Electronic Supplementary Material (ESI) for CrystEngComm

Supplementary Materials

Structural diversity of Ni(II) coordination polymers containing dipyridyl amide and angular dicarboxylate ligands: synthesis, structures and magnetism

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Fig. S1. TGA curves for **1** – **4**.

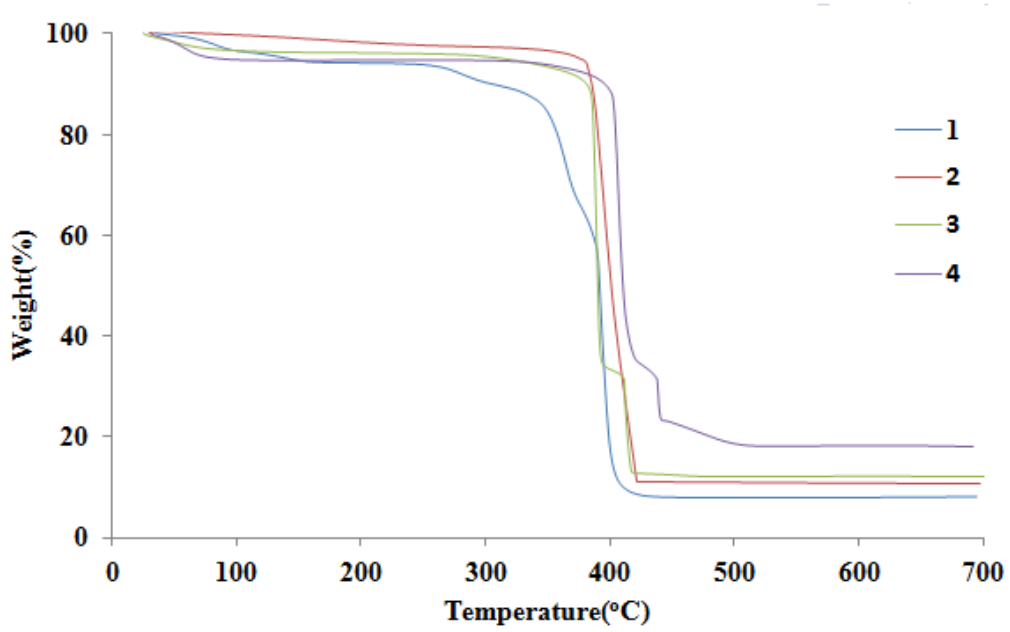

Fig. S2. χT -T curves of complexes (a) **1** (b) **2** (c) **3** and (d) **4**. Red curve shows empirical equation fitting result.

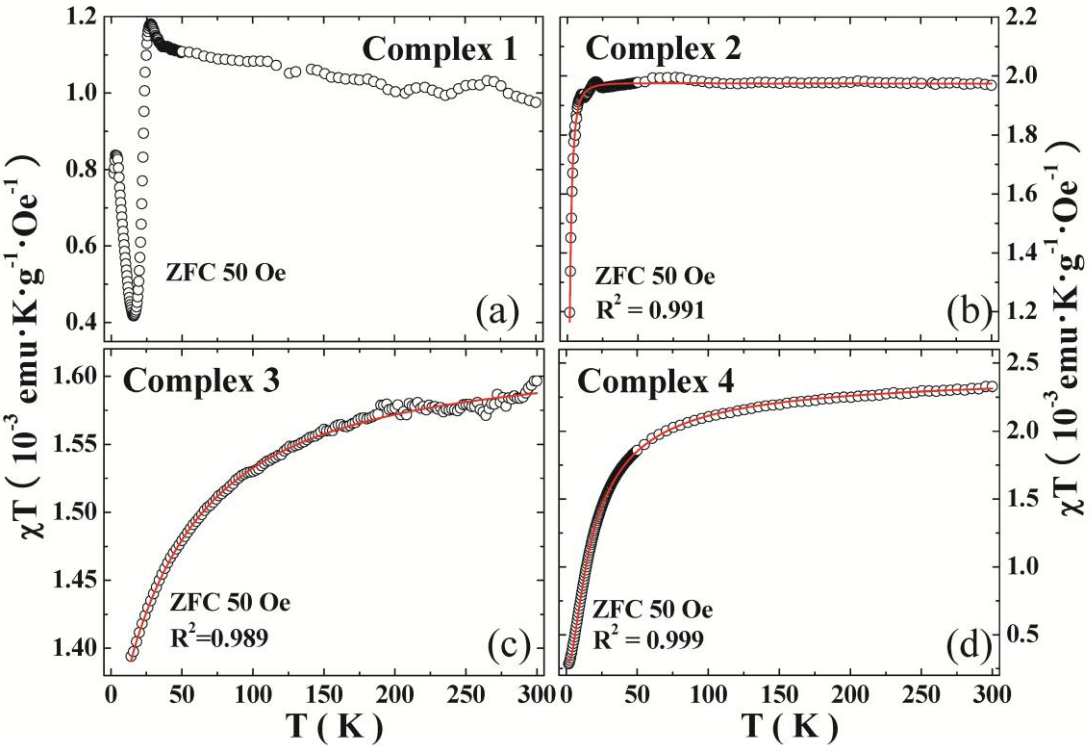

Table S1. Selected Bond lengths (Å) and Angles (°) for **1**.

Bond lengths

Ni-N(1)	2.045(3)	Ni-O(3)	2.052(2)
Ni-N(4A)	2.050(3)	Ni-O(6B)	2.070(2)
Ni-O(5B)	2.163(2)	Ni-O(4)	2.191(2)

Bond angles

N(1)-Ni-O(3)	98.48(10)	N(1)-Ni-N(4A)	97.74(10)
O(3)-Ni-N(4A)	93.57(9)	N(1)-Ni-O(6B)	94.48(10)
O(3)-Ni-O(6B)	161.54(9)	N(4A)-Ni-O(6B)	97.65(9)
N(1)-Ni-O(5B)	155.62(10)	O(3)-Ni-O(5B)	103.48(9)
N(4A)-Ni-O(5B)	91.38(9)	O(6B)-Ni-O(5B)	61.79(8)
N(1)-Ni-O(4)	90.89(9)	O(3)-Ni-O(4)	61.72(8)
N(4A)-Ni-O(4)	154.87(9)	O(6B)-Ni-O(4)	105.19(8)
O(5B)-Ni-O(4)	90.28(8)		

Symmetry transformations used to generate equivalent atoms:

(A) –x, y + 1/2, -z + 3/2 (B) x, y + 1, z.

Table S2. Selected Bond lengths (Å) and Angles (°) for **2**.

Bond lengths

Ni-N(1A)	2.0252(18)	Ni-N(1)	2.0252(18)
Ni-O(3)	2.0995(15)	Ni-O(3A)	2.0995(15)
Ni-O(2A)	2.1231(16)	Ni-O(2)	2.1232(16)

Bond angles

N(1A)-Ni-N(1)	87.38(11)	N(1A)-Ni-O(3)	98.20(7)
N(1)-Ni-O(3)	98.30(7)	N(1A)-Ni-O(3A)	98.30(7)
N(1)-Ni-O(3A)	98.20(7)	O(3)-Ni-O(3A)	157.12(9)
N(1A)-Ni-O(2A)	160.39(7)	N(1)-Ni-O(2A)	94.43(7)
O(3)-Ni-O(2A)	100.85(6)	O(3A)-Ni-O(2A)	62.11(6)
N(1A)-Ni-O(2)	94.43(7)	N(1)-Ni-O(2)	160.39(7)
O(3)-Ni-O(2)	62.11(6)	O(3A)-Ni-O(2)	100.85(6)
O(2A)-Ni-O(2)	90.37(10)		

Symmetry transformations used to generate equivalent atoms:

(A) x, -y + 1/2, -z + 1/2.

Table S3. Selected Bond lengths (Å) and Angles (^{o}) for **3**.

Bond lengths

Ni-N(1)	1.955(12)	Ni-O(2)	2.075(2)
Ni-O(2A)	2.075(2)	Ni-N(4B)	2.101(11)
Ni-O(1)	2.153(3)	Ni-O(1A)	2.153(3)

Bond angles

N(1)-Ni-O(2)	96.2(3)	N(1)-Ni-O(2A)	102.3(4)
O(2)-Ni-O(2A)	155.64(14)	N(1)-Ni-N(4B)	92.8(4)
O(2)-Ni-N(4B)	100.3(3)	O(2A)-Ni-N(4B)	94.5(3)
N(1)-Ni-O(1)	158.0(4)	O(2)-Ni-O(1)	62.07(9)
O(2A)-Ni-O(1)	99.68(9)	N(4B)-Ni-O(1)	87.7(3)
N(1)-Ni-O(1A)	98.9(3)	O(2)-Ni-O(1A)	99.68(9)
O(2A)-Ni-O(1A)	62.07(9)	N(4B)-Ni-O(1A)	155.5(3)
O(1)-Ni-O(1A)	89.31(15)		

Symmetry transformations used to generate equivalent atoms: (A) –x + 1, -y + 1, z (B) x - 1/2, -y + 1, z.

Table S4. Selected Bond lengths (Å) and Angles (°) for **4**.

Bond lengths

Ni-N(1)	2.004(2)	Ni-O(6C)	2.0070(19)
Ni-O(7B)	2.0240(19)	Ni-O(3A)	2.060(2)
Ni-O(2)	2.103(2)	Ni-O(2A)	2.345(2)
Ni-Ni(A)	2.7091(7)		

Bond angles

N(1)-Ni-O(6C)	96.25(9)	N(1)-Ni-O(7B)	96.17(9)
O(6C)-Ni-O(7B)	166.53(8)	N(1)-Ni-O(3A)	106.24(9)
O(6C)-Ni-O(3A)	90.58(9)	O(7B)-Ni-O(3A)	90.94(9)
N(1)-Ni-O(2)	88.94(9)	O(6C)-Ni-O(2)	88.33(9)
O(7B)-Ni-O(2)	86.71(8)	O(3A)-Ni-O(2)	164.81(8)
N(1)-Ni-O(2A)	165.86(9)	O(6C)-Ni-O(2A)	85.04(8)
O(7B)-Ni-O(2A)	84.19(8)	O(3C)-Ni-O(2A)	59.63(8)
O(2)-Ni-O(2A)	105.19(7)		

Symmetry transformations used to generate equivalent atoms: (A) –x + 1, -y + 1, -z + 1; (B) x - 1/2, y – 1/2, z; (C) –x + 3/2, -y + 3/2, -z + 1.

Table S5. C-X-C angles of MBA^{2-}, OBA^{2-} and SDA^{2-} ligands in known metal complexes.

Metal	Dicarboxylate	Co-Ligand	(C-X-C) angle	reference
Zn	MBA^{2-}		114.1	1
Zn	OBA^{2-}		122.5	2
Zn	OBA^{2-}	4,4'-bipy	118.7	3
Co	OBA^{2-}	4,4'-bipy	120.8	4
Ni	OBA^{2-}	N,N'-4-bipyridnylamine	117.6	5
Co	OBA^{2-}	N,N'-4-bipyridnylamine	117.3	5
Ni	OBA^{2-}	4,4'-Trimethylenedipyridine	117.6	6
Cu	OBA^{2-}	4,4'-Trimethylenedipyridine	117.8	6
Cu	SDA^{2-}	4,4'-bipy	103.1	7
Cu	SDA^{2-}	4,4'-bipy	101.4	8
Ni	SDA^{2-}	4,4'-bipy	102.7	9
Cd	SDA^{2-}	4,4'-bipy	104.8	10
Cd	SDA^{2-}	4,4'-bipy	104.9	11
Zn	SDA^{2-}	4,4'-bipy	102.9	12
Cd	SDA^{2-}	4,4'-Trimethylenedipyridine	103.3	13
Mn	SDA^{2-}	4,4'-Trimethylenedipyridine	105.1	14

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