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Structural analysis of {M_4O_4} cubanes where M = Mn and Fe

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Table S1. Geometric parameters for manganese(I) cubanes

Code	Mn-Mn (Å)	s.d.	distortion	Mn-O (Å)	Tet.par.	Mn-O-Mn (°)	O-O (Å)	Ligand coding	Ref.
FLOHMN	3.199	0.000		2.053	0.791	102.37	2.529	$Mn_4/0s_4/m_{12}$	1
FLOHMN01	3.197	0.000		2.052	0.791	102.35	2.529	$Mn_4/0s_4/m_{12}$	2
KUSGEK	3.159	0.006	L, S4-	2.033	0.798	101.95	2.519	$Mn_4/0s_4/m_{12}$	3
KUSGEK10	3.159	0.006	L, S4-	2.033	0.798	101.95	2.519	$Mn_4/0s_4/m_{12}$	2
PEGGUD	3.156	0.009	L, C3+	2.037	0.804	101.57	2.538	$Mn_4/0s_4/m_{12}$	4
PEGHAK	3.178	0.004	L	2.046	0.798	101.92	2.537	$Mn_4/0s_4/m_{12}$	4
PEHKIW	3.165	0.014	L, S4-	2.040	0.797	101.97	2.524	$Mn_4/0s_4/m_{12}$	5
PEHKIW10	3.165	0.014	L, S4-	2.039	0.797	101.97	2.524	$Mn_4/0s_4/m_{12}$	2
TITXID	3.172	0.016	L	2.051	0.796	102.08	2.524	$Mn_4/0s_4/m_{12}$	6
TITXOJ	3.173	0.012	L	2.052	0.793	102.21	2.517	$Mn_4/0s_4/m_{12}$	6
VOKFIK	3.194	0.002		2.058	0.791	102.33	2.528	$Mn_4/0s_4/m_{12}$	7
VOKFIK10	3.193	0.002		2.047	0.794	102.17	2.535	$Mn_4/0s_4/m_{12}$	2
ZEBFER	3.201	0.006	L, S4+	2.058	0.794	102.14	2.543	$Mn_4/0s_4/m_{12}$	2
ZEBFIV	3.196	0.001		2.056	0.787	102.61	2.515	$Mn_4/0s_4/m_{12}$	2
ZEBFOB	3.201	0.003	L, S4-	2.053	0.795	102.13	2.544	$Mn_4/0s_4/m_{12}$	2
ZEBFUH	3.200	0.005	L	2.042	0.794	102.20	2.540	$Mn_4/0s_4/m_{12}$	2
ZEBFUH	3.197	0.006	L, C3-	2.036	0.793	102.21	2.536	$Mn_4/0s_4/m_{12}$	2
ZEBGAO	3.166	0.010	L	2.048	0.802	101.67	2.541	$Mn_4/0s_4/m_{12}$	2
ZEBGES	3.158	0.005	L, S4-	2.039	0.801	101.74	2.531	$Mn_4/0s_4/m_{12}$	2
ZEBGOC	3.178	0.023	L, S4+	2.060	0.800	101.80	2.543	$Mn_4/0s_4/m_{12}$	2
ZEBHAP	3.156	0.017	L, S4-	2.047	0.807	101.40	2.546	$Mn_4/0s_4/m_{12}$	2
ZIZHIZ	3.205	0.001	0	2.083	0.795	102.10	2.548	$Mn_4/0s_4/m_{12}$	8
Mean value	3.180			2.048	0.796	102.04	2.532		
s.d	0.018			0.009	0.005	0.28	0.010		

Legend for tables:
Mn-Mn (Å): average Mn-Mn distance for the structure
s.d. : standard deviation of the Mn-Mn distances
distortion : classified as low (L), medium (M) or high (H) as s.d. < 0.030, 0.30 < s.d. < 0.100 , s.d. > 0.100, symmetry of the distortion, + elongation, - compression.
Mn-O (Å) : average Mn-O distance for the structure
Tet.par. : Tetrahedral parameter = O-O / Mn-Mn
Mn-O-Mn (°) : average Mn-O-Mn angle for the structure
O-O (Å) : average O-O distance for the structure
Ligand coding : metal/μ_3-bridging ligand/terminal ligand. $Mn_4/0s_4/m_{12}$ implies four manganese, four unsupported μ_3-bridging ligands, and twelve monodentate terminal ligands.
Macro: macrocyclic ligand
Ref. : Literature reference

Table S2. Geometric parameters for manganese(II) cubanes

Code	Mn-Mn (Å)	s.d.	distortion	Mn-O (Å)	Tet.par.	Mn-O-Mn (°)	O-O (Å)	Ligand coding	Ref.
CEHVOB	3.314	0.029	L,S4-	2.198	0.866	97.85	2.871	$Mn_4/3s_4/$	9
CUGKUK	3.361	0.064	M, S4-	2.204	0.840	99.41	2.823	macro	10
FUBMIY	3.370	0.059	M, S4-	2.206	0.836	99.61	2.819	macro	11
LEFXEZ[a]	3.231	0.076	M, S4-	2.167	0.888	96.41	2.870	$Mn_4/0s_4/m_2b_4$	12
MAWZIT	3.373	0.043	M	2.206	0.836	99.69	2.818	$Mn_4/2s_4/m_4$	13
MOFSAB	3.371	0.032	M, S4-	2.211	0.842	99.32	2.838	$Mn_4/2s_4/m_4$	14
OCIJAM	3.320	0.113	H,C3+	2.172	0.861	97.15	2.859		15
TAVNUZ	3.258	0.040	M, S4-	2.175	0.877	97.38	2.855	$Mn_4/0s_4/m_4b_4$	16
TAVPAH	3.267	0.046	M, S4-	2.201	0.847	100.36	2.767	$Mn_4/0s_4/m_4b_4$	16
TEZPUJ	3.379	0.166	H,S4+	2.198	0.817	100.43	2.761	macro	17
TEZQAQ	3.375	0.154	H,S4+	2.189	0.847	97.61	2.858	macro	17
VAFBIO	3.293	0.089	M, S4-	2.216	0.860	99.58	2.831	$Mn_4/1s2_4/m_4$	18
YAQXUK	3.384	0.076	M	2.195	0.836	98.74	2.831	$Mn_4/2s_4/m_4$	19
mean	3.330			2.195	0.850	98.735	2.831		
	0.053			0.015	0.019	1.307	0.035		

Table S3. Geometric parameters for manganese(III) and mixed valence cubanes

Code	O.N.	Mn-Mn (Å)	s.d.	distortion	Mn-O (Å)	Tet.par.	Mn-O-Mn (°)	O-O (Å)	Ligand coding	Ref.
VOKFUW	Mn1.25	3.228	0.030	L, C3+	2.083	0.804	97.6	2.595	$Mn_4/0s_4/m_{12}$	7
MABHIH	Mn2.5	3.199	0.191	H, C2	2.128	0.871	97.6	2.787		20
TEDPEX	Mn2.5	3.150	0.229	H, C2	2.113	0.883	96.7	2.782	$Mn_4/2s2_4/d_2$	21
mean		3.174			2.120	0.877	97.140	2.784		
LAHXEY	Mn(III)	3.070	0.167	H, C2	2.044	0.864	98.1	2.652	$Mn_4/0s_4/m_2d_5$	22
MOTFIK	Mn(III)	3.026	0.168	H, C2	2.039	0.882	97.0	2.670		23
mean		3.048			2.042	0.873	97.549	2.661		
UFAMAP	Mn3.25	3.008	0.243	H, C3-	2.013	0.875	97.6	2.633	$Mn_4/0s_4/b_3d_3$	24
VALROP	Mn3.25	2.965	0.183	H, C3-	1.979	0.876	96.2	2.597	$Mn_4/0s_4/b_3d_3$	25
VALRUV	Mn3.25	2.956	0.183	H, C3-	1.984	0.887	96.2	2.623	$Mn_4/0s_4/b_3d_3$	25
ZALSUA	Mn3.25	3.000	0.221	H, C3-	2.008	0.878	96.1	2.634	$Mn_4/0s_4/b_3d_3$	26
ZALSUA01	Mn3.25	3.000	0.221	H, C3-	2.008	0.878	97.4	2.634	$Mn_4/0s_4/b_3d_3$	27
mean		2.986			1.998	0.879	96.7	2.624		
LAHXIC	Mn3.5	2.920	0.056	M, C2	1.943	0.874	97.4	2.551	$Mn_4/0s_4/d_6$	22
LAHXIC	Mn3.5	2.921	0.034	M, C2	1.947	0.877	97.2	2.563	$Mn_4/0s_4/d_6$	22
LAHXOI	Mn3.5	2.911	0.095	M, C2	1.945	0.882	96.9	2.569	$Mn_4/0s_4/d_6$	22
NAYSUB	Mn3.5	2.930	0.019	L, C3-	1.953	0.876	97.3	2.567	$Mn_4/0s_4/d_6$	28
NAYSUB	Mn3.5	2.923	0.003	L, C3-	1.948	0.877	97.2	2.563	$Mn_4/0s_4/d_6$	28
NAYSUB	Mn3.5	2.931	0.028	L, C3+	1.948	0.872	97.5	2.554	$Mn_4/0s_4/d_6$	28
NAYSUB	Mn3.5	2.923	0.022	L, C3-	1.947	0.875	97.3	2.558	$Mn_4/0s_4/d_6$	28
NAYSUB01	Mn3.5	2.928	0.021	L, C3-	1.935	0.858	98.3	2.513	$Mn_4/0s_4/d_6$	29
NAYSUB01	Mn3.5	2.937	0.054	M, C3-	1.948	0.866	97.8	2.544	$Mn_4/0s_4/d_6$	29
NAYSUB01	Mn3.5	2.922	0.052	M, C3+	1.939	0.867	97.8	2.534	$Mn_4/0s_4/d_6$	29
NAYSUB01	Mn3.5	2.927	0.047	M, C3-	1.958	0.885	96.7	2.590	$Mn_4/0s_4/d_6$	29
mean		2.922			1.946	0.874	97.4	2.555		
HIRDIV	Mn3.75	2.888	0.057	M, C3+	1.922	0.873	97.4	2.522	$Mn_4/0s_4/d_6$	30
NECJAH	Mn3.75	2.885	0.050	M, C3+	1.920	0.873	97.4	2.519	$Mn_4/0s_4/d_6$	31
mean		2.886			1.921	0.873	97.4	2.520		

Table S4. Geometric parameters for manganese(IV) cubanes

Code	Mn-Mn (Å)	s.d.	distortion	Mn-O (Å)	Tet.par.	Mn-O-Mn (°)	O-O (Å)	Ref.
VOPRIB	2.859	0.061	M, S4-	1.915	0.886	96.6	2.534	32
ACIZUH	2.897	0.062	M, S4-	1.926	0.870	97.5	2.522	33
ACOBAV	2.864	0.061	M, S4-	1.912	0.879	97.0	2.517	33
AQACMN	2.860	0.064	M, S4-	1.908	0.877	97.1	2.508	34
AQACMN02	2.856	0.056	M, S4-	1.913	0.886	96.6	2.530	35
AQACMN03	2.848	0.056	M, S4-	1.906	0.885	96.7	2.519	36
BEDCIX	2.863	0.054	M, S4-	1.915	0.883	96.8	2.530	37

DAGJEB	2.847	0.022	L, S4-	1.907	0.887	96.6	2.525	38
DATVEA	2.873	0.081	M, S4-	1.914	0.874	97.3	2.511	39
ESIXEJ	2.865	0.066	M, S4-	1.909	0.875	97.2	2.508	40
FAQBUV	2.888	0.068	M, S4-	1.926	0.877	97.1	2.534	41
FERREA	2.858	0.057	M, S4-	1.913	0.885	96.7	2.530	42
FICSIU	2.862	0.064	M, S4-	1.913	0.882	96.8	2.525	43
IBIHUX	2.883	0.079	M, S4-	1.925	0.878	97.0	2.531	44
KAGLEJ	2.880	0.087	M, S4-	1.924	0.880	96.9	2.533	45
KAGLEJ10	2.880	0.087	M, S4-	1.924	0.880	96.9	2.533	46
KEQXEJ	2.870	0.066	M, S4-	1.916	0.879	97.0	2.524	47
LAYCIY	2.866	0.076	M, S4-	1.913	0.878	97.1	2.515	48
LAYCOE	2.872	0.079	M, S4-	1.919	0.881	96.9	2.529	48
MABGAY	2.865	0.057	M, S4-	1.915	0.883	96.8	2.530	49
MABGAY01	2.874	0.054	M, S4-	1.921	0.882	96.9	2.535	49
MABGEC	2.871	0.052	M, S4-	1.919	0.883	96.8	2.534	49
NEPZEN	2.860	0.063	M, S4-	1.913	0.883	96.8	2.525	50
NORXUN	2.872	0.078	M, S4-	1.918	0.879	97.0	2.524	51
PAKSIE	2.862	0.053	M, S4-	1.917	0.885	96.7	2.534	52
PATZOA	2.870	0.053	M, C3+	1.917	0.881	96.9	2.530	53
RALWUW	2.864	0.058	M, S4-	2.036	0.882	96.8	2.527	54
REZFIL	2.846	0.039	M, C3+	2.036	0.888	96.5	2.528	55
RUHSES	2.881	0.062	M, S4-	1.915	0.880	96.9	2.536	56
RUHSIW	2.880	0.056	M, S4-	1.907	0.889	96.5	2.559	56
SABNEP	2.854	0.044	M, S4-	1.924	0.884	96.7	2.523	57
SISYEY	2.873	0.057	M, S4-	1.931	0.880	97.0	2.527	58
SISYEY01	2.873	0.057	M, S4-	1.909	0.880	97.0	2.527	59
SUWZEP	2.855	0.071	M, S4-	1.918	0.882	96.8	2.517	60
SUWZEP01	2.869	0.082	M, S4-	1.918	0.879	97.0	2.521	61
TIMQAH	2.857	0.062	M, S4-	1.909	0.885	96.7	2.528	62
UDAVUQ	2.860	0.073	M, S4-	1.917	0.883	96.8	2.525	61
UJASED	2.853	0.069	M, S4-	1.913	0.882	96.9	2.515	63
UMETOV	2.866	0.064	M, S4-	1.913	0.879	97.0	2.520	64
UMETUB	2.865	0.059	M, S4-	1.906	0.883	96.8	2.531	64
VEDFUG	2.867	0.054	M, S4-	1.914	0.878	97.1	2.518	65
VEDGAN	2.867	0.067	M, S4-	1.917	0.881	96.9	2.527	65
VOQGAJ	2.882	0.059	M, S4-	1.913	0.871	97.5	2.511	66
VOQGAJ	2.871	0.045	M, S4-	1.917	0.866	97.8	2.486	66
VOQGEN	2.881	0.050	M, S4-	1.917	0.876	97.3	2.523	66
WAQTOY	2.867	0.066	M, S4-	1.905	0.875	97.2	2.508	67
WAQTUE	2.871	0.068	M, S4-	1.920	0.881	96.9	2.528	67
WAQVAM	2.876	0.059	M, S4-	1.911	0.878	97.1	2.525	67
WIMRIT	2.875	0.065	M, S4-	1.918	0.880	97.0	2.530	68
WIMRIT11	2.855	0.082	M	1.919	0.880	96.9	2.513	69
WOWTEH	2.861	0.072	M, S4-	1.920	0.880	96.9	2.518	70
WOWTIL	2.871	0.065	M, S4-	1.907	0.883	96.8	2.535	70
XAXSAR	2.874	0.070	M, S4-	1.911	0.872	97.4	2.505	71
XEHSOS	2.866	0.053	M, S4-	1.920	0.884	96.8	2.533	72
XUBXOH	2.866	0.066	M, S4-	1.913	0.884	96.7	2.533	73
mean	2.867(10)			1.920(23)	0.880(4)	96.9(3)	2.524(11)	

VOPRIB has coordination $Mn_4/0s_4/m_2d_5$. The other compounds are all of the Mn_{12} single molecule magnet family.

Table S5. Geometric parameters for iron cubanes

Code	Fe-Fe (Å)	s.d.	Distortion	Fe-O (Å)	Tet. parm	Fe-O-Fe (°)	O-O (Å)	Ligand coding	Ref.
CEHVER	3.216	0.041	M, S4-	2.143	0.876	97.29	2.816	$Fe_4/3s_4$	9
EBUSAW	3.244	0.000		2.122	0.836	99.68	2.712	$Fe_4/3s_4$	74
EBUVON	3.262	0.056	M, S4-	2.152	0.853	98.61	2.783	$Fe_4/1s2_4/m_4$	75
EBUVUT	3.267	0.037	M, S4-	2.158	0.857	98.43	2.798	$Fe_4/1s2_4/m_4$	75
EBUWAA	3.249	0.037	M, S4-	2.144	0.855	98.55	2.777	$Fe_4/1s2_4/m_4$	75
EBUWII	3.249	0.095		2.145	0.855	98.48	2.779	$Fe_4/1s2_4/m_4$	75
EBUWII	3.219	0.118	H, S4-	2.137	0.865	97.77	2.784	$Fe_4/1s2_4/m_4$	75
EBUWOO	3.222	0.100	H, S4-	2.137	0.864	97.89	2.785	$Fe_4/1s2_4/m_4$	75
KASCOX[a]	3.135	0.033	M, S4+	2.117	0.905	95.53	2.835	$Fe_4/0s_4/m_9b_1$	76
LEFWOI	3.198	0.043	M, S4-	2.126	0.872	97.50	2.788	$Fe_4/0s_4/m_4b_4$	12
LEFWUO	3.216	0.034	M	2.129	0.862	98.13	2.771	$Fe_4/0s_4/m_4b_4$	12
MESDET	3.161	0.082	M, C2	2.115	0.882	96.75	2.788	$Fe_4/0s_4/m_4b_4$	77
ODOZUC	3.214	0.138	H	2.147	0.877	97.06	2.820	$Fe_4/1s_32s22/m_3d$	78
ODUBAQ	3.172	0.127	H, S4+	2.132	0.890	96.21	2.821	$Fe_4/0s_21s2s22/m_3d_2$	78
QEFKOB	3.236	0.120	H, S4-	2.145	0.862	97.94	2.790	$Fe_4/1s2_4/m_4$	79
VUDNEN[b]	3.260	0.142	H	2.173	0.870	97.37	2.836	$Fe_4/1s_4/m_6$	80
mean	3.22(4)			2.14(2)	0.87(2)	97.7(10)	2.79(3)		
LEFXAV[c]	3.152	0.112	H, S4-	2.113	0.882	96.57	2.781	$Fe_4/0s_4/m_4d_4$	12
LEFXAV[c]	3.150	0.111	H, S4-	2.111	0.882	96.63	2.778	$Fe_4/0s_4/m_4d_4$	12
	3.151			2.112			2.78		
GOYGAC	3.073	0.012	L, C2	2.040	0.868	97.75	2.668	$Fe_4/3s_4$	81

Notes: [a] Contains one five-coordinate iron; [b] Contains two five-coordinate irons; [c] Contains one iron(III) and three iron(II)

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