

## Supporting Information

# Understanding and tuning the properties of redox-accumulating transition metal cluster compounds

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Table S1. Mulliken spin populations of the Mn ions and the central oxygen atom for the density functionals considered.

		PBE	TPSS	M06L	PBE0	TPSSh	M06	B3LYP
<b>1<sup>2+</sup></b>	Mn1	4.83	4.84	4.90	4.94	4.89	4.90	4.85
	Mn2	4.83	4.84	4.90	4.94	4.89	4.90	4.85
	Mn3	4.68	4.70	4.80	4.87	4.79	4.82	4.77
	Mn4	4.68	4.70	4.80	4.87	4.79	4.82	4.77
	Mn5	4.68	4.70	4.80	4.87	4.79	4.81	4.77
	O	0.14	0.12	0.06	0.10	0.11	0.11	0.16
<b>1<sup>3+</sup></b>	Mn1	4.81	4.83	4.89	4.94	4.89	4.91	4.85
	Mn2	4.81	4.83	4.89	4.94	4.89	4.91	4.85
	Mn3	4.65	4.67	4.77	4.86	4.77	4.81	4.76
	Mn4	4.65	4.67	4.76	4.86	4.77	4.81	4.76
	Mn5	4.23	4.24	4.39	4.28	4.26	4.33	4.19
	O	0.09	0.07	-0.04	-0.05	0.00	-0.08	0.02
<b>1<sup>4+</sup></b>	Mn1	4.78	4.80	4.86	4.93	4.87	4.90	4.84
	Mn2	4.78	4.80	4.86	4.93	4.87	4.90	4.84
	Mn3	4.30	4.31	4.45	4.49	4.39	4.50	4.37
	Mn4	4.28	4.29	4.43	4.46	4.37	4.48	4.34
	Mn5	4.28	4.29	4.43	4.46	4.37	4.48	4.34
	O	0.01	-0.01	-0.12	-0.19	-0.09	-0.23	-0.10
<b>1<sup>5+</sup></b>	Mn1	4.66	4.68	4.75	4.92	4.85	4.89	4.83
	Mn2	4.65	4.67	4.74	4.91	4.84	4.89	4.82
	Mn3	4.04	4.04	4.20	4.10	4.02	4.16	3.98
	Mn4	4.03	4.03	4.19	4.10	4.02	4.16	3.98
	Mn5	4.04	4.04	4.20	4.10	4.02	4.16	3.98
	O	0.07	0.06	-0.04	0.00	0.04	-0.05	0.06
<b>1<sup>6+</sup></b>	Mn1	4.27	4.29	4.37	4.75	4.40	4.58	4.45
	Mn2	4.20	4.25	4.37	4.23	4.35	4.41	4.32

	Mn3	4.09	4.14	4.23	4.24	4.23	4.36	4.18
	Mn4	3.95	3.91	4.13	4.07	3.99	4.14	3.95
	Mn5	3.97	3.91	4.11	4.08	3.99	4.14	3.96
	O	0.05	0.06	-0.04	-0.01	0.03	-0.06	0.06
<b>1<sup>7+</sup></b>	Mn1	3.91	3.91	4.06	4.10	4.00	4.17	3.98
	Mn2	3.91	3.91	4.06	4.10	4.00	4.17	3.98
	Mn3	3.86	3.86	4.04	4.06	3.96	4.11	3.94
	Mn4	3.88	3.88	4.04	4.07	3.97	4.13	3.95
	Mn5	3.88	3.88	4.04	4.07	3.97	4.13	3.95
	O	0.07	0.07	-0.01	0.00	0.04	-0.05	0.06
<b>1<sup>8+</sup></b>	Mn1	3.91						
	Mn2	2.69						
	Mn3	3.85						
	Mn4	3.86						
	Mn5	3.87						
	O	0.07						
<b>1<sup>9+</sup></b>	Mn1	2.70						
	Mn2	2.71						
	Mn3	3.85						
	Mn4	3.85						
	Mn5	3.85						
	O	0.06						

Table S2. Mn-N distances in Å. Full sets of Cartesian coordinates are given at the end of this file.

	<b>1<sup>2+</sup></b>	<b>1<sup>3+</sup></b>	<b>1<sup>4+</sup></b>	<b>1<sup>5+</sup></b>	<b>1<sup>6+</sup></b>	<b>1<sup>7+</sup></b>	<b>1<sup>8+</sup></b>	<b>1<sup>9+</sup></b>
Mn1-N	2.36	2.32	2.30	2.22	2.29	2.28	2.29	2.03
	2.36	2.37	2.30	2.27	2.14	2.05	2.06	2.03
	2.36	2.32	2.30	2.28	2.14	2.07	2.07	2.03
	2.17	2.17	2.18	2.18	2.09	2.00	2.02	1.95
	2.17	2.16	2.18	2.20	2.06	2.01	2.00	1.95
	2.17	2.20	2.18	2.15	2.20	2.22	2.19	1.95
Mn2-N	2.37	2.37	2.31	2.27	2.14	2.07	2.03	2.03
	2.36	2.32	2.30	2.27	2.13	2.05	2.03	2.03
	2.36	2.32	2.30	2.22	2.29	2.28	2.04	2.03
	2.17	2.16	2.18	2.15	2.20	2.21	1.95	1.95
	2.17	2.17	2.18	2.19	2.06	2.02	1.96	1.95
	2.17	2.20	2.19	2.17	2.08	2.00	1.94	1.95
Mn3-N	2.21	2.19	2.16	2.13	2.12	2.10	2.09	2.09
	2.14	2.12	2.01	1.97	1.99	1.95	1.94	1.95
	2.14	2.10	2.02	1.97	1.99	1.95	1.97	1.95
	2.21	2.21	2.16	2.13	2.12	2.10	2.10	2.09
Mn4-N	2.21	2.21	2.16	2.12	2.12	2.13	2.09	2.09
	2.14	2.10	2.01	1.97	1.96	1.96	1.95	1.95
	2.14	2.12	2.01	1.97	1.94	1.94	1.98	1.95
	2.21	2.19	2.16	2.13	2.11	2.08	2.11	2.09
Mn5-N	2.21	2.18	2.16	2.13	2.11	2.08	2.06	2.09
	2.14	2.02	2.01	1.97	1.94	1.93	1.92	1.95
	2.14	2.02	2.01	1.97	1.96	1.96	1.97	1.95
	2.21	2.18	2.16	2.13	2.12	2.13	2.12	2.09

Table S3. Experimentally determined  $E_{1/2}$  values in eV and computed energy differences  $\Delta E$  between reduced and oxidized species in eV for different density functionals.

	$\mathbf{1}^{3+}/\mathbf{1}^{2+}$	$\mathbf{1}^{4+}/\mathbf{1}^{3+}$	$\mathbf{1}^{5+}/\mathbf{1}^{4+}$	$\mathbf{1}^{6+}/\mathbf{1}^{5+}$	$\mathbf{1}^{7+}/\mathbf{1}^{6+}$
$\Delta E_{\text{PBE0}}$	3.86	4.61	5.20	6.34	5.64
$\Delta E_{\text{B3LYP}}$	3.62	4.32	5.01	6.01	5.50
$\Delta E_{\text{M06}}$	4.01	4.69	5.49	6.42	5.95
$\Delta E_{\text{TPSS}}$	3.17	3.58	4.66	5.05	5.35
$\Delta E_{\text{PBE}}$	3.28	3.68	4.76	5.23	5.41
$\Delta E_{\text{M06L}}$	3.55	4.13	5.32	5.83	5.99
$\Delta E_{\text{TPSSh}}$	3.42	3.96	4.91	5.51	5.44
exp. $E_{1/2}$	-0.58	0.13	0.61	1.21	1.33

Table S4. Mulliken spin populations of the Mn ions and the central oxygen atom in the bpp-OH and bpp-CN modifications.

	Mn1	Mn2	Mn3	Mn4	Mn5	O
<b>CN</b>						
$\mathbf{1}^{2+}$	4.84	4.84	4.66	4.66	4.66	0.13
$\mathbf{1}^{3+}$	4.82	4.82	4.64	4.64	4.25	0.08
$\mathbf{1}^{4+}$	4.77	4.77	4.30	4.30	4.29	0.01
$\mathbf{1}^{5+}$	4.36	4.35	4.25	4.25	4.34	0.00
$\mathbf{1}^{6+}$	3.92	3.92	4.32	4.20	4.20	-0.01
$\mathbf{1}^{7+}$	3.92	3.92	3.85	3.88	3.88	0.07
<b>OH</b>						
$\mathbf{1}^{2+}$	4.83	4.84	4.70	4.69	4.70	0.15
$\mathbf{1}^{3+}$	4.81	4.82	4.64	4.68	4.23	0.09
$\mathbf{1}^{4+}$	4.78	4.77	4.30	4.29	4.28	0.00
$\mathbf{1}^{5+}$	4.78	4.77	3.94	3.91	3.90	0.09
$\mathbf{1}^{6+}$	4.34	4.21	4.07	3.88	3.88	0.07
$\mathbf{1}^{7+}$	3.88	3.87	3.85	3.85	3.86	0.07

Table S5. Computed energy differences  $\Delta E$  between reduced and oxidized species in eV for the PBE density functional.

	$\mathbf{1}^{4-}/\mathbf{1}^{3-}$	$\mathbf{1}^{3-}/\mathbf{1}^{2-}$	$\mathbf{1}^{2-}/\mathbf{1}^{1-}$	$\mathbf{1}^{1-}/\mathbf{1}^0$
$\Delta E_{\text{PBE}}$	3.77	4.53	4.84	5.18

Table S6. Mulliken spin populations of the Mn ions and the central oxygen atom in the bbp helicate.

	Mn1	Mn2	Mn3	Mn4	Mn5	O
$\mathbf{1}^{4-}$	2.62	3.89	3.85	3.85	3.84	0.06
$\mathbf{1}^{3-}$	2.63	2.63	3.83	3.83	3.83	0.06
$\mathbf{1}^{2-}$	2.61	2.61	3.47	3.45	3.48	0.00
$\mathbf{1}^{-}$	2.59	2.59	2.86	3.34	2.88	0.03
$\mathbf{1}$	2.57	2.57	2.59	2.59	2.59	0.07

### Comment on the neglect of magnetic coupling

The uncertainty introduced by computing the redox potentials as the energy differences between the high spin determinants of the complexes can be estimated by taking the energy difference between the lowest-energy broken-symmetry solution and the high spin solution. The lowest-energy broken symmetry solution is the best approximation that can be obtained with DFT for the spin ground state of a system, but the broken symmetry formalism can only be applied to species with localized valences. In the present case, the only species for which BS-DFT is therefore unambiguously applicable are the  $\text{Mn(II)}_5$  and  $\text{Mn(III)}_5$  redox levels that do not suffer from any degree of valence delocalization (Table S1). For complexes  $\mathbf{1}^{2+}$  and  $\mathbf{1}^{7+}$  the energy differences are:

$$\mathbf{1}^{2+}: E(\text{HS})-E(\text{BS}) \approx 1518 \text{ cm}^{-1} = 0.19 \text{ eV}$$

$$\mathbf{1}^{7+}: E(\text{HS})-E(\text{BS}) \approx 722 \text{ cm}^{-1} = 0.09 \text{ eV}$$

Since the deviation between high spin and broken symmetry solution is of the same sign, the uncertainty due to this approximation is at most on the order of 0.10 eV. Even though this shows that there may be a small effect by computing the redox levels as energy differences between broken symmetry solutions, we stress that the broken-symmetry formalism cannot be used in valence-delocalized cases and hence currently the only valid way to study the redox properties of this series is to use the high spin energies.

### Jahn–Teller axes in the Mn(III)<sub>5</sub> complex

Figure S1 shows the Jahn–Teller axes for complex  $\mathbf{1}^{7+}$ , identified by the elongated Mn–N bond lengths. While the Jahn–Teller axes of the octahedrally coordinated apical manganese ions are readily identified by their significant Mn–N bond elongations, only two of the three pentacoordinate manganese ions in the central trimer of  $\mathbf{1}^{7+}$  show Jahn–Teller distortions. The reason lies in different local deviations from ideal trigonal-bipyramidal symmetry; the two equatorial oxygen–manganese–nitrogen angles of Mn3 (in the back in Figure S1) have almost identical values, whereas the equatorial oxygen–manganese–nitrogen angles for Mn4 and Mn5 deviate by  $16^\circ$  from each other ( $\mathbf{1}^{7+}$ : O–Mn–N ca.  $133^\circ$  for Mn3 vs.  $124^\circ$  and  $140^\circ$  for Mn4 and Mn5, all Mn–N–Mn ca.  $96^\circ$ ;  $\mathbf{1}^{6+}$ : all O–Mn–N ca.  $130^\circ$ , all N–Mn–N ca.  $96^\circ$ ).

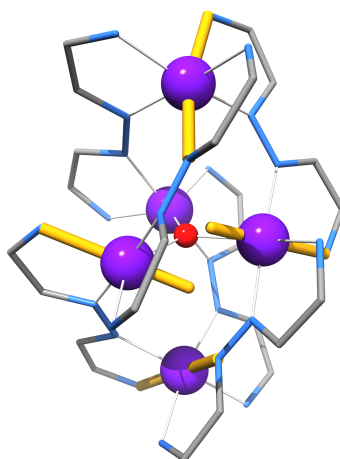


Figure S1. Complex  $\mathbf{1}^{7+}$  with truncated ligand system; the Jahn-Teller axes are shown as yellow lines.

### Cartesian coordinates of all optimized geometries (Å)

$\mathbf{1}^{2+}$

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Mn	2.14549060855556	10.77514327804733	3.85828829252228
Mn	-1.50069180287904	7.80227539689634	9.75225222651085
Mn	0.67604740334090	10.90134547431131	7.83436526594942
Mn	-1.29582457380320	9.14366016203972	5.73555503531164
Mn	1.59780415279619	7.81017190708670	6.84526385578519
O	0.32639487894103	9.28558232279036	6.80474925769062
N	2.15234632610277	13.05175989809974	3.24641616293291
N	4.47934879132663	10.69570189857895	3.49104618964862
N	1.80458392114330	10.20172568045467	1.59094521395803
N	0.12727162039945	11.52038063345764	4.13858014193000
N	3.11066769978827	11.11167257279245	5.77139528167059
N	1.90711652231220	8.61981610930489	3.76667367887602
N	-1.78113048484565	5.49266010272201	10.18627867518622
N	-3.77390379928050	8.14851250631790	10.28177201134465
N	-0.94851129918066	8.11934564969386	12.02237386214145
N	-1.92101073610639	6.83367131464406	7.85674450128666
N	-1.93230121234313	9.89622714874889	9.38847677222319
N	0.66282225993471	7.72255216689274	9.90342580101369
N	1.98904974555051	11.15384670733260	9.59343859504977
N	2.61686386322912	11.27259698298650	7.00800122775710
N	-1.18533195428919	10.89416028534081	8.89330299517549
N	-0.13785342631059	12.93406266208093	7.53795453978609
N	-3.19395489837001	10.25476745023579	5.93635609283892
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N	-1.97143496810611	7.30580502654241	6.60249022357861
N	-1.69150472408644	7.82540716600713	4.00516316484304
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180

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180

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