

Supporting information

With complements of the ligands: an unusual S-shaped [Mn₇]₂ assembly from tethered calixarenes

metal VBS	d(M-L1)	d(M-L2)	d(M-L3)	d(M-L4)	d(M-L5)	r(0)	beta
Mn1	1.891	1.934	1.953	1.916	2.083	1.76	0.37
	-0.131	-0.174	-0.193	-0.156	-0.323		
	-0.35405	-0.47027	-0.52162	-0.421622	-0.87297		
	0.701837	0.624833	0.593557	0.6559822	0.417708		
Mn1(Qx.State)	2.993918						

metal VBS	d(M-L1)	d(M-L2)	d(M-L3)	d(M-L4)	d(M-L5)	d(M-L6)	r(0)	beta
Mn2	2.206	2.204	1.946	1.937	1.917	1.94	1.76	0.37
	-0.446	-0.444	-0.186	-0.177	-0.157	-0.18		
	-1.20541	-1.2	-0.5027	-0.478378	-0.42432	-0.48649		
	0.299571	0.301194	0.604894	0.6197876	0.654212	0.614783		
Mn2(Qx.State)	3.09444							

metal VBS	d(M-L1)	d(M-L2)	d(M-L3)	d(M-L4)	d(M-L5)	d(M-L6)	r(0)	beta
Mn3	2.119	1.981	1.973	1.916	1.916	1.94	1.76	0.37
	-0.359	-0.221	-0.213	-0.156	-0.156	-0.18		
	-0.97027	-0.5973	-0.57568	-0.421622	-0.42162	-0.48649		
	0.378981	0.550297	0.562325	0.6559822	0.655982	0.614783		
Mn3(Qx.State)	2.803567							

metal VBS	d(M-L1)	d(M-L2)	d(M-L3)	d(M-L4)	d(M-L5)	r(0)	beta
Mn4	2.116	2.208	2.155	2.191	2.19	1.79	0.37
	-0.326	-0.418	-0.365	-0.401	-0.4		
	-0.88108	-1.12973	-0.98649	1.083784	-1.08108		
	0.414335	0.323121	0.372885	0.338313	0.339229		
Mn4(Qx.State)	1.787881						

metal VBS	d(M-L1)	d(M-L2)	d(M-L3)	d(M-L4)	d(M-L5)	r(0)	beta
Mn5	2.128	2.218	2.17	2.161	2.187	1.79	0.37
	-0.338	-0.428	-0.38	-0.371	-0.397		
	-0.91351	-1.15676	1.02703	-1.002703	1.07297		
	0.401112	0.314505	0.35807	0.3668865	0.34199		
Mn5(Qx.State)	1.782564						

metal VBS	d(M-L1)	d(M-L2)	d(M-L3)	d(M-L4)	d(M-L5)	d(M-L6)	r(0)	beta
Mn6	2.284	2.189	2.005	1.906	1.869	1.934	1.76	0.37
	-0.524	-0.429	-0.245	-0.146	-0.109	-0.174		
	-1.41622	-1.15946	-0.66216	-0.394595	-0.29459	-0.47027		
	0.24263	0.313656	0.515735	0.6739532	0.744833	0.624833		
Mn6(Qx.State)	3.115641							

metal VBS	d(M-L1)	d(M-L2)	d(M-L3)	d(M-L4)	d(M-L5)	d(M-L6)	r(0)	beta
Mn7	2.292	2.171	1.865	1.908	2.027	1.913	1.76	0.37
	-0.532	-0.411	-0.105	-0.148	-0.267	-0.153		
	-1.43784	-1.11081	-0.28378	-0.4	-0.72162	-0.41351		
	0.237441	0.329292	0.752929	0.67032	0.485964	0.661323		
Mn7(Qx.State)	3.137268							

Figure S1. Bond Valence Sum calculations for Mn centres in compound **6**.