

Electronic Supplementary Information

Expanding the 2, 2'-bipyrimidine bridged 1D homonuclear coordination polymers

family: $[M^{II}bpymCl_2]$ (M=Fe, Co) magnetic and structural characterization

Pablo Alborés^{* a,b} and Eva Rentschler^{* a}

^aDepartamento de Química Inorgánica, Analítica y Química Física/ INQUIMAE (CONICET), Facultad de Ciencias Exactas y Naturales Universidad de Buenos Aires, Pabellón 2, Ciudad Universitaria, C1428EHA Buenos Aires, Argentina Fax: +5411 / 4576-3341

*^bInstitute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University of Mainz, Duesbergweg 10-14 D-55128 Mainz-Germany
Fax: +49 6131 / 39-23922*

E-mail: albores@qi.fcen.uba.ar; rentschl@uni-mainz.de

Table S1 – Selected Bond Distances for compounds **1** and **2** (Å).

1			2	
Fe1-Cl2	2.3771(15)		Co1-Cl2	2.357(2)
Fe1-N1	2.215(4)		Co1-N1	2.161(6)
Fe1-N2	2.249(4)		Co1-N2	2.194(5)
Fe1-Cl2_a	2.3771(15)		Co1-Cl2_a	2.357(2)
Fe1-N1_a	2.215(4)		Co1-N1_a	2.161(6)
Fe1-N2_a	2.249(4)		Co1-N2_a	2.194(5)

Symmetry code: a: 0.25-x, 0.25-y, z

Table S2 – Selected Bond Angles for compounds **1** and **2** (Degrees)

1		2	
Cl2-Fe1-N1	100.02(9)	Cl2-Co1-N1	92.96(15)
Cl2-Fe1-N2	165.36(10)	Cl2-Co1-N2	167.96(14)
Cl2-Fe1-Cl2_a	97.77(5)	Cl2-Co1-Cl2_a	98.06(9)
Cl2-Fe1-N1_a	92.01(9)	Cl2-Co1-N1_a	95.15(15)
Cl2-Fe1-N2_a	89.74(9)	Cl2-Co1-N2_a	88.77(14)
N1-Fe1-N2	92.22(13)	N1-Co1-N2	76.49(19)
Cl2_a-Fe1-N1	92.01(9)	Cl2_a-Co1-N1	95.15(15)
N1-Fe1-N1_a	161.71(14)	N1-Co1-N1_a	167.6(2)
N1-Fe1-N2_a	74.25(13)	N1-Co1-N2_a	94.38(19)
Cl2_a-Fe1-N2	89.74(9)	Cl2_a-Co1-N2	88.77(14)

N1_a-Fe1-N2	74.25(13)	N1_a-Co1-N2	94.38(19)
N2-Fe1-N2_a	85.86(13)	N2-Co1-N2_a	86.3(2)
Cl2_a-Fe1-N1_a	100.02(9)	Cl2_a-Co1-N1_a	92.96(15)
Cl2_a-Fe1-N2_a	165.36(10)	Cl2_a-Co1-N2_a	167.96(14)
N1_a-Fe1-N2_a	92.22(13)	N1_a-Co1-N2_a	76.49(19)

Symmetry code: a: 0.25-x, 0.25-y, z

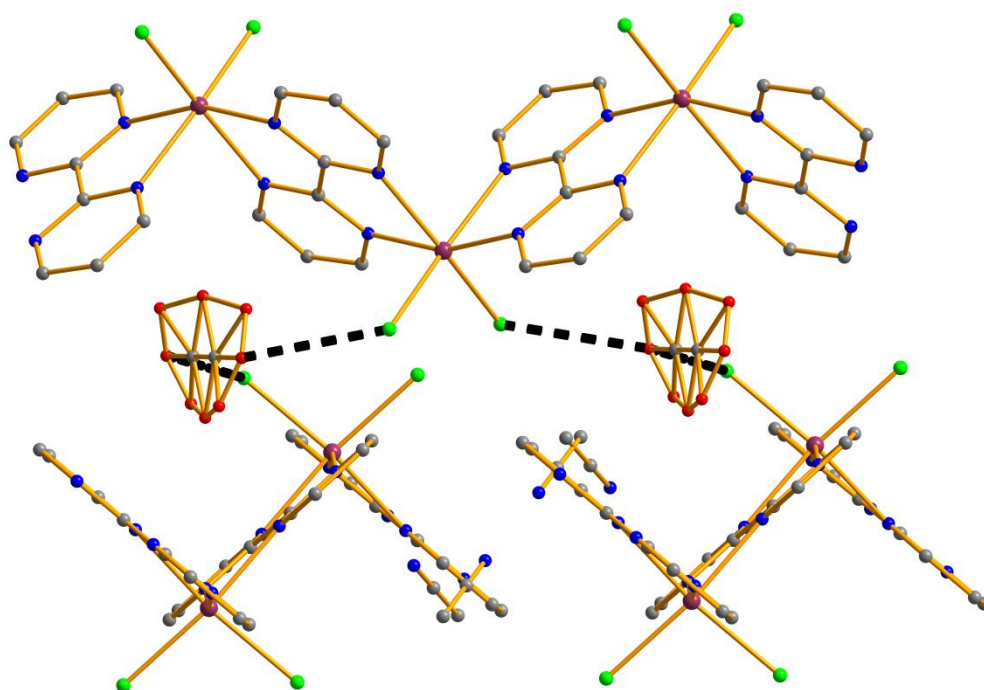


Figure S1. Short contact interactions between neighbouring chains mediated by H-interactions involving methanol solvent molecules and chloride ligands in compound **1** (same pattern is observed in compound **2**).

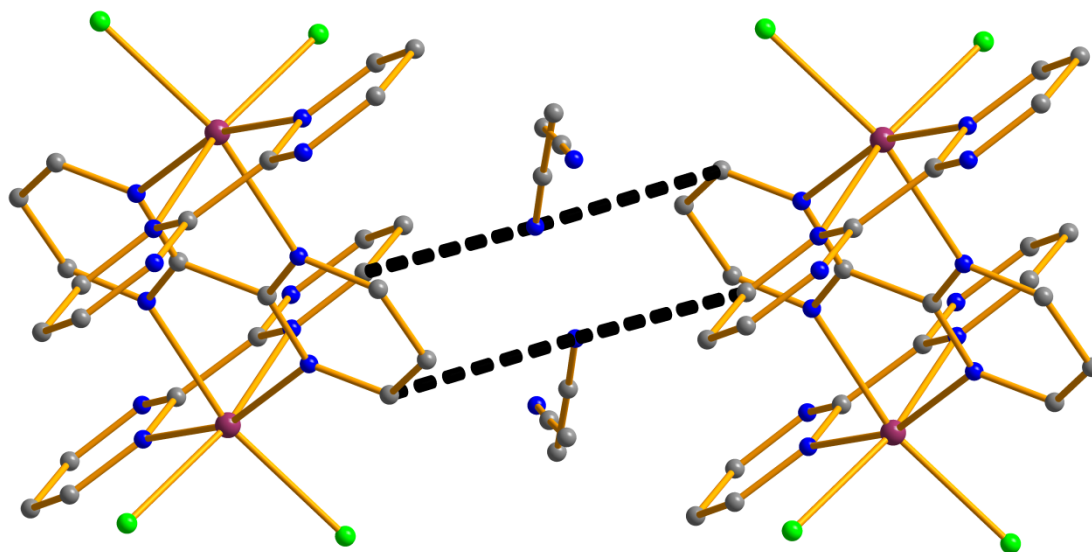


Figure S2. Short contact interactions between neighbouring chains mediated by C-H...N interactions involving acetonitrile solvent molecules and bipyrimidine ligands in compound **1** (same pattern is observed in compound **2**).

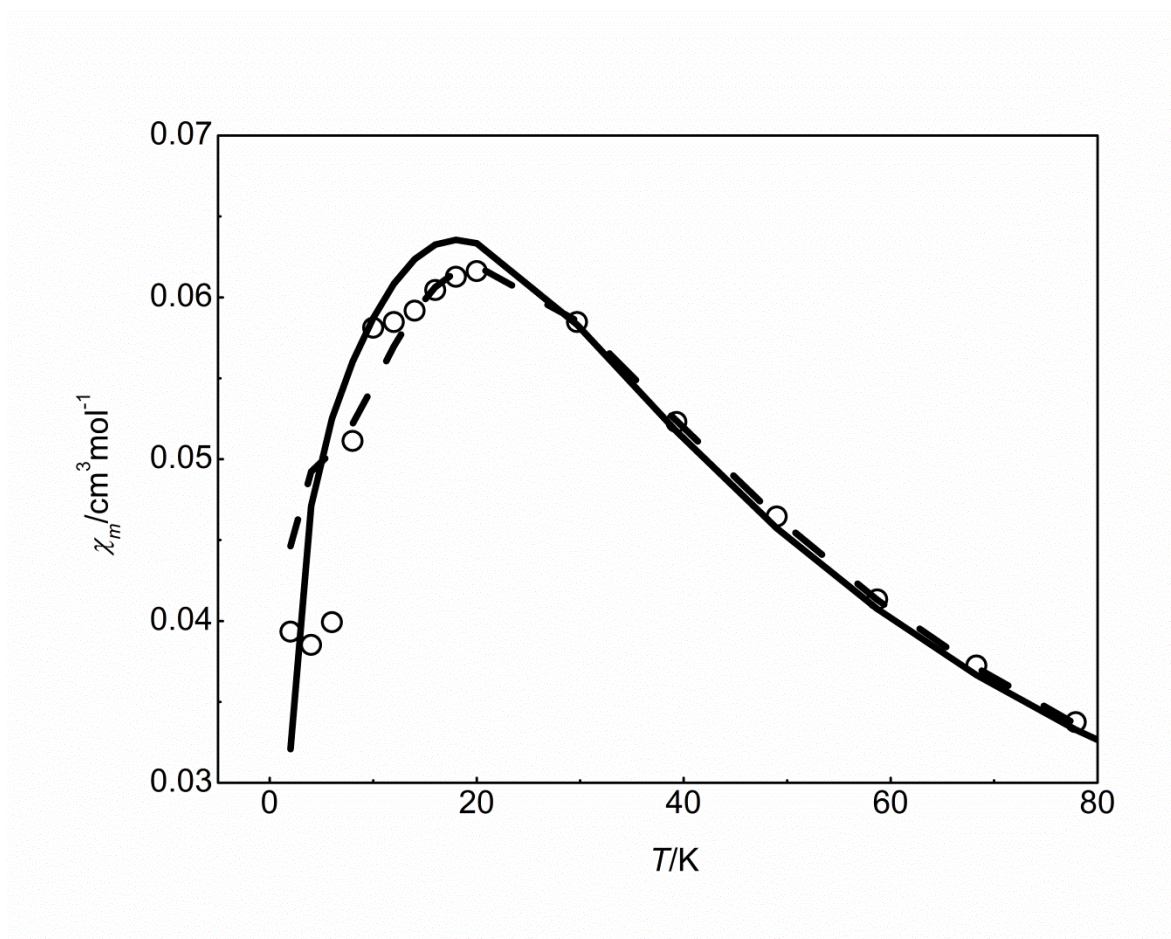


Figure S3. χ_m vs T plot in the range 2-80 K at 0.1 T of compound **1**. Open circles: experimental data; full line: best fitting without ZFS; dashed line: best fitting with ZFS (see text for details).