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Supporting information

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

				707000000		10000		
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(Ox.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	h c	
	-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(Ox.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(Ox.State)	2.803567	0.000201	0.002020	J.0003022	0.000002	0.014703		
WII3(OX.State)	2.003307							
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	
WITH		A CONTRACTOR OF THE	400,000	-0.401	-0.4	10	0.07	
	-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(Ox.State)	1.787881	0.020121	0.072000	0.000010	0.000220			
(90090909)	1.707001							
metal VRS	d(M-I 1)	d(M-L2)	d(M-I 3)	d(M-I 4)	d(M-I 5)	r(0) E	beta	
AND REPORT OF THE PROPERTY OF	d(M-L1)	d(M-L2)	d(M-L3)	d(M-L4)	-1		beta 0.37	
A CHARLEST AND A CHARLEST CO.	2.128	2.218	2.17	2.161	2.187	r(0) 1.79	0.37	
A CHARLEST AND A CHARLEST CO.					-1	Charles and the same of the sa	T. C. C. C.	
metal VBS Mn5	-0.338	2.218 -0.428	-0.38 -	2.161 -0.371	2.187 -0.397 -	Charles and the same of the sa	T. C. C. C.	
A CHECK AND CHECK CONT. II.	2.128 -0.338 -0.91351	-0.428 -1.15676	2.17 -0.38 - 1.02703	2.161 -0.371 -1.002703	2.187 -0.397 - 1.07297	Charles and the same of the sa	T. C. C. C.	
Mn5	2.128 -0.338 -0.91351 0.401112	2.218 -0.428	-0.38 -	2.161 -0.371	2.187 -0.397 -	Charles and the same of the sa	T. C. C. C.	
Mn5	2.128 -0.338 -0.91351	-0.428 -1.15676	2.17 -0.38 - 1.02703	2.161 -0.371 -1.002703	2.187 -0.397 - 1.07297	Charles and the same of the sa	T. C. C. C.	
Mn5 Mn5(Ox.State)	2.128 -0.338 -0.91351 0.401112 1.782564	2.218 -0.428 -1.15676 0.314505	2.17 -0.38 - 1.02703 0.35807	2.161 -0.371 -1.002703 0.3668865	2.187 -0.397 - 1.07297 0.34199	1.79	T. C. C. C.	beta
Mn5(Ox.State) metal VBS	2.128 -0.338 -0.91351 0.401112 1.782564	2.218 -0.428 -1.15676 0.314505	2.17 -0.38 - 1.02703 0.35807	2.161 -0.371 -1.002703 0.3668865	2.187 -0.397 -1.07297 0.34199	1.79 d(M-L6)	0.37	2000
Mn5(Ox.State) metal VBS	2.128 -0.338 -0.91351 0.401112 1.782564 d(M-L1) 2.284	2.218 -0.428 -1.15676 0.314505 d(M-L2) 2.189	2.17 -0.38 - 1.02703 0.35807 d(M-L3) 2.005	2.161 -0.371 -1.002703 0.3668865 d(M-L4) 1.906	2.187 -0.397 - 1.07297 0.34199 d(M-L5) 1.869	1.79 d(M-L6) 1.934	0.37	2000
Mn5(Ox.State) metal VBS	2.128 -0.338 -0.91351 0.401112 1.782564 d(M-L1) 2.284 -0.524	2.218 -0.428 -1.15676 0.314505 d(M-L2) 2.189 -0.429	2.17 -0.38 - 1.02703 0.35807 d(M-L3) 2.005 -0.245	2.161 -0.371 -1.002703 0.3668865 d(M-L4) 1.906 -0.146	2.187 -0.397 - 1.07297 0.34199 d(M-L5) 1.869 -0.109	1.79 d(M-L6) 1.934 -0.174	0.37	2000
Mn5(Ox.State) metal VBS	2.128 -0.338 -0.91351 0.401112 1.782564 d(M-L1) 2.284 -0.524 -1.41622	2.218 -0.428 -1.15676 0.314505 d(M-L2) 2.189 -0.429 -1.15946	2.17 -0.38 - 1.02703 0.35807 d(M-L3) 2.005 -0.245 -0.66216	2.161 -0.371 -1.002703 0.3668865 d(M-L4) 1.906 -0.146 -0.394595	2.187 -0.397 - 1.07297 0.34199 d(M-L5) 1.869 -0.109 -0.29459	1.79 d(M-L6) 1.934 -0.174 -0.47027	0.37	2000
Mn5(Ox.State) metal VBS Mn6	2.128 -0.338 -0.91351 0.401112 1.782564 d(M-L1) 2.284 -0.524 -1.41622 0.24263	2.218 -0.428 -1.15676 0.314505 d(M-L2) 2.189 -0.429	2.17 -0.38 - 1.02703 0.35807 d(M-L3) 2.005 -0.245	2.161 -0.371 -1.002703 0.3668865 d(M-L4) 1.906 -0.146	2.187 -0.397 - 1.07297 0.34199 d(M-L5) 1.869 -0.109	1.79 d(M-L6) 1.934 -0.174	0.37	2000
Mn5(Ox.State) metal VBS Mn6	2.128 -0.338 -0.91351 0.401112 1.782564 d(M-L1) 2.284 -0.524 -1.41622	2.218 -0.428 -1.15676 0.314505 d(M-L2) 2.189 -0.429 -1.15946	2.17 -0.38 - 1.02703 0.35807 d(M-L3) 2.005 -0.245 -0.66216	2.161 -0.371 -1.002703 0.3668865 d(M-L4) 1.906 -0.146 -0.394595	2.187 -0.397 - 1.07297 0.34199 d(M-L5) 1.869 -0.109 -0.29459	1.79 d(M-L6) 1.934 -0.174 -0.47027	0.37	2000
Mn5(Ox.State) metal VBS Mn6 Mn6(Ox.State)	2.128 -0.338 -0.91351 0.401112 1.782564 d(M-L1) 2.284 -0.524 -1.41622 0.24263 3.115641	2.218 -0.428 -1.15676 0.314505 d(M-L2) 2.189 -0.429 -1.15946 0.313656	2.17 -0.38 - 1.02703 0.35807 d(M-L3) 2.005 -0.245 -0.66216 0.515735	2.161 -0.371 -1.002703 0.3668865 d(M-L4) 1.906 -0.146 -0.394595 0.6739532	2.187 -0.397 - 1.07297 0.34199 d(M-L5) 1.869 -0.109 -0.29459 0.744833	1.79 d(M-L6) 1.934 -0.174 -0.47027 0.624833	0.37 r(0) 1.76	
Mn5(Ox.State) metal VBS Mn6 Mn6(Ox.State) metal VBS	2.128 -0.338 -0.91351 0.401112 1.782564 d(M-L1) 2.284 -0.524 -1.41622 0.24263 3.115641	2.218 -0.428 -1.15676 0.314505 d(M-L2) 2.189 -0.429 -1.15946 0.313656	2.17 -0.38 - 1.02703 0.35807 d(M-L3) 2.005 -0.245 -0.66216 0.515735	2.161 -0.371 -1.002703 0.3668865 d(M-L4) 1.906 -0.146 -0.394595 0.6739532	2.187 -0.397 - 1.07297 0.34199 d(M-L5) 1.869 -0.109 -0.29459 0.744833	d(M-L6) 1.934 -0.174 -0.47027 0.624833 d(M-L6)	0.37 r(0) 1.76	beta
Mn5(Ox.State) metal VBS Mn6 Mn6(Ox.State)	2.128 -0.338 -0.91351 0.401112 1.782564 d(M-L1) 2.284 -0.524 -1.41622 0.24263 3.115641 d(M-L1) 2.292	2.218 -0.428 -1.15676 0.314505 d(M-L2) 2.189 -0.429 -1.15946 0.313656 d(M-L2) 2.171	2.17 -0.38 - 1.02703 0.35807 d(M-L3) 2.005 -0.245 -0.66216 0.515735 d(M-L3) 1.865	2.161 -0.371 -1.002703 0.3668865 d(M-L4) 1.906 -0.146 -0.394595 0.6739532 d(M-L4) 1.908	2.187 -0.397 - 1.07297 0.34199 d(M-L5) 1.869 -0.109 -0.29459 0.744833 d(M-L5) 2.027	d(M-L6) 1.934 -0.174 -0.47027 0.624833 d(M-L6) 1.913	0.37 r(0) 1.76	beta
Mn5(Ox.State) metal VBS Mn6 Mn6(Ox.State) metal VBS	2.128 -0.338 -0.91351 0.401112 1.782564 d(M-L1) 2.284 -0.524 -1.41622 0.24263 3.115641 d(M-L1) 2.292 -0.532	2.218 -0.428 -1.15676 0.314505 d(M-L2) 2.189 -0.429 -1.15946 0.313656 d(M-L2) 2.171 -0.411	2.17 -0.38 - 1.02703 0.35807 d(M-L3) 2.005 -0.245 -0.66216 0.515735 d(M-L3) 1.865 -0.105	2.161 -0.371 -1.002703 0.3668865 d(M-L4) 1.906 -0.146 -0.394595 0.6739532 d(M-L4) 1.908 -0.148	2.187 -0.397 - 1.07297 0.34199 d(M-L5) 1.869 -0.109 -0.29459 0.744833 d(M-L5) 2.027 -0.267	d(M-L6) 1.934 -0.174 -0.47027 0.624833 d(M-L6) 1.913 -0.153	0.37 r(0) 1.76	beta
Mn5(Ox.State) metal VBS Mn6 Mn6(Ox.State) metal VBS	2.128 -0.338 -0.91351 0.401112 1.782564 d(M-L1) 2.284 -0.524 -1.41622 0.24263 3.115641 d(M-L1) 2.292 -0.532 -1.43784	2.218 -0.428 -1.15676 0.314505 d(M-L2) 2.189 -0.429 -1.15946 0.313656 d(M-L2) 2.171 -0.411 -1.11081	2.17 -0.38 - 1.02703 0.35807 d(M-L3) -0.245 -0.66216 0.515735 d(M-L3) -0.865 -0.105 -0.28378	2.161 -0.371 -1.002703 0.3668865 d(M-L4) 1.906 -0.146 -0.394595 0.6739532 d(M-L4) 1.908 -0.148 -0.4	2.187 -0.397 - 1.07297 0.34199 d(M-L5) 1.869 -0.109 -0.29459 0.744833 d(M-L5) 2.027 -0.267 -0.72162	d(M-L6) 1.934 -0.174 -0.47027 0.624833 d(M-L6) 1.913 -0.153 -0.41351	0.37 r(0) 1.76	beta
Mn5(Ox.State) metal VBS Mn6 Mn6(Ox.State) metal VBS	2.128 -0.338 -0.91351 0.401112 1.782564 d(M-L1) 2.284 -0.524 -1.41622 0.24263 3.115641 d(M-L1) 2.292 -0.532	2.218 -0.428 -1.15676 0.314505 d(M-L2) 2.189 -0.429 -1.15946 0.313656 d(M-L2) 2.171 -0.411	2.17 -0.38 - 1.02703 0.35807 d(M-L3) 2.005 -0.245 -0.66216 0.515735 d(M-L3) 1.865 -0.105	2.161 -0.371 -1.002703 0.3668865 d(M-L4) 1.906 -0.146 -0.394595 0.6739532 d(M-L4) 1.908 -0.148	2.187 -0.397 - 1.07297 0.34199 d(M-L5) 1.869 -0.109 -0.29459 0.744833 d(M-L5) 2.027 -0.267	d(M-L6) 1.934 -0.174 -0.47027 0.624833 d(M-L6) 1.913 -0.153	0.37 r(0) 1.76	

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