

Binuclear heterometallic M(III)–Mn(II) (M = Fe, Cr) oxalate-bridged complexes associated with a bisamidinium dication: a structural and magnetic study

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PXRD characterization for compounds 1-2

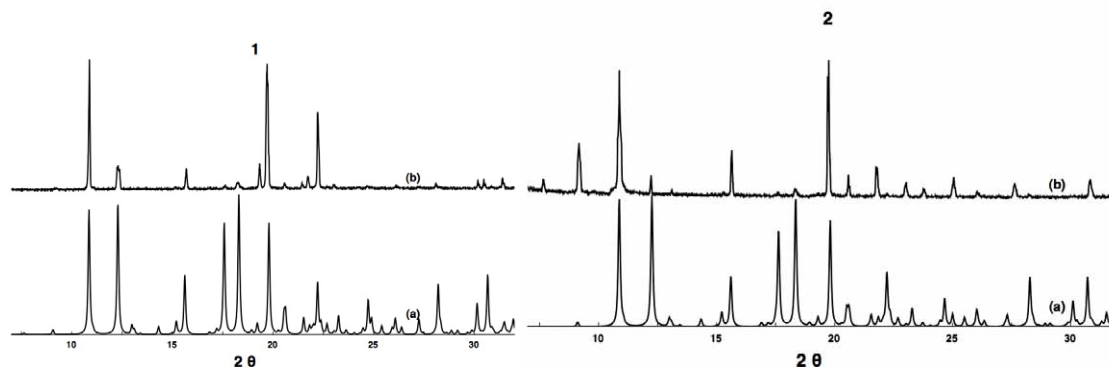


Figure S1 : Comparison of the simulated (a) and recorded (b) PXRD patterns for **1** (left) and **2** (right).

Thermal properties

Thermal analysis of the polycrystalline compounds reveals that **1** and **2** are stable up to 250 and 350°C respectively. The first weight loss of 19.6% for **1** (19.3% for **2**) between 30-147°C corresponds to the removal of 14 water molecules (calc.: 19.35%, 19.46% for **1** and **2** respectively); the analysis of the derivate of the curves in this area reveals, as expected by the different nature of the water molecules (6 lattice water molecules, 8 molecules as aqua ligands) a two steps loss process. At high temperature (250°C), **1** presents a decomposition process different from the one of **2**, related to the early decomposition of Fe(III) into oxydes.

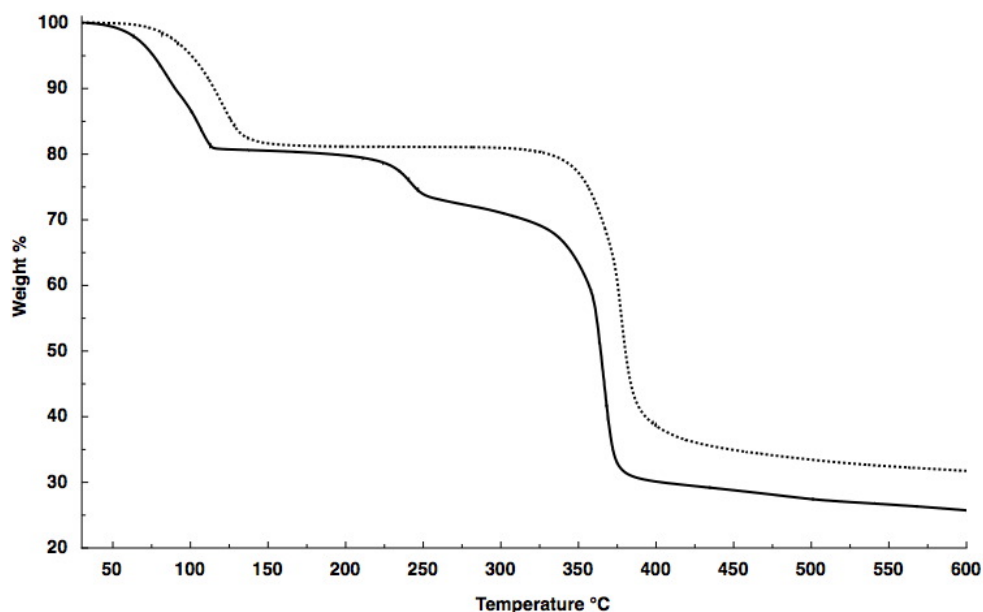


Figure S2 : TGA trace for **1** (—) and **2** (.....)

Table 2. Selected bond distances and angles for compounds 1 and 2.

1		2	
Fe-O(13)	1.9835(12)	Cr-O(13)	1.958(3)
Fe-O(1)	2.0072(12)	Cr-O(12)	1.972(3)
Fe-O(10)	2.0079(12)	Cr-O(1)	1.976(3)
Fe-O(12)	2.0114(12)	Cr-O(11)	1.981(3)
Fe-O(11)	2.0175(13)	Cr-O(10)	1.983(3)
Fe-O(2)	2.0314(12)	Cr-O(2)	1.989(3)
Mn-O(6)	2.1329(14)	Mn-O(6)	2.131(3)
Mn-O(7)	2.1416(13)	Mn-O(7)	2.147(3)
Mn-O(5)	2.1546(14)	Mn-O(5)	2.153(3)
Mn-O(8)	2.1660(14)	Mn-O(8)	2.167(3)
Mn-O(4)	2.2149(12)	Mn-O(4)	2.222(3)
Mn-O(3)	2.2425(13)	Mn-O(3)	2.239(3)
O(13)-Fe-O(1)	95.16(5)	O(13)-Cr-O(12)	82.90(12)
O(13)-Fe-O(10)	168.74(6)	O(13)-Cr-O(1)	91.11(13)
O(1)-Fe-O(10)	93.77(5)	O(12)-Cr-O(1)	92.63(13)
O(13)-Fe-O(12)	81.10(5)	O(13)-Cr-O(11)	93.32(13)
O(1)-Fe-O(12)	92.63(5)	O(12)-Cr-O(11)	93.63(14)
O(10)-Fe-O(12)	91.67(5)	O(1)-Cr-O(11)	172.74(12)
O(13)-Fe-O(11)	92.24(5)	O(13)-Cr-O(10)	173.48(14)
O(1)-Fe-O(11)	168.16(5)	O(12)-Cr-O(10)	92.96(13)
O(10)-Fe-O(11)	80.12(5)	O(1)-Cr-O(10)	94.12(13)
O(12)-Fe-O(11)	97.64(6)	O(11)-Cr-O(10)	81.89(13)
O(13)-Fe-O(2)	91.82(5)	O(13)-Cr-O(2)	92.01(12)
O(1)-Fe-O(2)	80.97(5)	O(12)-Cr-O(2)	173.09(12)
O(10)-Fe-O(2)	96.35(5)	O(1)-Cr-O(2)	82.77(13)
O(12)-Fe-O(2)	170.03(5)	O(11)-Cr-O(2)	91.32(12)
O(11)-Fe-O(2)	89.59(5)	O(10)-Cr-O(2)	92.52(13)
O(6)-Mn-O(7)	88.42(6)	O(6)-Mn-O(7)	88.27(13)
O(6)-Mn-O(5)	96.84(6)	O(6)-Mn-O(5)	97.09(15)
O(7)-Mn-O(5)	91.17(5)	O(7)-Mn-O(5)	91.20(12)
O(6)-Mn-O(8)	93.71(6)	O(6)-Mn-O(8)	93.19(14)
O(7)-Mn-O(8)	177.49(6)	O(7)-Mn-O(8)	177.74(14)

O(5)-Mn-O(8)	89.89(6)	O(5)-Mn-O(8)	90.33(14)
O(6)-Mn-O(4)	167.15(6)	O(6)-Mn-O(4)	167.12(13)
O(7)-Mn-O(4)	89.75(5)	O(7)-Mn-O(4)	90.37(12)
O(5)-Mn-O(4)	95.91(5)	O(5)-Mn-O(4)	95.75(12)
O(8)-Mn-O(4)	87.88(5)	O(8)-Mn-O(4)	87.82(12)
O(6)-Mn-O(3)	91.83(6)	O(6)-Mn-O(3)	91.77(13)
O(7)-Mn-O(3)	88.41(5)	O(7)-Mn-O(3)	88.03(12)
O(5)-Mn-O(3)	171.31(5)	O(5)-Mn-O(3)	171.08(13)
O(8)-Mn-O(3)	90.20(6)	O(8)-Mn-O(3)	90.20(14)
O(4)-Mn-O(3)	75.41(5)	O(4)-Mn-O(3)	75.38(11)