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; iii: x, -y+3/2, z-1/2.

Fig. S2. Details of hydrogen bonds formed between 4,4'-H$_2$bipy and In(III) coordination spheres (a). Schematic representation of the $\pi$-$\pi$ 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'-H₂bipy 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).
Table S1 Hydrogen bonds for 1-4 [Å and °].

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

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,z; (v): x,y+1/2,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.