Co-existence of ferro- and antiferromagnetic interactions in a hexanuclear mixed-valence $Co^{III}_2Mn^{II}_2Mn^{IV}_2$ cluster sustained by a multidentate Schiff base ligand

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Supplementary Information

Table S1. Bond Valence Sum calculations for complex **1**

Ion	BVS	Ro	B
Mn1	4.00	1.753	0.37
Mn2	2.05	2.133 (Cl); 1.765 (O)	
Co1	3.08	1.75 (N); 1.637 (O)	

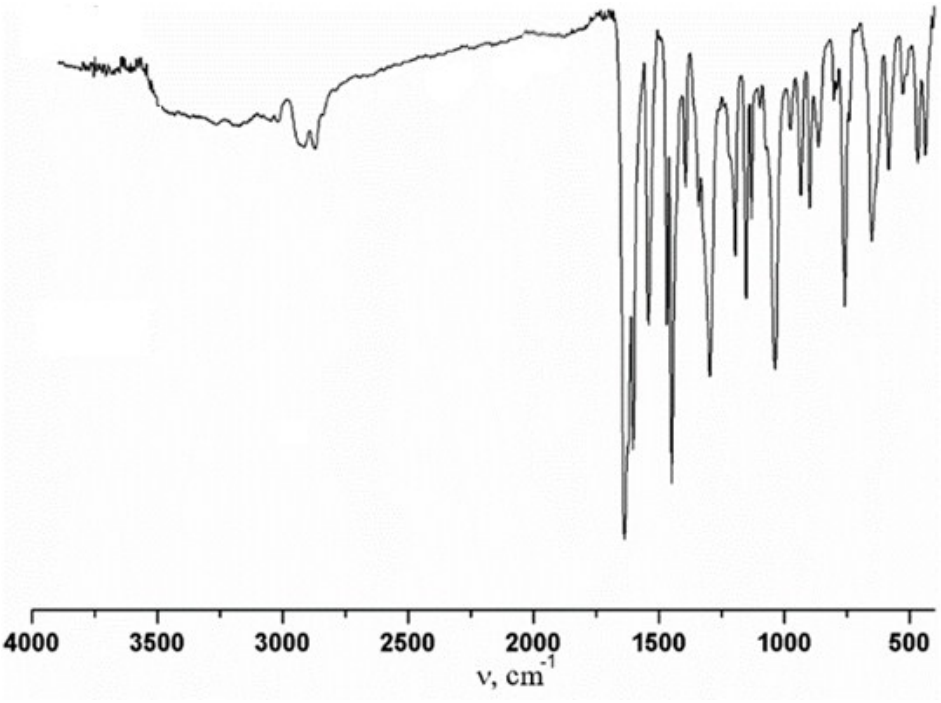

Figure S1. IR spectrum of complex **1**.

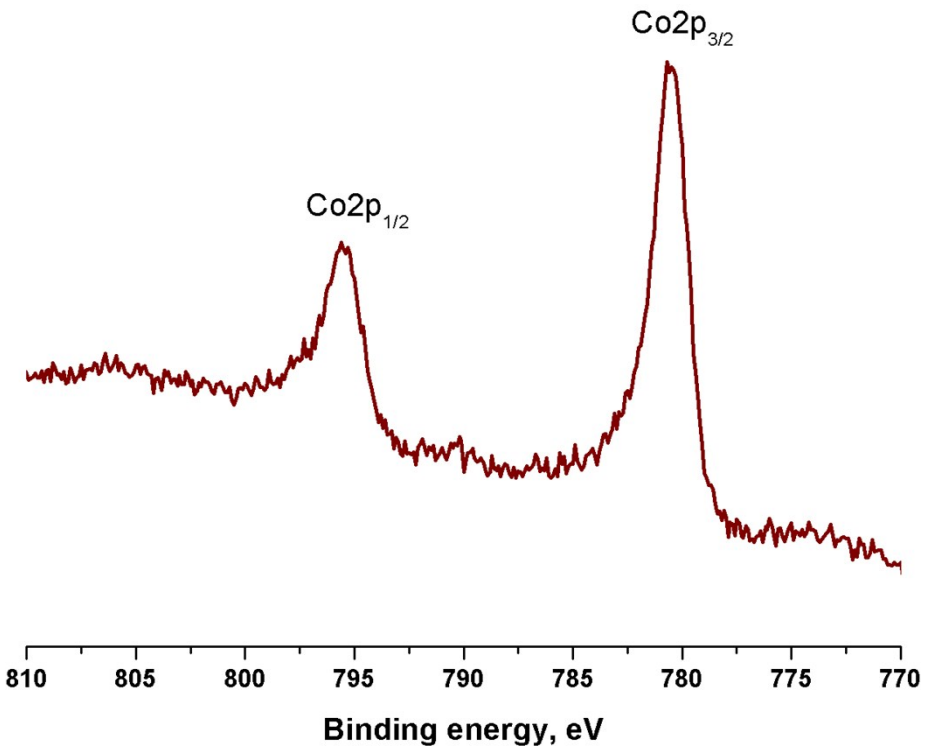

Figure S2. Co2p X-ray photoelectron spectrum of **1**.

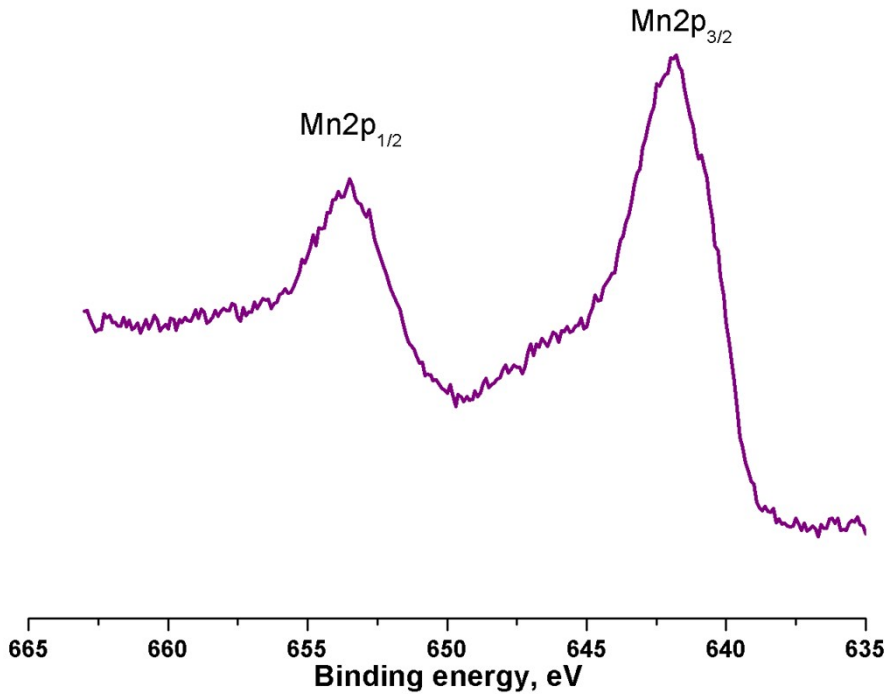

Figure S3. Mn2p X-ray photoelectron spectrum of **1**.

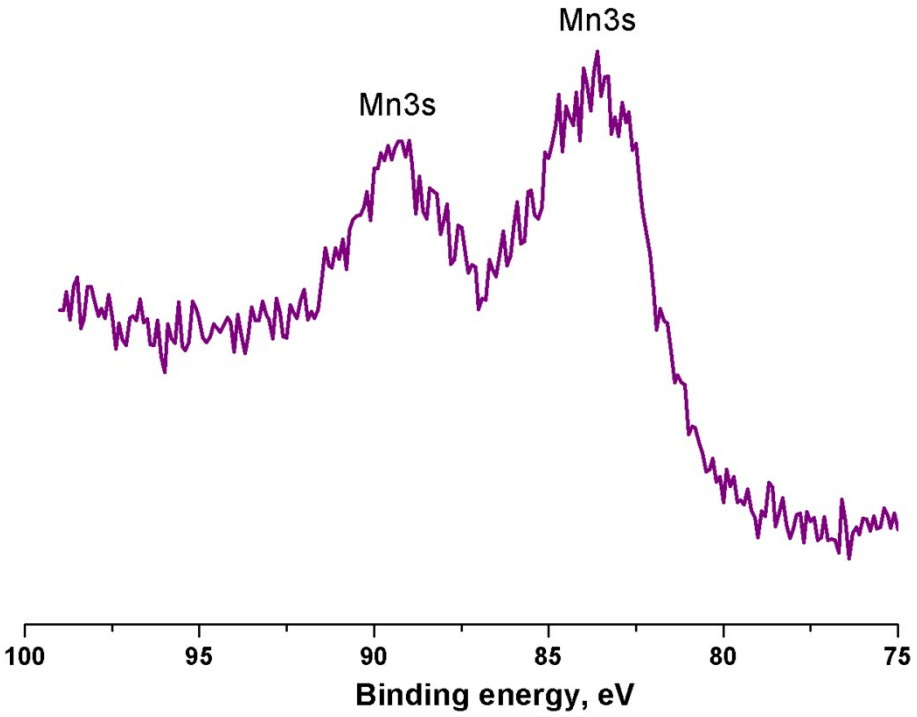

Figure S4. Mn3s X-ray photoelectron spectrum of **1**.

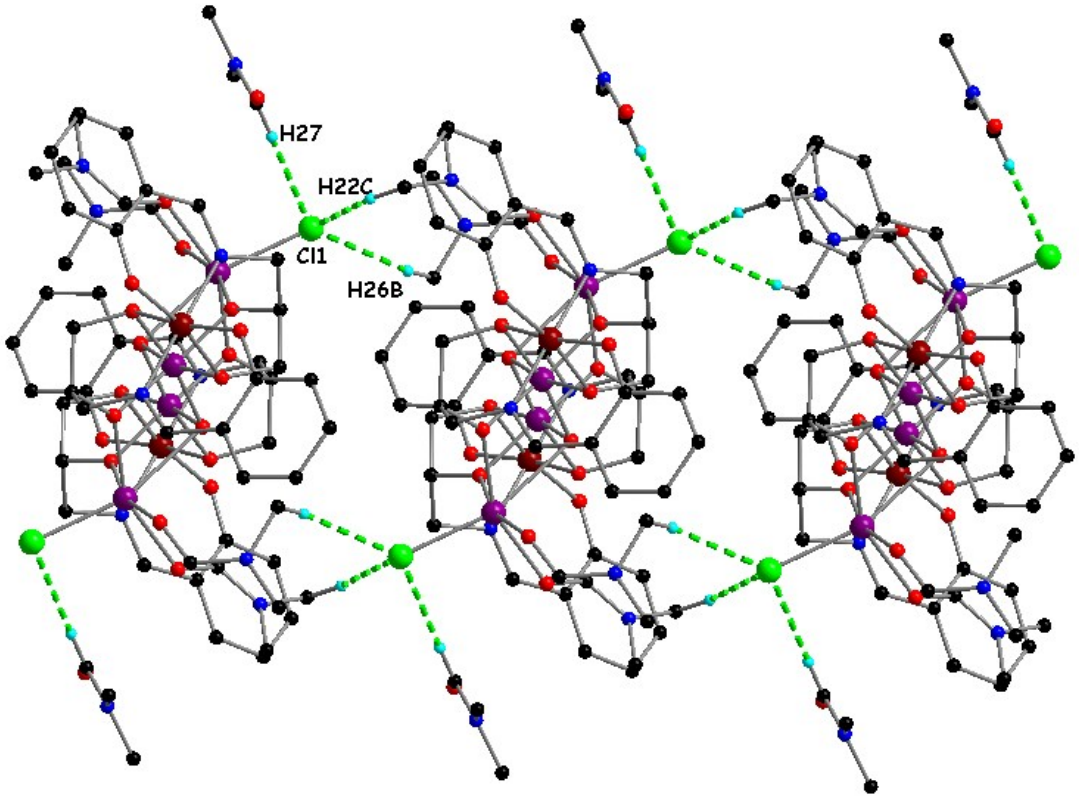

Figure S5. Hydrogen bonds (dashed green lines) in the crystal structure of **1**. Hydrogen atoms which are not involved in these interactions were omitted for clarity.

Table S2. Calculated spin configurations of the manganese atoms and their relative energies as a function of the different magnetic coupling parameters (J_i) for **1** including the interaction between second neighbours according to Scheme 1. The spin configuration used as a reference is that with the maximum multiplicity ($S = 8$) which is generated from the parallel alignment of all local spin moments. Only the centres with an inverted spin moment are noted.

Spin conf	S	J_1	J_2	J_3	j
{1}	5	6	9	9	0
{2}	3	0	9	9	15
{1, 2}	0	6	0	18	15
{1, 1^i}	2	0	18	18	0
{1, 2^i}	0	6	18	0	15