Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Electronic Supplementary Information

Ferromagnetism in polynuclear systems based on non-linear [$Mn^{II}_2Mn^{III}$] building blocks

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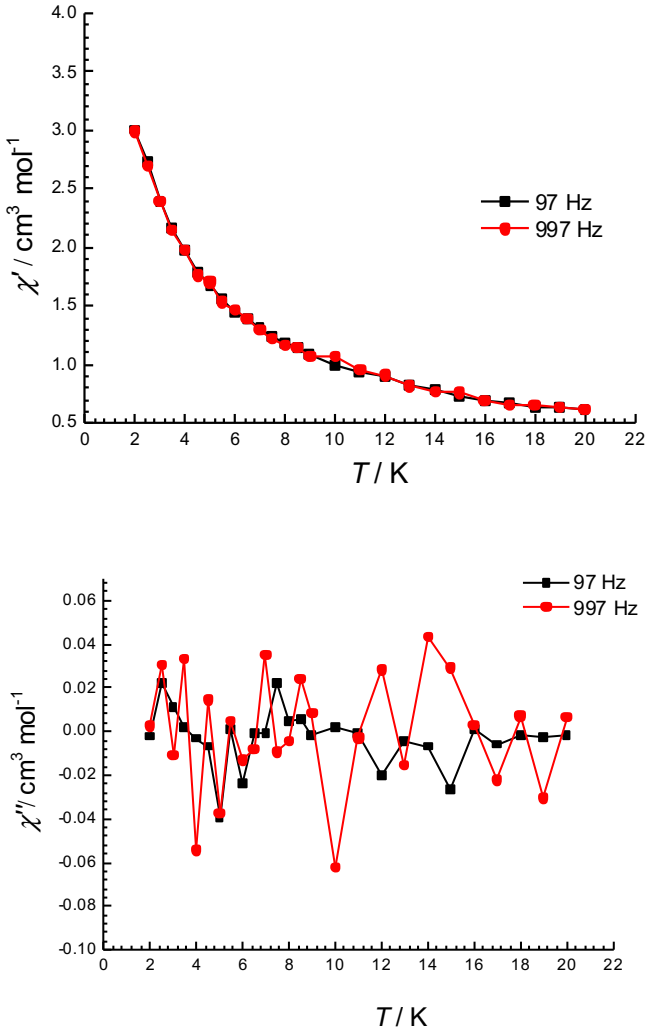

Fig. S1 AC susceptibilities under 0 Oe dc field for **4** at indicated frequencies.

Table S1 Spin distributions and energies for systems **1**, **3** and **4**

Complex 1

	Mn_1^{II}	Mn_2^{III}	Mn_3^{II}	Energy/a.u.
HS	4.85	3.84	4.85	-16093.4187913
SD1	4.83	-3.74	4.83	-16093.4175044
SD2	4.85	3.79	-4.83	-16093.4181215

Complex 3

	Mn_1^{II}	Mn_2^{III}	Mn_3^{II}	Mn_4^{II}	Mn_5^{III}	Mn_6^{II}	Energy/a.u.
HS	4.82	3.85	4.83	4.83	3.85	4.82	-15501.6921053
SD1	4.80	-3.84	4.81	4.81	-3.84	4.80	-15501.6885574
SD2	4.82	3.79	-4.81	-4.81	3.79	4.82	-15501.6906334
SD3	-4.80	3.88	4.83	4.83	3.87	-4.80	-15501.6899758
SD4	4.80	-3.72	4.78	-4.78	3.72	-4.80	-15501.6891663
SD5	4.81	3.94	4.81	-4.81	-3.93	-4.81	-15501.6927395
SD6	-4.82	-3.86	-4.81	4.81	3.94	4.82	-15501.6927395
SD7	4.80	-3.84	4.81	4.83	3.93	4.81	-15501.6903317
SD8	4.81	3.92	4.83	4.81	-3.84	4.81	-15501.6903323
SD9	-4.80	3.78	4.83	4.83	3.84	4.82	-15501.6910414
SD10	4.82	3.78	-4.78	4.81	3.86	4.82	-15501.6919915

Complex 4

	Mn_1^{II}	Mn_2^{III}	Mn_3^{II}	Energy/a.u.
HS	4.86	3.86	4.82	-7771.68120338
SD1	4.85	-3.74	4.81	-7771.67919897
SD2	4.86	3.80	-4.81	-7771.68030238
SD3	-4.82	3.80	4.82	-7771.68006868

Table S2 Experimental J values (in cm-1), Mn-O-Mn angles (in degrees), coordination number of the Mn^{II} and Mn^{III} centres of reported double-bridged alkoxo or phenoxo $Mn^{II}\cdots Mn^{III}$ complexes.

Compound	J_{exp}	Mn-O-Mn	Coord. Num.	Refcode	ref.
Dinuclear complexes					
Phenoxo-alkoxo bridging ligands					
$[Mn^{III}(L_1)(CH_3OH)(OCH_3)Mn^{II}Cl_2]\cdot CH_3OH$	+6.0	106.17/103.29	5/6	CAFHOG	[1]
$[Mn^{II}Mn^{III}(L)(\mu\text{-}OMe)Br_2]$	+2.9	103.67/104.17	6/6	RETWOE	[2]
$[Mn^{II}Mn^{III}(L)(\mu\text{-}OMe)Br_2]$	+3.7	104.11/105.12	6/6	RETWUK	[2]
$[Mn^{II}Mn^{III}(L)(\mu\text{-}OMe)Cl_2]$	+2.15	104.18/105.27	6/6	RETXEV	[2]
$[Mn^{II}Mn^{III}(L)(\mu\text{-}OMe)Cl_2]$	+4.2	103.42/104.38	6/6	RETXIZ	[2]
$[Mn^{II}Mn^{III}(L)(\mu\text{-}OMe)Cl_2]$	+3.44	103.76/103.96	6/6	RETXOF	[2]
$(TEA)[Mn^{II}Mn^{III}(2\text{-}OH(5\text{-}Clsal)pn)_2]$	+0.5	103.82/103.97	6/6	ROCRAC	[3]
Trinuclear					
Bisdialkoxo and bisalkoxophenoxo bridges					
$[Mn^{III}Mn_2^{II}(Hcht)_2(bpy)_4](ClO_4)_3\cdot Et_2O\cdot 2MeCN$	+3.2	102.00	6/6	WANHUP	[4]
$[Mn^{III}Mn_2^{II}(L)(\mu\text{-}OMe)_2](ClO_4)_3$	+3.6	96.62/107.68 96.83/107.97	6/6	QAXZUK	[5]

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