SUPPORTING INFORMATION

A mononuclear Mn^{III}/'bis-tris' complex and its conversion to a mixed-valence Mn$^{II/III}_5$ cluster

Theocharis C. Stamatatos, Khalil A. Abboud, and George Christou*

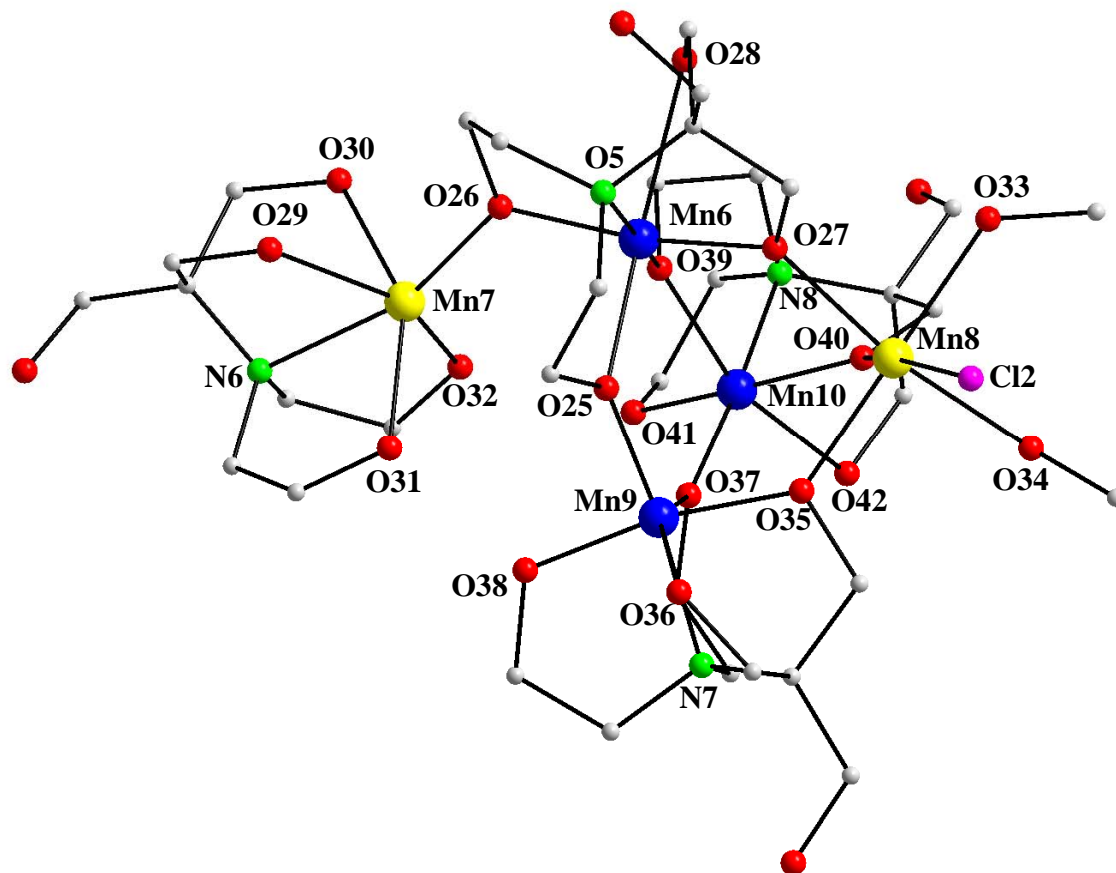Department of Chemistry, University of Florida, Gainesville, Florida, 32611-7200, USA.

Fig. S1 Labeled PovRay representation of complex **2b**, with H atoms omitted for clarity. Colour scheme: Mn^{II} yellow; Mn^{III} blue; Cl pink, O red; N green; C grey.

Table S1. Selected interatomic distances (Å) and angles (°) for **2b·2MeOH**

Mn(6)-O(25)	2.135(3)	Mn(8)-O(35)	2.158(3)
Mn(6)-O(26)	1.904(4)	Mn(8)-O(40)	2.189(4)
Mn(6)-O(27)	1.916(4)	Mn(8)-Cl(2)	2.501(2)
Mn(6)-O(28)	2.424(4)	Mn(9)-O(25)	1.893(3)
Mn(6)-O(39)	1.891(4)	Mn(9)-O(35)	1.924(4)
Mn(6)-N(5)	2.057(4)	Mn(9)-O(36)	2.396(4)
Mn(7)-O(26)	2.078(4)	Mn(9)-O(37)	2.140(3)
Mn(7)-O(29)	2.277(4)	Mn(9)-O(38)	1.887(4)
Mn(7)-O(30)	2.163(5)	Mn(9)-N(7)	2.053(4)
Mn(7)-O(31)	2.141(5)	Mn(10)-O(37)	1.885(3)
Mn(7)-O(32)	2.158(5)	Mn(10)-O(39)	2.150(4)
Mn(7)-N(6)	2.331(5)	Mn(10)-O(40)	1.926(4)
Mn(8)-O(27)	2.176(4)	Mn(10)-O(41)	1.877(4)
Mn(8)-O(33)	2.214(4)	Mn(10)-O(42)	2.381(4)
Mn(8)-O(34)	2.317(4)	Mn(5)-N(8)	2.059(4)
Mn(6)…Mn(7)	3.497(3)	Mn(7)…Mn(9)	4.718(2)
Mn(6)…Mn(8)	3.688(1)	Mn(7)…Mn(10)	4.728(2)
Mn(6)…Mn(9)	3.679(2)	Mn(8)…Mn(9)	3.726(2)
Mn(6)…Mn(10)	3.712(2)	Mn(8)…Mn(10)	3.704(3)
Mn(7)…Mn(8)	6.658(3)	Mn(9)…Mn(10)	3.742(2)
Mn(6)-O(26)-Mn(7)	122.8(2)	Mn(8)-O(35)-Mn(9)	131.7(2)
Mn(6)-O(27)-Mn(8)	128.6(2)	Mn(8)-O(40)-Mn(10)	128.3(2)
Mn(6)-O(25)-Mn(9)	131.8(2)	Mn(9)-O(37)-Mn(10)	136.7(2)
Mn(6)-O(39)-Mn(10)	133.3(2)		

Table S2. Bond Valence Sum (BVS)[a] calculations for Mn atoms in **2b**

Atom	Mn^{II}	Mn^{III}	Mn^{IV}
Mn6	3.169	<u>2.929</u>	3.026
Mn7	<u>2.000</u>	1.844	1.913
Mn8	<u>1.885</u>	1.724	1.810
Mn9	3.198	<u>2.956</u>	3.053
Mn10	3.199	<u>2.956</u>	3.054

[a] The underlined value is the one closest to the charge for which it was calculated. The oxidation state of a particular atom can be taken as the nearest whole number to the underlined value.
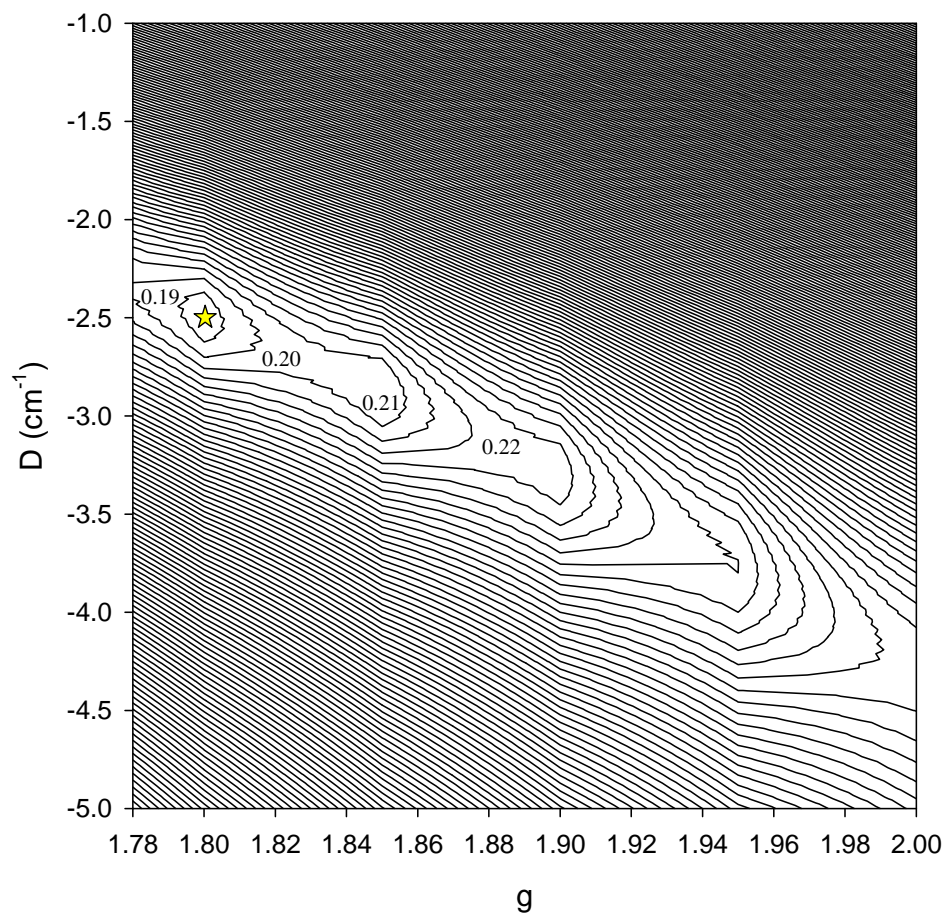
Fig. S2 Two-dimensional contour plot of the root-mean-square error surface for the *D* vs *g* fit for complex **1**. The asterisk indicates the best fit (error minimum); see the text for the fit parameters.