

Electronic Supplementary Material (ESI) for New Journal of Chemistry.
This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2016

The perylene complex with one-dimensional coordination polymer containing $[\text{Mn}_6\text{O}_2(\text{CHCl}_2\text{COO})_{10}(\text{H}_2\text{O})_2]$ cluster units linked by 3,10-perylenequinone bridges

Lyudmila A. Kushch,^{[a][‡]} Anna V. Kazakova,^{*[a]} Svetlana A. Mironova,^[a] Eduard B. Yagubskii,^{*[a]} Sergey V. Simonov,^[b] Leokadiya V. Zorina,^[b] Rimma P. Shibaeva,^[b] Andrei V. Sadakov,^[c] Vladimir S. Mironov^[d]

[a] Institute of Problems of Chemical Physics of Russian Academy of Sciences, Semenov's av., 1, Chernogolovka 142432, MD, Russian Federation, kazakova@icp.ac.ru, yagubski@icp.ac.ru

[b] Institute of Solid State Physics of Russian Academy of Sciences, Academician Ossipyan str., 2, Chernogolovka 142432, MD, Russian Federation, shibaeva@issp.ac.ru

[c] P.N. Lebedev Physical Institute of Russian Academy of Sciences, Leninskii av., 53, Moscow 119333, Russian Federation

[d] A.V. Shubnikov Institute of Crystallography of Russian Academy of Sciences, Leninskii av., 59, Moscow 119333, Russian Federation, mirsa@list.ru

[‡] Deceased

Electronic Supplementary Information (ESI)

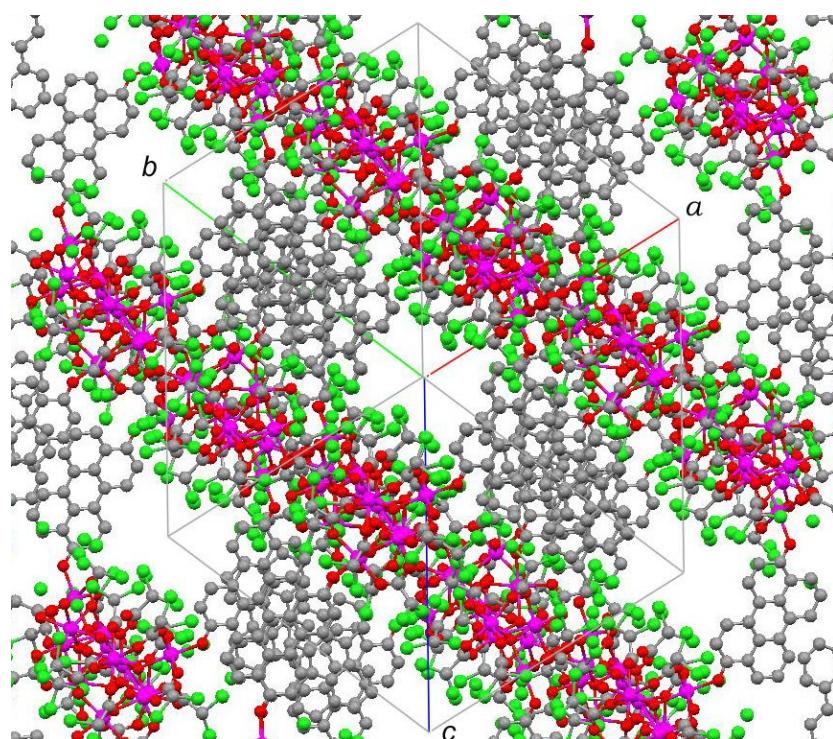


Figure S1. View of I along the [111] direction. (Cavities of 26% of the total crystal volume running along [111] are a reason for non-solvent composition of I)

Table S1. Selected Interatomic Distances (\AA) for **II**

Mn1 - O6	1.866(3)	Mn5 - O5	1.894(3)	Mn10 - O9	1.863(3)
Mn1 - O1	1.889(3)	Mn5 - O6	1.895(3)	Mn10 - O8	1.888(3)
Mn1 - O5	1.890(3)	Mn5 - O44	1.923(4)	Mn10 - O34	1.940(4)
Mn1 - O2	1.906(3)	Mn5 - O29	1.931(4)	Mn10 - O35	1.944(3)
Mn1 - O4	1.909(3)	Mn5 - O14	2.176(4)	Mn10 - O24	2.115(4)
Mn1 - O13	1.915(3)	Mn5 - O21	2.238(4)	Mn10 - O45	2.348(4)
Mn2 - O7	1.880(3)	Mn6 - O8	1.903(3)	Mn11 - O10	1.866(3)
Mn2 - O8	1.890(3)	Mn6 - O7	1.921(3)	Mn11 - O11	1.913(3)
Mn2 - O3	1.912(3)	Mn6 - O32	1.948(3)	Mn11 - O39	1.925(4)
Mn2 - O15	1.916(4)	Mn6 - O33	1.954(3)	Mn11 - O38	2.006(4)
Mn2 - O1	1.917(3)	Mn6 - O23	2.115(4)	Mn11 - O26	2.104(4)
Mn2 - O2	1.919(3)	Mn6 - O16	2.174(4)	Mn11 - O27	2.142(4)
Mn3 - O9	1.848(3)	Mn7 - O9	1.899(3)	Mn12 - O12	1.854(3)
Mn3 - O10	1.860(3)	Mn7 - O37	1.929(4)	Mn12 - O5	1.885(3)
Mn3 - O3	1.923(3)	Mn7 - O10	1.931(3)	Mn12 - O43	1.930(4)
Mn3 - O2	1.925(3)	Mn7 - O36	1.964(4)	Mn12 - O42	1.936(4)
Mn3 - O4	1.938(3)	Mn7 - O18	2.139(4)	Mn12 - O46	2.200(4)
Mn3 - O17	1.941(4)	Mn7 - O25	2.149(4)	Mn12 - O47	2.280(4)
Mn4 - O11	1.863(3)	Mn8 - O11	1.890(3)	Mn9 - O6	1.867(3)
Mn4 - O12	1.876(3)	Mn8 - O12	1.894(3)	Mn9 - O7	1.872(3)
Mn4 - O4	1.899(3)	Mn8 - O40	1.931(3)	Mn9 - O30	1.937(3)
Mn4 - O19	1.904(4)	Mn8 - O41	1.971(4)	Mn9 - O31	1.943(4)
Mn4 - O3	1.923(3)	Mn8 - O28	2.177(4)	Mn9 - O22	2.051(4)
Mn4 - O1	1.937(3)	Mn8 - O20	2.196(4)		

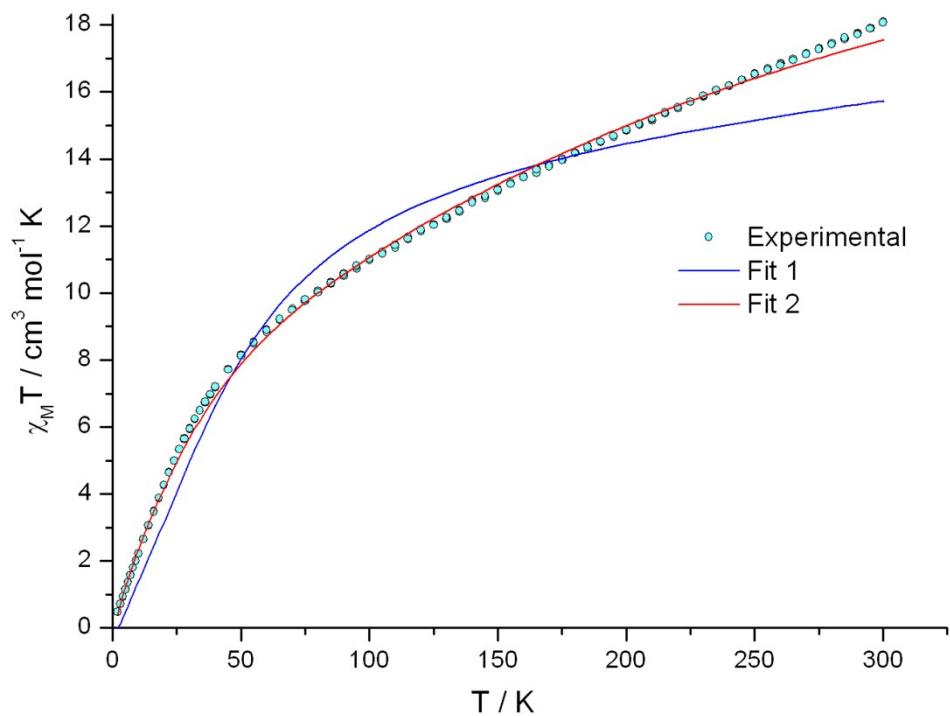


Figure S2. Comparison of the experimental and simulated temperature dependence of the $\chi_M T$ product of **I***. Fit 1 (blue solid curve): $J = -100$, $J_1 = -8$, $J_2 = J_3 = -12 \text{ cm}^{-1}$, $g_{\text{Mn}} = 2.00$; Fit 2 (red solid curve, obtained in terms of extended spin Hamiltonian (2)): $J_{12} = J_{56} = -7.5$, $J_{34} = -30$, $J_{13} = J_{46} = -40 \text{ cm}^{-1}$, and $g_{\text{Mn}} = 2.117$ (see Figure 6 in the main text for the spin coupling scheme).