Mn(III) Chain Coordination Polymers assembled by Salicylidene–2–ethanolamine Schiff Base Ligands: Synthesis, Crystal Structures and HFEPR Study

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Supplementary information

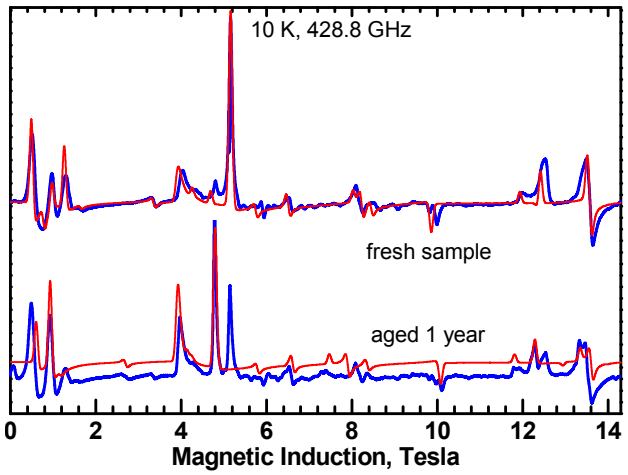

Figure S1. EPR spectra of **1**. Blue: experimental; red: simulated. The spin Hamiltonian parameters of the fresh sample are given in Table 4 (main text). The spectrum of an aged sample was simulated using $g_x = 1.976$, $g_y = 1.976$, $g_z = 2.002$, $D = -3.37$ cm^{-1}, $E = -0.68$ cm^{-1} , $B_4^0 = -0.00051$ cm^{-1}, $B_4^4 = -0.0073$ cm^{-1}.

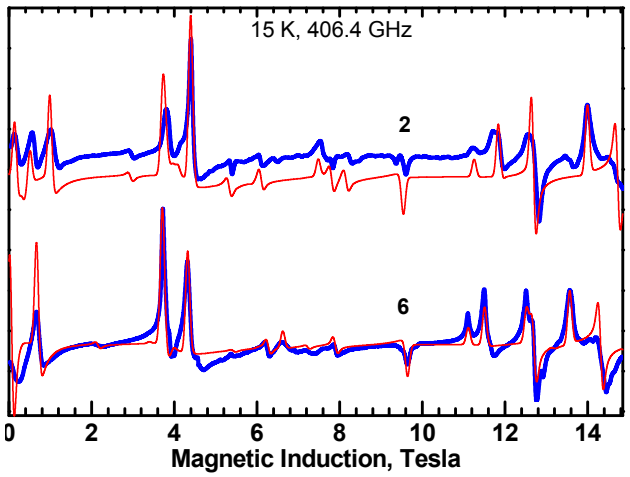

Figure S2. EPR spectra of the Br^- – containing complexes **2** (L1) and **6** (L2). Blue: experimental; red: simulated. The spin Hamiltonian parameters are given in Table 4 (main text).

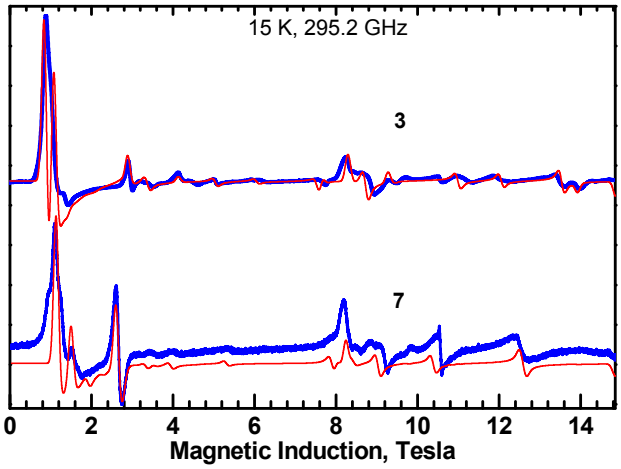

Figure S3. EPR spectra of the I^- – containing complexes **3** (L1) and **7** (L2). Blue: experimental; red: simulated. The spin Hamiltonian parameters are given in Table 4 (main text).

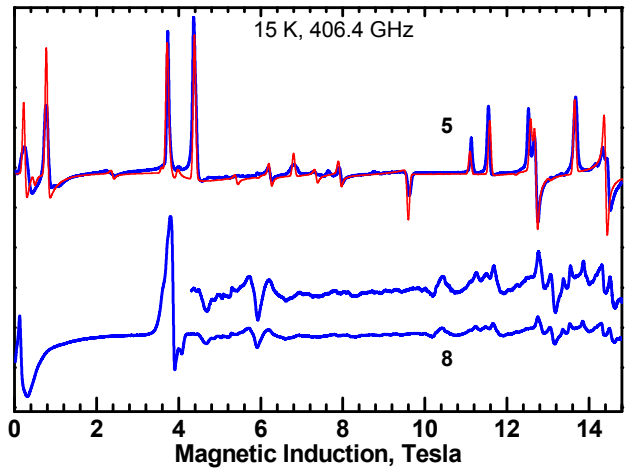

Figure S4. Comparison of the EPR spectra of the well-behaved complex **5** to ill-behaved **8**. Blue: experimental; red: simulated. The spin Hamiltonian parameters are given in Table 4 (main text). The additional splittings seen in **8** are most likely due to the metal-metal interactions.

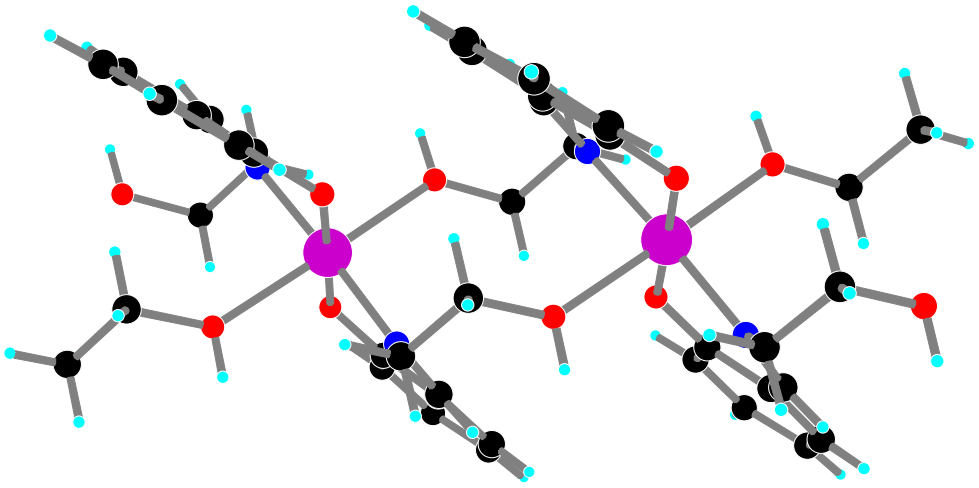

Figure S5. The arrangement of Mn moieties in **4** used to calculate the exchange integral *J* in the polymer chain. J= 0.02 cm^{-1} (antiferromagnetic, for $H = JS_1S_2$) was obtained.. The moieties are related by the symmetry operation x+1, y, z (a translation).

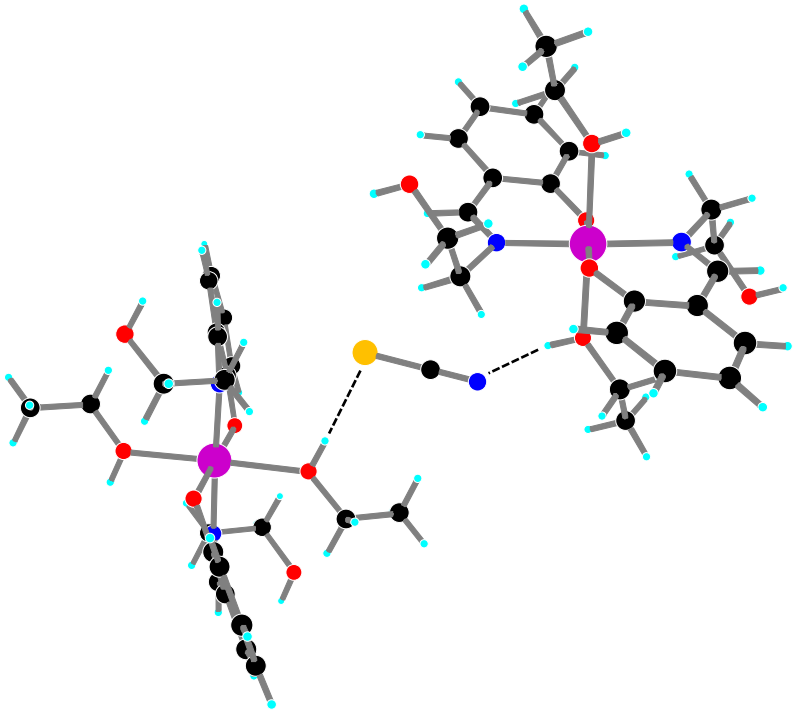

Figure S6. The arrangement of Mn moieties in **4,** used to calculate the exchange integral *J* due to the hydrogen bonds. J= 0.02 cm^{-1} (antiferromagnetic) was obtained. The moieties are related by the symmetry operation –x+3/2, -y+1, z-1/2 (a 2-fold axis) and they belong to different chains.

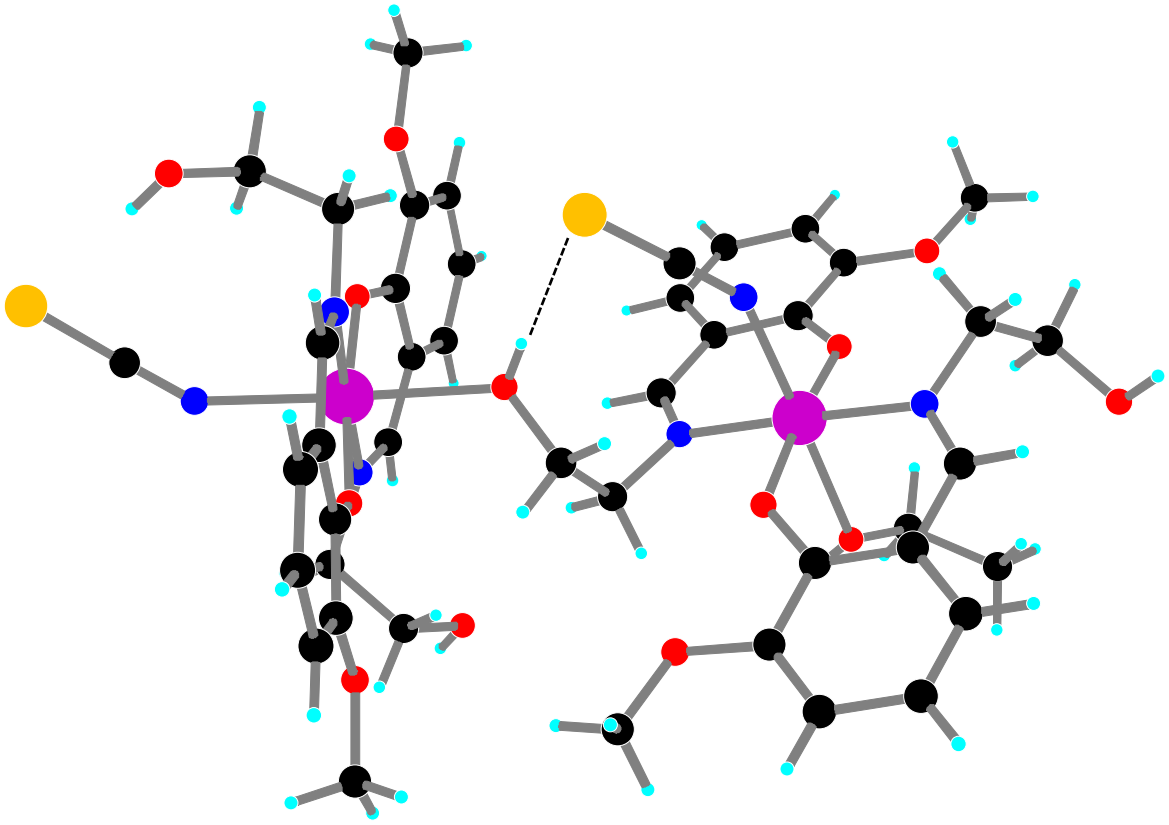

Figure S7. The arrangement of Mn moieties in **8** used to calculate the exchange integral J in the polymer chain. J= 0.04 cm^{-1} (antiferromagnetic) was obtained. Note that the Mn moieties in the polymer chain of **8** are not parallel to each other, opposite to all other complexes. The two moieties are related by the symmetry operation –x+3/2, y-1/2, -z+3/2, (a 2-fold axis).