Electronic Supplementary Material (ESI) for Dalton Transactions

SUPPLEMENTARY INFORMATION FOR

Synthesis of *closo*- and *nido*-Biscarboranes with Rigid Unsaturated Linkers as Precursors to Linear Metallacarborane-Based Molecular Rods

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Table S1. Crystallographic details for **3**, **6**, **9**, **14, 15**, and **17**.

compound	**3**	**6**	**9**	**14**	**15**	**17**
empirical formula	$C_6H_{22}B_{20}$	$C_{10}H_{26}B_{20}$	$C_{15}H_{27}B_{20}Cl_3$	$C_8H_{22}B_{20}$	$C_{38}H_{94}B_{18}N_2$	$C_{46}H_{98}B_{18}N_2$
Fw	310.44	362.51	529.92	334.46	773.73	873.84
crystal size (mm^3)	0.26 × 0.16× 0.14	0.20 × 0.14× 0.10	0.86 × 0.20× 0.16	0.42 × 0.26× 0.22	0.36 × 0.06× 0.06	0.36 × 0.22× 0.18
crystal system	orthorhombic	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
space group	*Pnn*2	$P2_1/c$	$P2_1/c$	$P2_1/n$	$P2_1/c$	$P2_1/n$
a (Å)	11.4869(10)	7.1373(5)	23.4549(9)	6.7200(8)	14.8236(17)	10.9742(16)
b (Å)	11.6934(11)	11.1008(8)	11.1387(4)	12.6135(15)	18.229(2)	15.710(2)
c (Å)	6.8962(6)	13.1767(10)	23.2584(9)	12.0553(14)	19.262(2)	16.935(3)
β (deg)		92.339(1)	111.488(2)	100.506(2)	100.120(2)	90.556(3)
V ($Å^3$)	926.30(14)	1043.12(13)	5654.1(4)	1004.7(2)	5124.1(10)	2919.7(7)
Z	2	2	8	2	4	2
T (K)	173(2)	173(2)	173(2)	173(2)	173(2)	173(2)
λ (Å)	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
d_{calc} ($g \cdot cm^{-3}$)	1.113	1.154	1.245	1.106	1.003	0.994
μ (mm^{-1})	0.046	0.051	0.333	0.047	0.051	0.051
θ_{max} (deg)	27.14	25.00	29.91	27.13	25.00	27.12
unique data	7733	7616	51767	8555	49669	25157
observed data [$I > 2\sigma(I)$]	996	1400	8798	1753	3826	3048
parameters	162	162	930	171	682	383
GOF[a] on F^2	1.189	1.057	1.040	1.079	1.001	1.048
$R1$[b], $wR2$[c] [$I > 2\sigma(I)$]	0.0687, 0.1714	0.0489, 0.1145	0.0582, 0.1481	0.0518, 0.1354	0.0770, 0.1491	0.0702, 0.1771
$R1$[b], $wR2$[c] (all data)	0.0760, 0.1791	0.0713, 0.1257	0.1176, 0.1800	0.0650, 0.1443	0.1974, 0.2024	0.1580, 0.2187
$\Delta\rho_{max,min}$ ($e \cdot A^{-3}$)	0.473, –0.202	0.205, –0.199	0.530, –0.384	0.283, –0.107	0.216, –0.289	0.444, –0.139
T_{min}/T_{max}	0.75 /0.99	0.75 /0.99	0.76 /0.95	0.71 /0.99	0.67 /0.75	0.81 /0.99

[a] $GOF = [\Sigma[w(F_o^2 - F_c^2)^2]/(N_{obs} - N_{params})]^{1/2}$. [b] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [c] $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$.

Table S2. Selected bond distances (Å) and angles (°) in **3**, **6**, **9**, **14**, **15**, and **17**.

	3	**6**	**9**	**14**	**15**	**17**
B–C	1.527(5)	1.584(3)	1.542(3) 1.544(3) 1.545(3) 1.545(3)	1.5450(16)	1.552(12) 1.553(12)	1.550(4)
C≡C	1.220(7)	-	1.195(2) 1.200(2) 1.200(2) 1.200(3)	1.2051(16)	1.215(10)	1.190(3)
C_{arom}–C_{arom}	-	1.392(2) 1.396(2) 1.397(2)	1.395(3) 1.388(3) 1.388(3) 1.389(3) 1.381(3) 1.384(3) 1.390(3) 1.396(2) 1.384(2) 1.396(2) 1.389(3) 1.387(2)	-	-	1.386(4) 1.380(4) 1.375(4)
B–C_B≡C_X	174.2(2)	-	177.4(2) 177.8(2) 176.1(2) 178.4(2)	178.74(14)	177.9(8)	178.7(3)
C_B≡C_X–X, X = B or C	174.2(2)	-	178.1(2) 178.4(2) 177.3(2) 177.8(3)	179.38(17)	178.8(8)	178.9(3)