Supporting Information

Synthesis, Crystal Structures and Magnetic Properties of Two Novel Cyanido-Bridged Heterotrimetallic $\{Cu^{II}Mn^{II}Cr^{III}\}$ Complexes

Maria-Gabriela Alexandru,[*,†] Diana Visinescu,[‡] Sergiu Shova,[&] Marius Andruh,[*,#] Francesc Lloret,[||] and Miguel Julve*[,||]

[†]Department of Inorganic Chemistry, Physical Chemistry and Electrochemistry, Faculty of Applied Chemistry and Materials Science, University Politehnica of Bucharest, 1-7 Gh. Polizu Street, 01106, Bucharest, Romania [‡]Coordination and Supramolecular Chemistry Laboratory, "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, Splaiul Independentei 202, Bucharest-060021, Romania

[&] "Petru Poni" Institute of Macromolecular Chemistry of the Romanian Academy, Aleea Grigore Ghica Vodă 41-A, RO-700487 Iasi, Romania.

[#]Inorganic Chemistry Laboratory, Faculty of Chemistry, University of Bucharest, Str. Dumbrava Rosie 23, 020464-Bucharest, Romania

[||]Departament de Química Inorgànica/Instituto de Ciencia Molecular (ICMol), Facultat de Química de la Universitat de València, C/ Catedrático José Beltrán 2, 46980 Paterna, València, Spain

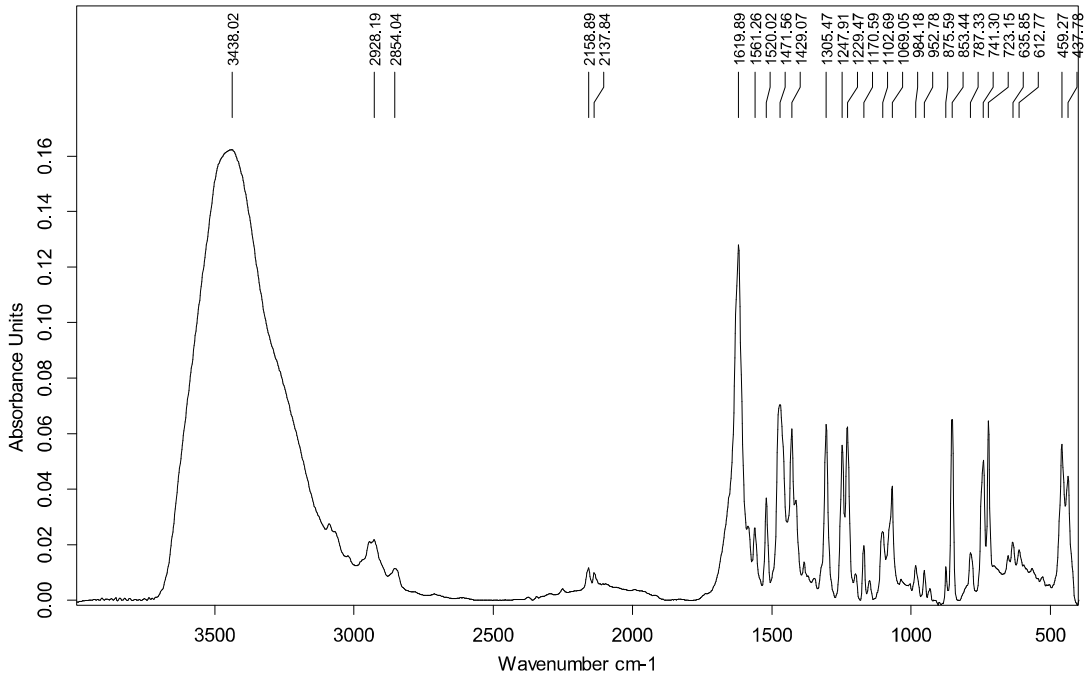

Figure S1. FTIR spectrum of **1**

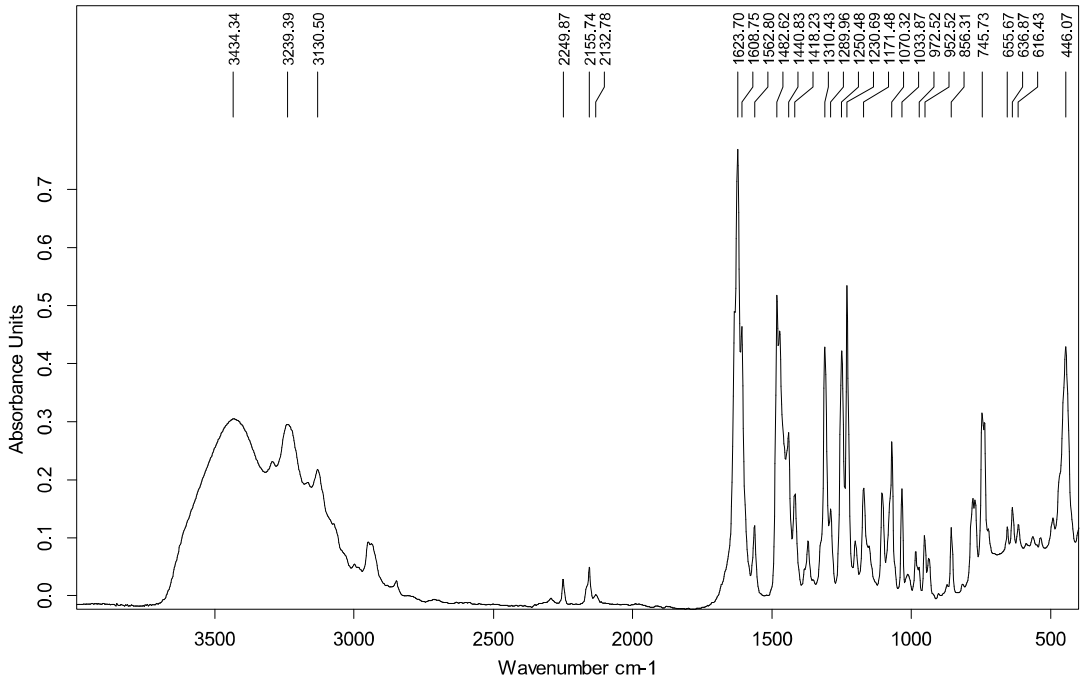

Figure S2. FTIR spectrum of **2**

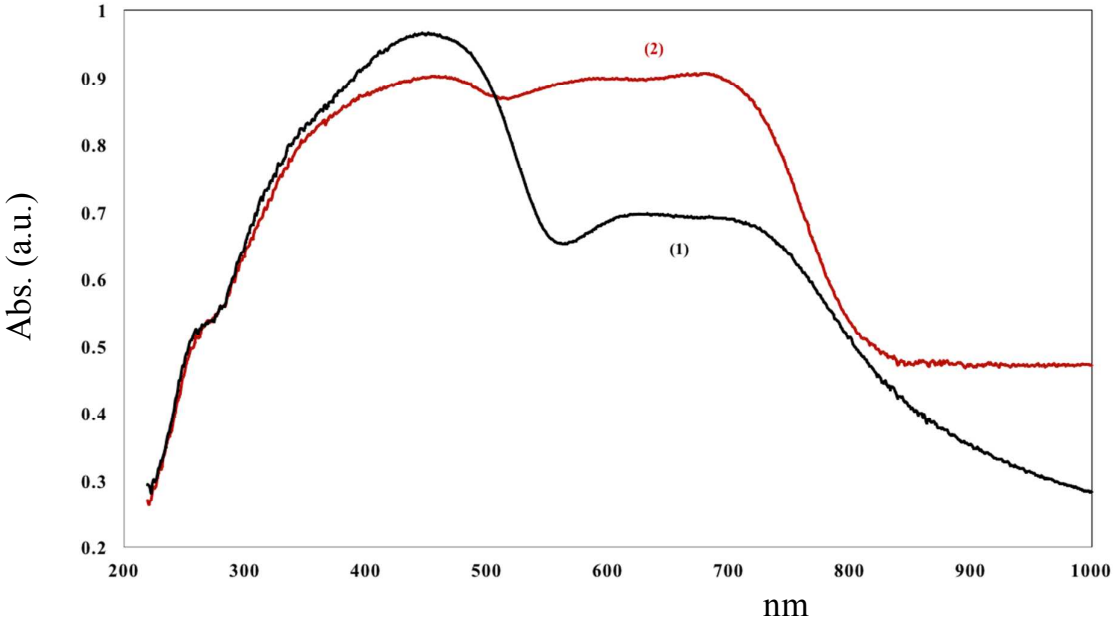

Figure S3. UV-Vis spectra of **1** and **2**

Tabel S1. Selected Bond Lengths(Å) and Angles (deg) for **1** and **2**[&]

	1	**2**		**1**	**2**		**1**	**2**		**1**	**2**
Cu1-N1	1.983(3)	1.967(4)	O1-Cu1-O2	77.82(10)	78.75(12)	O3-Mn1-N3	79.98(10)	77.69(12)	C20-Cr1-C22	94.88(14)	91.81(18)
Cu1-N2	1.996(3)	1.969(4)	N1-Cu1-N2	96.82(14)	96.47(18)	O1W-Mn1-N3	80.08(11)		C20-Cr1-C23	90.90(14)	93.18(17)
Cu1-N7	2.330(3)		Cu1-N7-C24	138.2(3)		O4-Mn1-N3	82.26(10)	78.40(13)	C20-Cr1-C21	87.58(13)	90.97(17)
Cu1-N6a[**]		2.7787(32)	Cu1-N6a-C23a[**]		135.23	O1W-Mn1-N4a[*]	167.39(11)		C22-Cr1-C23	90.95(15)	85.65(17)
Cu1-O1	1.966(2)	1.963(3)	N1-Cu1-O1	91.59(12)	91.63(15)	N3-Mn1-N4a[*]	93.07(11)		C22-Cr1-C21	177.35(13)	174.58(18)
Cu1-O2	1.949(2)	1.919(3)	N1-Cu1-O2	165.39(12)	167.00(13)	N3-Mn1-N7		86.75(13)	C23-Cr1-C21	90.00(14)	89.50(17)
Mn1-N3	2.205(3)	2.245(4)	N2-Cu1-O1	169.90(12)	170.67(15)	N7-Mn1-N10b		173.52(15)	Cr1-C20-N3	175.5(3)	177.1(4)
Mn1-N4a[*]	2.226(3)		N2-Cu1-O2	92.89(12)	92.53(15)	N10b[*]-Mn1-N3		93.51(13)	Cr1-C21-N4	176.8(3)	179.5(5)
Mn1-N10b		2.201(3)	N1-Cu1-N7	98.36(12)		N10b[*]-Mn1-O2		88.85(12)	Cr1-C22-N5	174.5(3)	169.8(4)
Mn1-N7		2.191(3)	N2-Cu1-N7	86.01(12)		O1-Mn1-N4a[*]	104.26(10)		Cr1-C23-N6	179.2(4)	177.6(4)
Mn1-O1	2.192(2)	2.202(3)	N7-Cu1-O1	98.32(11)		O2-Mn1-N4a[*]	96.43(10)		N13-Cr2-N14	79.79(12)	81.17(17)
Mn1-O2	2.235(2)	2.206(3)	N7-Cu1-O2	93.16(11)		O3-Mn1-N4a[*]	82.67(10)		N13-Cr2-C25	171.24(13)	96.84(18)
Mn1-O3	2.458(3)	2.492(3)	Cu1-O1-Mn1	106.86(10)	105.87(13)	O4-Mn1-N4a[*]	80.62(10)		N13-Cr2-C24	87.17(13)	86.53(16)
Mn1-O4	2.404(2)	2.420(3)	Cu1-O2-Mn1	105.82(10)	107.29(14)	N7-Mn1-O1		86.94(12)	N13-Cr2-C27	93.13(13)	88.93(15)
Mn1-O1W	2.187(3)		O1-Mn1-O2	67.47(9)	67.92(11)	N7-Mn1-O2		87.38(12)	N13-Cr2-C26	93.39(14)	174.39(19)
Cr1-C20	2.059(4)	2.053(5)	O1-Mn1-O3	67.47(9)	67.58(10)	N7-Mn1-O3		91.68(12)	N14-Cr2-C25	92.20(13)	177.93(17)
Cr1-C21	2.100(4)	2.076(5)	O1-Mn1-O4	135.21(9)	136.80(11)	N7-Mn1-O4		92.35(13)	N14-Cr2-C24	85.91(12)	90.90(15)
Cr1-C22	2.067(4)	2.087(5)	O1-Mn1-O1W	87.57(10)		N10b-Mn1-O1		96.52(15)	N14-Cr2-C27	96.60(13)	87.51(15)
Cr1-C23	2.065(4)	2.076(5)	O2-Mn1-O3	133.13(9)	135.48(11)	N10b-Mn1-O2		88.85(12)	N14-Cr2-C26	171.59(14)	93.61(18)
Cr1-N12	2.078(3)	2.071(3)	O2-Mn1-O4	67.75(8)	68.90(11)	N10b-Mn1-O3		94.71(12)	C24-Cr2-C25	88.75(14)	88.45(16)
Cr1-N11	2.075(3)	2.062(2)	O2-Mn1-O1W	83.97(10)		N10b-Mn1-O4		81.37(12)	C24-Cr2-C27	177.49(14)	175.37(18)
Cr2-C24	2.072(4)	2.080(4)	O3-Mn1-O4	154.82(9)	155.48(11)	N12-Cr1-C22	87.68(13)	94.19(15)	C24-Cr2-C26	88.86(14)	91.52(18)
Cr2-C25	2.060(4)	2.067(5)	O3-Mn1-O1W	106.29(10)		N12-Cr1-N11	79.93(12)	80.47(13)	C25-Cr2-C27	91.28(14)	92.99(16)
Cr2-C26	2.060(4)	2.030(6)	O4-Mn1-O1W	87.93(10)		N12-Cr1-C21	91.17(12)	90.58(15)	C25-Cr2-C26	94.27(15)	88.37(19)
Cr2-C27	2.074(4)	2.086(4)	Mn1-N3-C20	177.1(3)	170.3(3)	N12-Cr1-C20	93.89(13)	88.72(16)	C27-Cr2-C26	88.64(15)	92.92(17)
Cr2-N13	2.077(3)	2.057(4)	Mn1-N4a-C21a[*]	168.2(3)		N12-Cr1-C23	175.11(13)	178.09(17)	Cr2-C24-N7	173.7(3)	173.5(4)
Cr2-N14	2.087(3)	2.077(4)	Mn1-N7-C24		168.0(4)	N11-Cr1-C21	89.86(12)	92.53(14)	Cr2-C25-N8	173.1(3)	175.0(4)
			Mn1-N10b-C27b		159.7(4)	N11-Cr1-C20	173.27(13)	168.70(14)	Cr2-C27-N10	175.1(4)	174.3(4)
			O1-Mn1-N3	140.27(10)	144.46(13)	N11-Cr1-C22	87.59(12)	85.73(14)	Cr2-C26-N9	177.8(4)	174.0(5)
			O2-Mn1-N3	146.42(10)	146.47(13)	N11-Cr1-C23	95.33(13)	97.62(15)			

[&]Symmetry code: (*a**) = 1-*x*, 1-*y*, -*z*; (*a***) = -3/2-*x*, ½+*y*, ½-*z*; (*b*) = 1+*x*, *y*, *z*.

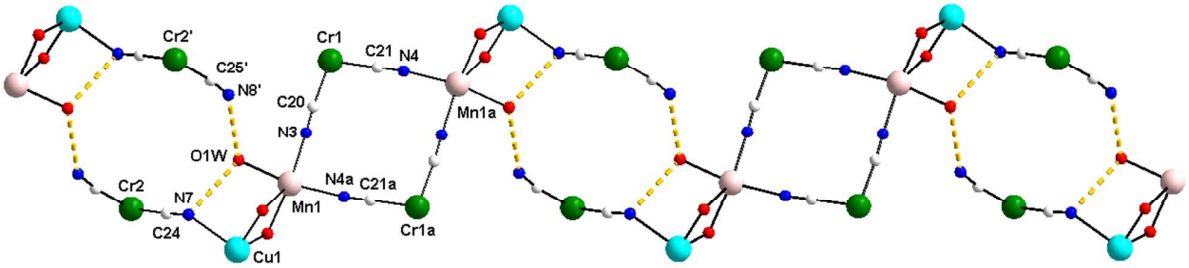

Figure S4. Fragment of the structure packing of **1** showing hydrogen bonds established between the aqua oxygen atoms and cyanide N atoms: O1W···N7, of 2.938(4) Å and O1W···N8', of 2.838(4) Å; *a* = 1-*x*, 1-*y*, -*z*; ' = 1-*x*, 1-*y*, 1-*z*.

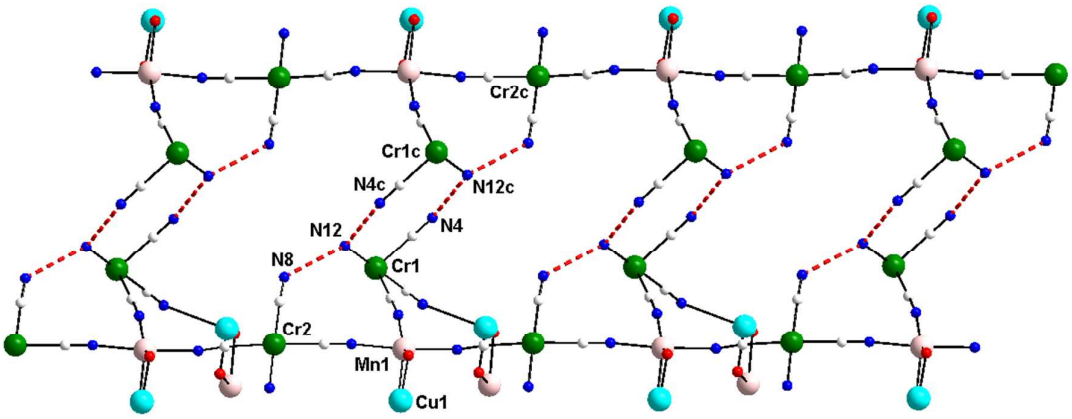

Figure S5. Fragment of the structure packing of **2** showing hydrogen bonds established between Nampy and Ncyanide: N2···N9, of 3.076(5) Å and N2···N3c, of 3.072(5) Å; *c* = -x, 1-*y*, -*z*.