Electronic Supplementary Material for CrystEngComm

Supplementary Information

Indium(III)-2,5-Pyridine Dicarboxylate Complexes with Mononuclear, 1D Chain, 2D Layer and 3D Chiral Frameworks

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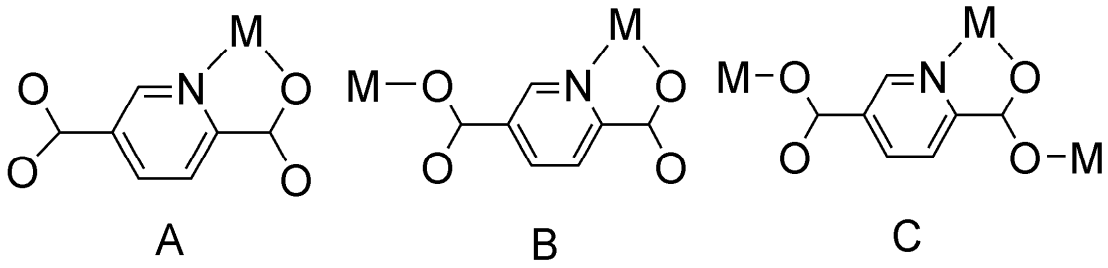

Scheme.S1. Schematic representation of the observed coordination modes of 2,5-pdc for compounds **1**-**5**.

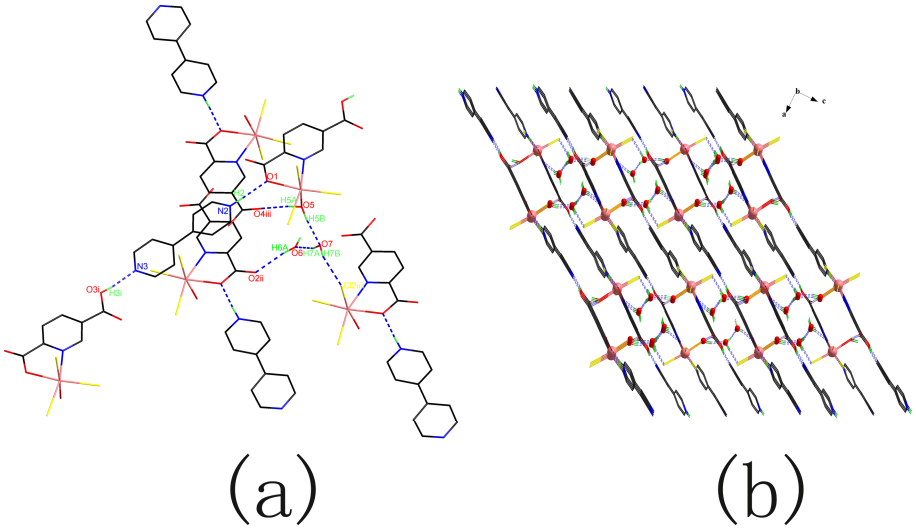

Fig. S1. Details of hydrogen bonds formed in **1** (a). Stick representation of the 3D network of **1** (b). Hydrogen bonds are shown in dashed blue lines. Symmetry code: i: x-1, y+1, z-1; ii: x, -y+5/2, z-1/2; iii: -x+1, y+1/2, -z+1/2; iiii: x, -y+3/2, z-1/2.

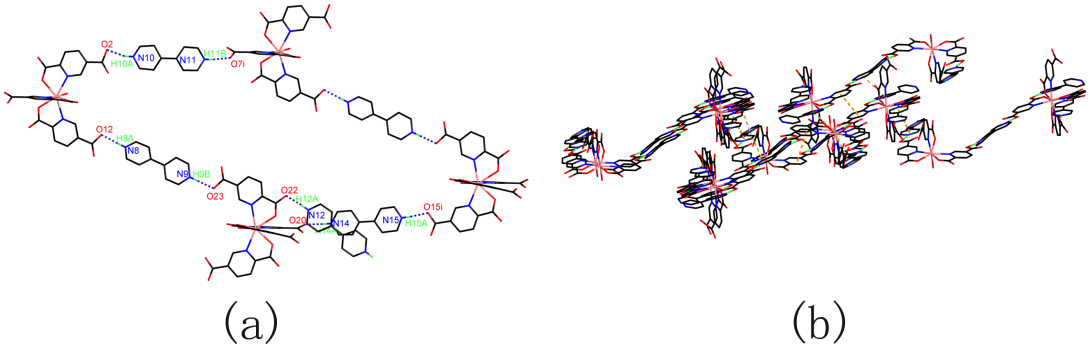

Fig. S2. Details of hydrogen bonds formed between 4,4'- H_2bipy and In(III) coordination spheres (a). Schematic representation of the π-π interaction **2** along [110] direction, indicated by dashed yellow lines (b). Hydrogen bonds are shown in dashed blue lines. Symmetry code: i: x+1, y+1, z.

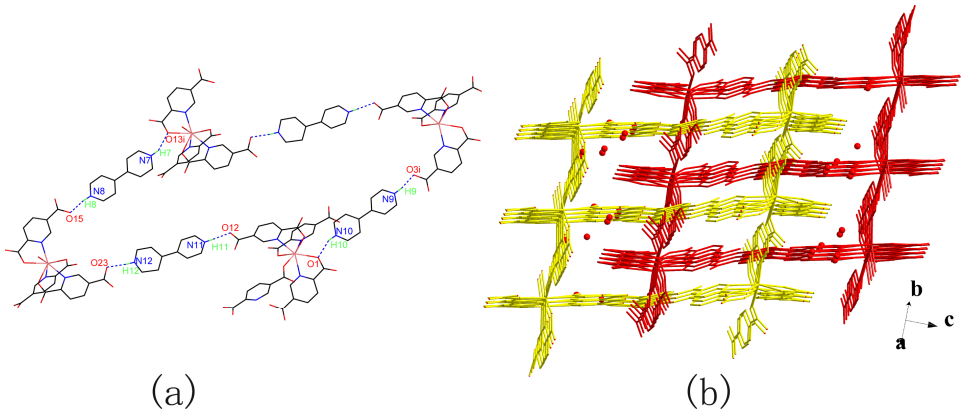

Fig. S3. Details of hydrogen bonds formed between 4,4'- H_2bipy and In(III) coordination spheres.

Hydrogen bonds are shown in dashed blue lines (a) Interpenetration of two bilayers in **3** (b).

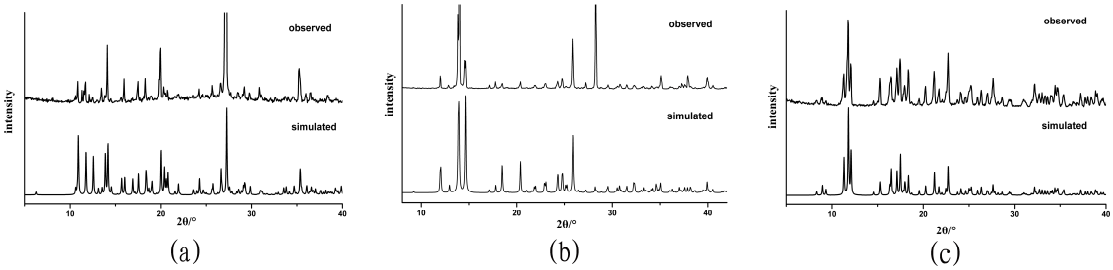

Fig. S4. X-ray powder diffraction (XPD) patterns of compounds **1** (a), **4** (b) and **5** (a).

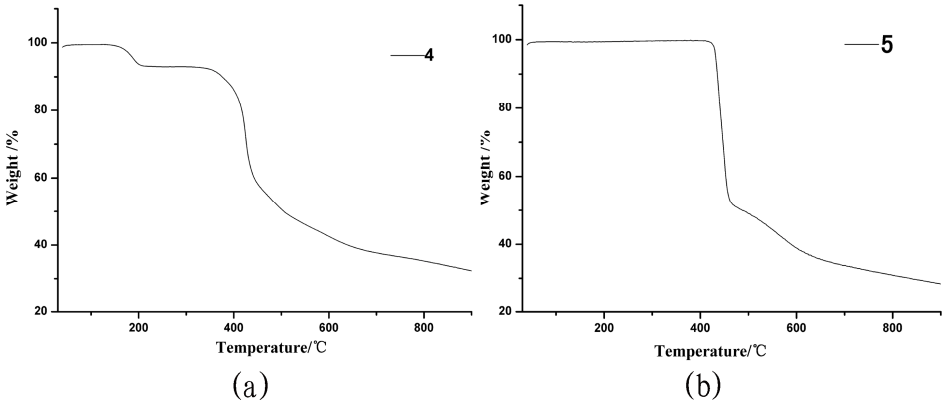

Fig. S5. The TG curves of compounds **4** (a) and **5** (b).

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Table S1 Hydrogen bonds for **1**- **4** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
		1		
O(5)-H(5B)...O(7)^{i}	0.88	1.76	2.624(3)	165.2
N(2)-H(2)...O(1)^{i}	0.90	1.81	2.710(2)	177.3
O(6)-H(6B)...O(2)^{i}	0.85	2.05	2.872(3)	164.3
O(3)-H(3A)...N(3)^{ii}	0.81	1.76	2.566(3)	172.6
O(5)-H(5A)...O(4)^{iii}	0.89	2.00	2.885(3)	171.0
O(7)-H(7A)...O(6)^{iv}	0.84	1.94	2.759(4)	165.0
O(7)-H(7B)...Cl(2)^{v}	0.86	2.44	3.280(2)	165.3
		2		
N8—H8A...O12^{i}	0.86	1.80	2.654 (9)	174.9
N10—H10A...O2^{ii}	0.86	1.85	2.688 (14)	163.9
N11—H11B...O7^{iii}	0.86	1.71	2.562 (9)	172.6
N15—H15B...O15^{iv}	0.86	1.79	2.646 (11)	174.4
N9—H9B...O23	0.86	1.75	2.610 (8)	175.6
N12—H12A...O22	0.86	1.74	2.601 (7)	174.8
N14—H14A...O20	0.86	1.76	2.601 (9)	165.5
		3		
N10—H10...O1^{i}	0.86	2.02	2.819 (9)	154.6
N7—H7...O13^{ii}	0.86	2.07	2.844 (9)	149.0
N8—H8...O15^{iii}	0.86	1.75	2.598 (7)	169.3
N9—H9...O3^{iv}	0.86	1.74	2.593 (9)	168.8
N12—H12...O23^{iv}	0.86	1.81	2.670 (11)	173.4
N11—H11...O12^{v}	0.86	1.74	2.603 (8)	178.3
		4		
O7—H7B...O4^{i}	0.88	2.02	2.844 (3)	156.7
O7—H7A...Cl1^{ii}	0.91	2.32	3.216 (2)	167.0
O6—H6B...O7^{iii}	0.87	1.77	2.634 (3)	174.7
O6—H6A...O2^{iv}	0.87	1.76	2.626 (3)	169.2

Symmetry Codes: for 1, (i): x,y,z; (ii): x+1,y-1,z+1; (iii): -x+1,y+1/2,-z+1/2, (iv): x,-y+5/2,z-1/2; (v): x,-y+3/2,z-1/2, for 2, (i) x, y, 1+z; (ii) -1+x, y, z; (iii) x, 1+y, z; (iv) 1+x, 1+y, z, for 3, (i): x, y, z; (ii): 1-x, 1-y, 1-z; (iii): 2-x, 2-y, 1-z; (iv): -1+x, -1+y, z; (v): 1-x, 1-y, -z, for 4, (i): -1+x, 1/2-y, -1/2+z; (ii): 1-x, 1/2+y, 1/2-z; (iii): 1+x, y, z; (iv) 2-x, -1/2+y, 1/2-z.