Geometric, Electronic and Magnetic Structures of S=19/2 and S=20/2 Thiophene-2-carboxylate Functionalized Mn_{12} Single Molecule Magnets

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Supplementary Material

I. Structural analysis

Structurally, the Mn atoms in both clusters can be divided into two types. The core of the cluster is composed of a cubane in which Mn_{1-4} occupy alternating corners (defining a tetrahedron) with oxo atoms making up the rest of the cubane. The remaining eight ions, Mn_{5-12}, comprise the outer ring of the cluster. Within this ring there are two types of manganese positions, namely those engaged in diamond type interactions with cubane manganese atoms and those that bridge these cubane segments. Water molecules are bound to Mn atoms in the latter positions.
Four of the eight manganese atoms that comprise the ring in the periphery of the clusters interact with the cubane manganese atoms via μ-oxo bridged diamond shaped structures. The diamond bond lengths in **I** typically range from ≈1.93 to 1.98 Å, but two of the opposing diamonds in the cluster have a more asymmetric arrangement of bonds, comprised of two short and one long Mn-O interaction (1.908, 1.911 and 2.013 Å for one and 1.899, 1.908 and 2.036 Å for the second). The fourth bond completing these diamonds is of intermediate length. In **II**, this same asymmetry is observed in each of the four diamonds, with each having a long bond (2.032, 2.019, 2.019, 2.037 Å), two short bonds (1.883, 1.926, 1.871, 1.930, 1.866, 1.923, 1.877, 1.914 Å) and one *intermediate bond* (1.939, 1.935, 1.927, 1.953 Å), although the latter are closer in length to the short bonds of the cubanes. The remaining four periphery ions ($Mn_{9,10,11,12}$) bridge the diamonds themselves. In **I**, the Mn-O bonds that connect the diamonds to the rest of the manganese ring are fairly uniform, ranging between 1.938 and 1.953 Å. Two bonds, however, lie outside this range. For each of the manganese atom sites with bound water molecules, there is a much longer Mn-O bond (2.033 and 2.055 Å). In **II**, the corresponding bonds are much more symmetric, with one short (≈1.95 Å) and one long bond (≈2.02 Å) per manganese. Notably, the long-short arrangement is chiral, i.e. they exhibit a clockwise/counterclockwise orientation, in a fashion similar to the orientations of the water molecules.

In contrast to their bond lenghts, the Mn-O-Mn angles in the cubane units of the two clusters do not differ significantly. Each oxygen atom of the cubane is surrounded by one larger angle of ≈98-100° and two slightly more acute angles of ≈93-98°. In the diamond moieties, the structure of **II** has a more regular pattern of Mn-O-Mn bonds, with each diamond containing one ≈100° angle and a smaller ≈94 degrees angle. The structure of **I** exhibits greater diversity in these bond angles, which range from ≈92° to ≈98°. Around the exterior of the manganese ring, the Mn-O-Mn bonds in **I** also show a wider degree of variance, ranging from ≈125° to ≈130°, than seen in **II**, which exhibits exterior Mn-O-Mn bond angles that vary in a chiral pattern, between a smaller (≈123-126°) and a larger (≈130-132°) angle. Thus, as expected for two *versus* four water-bound structures, **I** shows more bonding angle variance and asymmetry than **II**.

In addition to visualizing the clusters as cubane-ring structures, one can take a different perspective, namely that of a *sandwich*. The clusters are terminated by two arrangements of fairly *planar* Mn_4O_6 units (see Fig. S1) which sandwich the remaining four (not shown) *interstitial* atoms (Mn_{9-12}). The degree of asymmetry of each cluster can then be assessed by the relative positions of the latter. In **I**, each of the two waters are bound to an *interstitial* manganese site whereas the other two sites remain unsaturated. In **II**, each of the four waters is bound to one of the four interstitial sites. Such interstitial atoms alternatively lie closer to one of the two Mn_4O_6 planes. In **II**, each interstitial manganese lies ≈0.5 Å to the closest plane (0.515, 0.510, 0.500 and 0.528 Å), resulting in a highly symmetric structure. By contrast, in **I** the arrangements of the corresponding atoms are more variable, with distances ranging between 0.57 and 0.71 Å (0.709, 0.701, 0.571 and 0.677 Å). Thus, the arrangement of the *interstitial* metal positions in **I** is more variable and, consequently, the relative Mn-Mn positions in this cluster show greater structural disorder.

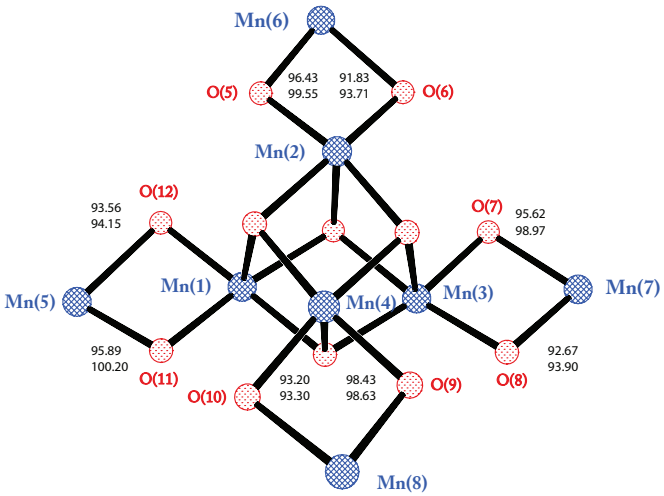

Figure S1: Optimized Mn-O-Mn bonding angles (degrees) of *planar* Mn_4O_6 units. Numbers on top and bottom correspond to angles of **I** and **II**, respectively.

II. Computational Details

The optimized geometries reported in Tables S1 and S2 were obtained using the PBE functional as implemented in the Siesta 3.1 package in conjunction with DZP basis functions and associated pseudopotentials. Spin polarized calculations were performed to converge to the ferrimagnetic states S = 19/2 and S = 20/2 of **I** and **II**, respectively. The default convergence criteria implemented in Siesta 3.1 was used to carry out all geometry optimizations.

Further single point calculations were carried out on the optimized geometries with Gaussian 09 to compute partial charges and magnetic moments *via* Mulliken and NBO population analyses. These quantities are based on spin unrestricted (U) PBE-PBE (referred to in the main text as PBE), B3-LYP,a and mPW1-PW91 calculations with several combinations of all-electron basis sets. For **I**, atomic centers 1-58 reported in Table S3 were treated with the 6-311G* (5D, 7F) basis whereas for atomic centers 59-206 several alternative basis sets were used (STO-3G, 3-21G* and 6-311G*). The main trends produced by the various combinations of basis sets were similar since the larger basis (6-311G*) was used for the Mn inner and outer cores in all cases. For **II**, atomic centers 1-60 reported in Table S4 were treated with the 6-311G* (5D, 7F) basis whereas for atomic centers 61-212 we also used all the combinations mentioned above.

III. Tables of structural parameters

Table S1: Mn-O bond lenghts (Å) for the ferrimagnetic ($\Phi^{KS}_{S=19/2}$) state of **I**.

Mn1-O1	2.093	Mn6-O37	2.085
Mn1-O2	1.944	Mn7-O7	1.941
Mn1-O4	1.962	Mn7-O8	1.980
Mn1-O11	1.930	Mn7-O20	2.220
Mn1-O12	1.963	Mn7-O22	2.009
Mn1-O42	2.021	Mn7-O23	1.976
Mn2-O1	1.970	Mn7-O44	2.175
Mn2-O2	1.997	Mn8-O9	1.908
Mn2-O3	1.969	Mn8-O10	2.036
Mn2-O5	1.908	Mn8-O26	2.062
Mn2-O6	1.951	Mn8-O28	2.095
Mn2-O38	2.034	Mn8-O29	2.017
Mn3-O2	1.960	Mn8-O40	2.114
Mn3-O3	2.127	Mn9-O5	2.033
Mn3-O4	1.967	Mn9-O12	1.941
Mn3-O7	1.931	Mn9-O13	2.018
Mn3-O8	1.986	Mn9-O15	2.103
Mn3-O43	2.026	Mn9-O36	2.073
Mn4-O1	1.969	Mn9-O45	2.163
Mn4-O3	1.966	Mn10-O6	1.944
Mn4-O4	1.977	Mn10-O7	1.953
Mn4-O9	1.899	Mn10-O18	2.032
Mn4-O10	1.930	Mn10-O19	2.113
Mn4-O39	1.960	Mn10-O21	2.038
Mn5-O11	1.943	Mn11-O8	1.945
Mn5-O12	1.983	Mn11-O9	2.055
Mn5-O32	2.199	Mn11-O24	2.107
Mn5-O34	2.016	Mn11-O25	2.005
Mn5-O35	1.992	Mn11-O27	2.090
Mn5-O41	2.167	Mn11-O46	2.121
Mn6-O5	1.911	Mn12-O10	1.953
Mn6-O6	2.013	Mn12-O11	1.938
Mn6-O14	2.029	Mn12-O30	2.010
Mn6-O16	2.079	Mn12-O31	2.110
Mn6-O17	2.005	Mn12-O33	2.054

Table S2: Mn-O bond lenghts (Å) for the ferrimagnetic ($\Phi^{KS}_{S=20/2}$) state of **II**.

Mn1-O1	1.978	Mn7-O7	1.930
Mn1-O2	2.113	Mn7-O8	2.019
Mn1-O4	2.004	Mn7-O20	2.198
Mn1-O11	1.877	Mn7-O22	2.041
Mn1-O12	1.953	Mn7-O23	1.990
Mn1-O42	1.941	Mn7-O44	2.186
Mn2-O1	1.985	Mn8-O9	1.926
Mn2-O2	1.990	Mn8-O10	2.032
Mn2-O3	1.983	Mn8-O26	2.042
Mn2-O5	1.866	Mn8-O28	2.191
Mn2-O6	1.927	Mn8-O29	1.985
Mn2-O38	1.934	Mn8-O40	2.173
Mn3-O2	1.846	Mn9-O5	2.050
Mn3-O3	1.972	Mn9-O12	1.967
Mn3-O4	1.977	Mn9-O13	2.001
Mn3-O7	1.871	Mn9-O15	2.064
Mn3-O8	1.935	Mn9-O36	2.098
Mn3-O43	1.938	Mn9-O45	2.114
Mn4-O1	1.985	Mn10-O6	1.946
Mn4-O3	1.999	Mn10-O7	2.020
Mn4-O4	1.971	Mn10-O18	2.062
Mn4-O9	1.883	Mn10-O19	2.096
Mn4-O10	1.939	Mn10-O21	1.987
Mn4-O39	1.943	Mn10-O46	2.156
Mn5-O11	1.914	Mn11-O8	1.953
Mn5-O12	2.019	Mn11-O9	2.015
Mn5-O32	2.216	Mn11-O24	2.057
Mn5-O34	2.036	Mn11-O25	1.991
Mn5-O35	1.976	Mn11-O27	2.098
Mn5-O41	2.194	Mn11-O47	2.166
Mn6-O5	1.923	Mn12-O10	1.955
Mn6-O6	2.037	Mn12-O11	2.003
Mn6-O14	2.048	Mn12-O30	2.050
Mn6-O16	2.205	Mn12-O31	2.099
Mn6-O17	1.988	Mn12-O33	1.994
Mn6-O37	2.180	Mn12-O48	2.148

Table S3: Optimized Cartesian coordinates of $Mn_{12}O_{12}(O_2CC_4H_3S)_{16}(H_2O)_2\}^{-1}$ (**I**) for its ferrimagnetic state S = 19/2. Optimization performed at the U-PBE/DZP level of theory.

Mn	-1.115538	1.057401	0.932101
Mn	-1.035835	-1.008032	-1.273422
Mn	0.981729	-1.019720	0.950238
Mn	1.005388	1.153935	-1.127098
Mn	-2.976414	3.232465	1.207415
Mn	-3.197296	-2.861687	-1.225015
Mn	2.801124	-3.224798	1.188197
Mn	3.196325	3.026841	-1.097900
Mn	-4.251866	0.388412	-0.408692
Mn	-0.280019	-4.183615	0.085131
Mn	4.144915	-0.357490	-0.376636
Mn	0.142702	4.263687	0.199043
O	-0.953782	0.956501	-1.151698
O	-0.958109	-0.868212	0.717396
O	0.921057	-0.820594	-1.166347
O	0.839718	0.937372	0.819484
O	-2.940786	-0.969048	-1.163844
O	-1.189673	-2.945980	-1.106576
O	0.885918	-2.946232	1.046663
O	2.947485	-1.279825	0.847108
O	2.902302	1.143340	-1.030592
O	1.167737	3.066934	-0.929950
O	-1.055794	2.982620	1.056567
O	-3.063038	1.286503	0.835970
O	-5.695965	-0.373475	-1.593884
O	-5.175258	-2.629870	-1.611648
O	-4.730169	-1.039843	1.059190
O	-3.467894	-2.958261	0.833552
O	-3.491360	-4.826741	-1.493787
O	-1.696460	-5.597775	-0.263439
O	1.057444	-5.059583	-1.297168
O	2.956900	-3.824330	-0.943380
O	0.347201	-5.619135	1.389227
O	2.609300	-5.176397	1.623330
O	4.741516	-3.584368	1.288861
O	5.596044	-1.826220	0.044655
O	5.618390	0.425259	-1.488943
O	5.172045	2.711510	-1.595723
O	4.703629	0.947981	1.156896
O	3.706494	3.037538	0.933868
O	3.485689	5.022545	-1.154424
O	1.613399	5.626594	0.064957
O	-1.196653	5.153195	-1.167022
O	-3.149120	3.963714	-0.859519
O	-0.481233	5.609104	1.620399
O	-2.743827	5.165015	1.732789
O	-4.942218	3.497248	1.392492
O	-5.739721	1.722056	0.142214
O	-2.945901	-2.624233	-3.281506
O	-1.253130	-1.048847	-3.295394
O	1.152285	1.266409	-3.077902
O	2.840125	2.848773	-3.174296
O	-2.831570	2.599584	3.274874
O	-1.273231	0.918618	2.942427

O	1.061754	-0.919647	2.971987
O	2.621937	-2.605113	3.265852
O	-3.389043	1.624838	-1.959435
O	3.291868	-1.490160	-1.953501
S	-4.860926	5.643623	-2.680557
S	-1.583502	-0.489297	5.476881
S	-1.607875	-0.369683	-6.297714
S	3.114510	-2.052590	6.197593
S	3.265330	2.616050	-6.179150
S	-3.412269	-3.699425	3.728697
S	4.529447	-4.924096	-3.268503
S	3.629750	3.710964	3.828060
S	-2.072736	-8.473624	-0.719807
S	-7.279007	-3.461110	-3.532365
S	3.366897	-7.725576	2.911751
S	8.446112	-2.534883	0.264346
S	7.604448	3.544292	-2.932529
S	4.772329	7.733706	-1.139466
S	-0.431841	7.611339	3.845566
S	-7.596740	4.515100	2.302363
C	-4.783982	7.069845	-3.750161
C	-3.107724	5.816697	-2.333976
C	-2.565852	6.894032	-3.012735
C	-3.512046	7.602617	-3.812648
C	-2.427834	4.908154	-1.390580
C	-2.160731	1.576204	3.628437
C	-2.383163	1.039871	4.984088
C	-2.330117	-0.344554	7.085585
C	-3.126647	0.778393	7.195442
C	-3.160519	1.561778	6.003131
C	-2.216470	-1.732314	-3.830692
C	-2.550779	-1.472271	-5.243956
C	-2.728462	-0.701516	-7.642986
C	-3.736258	-1.567363	-7.273439
C	-3.637528	-2.002117	-5.918552
C	1.933802	-1.600042	3.648717
C	2.120504	-1.115995	5.028526
C	2.790076	-0.816696	7.445236
C	2.006609	0.212010	6.964888
C	1.634234	0.047398	5.595783
C	2.069889	1.967601	-3.676184
C	2.194407	1.658282	-5.106256
C	2.808905	1.562407	-7.545540
C	1.924646	0.572734	-7.168429
C	1.580653	0.623918	-5.785294
C	-4.103081	-2.058638	1.508129
C	-4.160022	-2.256101	2.969173
C	-4.015988	-3.164307	5.319188
C	-4.715809	-1.977962	5.236305
C	-4.791894	-1.460484	3.908237
C	2.233982	-4.679102	-1.601190
C	2.831725	-5.280907	-2.805609
C	2.241078	-6.156252	-3.698900
C	3.105287	-6.559946	-4.759789
C	4.361800	-5.995863	-4.683008
C	4.193909	2.042326	1.595817
C	4.211330	2.193548	3.063734
C	4.623515	1.274288	4.011017
C	4.510926	1.750714	5.352325

C	3.999225	3.029071	5.435615
C	-2.728887	-5.743157	-1.007634
C	-3.087224	-7.128765	-1.342332
C	-4.118958	-7.596643	-2.136576
C	-4.131042	-9.018563	-2.267802
C	-3.112269	-9.641776	-1.575057
C	-5.876405	-1.606634	-1.913459
C	-7.067131	-1.867581	-2.736586
C	-8.117760	-1.017302	-3.011387
C	-9.115859	-1.595942	-3.851388
C	-8.820316	-2.889696	-4.226958
C	1.552452	-5.905286	1.718191
C	1.757087	-7.252153	2.271556
C	0.843434	-8.285822	2.369967
C	1.386657	-9.465949	2.961415
C	2.714779	-9.337269	3.314330
C	5.687850	-2.886765	0.741106
C	7.044898	-3.410654	0.966503
C	7.446115	-4.523307	1.681899
C	8.861499	-4.708473	1.689933
C	9.543887	-3.740816	0.981261
C	5.889710	1.663926	-1.742576
C	7.235222	1.905637	-2.296836
C	8.322682	1.058154	-2.408939
C	9.460979	1.683888	-3.006119
C	9.245441	3.002140	-3.350756
C	2.735805	5.851491	-0.511568
C	3.210388	7.237706	-0.410417
C	4.505115	9.393611	-0.544714
C	3.316792	9.520192	0.144471
C	2.583770	8.297883	0.224573
C	-1.671069	5.786812	2.064410
C	-1.853650	6.846476	3.068366
C	-1.525052	8.631772	4.821767
C	-2.851297	8.372399	4.550488
C	-3.038486	7.355596	3.565145
C	-5.869378	2.755626	0.874556
C	-7.253205	3.164005	1.170008
C	-9.345182	4.262910	2.055735
C	-9.604442	3.236013	1.171792
C	-8.421951	2.613436	0.672568
H	2.978041	10.462830	0.587282
H	1.622102	8.167664	0.736766
H	5.251604	10.165965	-0.747556
H	-4.009481	6.989557	3.213324
H	-1.103760	9.349574	5.530296
H	-3.677822	8.895661	5.044441
H	-8.412471	1.781623	-0.040811
H	-10.060553	4.894654	2.589629
H	-10.616172	2.931299	0.879096
H	-8.139311	-0.004611	-2.594083
H	-10.024658	-1.070784	-4.167552
H	-9.406135	-3.556317	-4.864810
H	6.722289	-5.176542	2.182416
H	9.361060	-5.535715	2.207894
H	10.622148	-3.647565	0.829013
H	8.289069	0.020559	-2.053338
H	10.414337	1.177642	-3.183659
H	9.944094	3.696733	-3.824624

H	-0.185792	-8.180679	2.006042
H	0.815624	-10.389105	3.113549
H	3.369418	-10.091536	3.759688
H	-4.834258	-6.913229	-2.608552
H	-4.870804	-9.574164	-2.856191
H	-2.899781	-10.712847	-1.513202
H	-3.725182	2.492329	5.875065
H	-2.140038	-1.111214	7.841127
H	-3.671849	1.042256	8.109928
H	-4.533966	-1.883425	-7.956012
H	1.527016	-0.177619	-7.862002
H	3.232576	1.750927	-8.535460
H	-3.796828	-3.757325	6.211245
H	-5.153439	-1.474554	6.106370
H	-5.292238	-0.528692	3.623297
H	1.040289	0.760011	5.013729
H	1.706155	1.074485	7.572129
H	3.207794	-0.937075	8.448567
H	4.982484	0.279455	3.724090
H	4.784246	1.153537	6.229626
H	3.802180	3.620064	6.334198
H	-1.504819	7.150600	-2.925823
H	-3.255607	8.485075	-4.410801
H	-5.685197	7.418591	-4.262062
H	1.204850	-6.487090	-3.571440
H	2.804650	-7.249521	-5.557537
H	5.208179	-6.136276	-5.360756
H	-4.345454	-2.668930	-5.411644
H	-2.564251	-0.222300	-8.611601
H	0.903857	-0.064627	-5.267657
H	3.308198	-2.473034	-1.667074
H	2.288943	-1.277648	-1.809797
H	-2.392161	1.441683	-1.803548
H	-3.436912	2.597736	-1.665490

Table S4: Optimized Cartesian coordinates of $Mn_{12}O_{12}(O_2CC_4H_3S)_{16}(H_2O)_4$ (**II**) for its ferrimagnetic state S = 20/2. Optimization performed at the U-PBE/DZP level of theory.

Mn	0.068143	-1.527485	-1.017519
Mn	-1.595804	-0.200372	1.031968
Mn	-0.297974	1.486551	-1.007097
Mn	1.408368	0.169595	1.005966
Mn	0.836575	-4.328927	-1.163940
Mn	-4.375477	-0.991341	1.164887
Mn	-1.053815	4.274921	-1.068145
Mn	4.210411	0.866358	1.077209
Mn	-2.147499	-3.697598	0.502077
Mn	-3.740258	2.078902	-0.367551
Mn	2.040792	3.609058	0.422945
Mn	3.513803	-2.122358	-0.531304
O	0.061949	-1.287928	0.945927
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O	1.159796	0.152172	-0.949099
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O	-3.288395	0.717128	0.947286
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O	1.612265	-2.592840	-0.947131
O	-0.848932	-3.247657	-0.905607
O	-3.487125	-4.386744	1.819352
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O	-3.623239	-3.627338	-0.938604
O	-4.716458	-1.590705	-0.929914
O	-6.154941	-0.129667	1.376607
O	-5.727041	1.713173	0.045617
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O	-0.168758	6.053874	-1.170644
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O	5.132175	2.612270	1.599770
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O	4.509452	1.401759	-1.026164
O	5.949054	-0.069984	1.280738
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O	-0.616532	-3.607110	1.957622
O	-3.715323	0.599262	-1.935820
O	0.591771	3.510452	2.029595
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