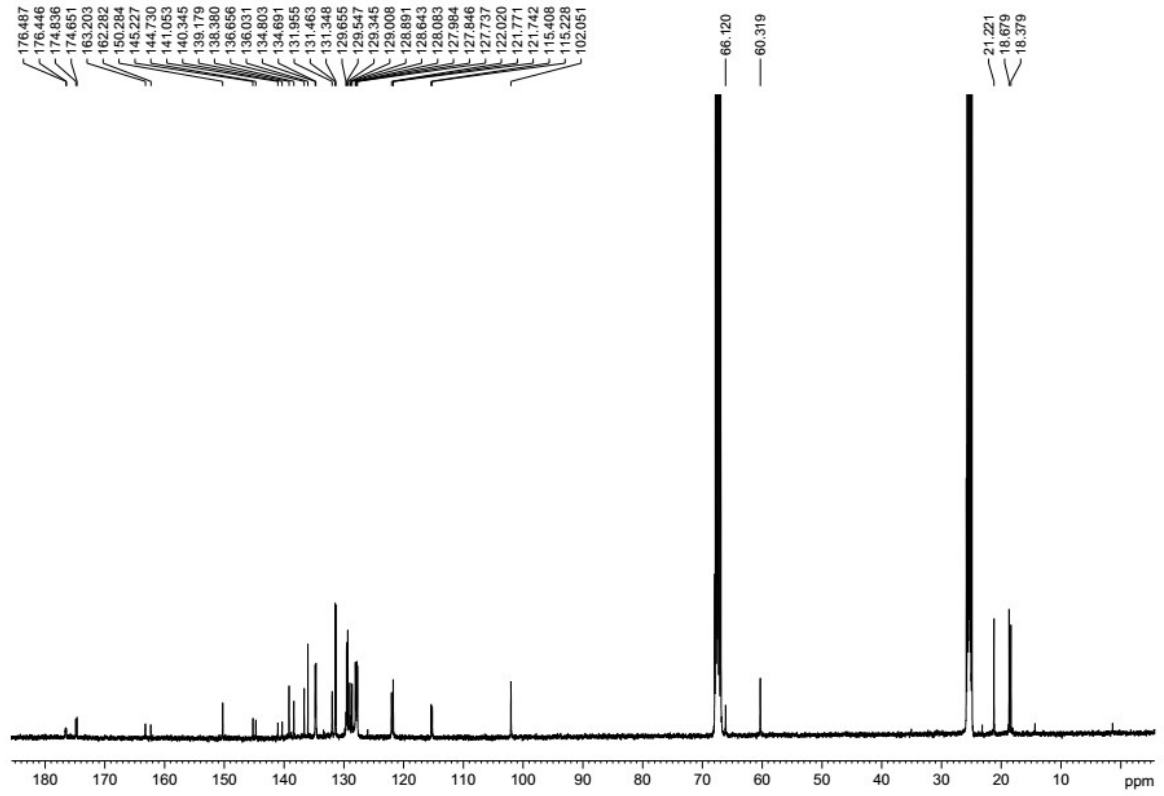


Figure S9. ^{13}C{^{1}H} NMR spectrum (101 MHz, THF-d_8) of complex **4**.

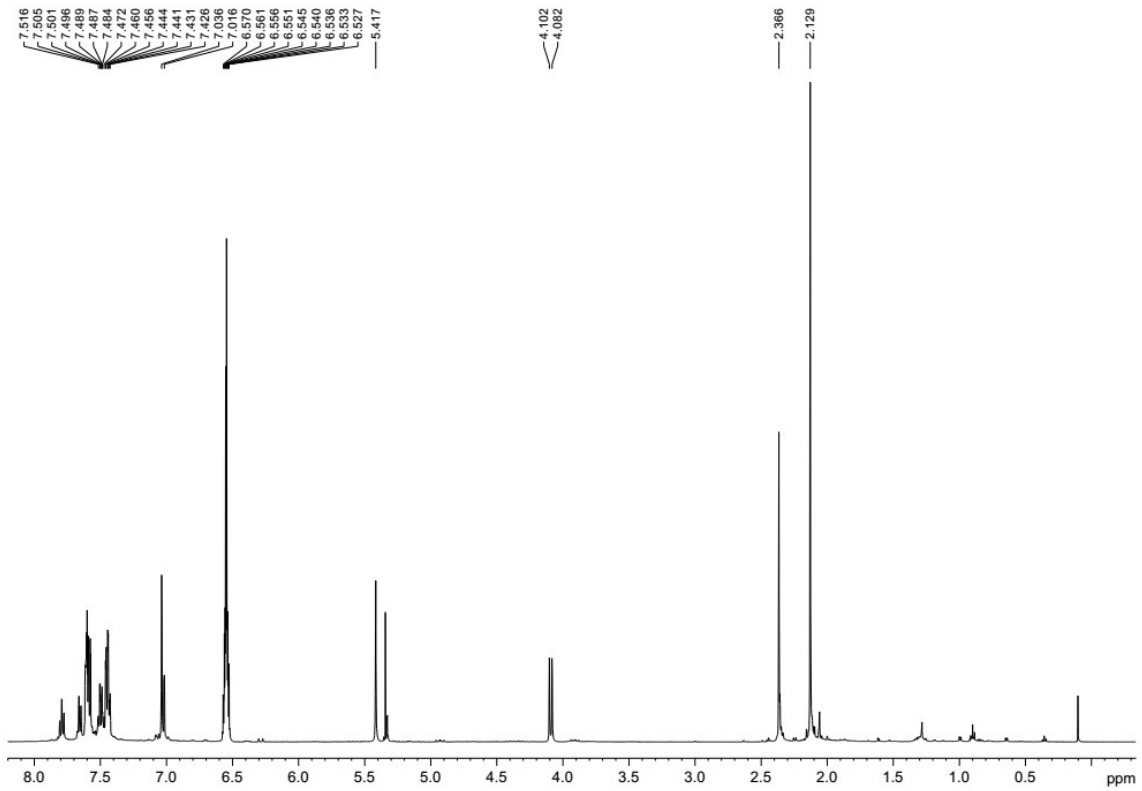


Figure S10. ^{1}H NMR spectrum (500 MHz, CD_2Cl_2) of complex **1(Bcat$_2$)**.

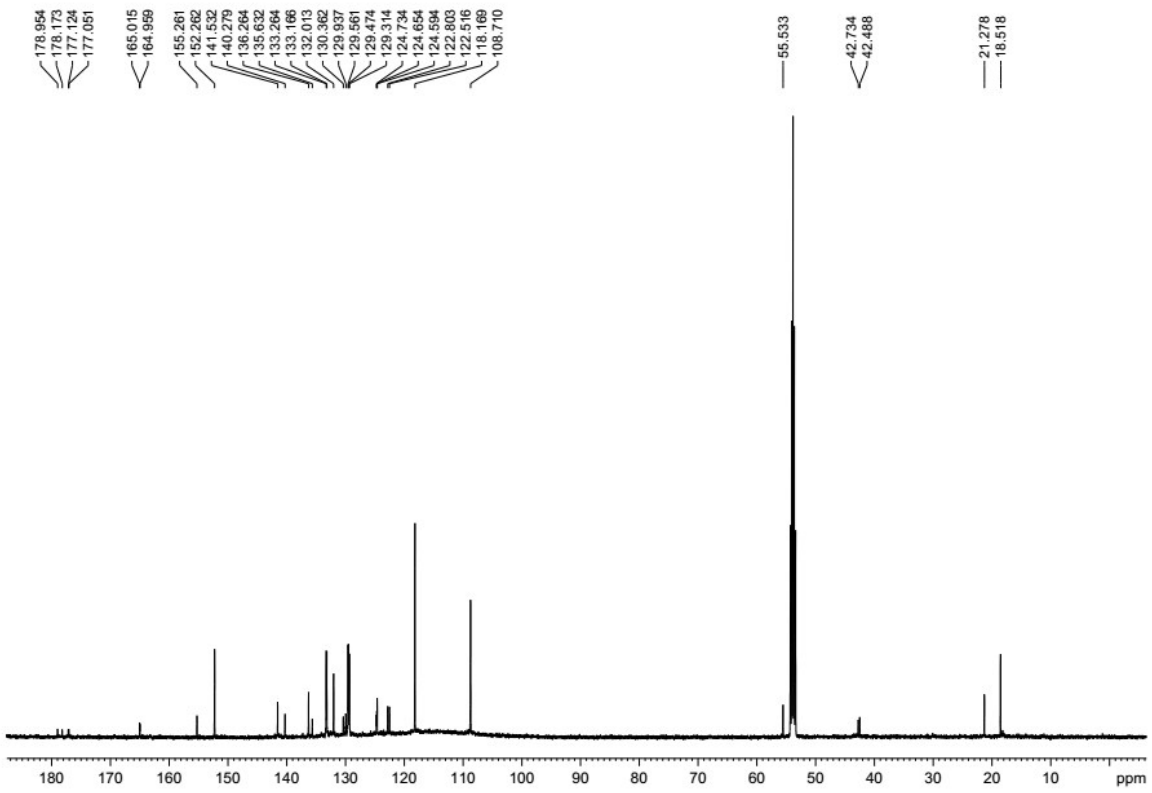


Figure S11. $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, CD_2Cl_2) of complex **1(Bcat$_2$)**.

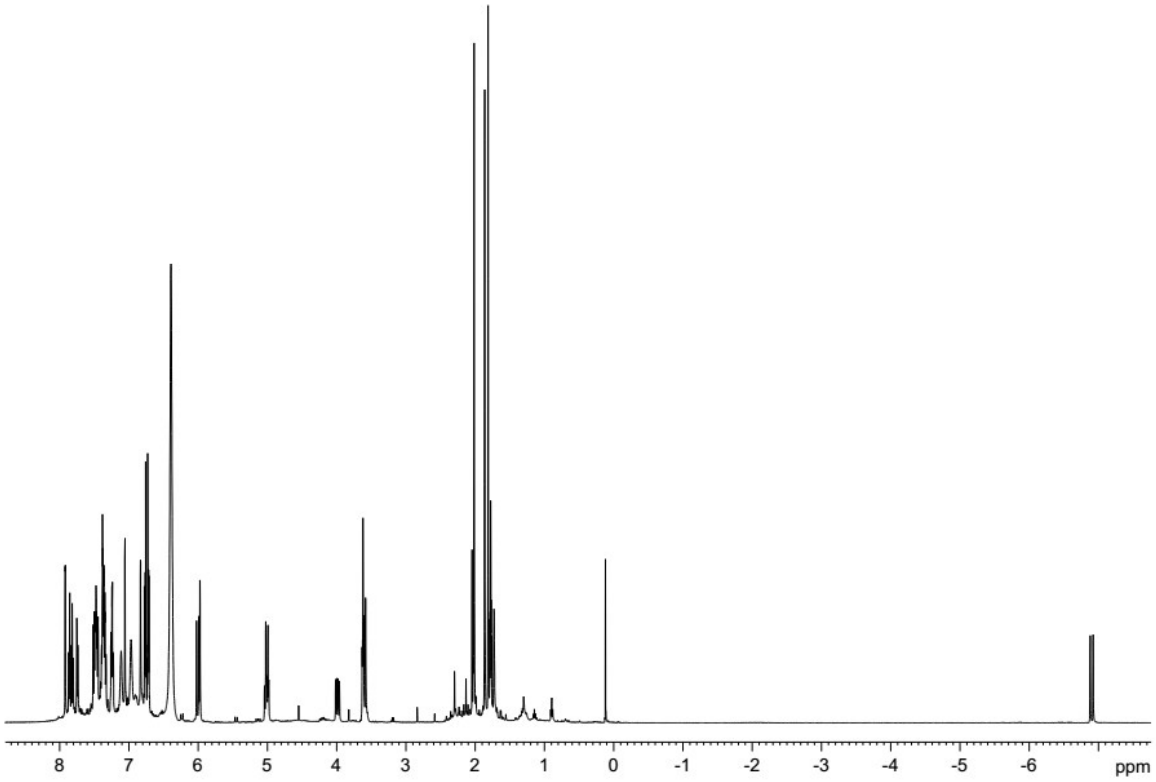


Figure S12. ^{1}H NMR spectrum (500 MHz, THF-d_8) of the reaction of **1(Bcat$_2$)** with HBcat (1.2 equiv) to yield **5(Bcat$_2$)**.

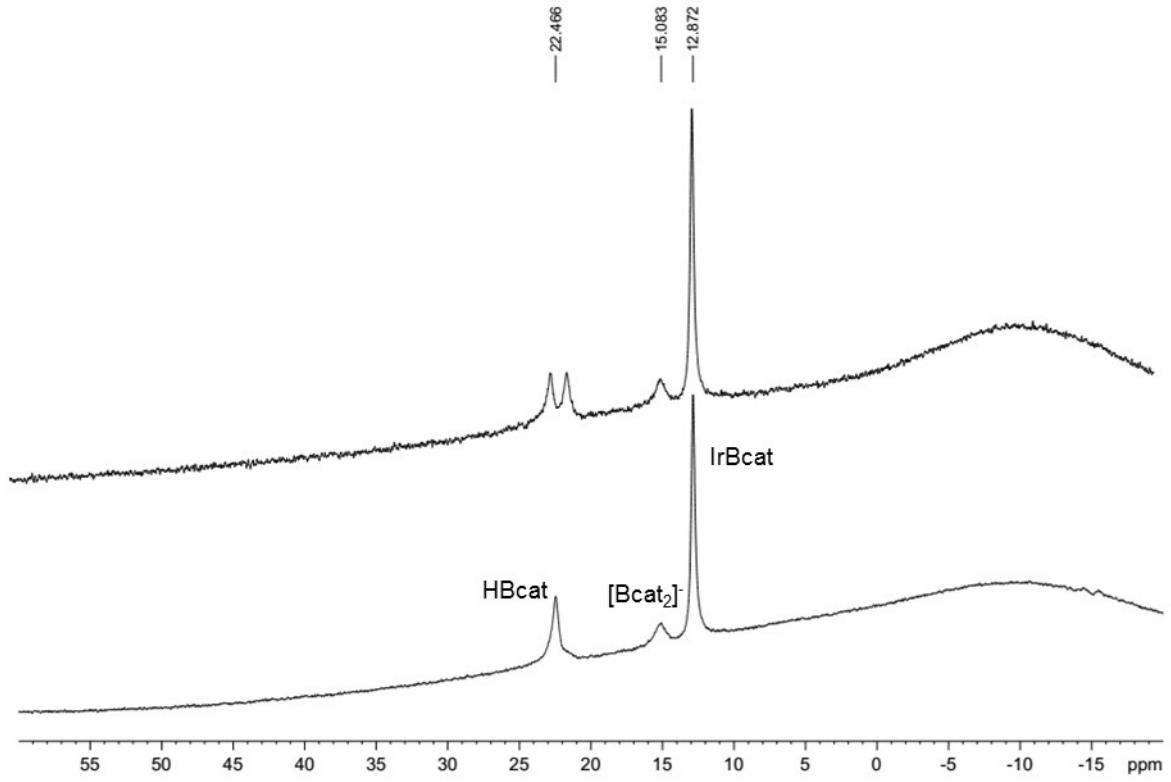


Figure S13. ^{11}B{^{1}H} (down) and ^{11}B NMR (top) spectra (160 MHz, THF-d_8) of the reaction of **1(Bcat$_2$)** with HBcat (1.2 equiv) to yield **5(Bcat$_2$)**.

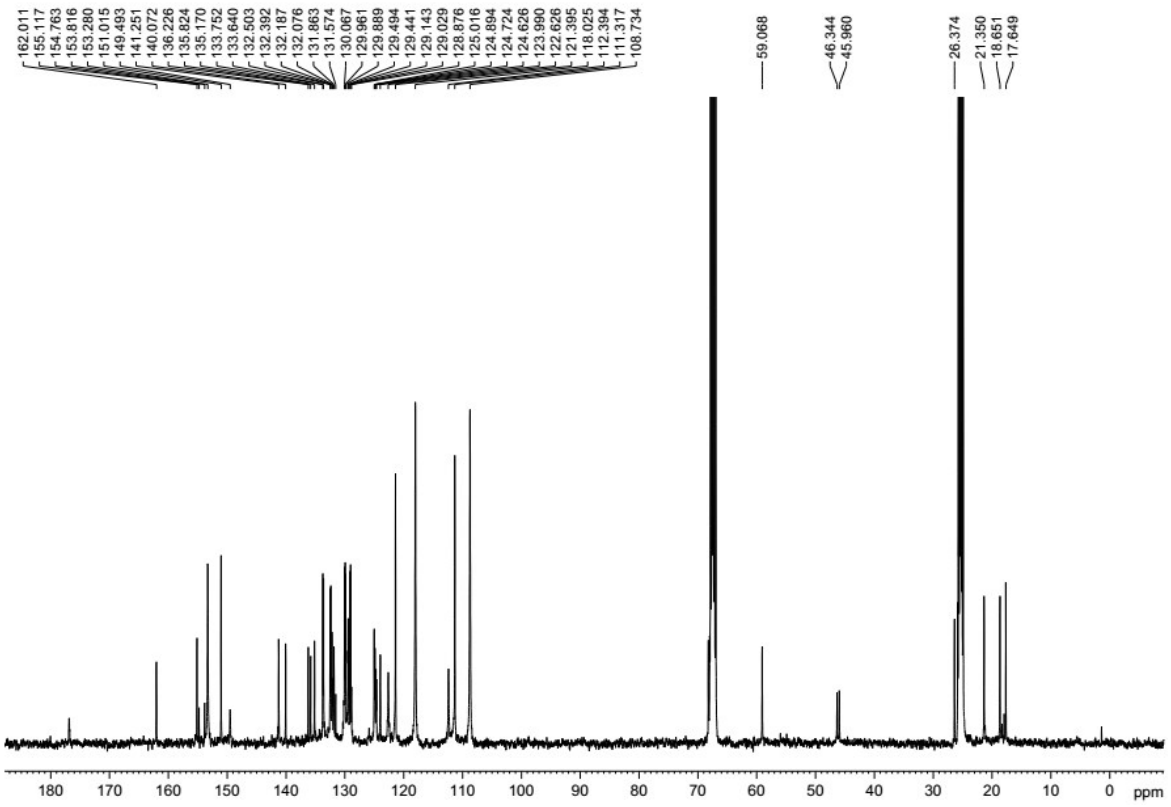


Figure S14. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, THF-d_8) of the reaction of **1(Bcat$_2$)** with HBcat (1.2 equiv) to yield **5(Bcat$_2$)**.

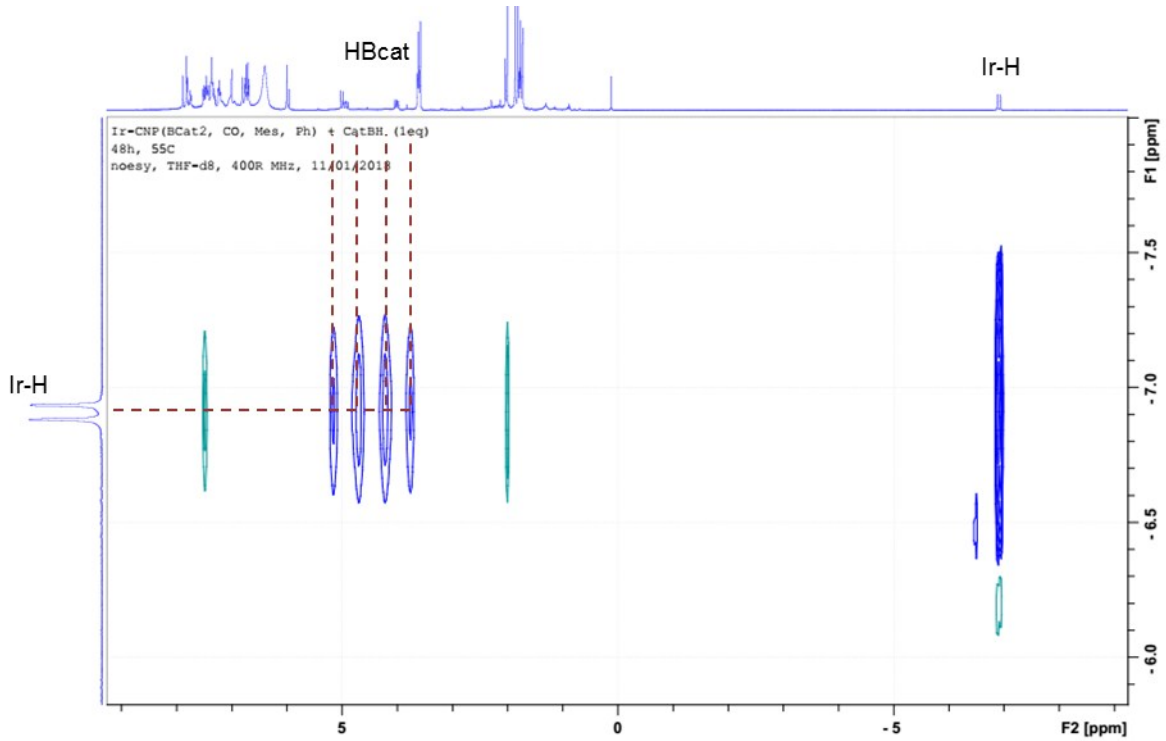


Figure S15. ^{1}H-^{1}H NOESY spectrum (400 MHz, THF-d_8, 328 K) of the reaction of **1(Bcat$_2$)** with HBcat (1.2 equiv) to yield **5(Bcat$_2$)** (mixing time = 800 ms). (Blue signals: exchange cross-peaks; green signals: NOE cross-peaks).

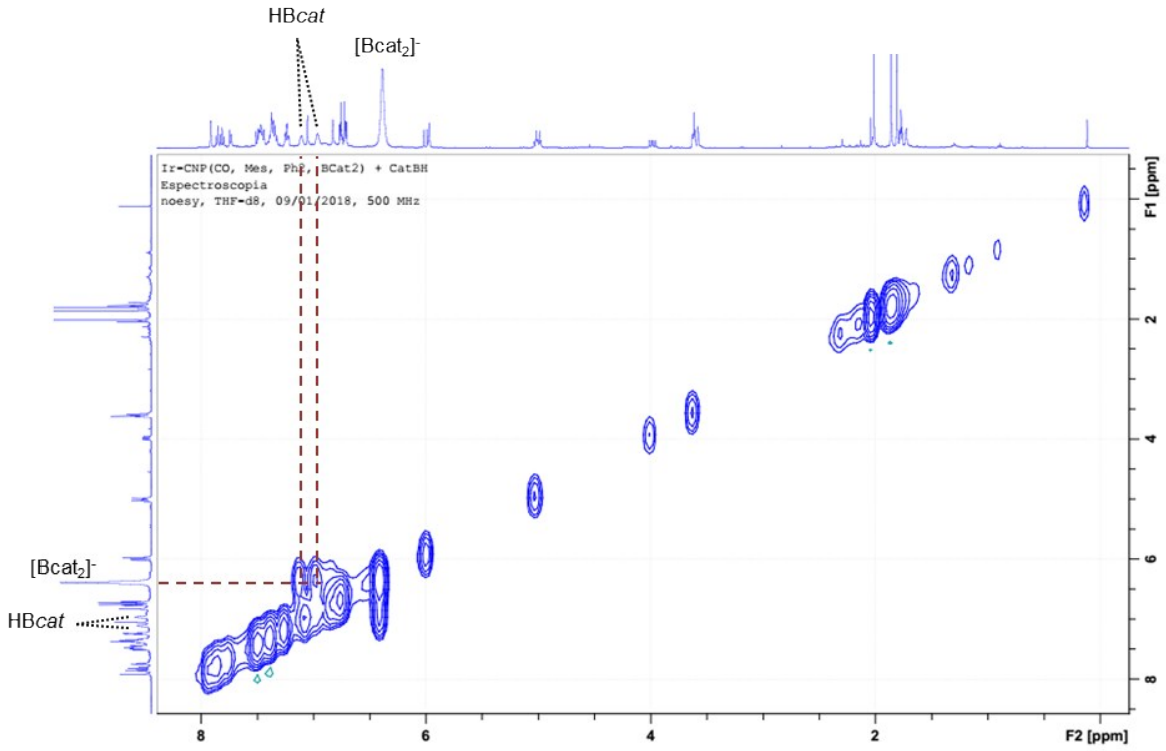


Figure S16. ^{1}H-^{1}H EXSY spectrum (500 MHz, THF-d_8) of the reaction of **1(Bcat$_2$)** with HBcat (1.2 equiv) to yield **5(Bcat$_2$)** (mixing time = 800 ms).

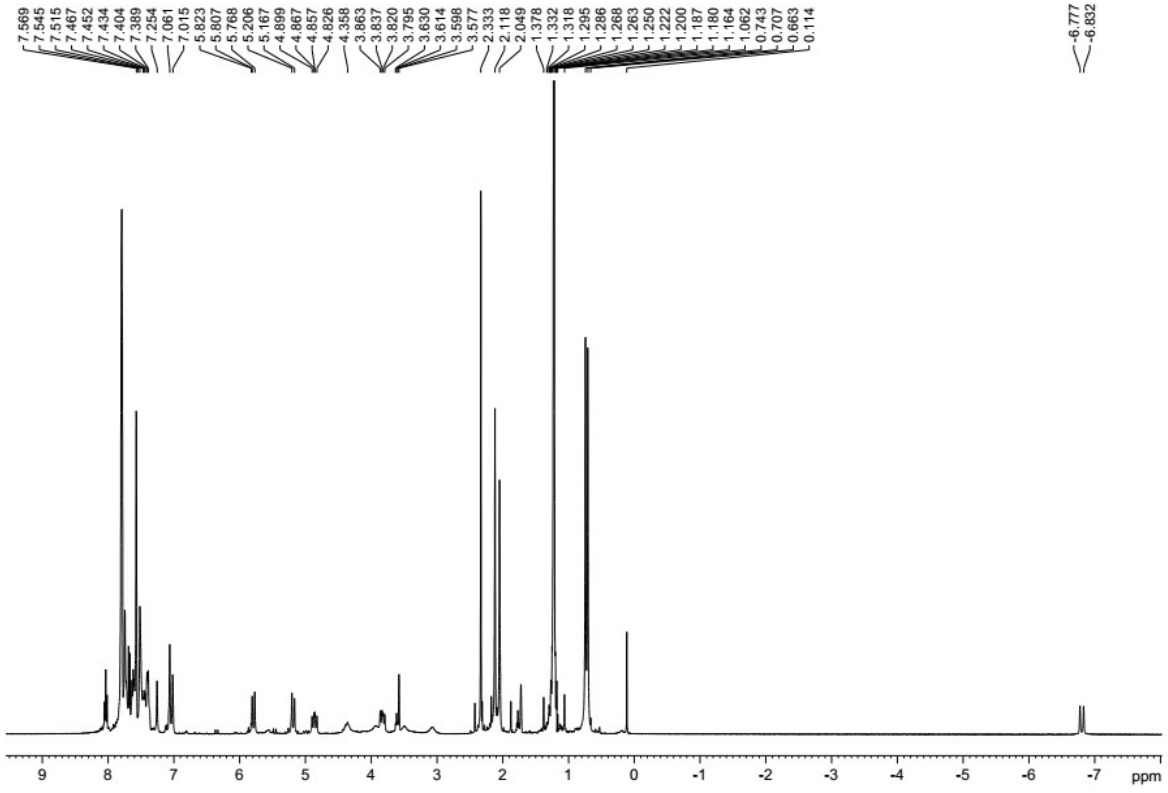


Figure S17. ^{1}H NMR spectrum (400 MHz, THF-d_8) of the reaction of **1(BAr$_F$)** with HBpin (2.4 equiv) to yield **6(BAr$_F$)**.

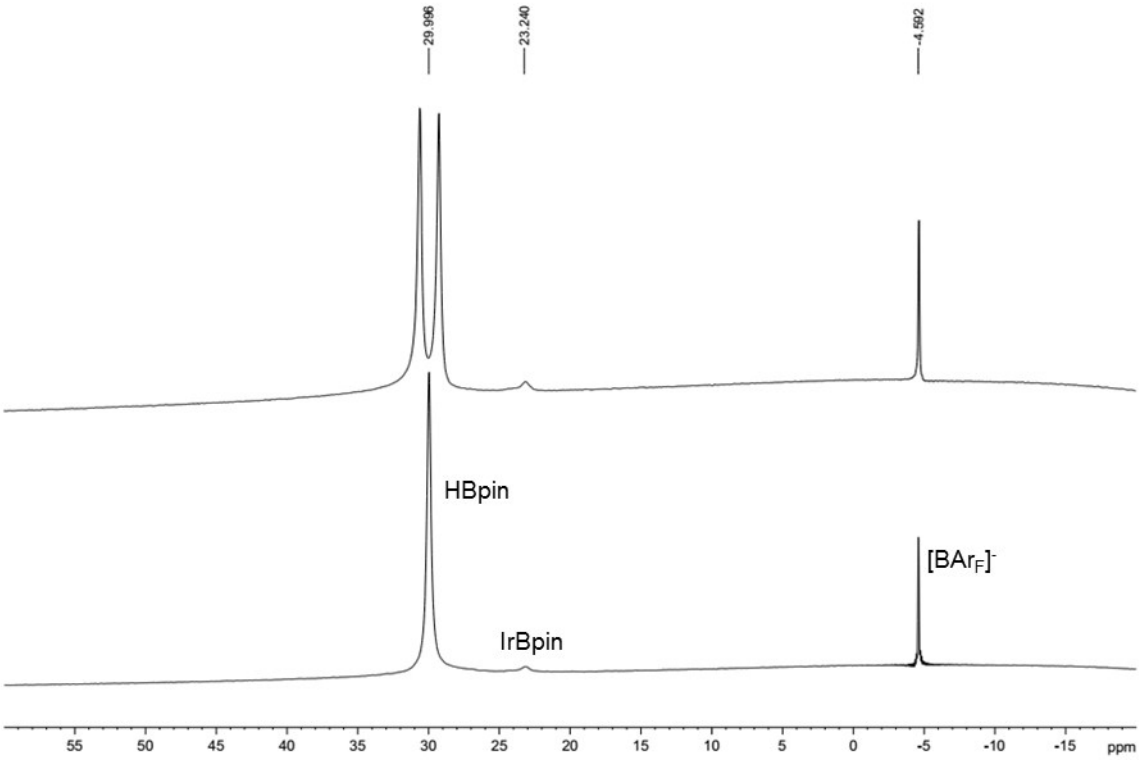


Figure S18. $^{11}B\{^1H\}$ (down) and ^{11}B NMR (top) spectra (160 MHz, THF-d_8) of the reaction of **1(BAr$_F$)** with HBpin (2.4 equiv) to yield **6(BAr$_F$)**.

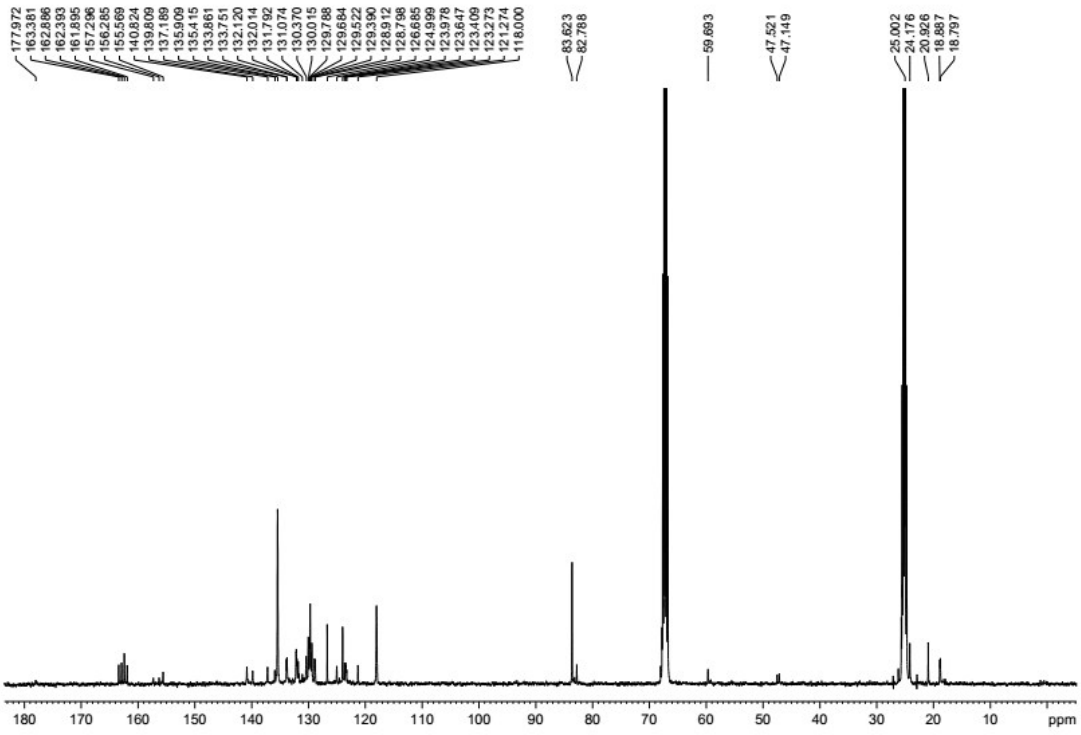


Figure S19. $^{13}C\{^1H\}$ NMR spectrum (101 MHz, THF-d_8) of the reaction of **1(BAr$_F$)** with HBpin (2.4 equiv) to yield **6(BAr$_F$)**.

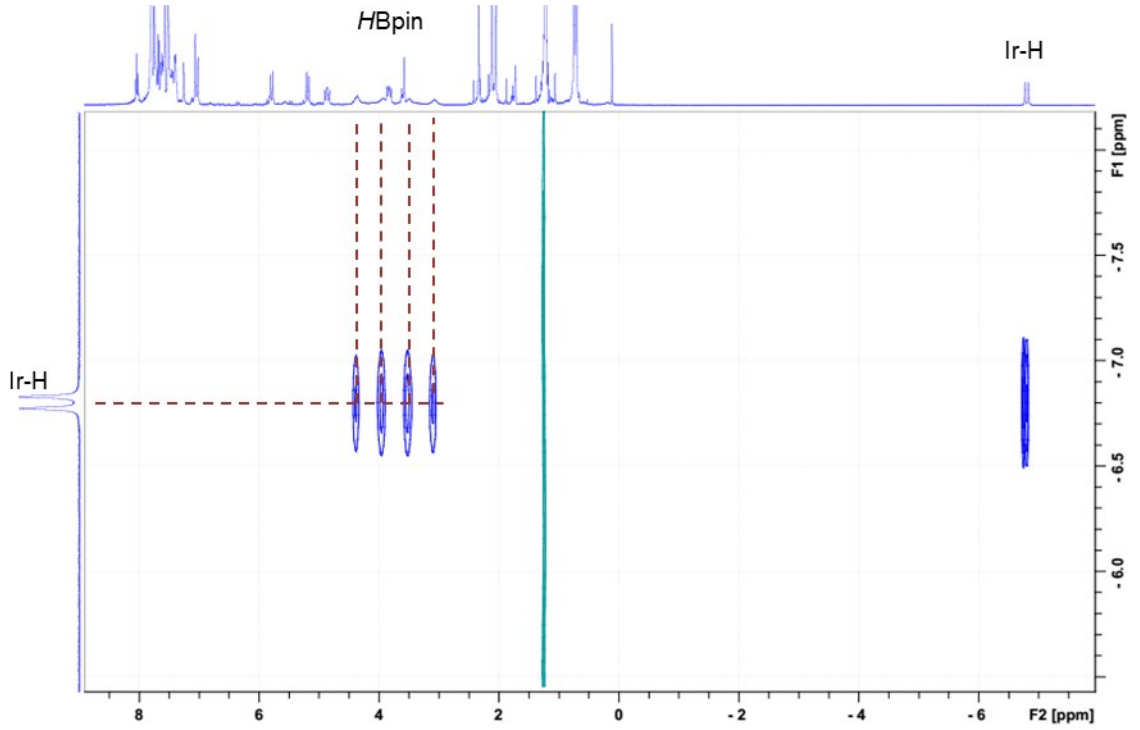


Figure S20. ^{1}H-^{1}H NOESY spectrum (400 MHz, THF-d_8) of the reaction of **1(BAr$_F$)** with HBpin (2.4 equiv) to yield **6(BAr$_F$)** (mixing time = 800 ms). (Blue signals: exchange cross-peaks; green signals: NOE cross-peaks).

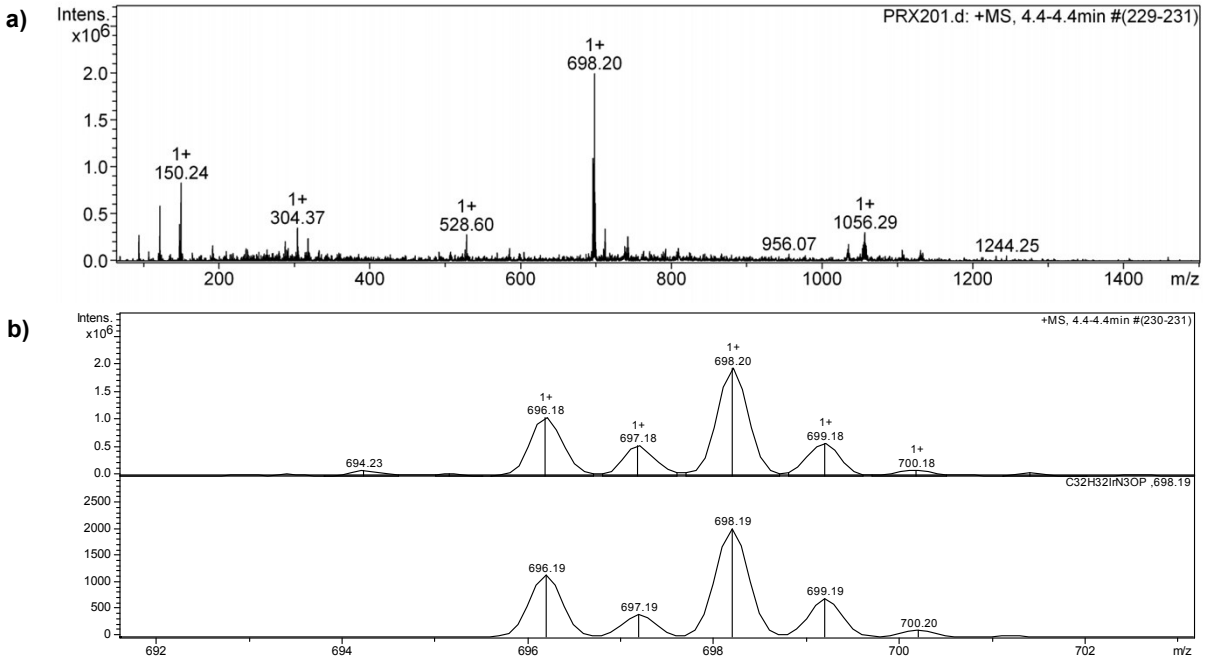


Figure S21. a) ESI-MS spectrum (positive mode) of the reaction of **2a/2b** with HBcat (5 equiv) under CO_2 (2 bar); b) experimental (top) and simulated (bottom) isotope patterns for *m/z* 698.

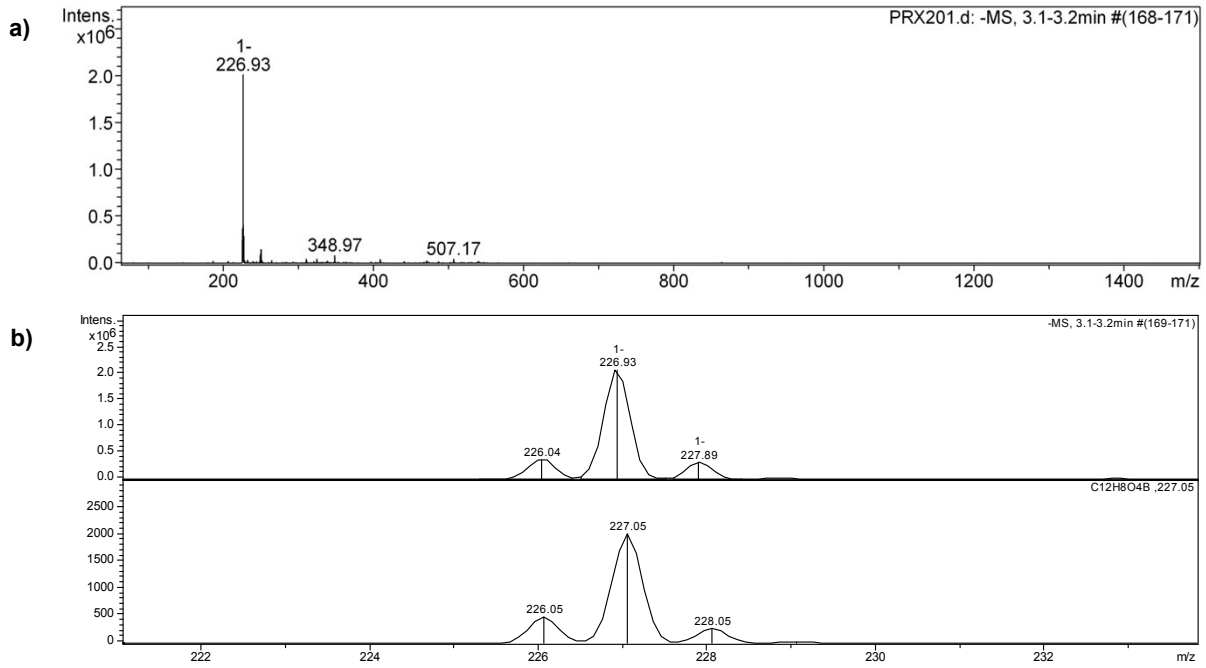


Figure S22. a) ESI-MS spectrum (negative mode) of the reaction of **2a/2b** with HBcat (5 equiv) under CO_2 (2 bar); b) experimental (top) and simulated (bottom) isotope patterns for *m/z* 227.

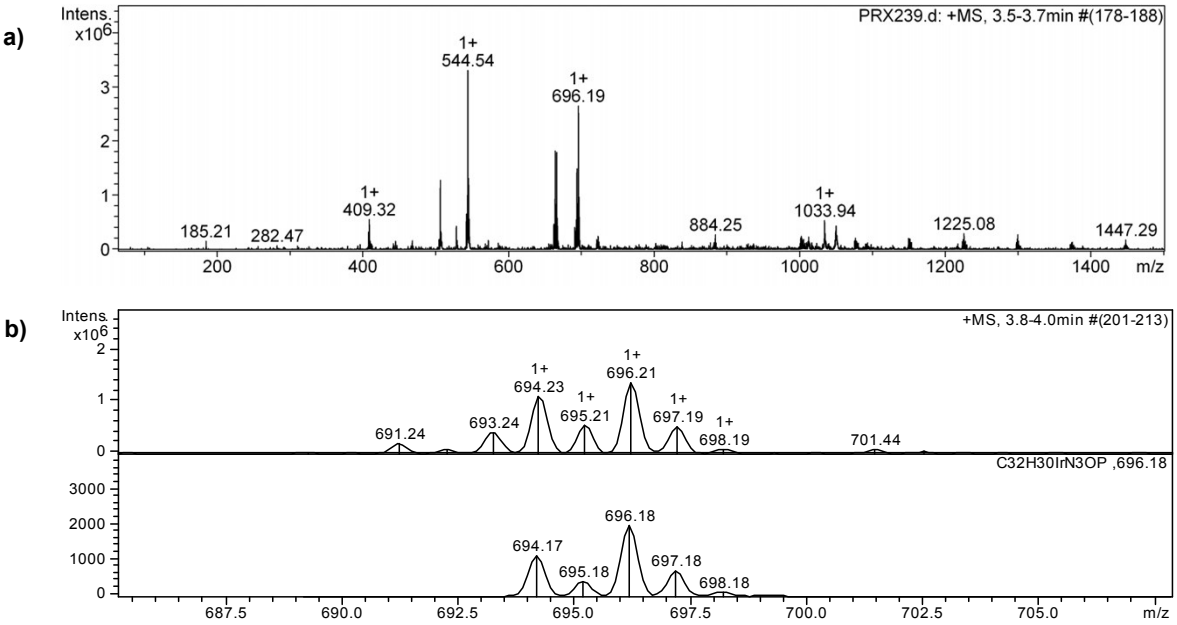


Figure S23. a) ESI-MS spectrum (positive mode) of the reaction of **2a/2b** with HBpin (5 equiv) under CO_2 (2 bar); b) experimental (top) and simulated (bottom) isotope patterns for *m/z* 696.

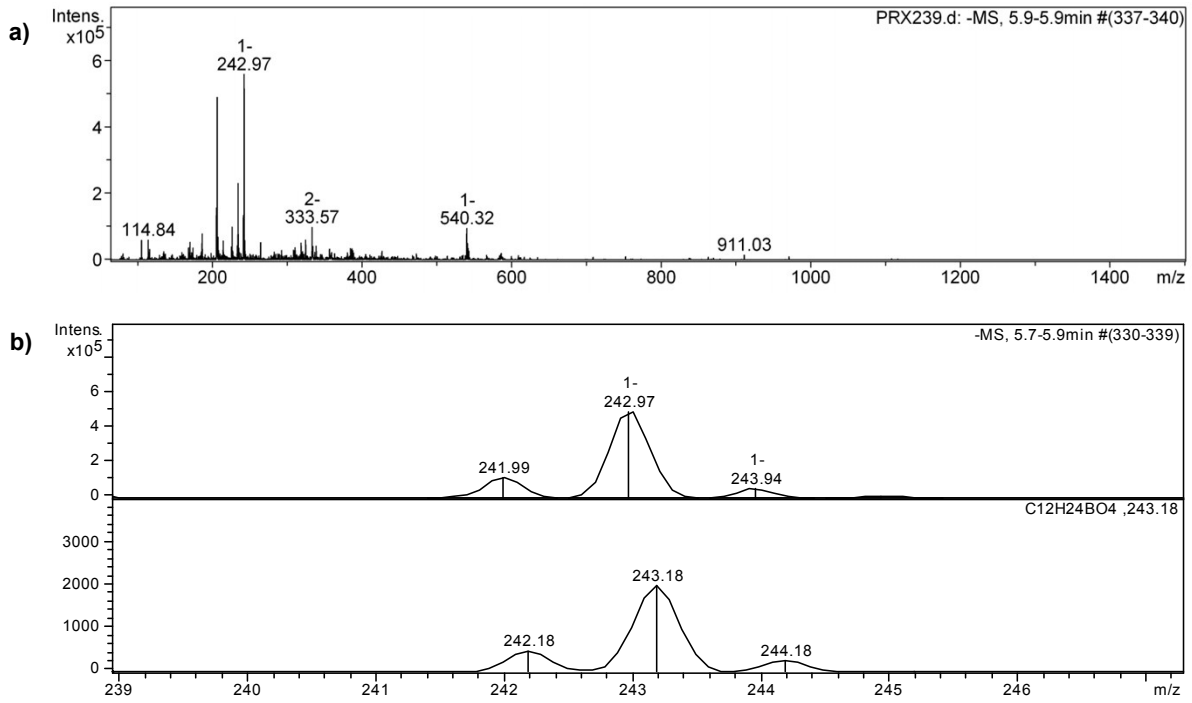


Figure S24. a) ESI-MS spectrum (negative mode) of the reaction of **2a/2b** with HBpin (5 equiv) under CO_2 (2 bar); b) experimental (top) and simulated (bottom) isotope patterns for *m/z* 243.

2. X-Ray structure analysis of 2a

One crystal of suitable size for X-ray diffraction analysis of **2a** was coated with dry perfluoropolyether and mounted on glass fibre and fixed in a cold nitrogen stream (T = 213 K) to the goniometer head. Data collection was performed on a Bruker-Nonius X8Apex-II CCD diffractometer, using monochromatic radiation λ(Mo K_α) = 0.71073 Å, by means of ω and φ scans with a width of 0.50 degree. The data were reduced (SAINT)[1] and corrected for absorption effects by the multi-scan method (SADABS).[2] The structure was solved by direct methods (SIR-2002)[3] and refined against all F^2 data by full-matrix least-squares techniques (SHELXL-2016/6)[4] minimizing $w[F_o^2-F_c^2]^2$. All non-hydrogen atoms were refined anisotropically. The hydrogen atoms were included from calculated positions and refined riding on their respective carbon atoms with isotropic displacement parameters. A summary of cell parameters, data collection, structure solution, and refinement for this crystal structure is given in Table S25. CCDC 1856145 (**2a**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

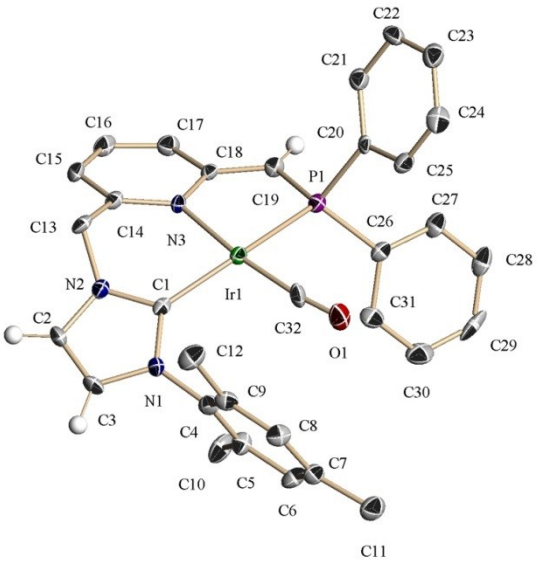


Figure S25. ORTEP view of molecular structure of salt complex **2a** with thermal ellipsoids drawn at the 30% level. Most of the hydrogen atoms are omitted for clarity.

[1] Bruker. SAINT. *APEX2* 2007, Bruker AXS Inc., Madison, Wisconsin, USA.

[2] a) G. M. Sheldrick, SADABS, Programs for Scaling and Absorption Correction of Area Detector Data. SADABS, Programs Scaling Absorpt. Correct. Area Detect. Data 1997, University of Göttingen: Göttingen, Germany. b) Bruker. SADABS. APEX2 2007, Bruker AXS Inc., Madison, Wisconsin, USA.

[3] M. C. Burla, M. Camalli, B. Carrozzini, G. L. Cascarano, C. Giacovazzo, G. Polidori, R. Spagna, SIR2002 : The Program. *J. Appl. Crystallogr.*, 2003, **36**, 1103–1103 DOI: 10.1107/S0021889803012585.

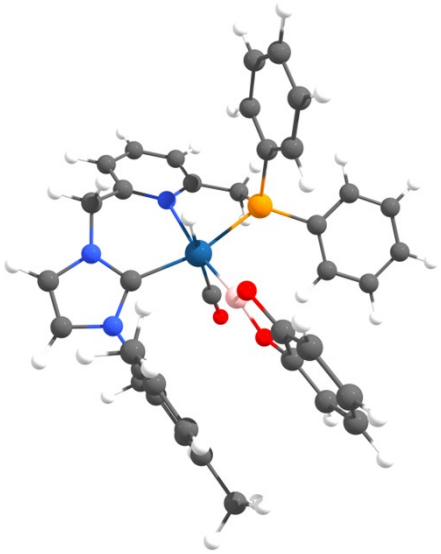
[4] a) G. M. Sheldrick, A Short History of SHELX. *Acta Crystallographica Section A: Foundations of Crystallography*. 2008, pp 112–122. DOI: 10.1107/S0108767307043930; b) G. M. Sheldrick, *Acta Cryst.,* 2015, **C71**, 3-8. DOI: 10.1107/S2053229614024218.

Table S1. Crystal data and structure refinement for **2a**

Empirical formula	$C_{36}H_{37}IrN_3O_2P$	
	$[C_{32}H_{29}IrN_3OP, C_4H_8O]$	
Formula weight	766.86	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2_1/n	
Unit cell dimensions	a = 11.5322(5) Å	a= 90°.
	b = 10.5191(6) Å	b= 100.875(3)°.
	c = 26.4134(12) Å	g = 90°.
Volume	3146.6(3) $Å^3$	
Z	4	
Density (calculated)	1.619 Mg/m^3	
Absorption coefficient	4.331 mm^{-1}	
F(000)	1528	
Crystal size	0.050 x 0.030 x 0.020 mm^3	
Theta range for data collection	2.089 to 25.249°.	
Index ranges	-13<=h<=13, -12<=k<=7, -31<=l<=29	
Reflections collected	21544	
Independent reflections	5648 [R(int) = 0.0959]	
Completeness to theta = 25.242°	98.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9184 and 0.8126	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5648 / 238 / 436	
Goodness-of-fit on F^2	0.959	
Final R indices [I>2sigma(I)]	R1 = 0.0460, wR2 = 0.0785	
R indices (all data)	R1 = 0.0904, wR2 = 0.0880	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.956 and -0.888 $e.Å^{-3}$	

3. DFT calculations

Tables of the optimized geometries (cartesian coordinates, in Angstroms) for the calculated species with B3LYP SCF uncorrected Energies in THF (in Hartrees) in parenthesis.



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N	-2.425415000	-1.804606000	-0.395679000
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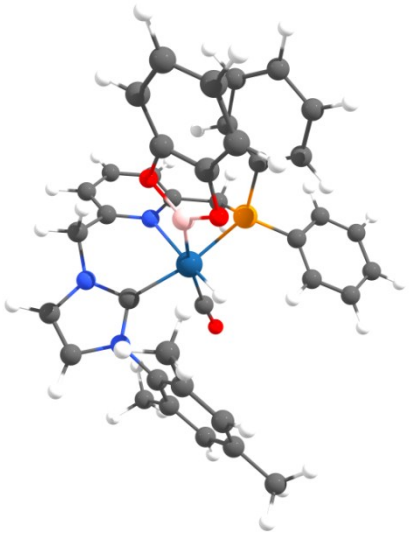
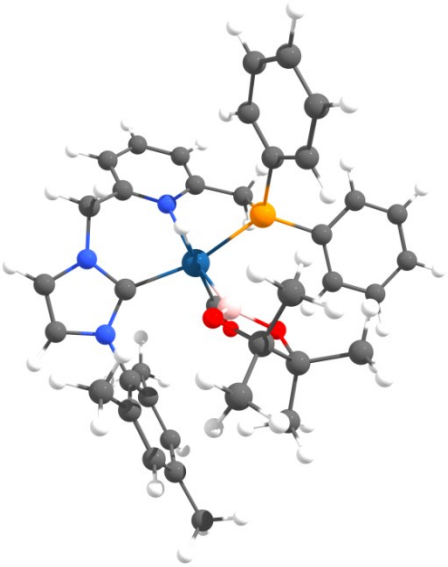
B	1.060561000	0.618091000	0.426442000
O	1.937229000	1.225013000	-0.503432000
O	1.347196000	1.129622000	1.708094000



5-II (-2329.395538)

Ir	-0.444417000	-0.090735000	0.478800000
P	1.156433000	1.597484000	0.749977000
N	-2.831202000	-2.021511000	-0.106105000
N	-1.288505000	-2.933453000	1.084966000
N	0.630035000	-0.884905000	2.276039000
C	-1.604647000	-1.789466000	0.430797000
C	-2.299822000	-3.880241000	0.954750000
H	-2.221828000	-4.861537000	1.394786000
C	-3.273327000	-3.305005000	0.206966000
H	-4.228277000	-3.673039000	-0.130976000
C	-3.593794000	-1.048848000	-0.839244000
C	-4.578350000	-0.321499000	-0.158585000
C	-5.265918000	0.666317000	-0.871975000
H	-6.026121000	1.249654000	-0.359270000
C	-4.998679000	0.919327000	-2.220700000
C	-4.024385000	0.148388000	-2.867778000
H	-3.816285000	0.324758000	-3.920101000
C	-3.308288000	-0.846298000	-2.197767000
C	-4.906848000	-0.599850000	1.285721000
H	-5.541669000	-1.489247000	1.378077000
H	-5.447877000	0.240404000	1.726841000
H	-4.010692000	-0.784262000	1.883672000
C	-5.762410000	1.976908000	-2.976413000
H	-6.285260000	2.654372000	-2.295830000
H	-6.512591000	1.522220000	-3.635034000
H	-5.096410000	2.571672000	-3.609774000
C	-2.255562000	-1.654863000	-2.908467000
H	-1.251131000	-1.299001000	-2.657670000
H	-2.377583000	-1.575269000	-3.991511000
H	-2.305108000	-2.712894000	-2.633275000
C	0.009120000	-3.213265000	1.693353000
H	0.743028000	-3.332495000	0.890403000
H	-0.083846000	-4.163669000	2.216163000
C	0.559313000	-2.181318000	2.651705000
C	1.135453000	-2.622529000	3.841122000
H	1.052361000	-3.667027000	4.118599000
C	1.834593000	-1.721488000	4.639262000
H	2.296454000	-2.047782000	5.565192000
C	1.948477000	-0.402086000	4.218889000
H	2.505612000	0.325975000	4.797021000
C	1.329355000	-0.002858000	3.034319000
C	1.435314000	1.431106000	2.575824000
H	2.386623000	1.862884000	2.895022000
C	2.783635000	1.377318000	-0.038949000
C	3.692987000	0.440918000	0.474311000
H	3.474943000	-0.093112000	1.392983000
C	4.879929000	0.175147000	-0.207872000
H	5.576535000	-0.555447000	0.191053000
C	5.165962000	0.837891000	-1.402639000
H	6.083972000	0.618674000	-1.938708000
C	4.265809000	1.776133000	-1.911595000
H	4.485127000	2.294384000	-2.839967000
C	3.077673000	2.047579000	-1.234596000
H	2.377924000	2.771766000	-1.638903000
C	0.701855000	3.331888000	0.469373000
C	1.471112000	4.367434000	1.022937000
H	2.345724000	4.135902000	1.623472000
C	1.113900000	5.694679000	0.796619000

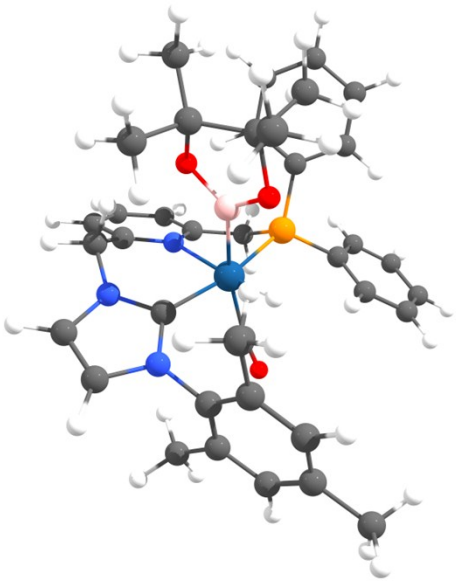
H	1.705933000	6.494711000	1.230280000
C	-0.002471000	5.994696000	0.009774000
H	-0.276918000	7.030404000	-0.166169000
C	-0.761680000	4.967431000	-0.551873000
H	-1.625719000	5.199960000	-1.166640000
C	-0.413299000	3.635037000	-0.323142000
H	-0.999076000	2.832422000	-0.759306000
H	0.634541000	2.022085000	3.038573000
H	-1.077201000	0.421587000	-0.875939000
C	-1.799806000	0.981550000	1.436460000
O	-2.578004000	1.703188000	1.883409000
C	2.257360000	-1.222555000	-2.630813000
C	2.673398000	-2.121191000	-1.648905000
C	2.923905000	-1.095920000	-3.836522000
C	3.774118000	-2.941137000	-1.820266000
C	4.045962000	-1.918658000	-4.023975000
H	2.599711000	-0.387324000	-4.590919000
C	4.461921000	-2.821255000	-3.038646000
H	4.093373000	-3.631571000	-1.046803000
H	4.602700000	-1.849225000	-4.953224000
H	5.335294000	-3.440834000	-3.216454000
B	0.922189000	-0.970395000	-0.854058000
O	1.843182000	-2.000627000	-0.555490000
O	1.162687000	-0.528960000	-2.169881000



6-I (-2334.160532)

Ir	0.223725000	-0.687375000	0.040563000
P	2.216223000	0.470783000	0.537746000
N	-2.517722000	-2.273404000	-0.315274000
N	-0.772580000	-3.353264000	-0.947854000
N	1.735058000	-2.396454000	0.392036000
C	-1.171846000	-2.136670000	-0.484087000
C	-1.839776000	-4.234196000	-1.061594000
H	-1.711417000	-5.242891000	-1.420117000
C	-2.939948000	-3.553733000	-0.664652000
H	-3.976509000	-3.841138000	-0.597625000
C	-3.443635000	-1.276419000	0.148566000
C	-3.704974000	-1.180431000	1.521042000
C	-4.625470000	-0.212714000	1.940989000
H	-4.825876000	-0.106443000	3.003812000
C	-5.307742000	0.595016000	1.027914000
C	-5.076135000	0.404567000	-0.340967000
H	-5.632516000	0.996727000	-1.062569000
C	-4.145567000	-0.525246000	-0.808306000
C	-3.103028000	-2.144887000	2.510986000
H	-3.716408000	-3.053013000	2.566233000
H	-3.069656000	-1.708016000	3.511338000
H	-2.094090000	-2.457342000	2.235889000
C	-6.257288000	1.666895000	1.495633000
H	-6.600447000	1.482816000	2.517370000
H	-7.132903000	1.737894000	0.842739000
H	-5.764045000	2.647185000	1.483373000
C	-3.924387000	-0.735650000	-2.282455000
H	-2.914107000	-0.431435000	-2.566384000
H	-4.634856000	-0.142971000	-2.863358000
H	-4.053668000	-1.787379000	-2.559345000
C	0.591813000	-3.692047000	-1.329878000
H	0.902560000	-3.007639000	-2.126992000
H	0.580444000	-4.705872000	-1.727129000
C	1.603131000	-3.591192000	-0.215010000
C	2.460757000	-4.650483000	0.067805000
H	2.321267000	-5.602722000	-0.431459000
C	3.504836000	-4.451925000	0.969602000
H	4.186292000	-5.261426000	1.209416000
C	3.686315000	-3.189800000	1.525046000
H	4.519420000	-2.980591000	2.186401000
C	2.786025000	-2.170112000	1.210654000
C	2.989995000	-0.762064000	1.698009000
H	4.050820000	-0.554734000	1.860392000
C	3.361586000	0.663641000	-0.865817000
C	4.299658000	-0.320637000	-1.200870000
H	4.417386000	-1.206859000	-0.587282000
C	5.099763000	-0.164643000	-2.334718000
H	5.827565000	-0.930085000	-2.586328000
C	4.969773000	0.970292000	-3.135974000
H	5.593455000	1.088403000	-4.016743000

C	4.040510000	1.958381000	-2.798964000
H	3.941448000	2.847614000	-3.413907000
C	3.239692000	1.807953000	-1.668987000
H	2.528469000	2.584017000	-1.403582000
C	2.393141000	2.029683000	1.471565000
C	3.683250000	2.560295000	1.645601000
H	4.537917000	2.082433000	1.177092000
C	3.869957000	3.707060000	2.413628000
H	4.868968000	4.112552000	2.541583000
C	2.773848000	4.333388000	3.013788000
H	2.920459000	5.229746000	3.608941000
C	1.492639000	3.809626000	2.842086000
H	0.637374000	4.298431000	3.298937000
C	1.297505000	2.660290000	2.073058000
H	0.297263000	2.289014000	1.904948000
H	2.477027000	-0.604397000	2.655062000
H	0.713605000	-0.739517000	-1.516849000
C	-0.469253000	-0.340273000	1.817131000
O	-0.862285000	0.005658000	2.846506000
C	-1.567605000	3.158087000	-0.729592000
C	-1.578397000	2.536072000	-2.179585000
B	-0.787840000	0.972524000	-0.676426000
O	-0.849408000	2.154154000	0.036907000
O	-1.341355000	1.118568000	-1.931197000
C	-2.898816000	2.688493000	-2.923604000
H	-3.727026000	2.246221000	-2.369144000
H	-3.119578000	3.746255000	-3.098214000
H	-2.833684000	2.192660000	-3.896596000
C	-0.421703000	3.013664000	-3.059183000
H	0.540391000	2.872299000	-2.560502000
H	-0.411671000	2.425374000	-3.981329000
H	-0.526282000	4.068922000	-3.326391000
C	-0.812182000	4.476927000	-0.603576000
H	-1.283784000	5.254053000	-1.213134000
H	-0.828153000	4.809079000	0.438614000
H	0.230929000	4.377858000	-0.909178000
C	-2.952734000	3.285410000	-0.097942000
H	-3.489422000	2.337647000	-0.140972000
H	-2.837010000	3.564368000	0.953761000
H	-3.552031000	4.055473000	-0.592348000



6-II **(-2334.163827)**

Ir	-0.302674000	0.057349000	0.499174000
P	1.517204000	1.521827000	0.451050000
N	-2.975179000	-1.564374000	0.385820000
N	-1.415429000	-2.588877000	1.457641000
N	0.834573000	-0.709519000	2.265732000
C	-1.666676000	-1.463422000	0.743323000
C	-2.548415000	-3.392322000	1.542796000
H	-2.538883000	-4.336330000	2.063695000
C	-3.531657000	-2.746285000	0.869430000
H	-4.563323000	-3.000619000	0.689023000
C	-3.711883000	-0.543725000	-0.307813000
C	-4.466995000	0.360335000	0.448706000
C	-5.133221000	1.383592000	-0.235465000
H	-5.714895000	2.103061000	0.334472000
C	-5.064870000	1.501342000	-1.626276000
C	-4.323209000	0.553909000	-2.345082000
H	-4.277477000	0.622565000	-3.429085000
C	-3.639339000	-0.483214000	-1.707706000
C	-4.582917000	0.228331000	1.945762000
H	-5.292482000	-0.563623000	2.213764000
H	-4.942213000	1.160118000	2.388270000
H	-3.628228000	-0.029095000	2.412110000
C	-5.786242000	2.610317000	-2.349117000
H	-6.271637000	3.294334000	-1.648026000
H	-6.556718000	2.208686000	-3.017699000
H	-5.095416000	3.191795000	-2.969702000
C	-2.845366000	-1.492435000	-2.493057000
H	-1.770447000	-1.327062000	-2.375193000
H	-3.082537000	-1.419530000	-3.557509000
H	-3.061225000	-2.514297000	-2.163434000

C	-0.099771000	-2.978952000	1.960147000
H	0.531147000	-3.226557000	1.101236000
H	-0.239624000	-3.873498000	2.565216000
C	0.648669000	-1.948249000	2.772732000
C	1.269579000	-2.347660000	3.954332000
H	1.090230000	-3.344623000	4.340207000
C	2.133072000	-1.470378000	4.604583000
H	2.632794000	-1.766019000	5.521163000
C	2.360009000	-0.217252000	4.048499000
H	3.044098000	0.486584000	4.508313000
C	1.690477000	0.146332000	2.879762000
C	1.911789000	1.508483000	2.270224000
H	2.924928000	1.860041000	2.477171000
C	3.089778000	1.081205000	-0.366332000
C	3.816411000	-0.031192000	0.087904000
H	3.440358000	-0.640750000	0.901376000
C	5.030190000	-0.364994000	-0.510495000
H	5.590032000	-1.221175000	-0.147009000
C	5.521522000	0.395067000	-1.575598000
H	6.466242000	0.131436000	-2.041111000
C	4.792212000	1.488876000	-2.043070000
H	5.164775000	2.078641000	-2.874849000
C	3.580841000	1.833822000	-1.441587000
H	3.025895000	2.691675000	-1.804735000
C	1.232355000	3.267302000	0.035184000
C	2.108027000	4.266801000	0.487664000
H	2.973901000	4.003110000	1.087266000
C	1.870585000	5.599910000	0.159576000
H	2.545734000	6.371971000	0.515643000
C	0.767392000	5.941014000	-0.628719000
H	0.585773000	6.980774000	-0.883450000
C	-0.098844000	4.948632000	-1.089392000
H	-0.954458000	5.212153000	-1.703426000
C	0.129811000	3.611987000	-0.758131000
H	-0.543552000	2.836584000	-1.109152000
H	1.215034000	2.227217000	2.720463000
H	-1.015749000	0.533599000	-0.827411000
C	-1.389710000	1.420299000	1.434025000
O	-2.025192000	2.308619000	1.803212000
B	0.667108000	-1.188828000	-0.915148000
O	1.468193000	-2.280218000	-0.613168000
O	0.529953000	-1.043349000	-2.282241000
C	0.634403000	-4.188909000	-1.798977000
H	0.739620000	-4.854348000	-2.660497000
H	0.780490000	-4.784625000	-0.893003000
H	-0.385751000	-3.794820000	-1.789124000
C	3.078163000	-3.634233000	-1.810937000
H	3.828457000	-2.851895000	-1.686697000
H	3.176843000	-4.337973000	-0.978531000
H	3.287781000	-4.177954000	-2.737574000
C	0.659744000	-2.536583000	-4.178970000
H	0.490837000	-1.721702000	-4.889277000
H	1.254082000	-3.305332000	-4.683076000
H	-0.310323000	-2.962903000	-3.916770000
C	2.649616000	-1.239361000	-3.388104000
H	3.323557000	-1.874448000	-3.970454000
H	2.354227000	-0.391752000	-4.012904000
H	3.193426000	-0.853176000	-2.526518000
C	1.668196000	-3.060499000	-1.831406000
C	1.397206000	-2.001292000	-2.957800000