Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information

Table S1. Crystallographic data of the Et_4N^+ salt of clusters **2**−**6**.

Complex	$(Et_4N)_2$•**[2]**	$(Et_4N)_2$•**[3]**	$(Et_4N)_2$•**[4]**•DMF	$(Et_4N)_2$•**[5]**•2DMF	$(Et_4N)_2$•**[6]**•8DMF
Empirical formula	$C_{54}H_{104}B_2Fe_6N_{16}S_{10}W_2$	$C_{70}H_{104}B_2Fe_6N_{16}S_{10}W_2$	$C_{77}H_{119}B_2Fe_6N_{17}OS_{10}W_2$	$C_{52}H_{98}B_2Fe_6N_{30}O_2S_6W_2$	$C_{74}H_{149}B_2Fe_6N_{24}O_{12}S_6W_2$
Formula weight	2022.55	2214.71	2343.9	2092.38	2483.94
Crystal system	Monoclinic	Monoclinic	Triclinic	Triclinic	Orthorhombic
Space group	$P2_1/n$	$C2/c$	P-1	P-1	$Ibam$
Z	2	4	4	1	4
a (Å)	12.814(5)	27.096(4)	14.222(3)	10.9698(17)	24.0221(8)
b (Å)	18.930(8)	19.118(3)	25.989(5)	11.9853(18)	18.0186(6)
c (Å)	15.716(6)	20.286(3)	28.267(5)	15.905(2)	23.9879(7)
α (°)	90	90	76.250(2)	72.820(2)	90
β (°)	95.057(9)	98.477(2)	89.471(2)	83.033(2)	90
γ (°)	90	90	88.082(2)	81.869(2)	90
V (Å^3)	3797(3)	10393(3)	10142(3)	1970.7(5)	10383.0(6)
D_{calcd} (g cm^{-3})	1.769	1.415	1.535	1.763	1.589
μ (mm^{-1})	4.449	3.258	3.344	4.194	3.203
F (000)	2028.0	4440.0	4728.0	1046.0	5068.0
GOF on F^2	0.962	1.008	1.019	1.030	1.083
R_1[a], wR_2[b] ([c])	0.0462, 0.1213	0.0366, 0.0927	0.0440, 0.0926	0.0364, 0.0785	0.0442, 0.1235
R_1[a], wR_2[b] ([d])	0.0524, 0.1259	0.0575, 0.1026	0.0777, 0.1072	0.0527, 0.0855	0.0465, 0.1261
($\Delta\rho$)max / ($\Delta\rho$)min[e]	1.57 / -0.59	0.81 / -0.42	1.53 / -1.15	1.45 / -0.78	0.98 / -1.38

[a] $R_1 = \sum(|F_o| - |F_c|)/\sum|F_o|$. [b] $wR_2 = \{\sum[w(F_o^2 - F_c^2)^2]/\sum[w(F_o^2)^2]\}^{1/2}$. [c] [$I \geq 2\sigma(I)$]. [d] [all data]. [e] unit (e·Å^{-3})