SUPPORTING MATERIAL

Synthesis and Characterization of New Coordination Compounds by the Use of 2-Pyridinemethanol and Di- or Tricarboxylic Acids

Ioannis Mylonas-Margaritis,^a Júlia Mayans,^b Wenming Tong,^c Pau Farràs,^c Albert

Escuer,^d Patrick McArdle,^a and Constantina Papatriantafyllopoulou * ^a

Table S1. Selected interatomic distances (Å) and angles (°) for 1.

Bonds			
Co1-N1	2.115	Co1-O1	2.168
Co1-O2	2.043		
Angles			
N1-Co1-O2	96.5(1)	N1-Co1-O1	90.2(4)
N1-Co1-O1	77.1(2)	N1-Co1-O2	95.7(5)

a. School of Chemistry, College of Science and Engineering, National University of Ireland Galway, H91 TK 33 Galway, Ireland; E-mail address: <u>constantina.papatriantafyllopo@nuigalway.ie</u>; Tel: +353 91 493462

^hInstituto de Ciencia Molecular (ICMol), Universidad de Valencia, Catedrático José Beltran 2, 46980 Paterna (Valencia), Spain

^{c.} School of Chemistry, Energy Research Centre, Ryan Institute, National University of Ireland, Galway (NUI Galway), University Road, H91 CF50 Galway, Ireland

^{d.} Departament de Química Inorgànica i Orgànica, Secció Inorgànica and Institute of Nanoscience (IN2UB) and Nanotecnology, Universitat de Barcelona, Marti i Franques 1-11, Barcelona-08028, Spain.

Bonds			
Ni1-01	2.104	Ni1-02	2.040
Ni1-N1	2.058		
Angles			
01-Ni1-02	92.91	02-Ni1-02	86.78
01-Ni1-N1	79.82	O2-Ni1-N1	94.50
01-Ni1-01	87.97	O2-Ni1-N1	95.15
01-Ni1-N1	90.58		

Table S2. Selected interatomic distances (Å) and angles (°) for 2.

Table S3. Selected interatomic distances (Å) and angles (°) for 3.

Bonds			
Ni1-02	2.058	Ni1-N1	2.052
Ni1-01	2.085		
Angles			
01-Ni1-02	92.48	N1-Ni1-O2	92.88
02-Ni1-01	87.52	N1-Ni1-O1	99.75
N1-Ni1-O1	80.25	N1-Ni1-O2	87.12

Bonds			
Zn1 - N2	2.130(3)	Zn2 - 05	1.957(5)
Zn1 - 06	2.010(5)	Zn2 - 01	1.906(4)
Zn1 - O3	2.137(3)	Zn2 - O6	1.915(4)
Zn1 - 01	2.012(4)	Zn2 - O2	1.960(5)
Zn1 - O4	2.149(3)		
Angles			
04-Zn1-01	92.8(2)	N2-Zn1-O4	89.8(1)
04-Zn1-06	92.1(1)	02-Zn2-O5	103.6(2)
06-Zn1-01	173.0(2)	05-Zn2-O1	112.4(2)
03-Zn1-06	93.8(2)	01-Zn2-O6	116.7(2)
03-Zn1-O4	91.6(1)	06-Zn2-O2	111.8(2)
03-Zn1-01	91.0(2)	02-Zn2-O1	107.8(2)
N2-Zn1-O6	78.5(2)	05-Zn2-O6	103.9(2)
N2-Zn1-O1	96.6(2)		

Table S4. Selected interatomic distances (Å) and angles (°) for 4.

Table S5. Selected interatomic distances (Å) and angles (°) for 5.

Bonds			
Fe1-06	2.149(4)	Fe2-02	2.089(0)
Fe1-01	2.073(3)	Fe2-O3	1.969(9)
Fe1-O4	2.187(7)	Fe2-O6	2.321(9)
Fe2-07	2.314(6)	Fe2-O5	2.121(2)
Fe2-N1	2.166(8)		
Angles			
06-Fe1-O4	92.23	03-Fe2-05	158.72
06-Fe1-O4	87.07	02-Fe2-O6	99.08
06-Fe1-01	89.64	02-Fe2-N1	98.15
06-Fe1-01	90.36	02-Fe2-O5	96.99
04-Fe1-01	90.46	N1-Fe2-O5	87.62
04-Fe1-01	89.54	N1-Fe2-O7	76.92
03-Fe2-06	100.74	05-Fe2-07	87.32
03-Fe2-O2	85.88	07-Fe2-O6	87.48
03-Fe2-N1	112.94	06-Fe2-O2	99.08
3-Fe2-07	91.93		



Fig. S1. Representation of the molecular structure of 2·DMF. Color code: Ni^{II}, purple; N, navy blue; O, red; C, grey. The hydrogen atoms and the solvate molecules are omitted for clarity.







Figure S3. The TGA diagram for 3.







Figure S5. The TGA diagram for 5.



Figure S6. Comparison of the pxrd patterns for 4 DMF (theoretical, blue; experimental, red).



Figure S7. Comparison of the pxrd patterns for 5 (theoretical, blue; experimental, red).