
Supplementary Information

Co-Crystallization of Achiral Components into Chiral Network by Supramolecular Interactions: Coordination Complexes - Organic Radical

Yan Li Gao,[†] Kseniya Yu Maryunina,[†] Sayaka Hatano,[†] Sadafumi Nishihara,[†] Katsuya Inoue,^{†,‡,*} Mohamedally Kurmoo^{†,‡,*}

[†] Department of Chemistry, Hiroshima University, Higashi-Hiroshima, Hiroshima 739-8526, Japan. Email: kxi@hiroshima-u.ac.jp

[‡] Center for Chiral Science, Hiroshima University, 1-3-1, Kagamiyama, Higashihiroshima, Hiroshima 739-8526, Japan.

[‡] Institut de Chimie de Strasbourg, CNRS-UMR7177, Université de Strasbourg, 4 rue Blaise Pascal, 67070 Strasbourg, France. Email: kurmoo@unistra.fr

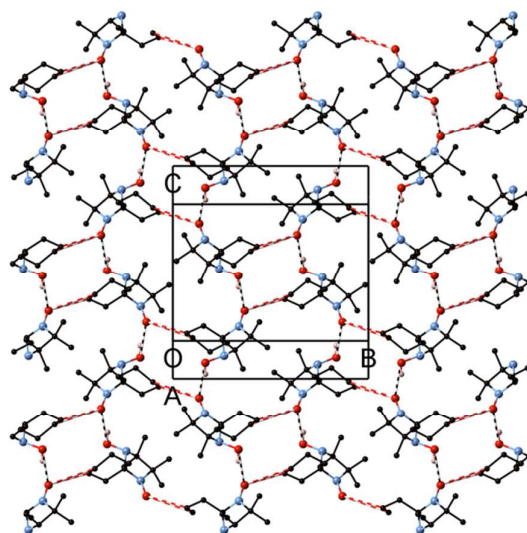


Figure S1. Structure of **2** highlighting the H-bonds between N-O $\cdots$ H-O-N connected chains along the *c*-axis and their (hexane)CH₂ $\cdots$ O-N interchain connections in the formation of layers.

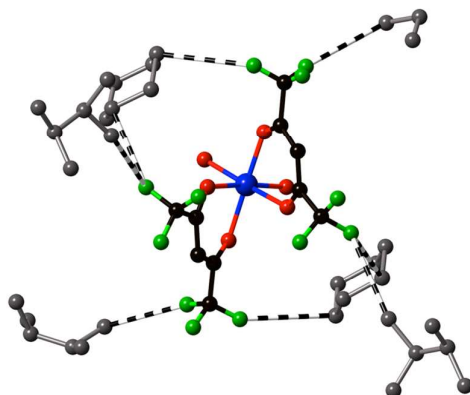


Figure S2. Structure of **1**·Co highlighting the F $\cdots$ C bonds between the inorganic cluster and the radicals.

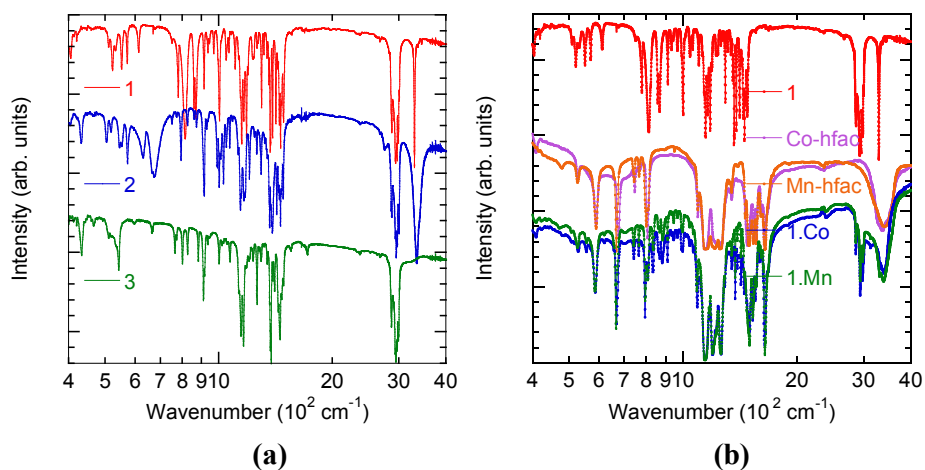


Figure S3. Infrared spectra of (a) radical **1**, **2**, **3**, (b) and *cis*-M(hfac)₂(H₂O)₂ and co-crystals **1**·Co and **1**·Mn.

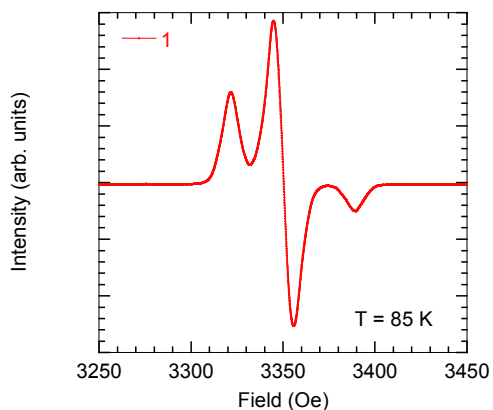


Figure S4. First derivative ESR spectrum of **1** in a frozen solution of 2-methyl tetrahydrofuran at 85 K.

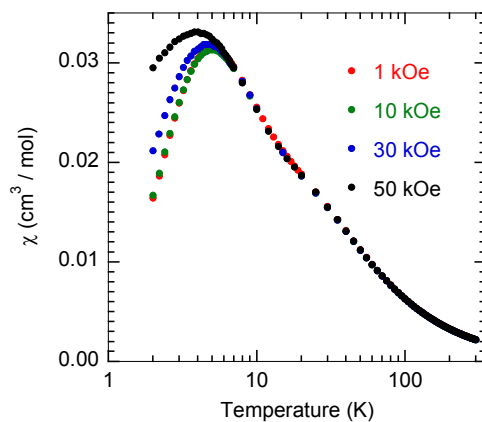


Figure S5. Temperature dependence of the magnetic susceptibility of **3** on cooling in different applied fields.

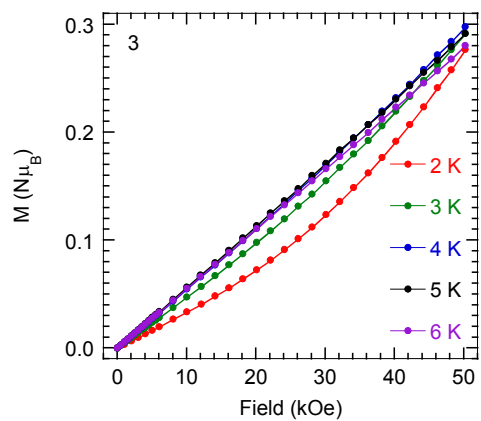


Figure S6. Field dependence of the magnetization of **3** at different temperatures.

Table S1. Crystal and refinement data for **1'Co** and **1'Mn** at 296 and 173 K.

	1'Co	1'Co	1'Mn	1'Mn
T (K)	296(2)	173(2)	296(2)	173(2)
formula	C ₁₇ H ₂₆ Co _{0.5} F ₆ N ₂ O ₄	C ₁₇ H ₂₆ Co _{0.5} F ₆ N ₂ O ₄	C ₁₇ H ₂₆ Mn _{0.5} F ₆ N ₂ O ₄	C ₁₇ H ₂₆ Mn _{0.5} F ₆ N ₂ O ₄
fw	465.86	465.86	463.87	463.87
cryst syst	Rhombohedral	Rhombohedral	Rhombohedral	Rhombohedral
space group	<i>P</i> 3 ₁ 21	<i>P</i> 3 ₁ 21	<i>P</i> 3 ₁ 21	<i>P</i> 3 ₁ 21
a (Å)	16.585(3)	16.409(1)	16.689(1)	16.479(1)
b (Å)	16.585(3)	16.409(1)	16.689(1)	16.479(1)
c (Å)	13.565(3)	13.483(1)	13.602(1)	13.562(1)
α (°)	90.00	90.00	90.00	90.00
β (°)	90.00	90.00	90.00	90.00
γ (°)	120.00	120.00	120.00	120.00
<i>V</i> (Å ³)	3231.2(1)	3143.8(2)	3280.8(5)	3189.3(2)
Z	6	6	6	6
Refls.				
Total	17499	17042	49508	49103
Unique	5342	5193	5445	5288
Param.	327	324	327	327
R _{int}	0.0448	0.0317	0.0485	0.0351
R ₁ /wR ₂	0.0585	0.0452	0.0519	0.0349
[<i>I</i> > 2σ(<i>I</i>)]	0.1361	0.1030	0.1274	0.0865
R ₁ /wR ₂	0.1139	0.0665	0.0878	0.0436
(all data)	0.1573	0.1116	0.1445	0.0912
GoF	1.023	1.021	1.027	1.039