Supporting Information

Reaction of Zirconocene-Carboryne Complex with Pyridines: Ligand C–H Activation

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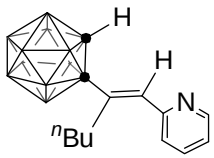
Table S1. Crystal Data and Summary of Data Collection and Refinement for 2, 4-7, 8a and 10

compd	**2**	**4**	**5**	**6**	**7**	**8a**	**10**
formula	$C_{17}H_{25}B_{10}NZr$	$C_{19}H_{29}B_{10}NZr$	$C_{21}H_{27}B_{10}NZr$	$C_{25}H_{29}B_{10}NZr$	$C_{23}H_{33}B_{10}NZr$	$C_{23}H_{33}B_{10}NZr$	$C_{25}H_{29}B_{10}NZr$
cryst size (mm)	0.40x0.30x0.20	0.50x0.4x0.30	0.40x0.3x0.10	0.40x0.30x0.20	0.40x0.30x0.20	0.40x0.30x0.20	0.50x0.20x0.20
fw	442.70	470.75	492.76	542.81	522.82	522.82	542.81
cryst syst	orthorhombic	monoclinic	monoclinic	orthorhombic	monoclinic	monoclinic	monoclinic
space group	*P*bca	$P2_1/m$	$P2_1/m$	*P*nma	*C*c	$P2_1/n$	*P*c
a, Å	14.383(3)	10.490(1)	10.811(3)	15.571(3)	12.806(1)	11.020(2)	10.375(1)
b, Å	14.605(3)	10.605(2)	10.573(3)	15.993(3)	28.139(1)	19.964(3)	23.269(3)
c, Å	20.451(4)	11.092(2)	14.089(4)	10.228(2)	8.488(1)	13.013(2)	11.481(1)
α, deg	90	90	90	90	90	90	90
β, deg	90	109.05(1)	112.16(1)	90	120.85(1)	111.46(1)	108.18(1)
γ, deg	90	90	90	90	90	90	90
V, $Å^3$	4295.9(13)	1166.5(3)	1491.6(7)	2546.9(8)	2625.8(1)	2664.2(8)	2633.3(5)
Z	8	2	2	4	4	4	4
D_{calcd}, Mg/m^3	1.369	1.340	1.097	1.416	1.322	1.303	1.369
radiation (λ), Å	Mo Kα (0.71073)	Mo Kα (0.71073)	Mo Kα (0.71073)	Mo Kα (0.71073)	Mo Kα (0.71073)	Mo Kα (0.71073)	Mo Kα (0.71073)
2θ range, deg	4.0 to 56.1	3.9 to 50.0	3.1 to 50.0	4.7 to 50.0	4.0 to 56.0	3.9 to 56.1	1.7 to 50.6
μ, mm^{-1}	0.515	0.479	0.377	0.449	0.433	0.427	0.435
F(000)	1792	480	500	1104	1072	1072	1104
no. of obsd	5205	2175	2771	2328	5335	6435	11224

reflns							
no. of params refnd	262	160	172	178	316	316	667
goodness of fit	1.036	1.194	1.088	1.044	1.014	1.018	0.997
R1	0.041	0.044	0.052	0.031	0.026	0.052	0.060
wR2	0.097	0.116	0.134	0.078	0.067	0.135	0.100



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rsk0421-H-CDCl3

8.6092 8.5993 7.7167 7.6943 7.6898 7.6749 7.6707 7.6556 7.6513 7.2602 7.2415 7.2078 7.1879 7.1702 7.1639 7.1516 7.7205 6.6027 3.9089 2.7034 2.6831 2.6744 2.6624 1.5577 1.5401 1.5275 1.5189 1.5093 1.5001 1.4802 1.3980 1.3799 1.3616 1.3433 1.3251 1.3070 1.2846 1.2546 0.9637 0.9295 0.9112 0.8930 0.0717

Bruker Advance III 400

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PROCNO	1
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TD	65536
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FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	128
DW	60.800 usec
DE	6.50 usec
TE	298.5 K
D1	1.00000000 sec
TD0	1
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P1	14.83 usec
PL1	0.00 dB
PL1W	8.31434441 W
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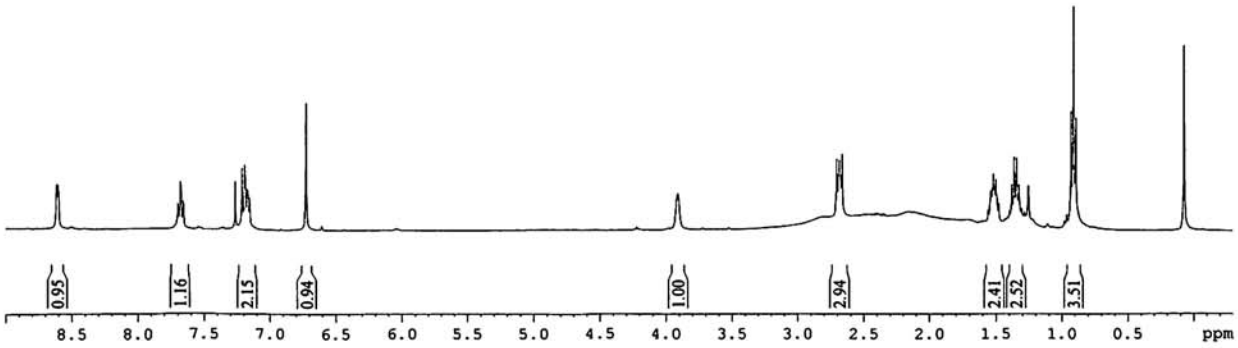

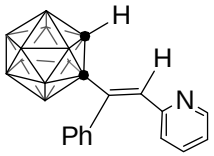

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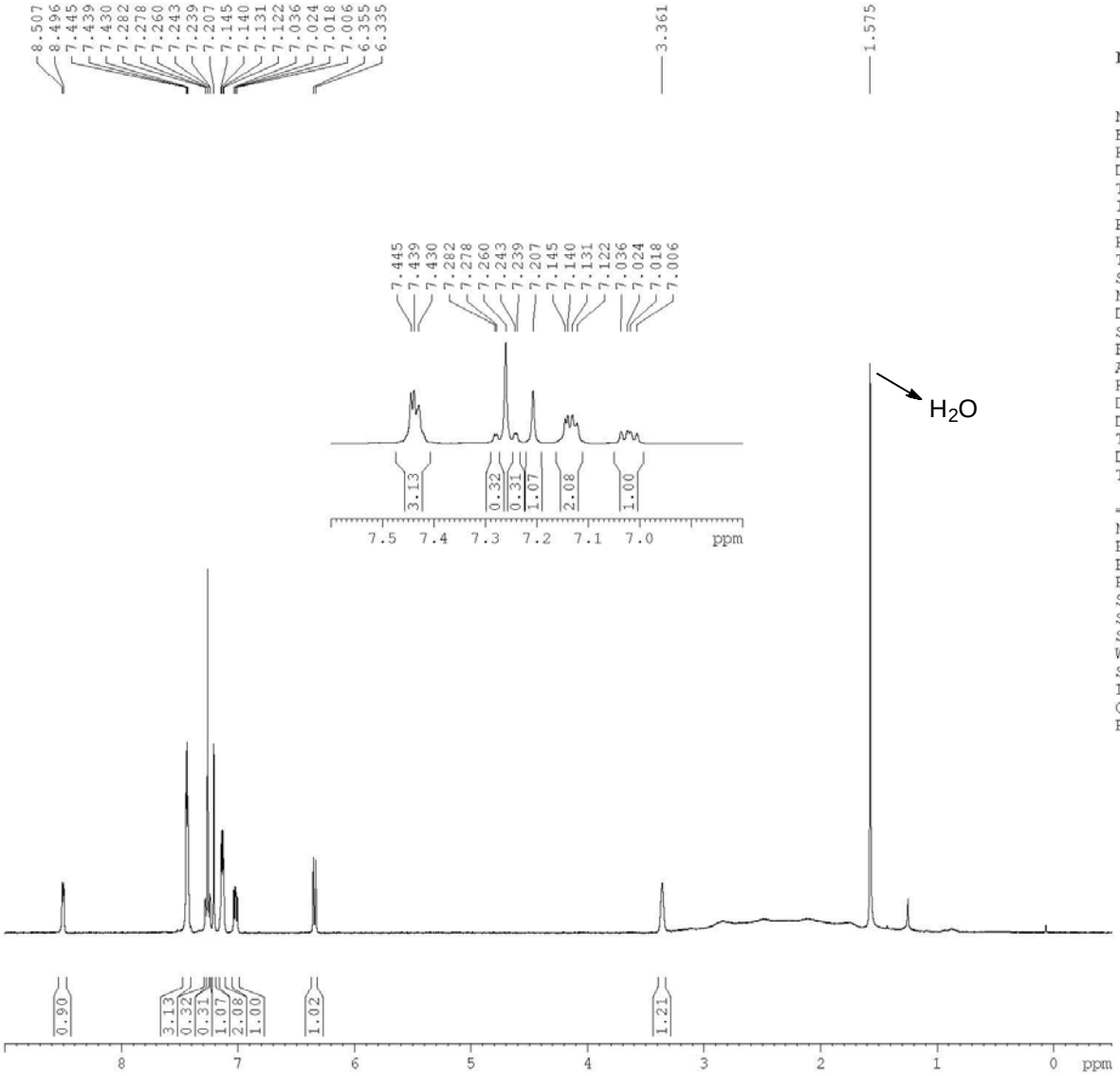

rsk0293-H-CDCl3

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PULPROG                  zg
TD                    65536
SOLVENT               CDCl3
NS                        8
DS                        0
SWH             10000.000 Hz
FIDRES           0.152588 Hz
AQ              3.2768500 sec
RG                      203
DW                   50.000 usec
DE                     6.50 usec
TE                    295.4 K
D1             1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                    14.83 usec
PL1                    0.00 dB
PL1W           8.31434441 W
SFO1          400.1318000 MHz
SI                    65536
SF            400.1300097 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
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