Supplementary Material

Assembly, Structure and Properties of Six Coordination Polymers Based on 1,3,5-Tri-4-pyridyl-1,2-ethenylbenzene

Chen Cao,*a,b Tian-Yi Gu, a Jian-Guo Zhang, a Ming Dai, c Chun-Yan Ni,*a Zhi-Gang Yao,*d and Jian-Ping Lang,*a,b

*aCollege of Chemistry, Chemical Engineering and Materials Science, Soochow University, Suzhou 215123, People’s Republic of China
*bState Key Laboratory of Organometallic Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai 200032, People’s Republic of China
*cSuzhou Clean Environment Institute, Jiangsu Sujing Group Co., Ltd., Suzhou 215122, People’s Republic of China
*dAnalysis and Testing Center, Soochow University, Suzhou 215123, People’s Republic of China

*To whom correspondence should be addressed. E-mail: chunyan89.ok@163.com, zhgyao@suda.edu.cn, jplang@suda.edu.cn
Table of Contents

Fig. S1. View of the 3D supramolecular structure of 1. All red dotted lines in 1 represent π−π interactions.................................53

Fig. S2. View of two different alignments of olefinic bonds in 1. The red dotted lines represent the parallel alignment while the pink dotted lines represent the anti-parallel arrangement..........................................................53

Fig. S3. (a) PXRD patterns of 1 (from single crystal data: black; as-synthesized: red; immersed in H2O: blue). (b) PXRD patterns of 2 (from single crystal data: black; as-synthesized: red; immersed in H2O: blue). (c) PXRD patterns of 3 (from single crystal data: black; as-synthesized: red; immersed in H2O: blue). (d) PXRD patterns of 4 (from single crystal data: black; as-synthesized: red; immersed in H2O: blue). (e) PXRD patterns of 5 (from single crystal data: black; as-synthesized: red; immersed in H2O: blue). (f) PXRD patterns of 6 (from single crystal data: black; as-synthesized: red; immersed in H2O: blue). ........................................................54

Fig. S4. Thermogravimetric analysis (TGA) curves for 1−4 ..................................................55

Fig. S5. Thermogravimetric analysis (TGA) curves for 5 and 6 ........................................55

Fig. S6. The emission spectra of 1−4 and tpeb ligand in the solid state at ambient temperature.............................................................................................................................56

Fig. S7. The emission spectra of 5, tpeb and H2dpa ligands in the solid state at ambient temperature.............................................................................................................................56

Fig. S8. UV-vis spectra of the RhB solutions under UV light irradiation without any catalysts with a time interval of 0.5 h.................................................................57

Fig. S9. PXRD patterns of 2 (from single crystal data: black; after degradation: red). .................................................................................................................................57

Table S1. Selected bond lengths (Å) and angles (°) for 1−6........................................58
Fig. S1. View of the 3D supramolecular structure of 1. All red dotted lines in 1 represent π–π interactions.

Fig. S2. View of two different alignments of olefinic bonds in 1. The red dotted lines represent the parallel alignment while the pink dotted lines represent the anti-parallel arrangement.
Fig. S3. (a) PXRD patterns of 1 (from single crystal data: black; as-synthesized: red; immersed in H₂O: blue). (b) PXRD patterns of 2 (from single crystal data: black; as-synthesized: red; immersed in H₂O: blue). (c) PXRD patterns of 3 (from single crystal data: black; as-synthesized: red; immersed in H₂O: blue). (d) PXRD patterns of 4 (from single crystal data: black; as-synthesized: red; immersed in H₂O: blue). (e) PXRD patterns of 5 (from single crystal data: black; as-synthesized: red; immersed in H₂O: blue). (f) PXRD patterns of 6 (from single crystal data: black; as-synthesized: red; immersed in H₂O: blue).
Fig. S4. Thermogravimetric analysis (TGA) curves for 1 – 4.

Fig. S5. Thermogravimetric analysis (TGA) curves for 5 and 6.
Fig. S6. The emission spectra of 1–4 and tpeb ligand in the solid state at ambient temperature.

Fig. S7. The emission spectra of 5, tpeb and H$_2$dpa ligands in the solid state at ambient temperature.
Fig. S8. UV-vis spectra of the RhB solutions under UV light irradiation without any catalysts with a time interval of 0.5 h.

Fig. S9. PXRD patterns of 2 (from single crystal data: black; after degradation: red).
Table S1. Selected bond lengths (Å) and angles (°) for 1–6

<table>
<thead>
<tr>
<th></th>
<th>Bond Lengths</th>
<th></th>
<th>Bond Lengths</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Cd(1)-N(1) 2.264(3) Cd(1)-N(2)#1 2.248(3)</td>
<td>Cd(1)-Br(2) 2.5385(6) Cd(1)-Br(1) 2.5396(7)</td>
<td>N(1)-Cd(1)-N(2)#1 107.49(12) N(2)#1-Cd(1)-Br(2) 108.26(8)</td>
</tr>
<tr>
<td></td>
<td>N(1)-Cd(1)-N(2) 107.49(12) N(2)#1-Cd(1)-Br(2) 108.26(8)</td>
<td>Br(2)-Cd(1)-N(1) 110.75(9) N(2)#1-Cd(1)-Br(1) 111.00(9)</td>
<td>Br(1)-Cd(1)-N(1) 100.14(10) Br(2)-Cd(1)-Br(1) 118.56(2)</td>
</tr>
<tr>
<td>2</td>
<td>Cd(1)-N(2)#1 2.266(5) Cd(1)-N(1) 2.258(5)</td>
<td>Cd(1)-I(1) 2.7128(8) Cd(1)-I(2) 2.7224(8)</td>
<td>N(2)#1-Cd(1)-N(1) 108.8(2) I(1)-Cd(1)-N(1) 108.43(14)</td>
</tr>
<tr>
<td></td>
<td>Cd(1)-I(1) 2.7128(8) Cd(1)-I(2) 2.7224(8)</td>
<td>N(2)#1-Cd(1)-N(1) 108.8(2) I(1)-Cd(1)-N(1) 108.43(14)</td>
<td>N(2)#1-Cd(1)-I(1) 112.55(14) I(2)-Cd(1)-I(2) 116.38(3)</td>
</tr>
<tr>
<td>3</td>
<td>Cu(1)-N(1) 1.998(3) Cu(1)-N(3)#1 1.981(3)</td>
<td>Cu(1)-N(5)#2 1.984(3) Cu(2)-N(4) 1.974(3)</td>
<td>N(1)-Cu(1)-N(3)#1 117.61(12) I(1)-Cu(1)-N(3)#1 95.75(8)</td>
</tr>
<tr>
<td></td>
<td>Cu(1)-I(1) 2.4927(6) Cu(2)-I(1) 2.5650(5)</td>
<td>N(1)-Cu(1)-N(3)#1 117.61(12) I(1)-Cu(1)-N(3)#1 95.75(8)</td>
<td>N(1)-Cu(1)-N(5)#2 116.09(9) N(5)#2-Cu(2)-N(4) 130.76(12)</td>
</tr>
<tr>
<td></td>
<td>N(1)-Cu(1)-N(3)#1 117.61(12) I(1)-Cu(1)-N(3)#1 95.75(8)</td>
<td>N(1)-Cu(1)-N(5)#2 116.09(9) N(5)#2-Cu(2)-N(4) 130.76(12)</td>
<td>N(1)-Cu(1)-O(1) 98.66(8) N(2)#2-Cd(1)-O(2) 91.43(8)</td>
</tr>
<tr>
<td>4</td>
<td>Cd(1)-N(2)#2 2.362(3) Cd(1)-N(3)#1 2.391(3)</td>
<td>Cd(1)-N(1) 2.417(3) Cd(1)-O(1) 2.513(3)</td>
<td>O(4)#1-Co(1)-N(3)#2 176.96(10) N(3)#2-Co(1)-O(2) 93.81(11)</td>
</tr>
<tr>
<td></td>
<td>Cd(1)-N(1) 2.417(3) Cd(1)-O(1) 2.513(3)</td>
<td>Cd(1)-N(1) 2.417(3) Cd(1)-O(1) 2.513(3)</td>
<td>N(1)-Co(1)-N(1) 175.93(11) O(1)-Co(1)-N(2)#3 93.81(11)</td>
</tr>
<tr>
<td></td>
<td>I(1)-Cd(1)-N(2)#2 109.75(8) I(1)-Cd(1)-N(3)#1 95.75(8)</td>
<td>N(1)-Cd(1)-O(1) 81.53(10) N(2)#2-Cd(1)-O(2) 140.01(11)</td>
<td>N(1)-Co(1)-N(3)#1 95.75(8) O(1)-Co(1)-N(2)#3 83.44(11)</td>
</tr>
<tr>
<td></td>
<td>N(1)-Cd(1)-O(1) 81.53(10) N(2)#2-Cd(1)-O(2) 140.01(11)</td>
<td>N(1)-Cd(1)-O(1) 81.53(10) N(2)#2-Cd(1)-O(2) 140.01(11)</td>
<td>N(1)-Co(1)-O(2) 88.61(10) N(3)#2-Co(1)-O(2) 148.48(11)</td>
</tr>
<tr>
<td></td>
<td>N(3)#1-Cd(1)-O(2) 94.09(11) N(1)-Cd(1)-O(2) 91.16(11)</td>
<td>N(3)#1-Cd(1)-O(2) 94.09(11) N(1)-Cd(1)-O(2) 91.16(11)</td>
<td>N(1)-Co(1)-O(2) 90.41(10) O(1)-Co(1)-O(2) 58.25(10)</td>
</tr>
<tr>
<td>5</td>
<td>Co(1)-O(4)#1 2.033(3) Co(1)-N(3)#2 2.139(3)</td>
<td>Co(1)-N(1) 2.159(3) Co(1)-O(1) 2.170(3)</td>
<td>O(4)#1-Co(1)-N(3)#2 88.95(11) O(4)#1-Co(1)-N(1) 88.35(11)</td>
</tr>
<tr>
<td></td>
<td>Co(1)-N(2)#3 2.173(3) Co(1)-O(2) 2.316(3)</td>
<td>Co(1)-N(2)#3 2.173(3) Co(1)-O(2) 2.316(3)</td>
<td>N(3)#1-Co(1)-N(1) 97.80(11) O(4)#1-Co(1)-N(1) 88.35(11)</td>
</tr>
<tr>
<td></td>
<td>O(4)#1-Co(1)-N(3)#2 88.95(11) O(4)#1-Co(1)-N(1) 88.35(11)</td>
<td>N(3)#2-Co(1)-N(1) 91.43(11) N(1)-Co(1)-O(1) 88.61(10)</td>
<td>N(3)#2-Co(1)-N(2)#3 85.43(11) N(1)-Co(1)-N(2)#3 85.43(11)</td>
</tr>
<tr>
<td></td>
<td>N(3)#2-Co(1)-O(1) 91.43(11) N(1)-Co(1)-O(1) 88.61(10)</td>
<td>O(4)#1-Co(1)-N(3)#2 88.95(11) O(4)#1-Co(1)-N(1) 88.35(11)</td>
<td>O(4)#1-Co(1)-N(2)#3 85.43(11) N(1)-Co(1)-N(2)#3 85.43(11)</td>
</tr>
<tr>
<td></td>
<td>O(4)#1-Co(1)-N(2)#3 89.22(11) N(3)#2-Co(1)-N(2)#3 85.43(11)</td>
<td>O(4)#1-Co(1)-N(2)#3 89.22(11) N(3)#2-Co(1)-N(2)#3 85.43(11)</td>
<td>N(1)-Co(1)-N(2)#3 175.93(11) O(1)-Co(1)-N(2)#3 93.81(11)</td>
</tr>
<tr>
<td></td>
<td>N(1)-Co(1)-N(2)#3 175.93(11) O(1)-Co(1)-N(2)#3 93.81(11)</td>
<td>O(4)#1-Co(1)-N(2)#3 175.93(11) O(1)-Co(1)-N(2)#3 93.81(11)</td>
<td>N(2)#3-Co(1)-O(2) 121.80(10) N(3)#2-Co(1)-O(2) 148.48(11)</td>
</tr>
<tr>
<td></td>
<td>O(4)#1-Co(1)-O(2) 121.80(10) N(3)#2-Co(1)-O(2) 148.48(11)</td>
<td>O(4)#1-Co(1)-O(2) 121.80(10) N(3)#2-Co(1)-O(2) 148.48(11)</td>
<td>N(1)-Co(1)-O(2) 90.41(10) O(1)-Co(1)-O(2) 58.25(10)</td>
</tr>
<tr>
<td></td>
<td>N(2)#3-Co(1)-O(2) 90.41(10) O(1)-Co(1)-O(2) 58.25(10)</td>
<td>N(2)#3-Co(1)-O(2) 90.41(10) O(1)-Co(1)-O(2) 58.25(10)</td>
<td></td>
</tr>
<tr>
<td>Bond</td>
<td>Distance</td>
<td>Bond</td>
<td>Distance</td>
</tr>
<tr>
<td>-----------------------------</td>
<td>----------</td>
<td>-----------------------------</td>
<td>----------</td>
</tr>
<tr>
<td>Ni(1)-O(5)#1</td>
<td>2.022(6)</td>
<td>Ni(1)-N(1)</td>
<td>2.084(6)</td>
</tr>
<tr>
<td>Ni(1)-N(4)</td>
<td>2.067(8)</td>
<td>Ni(1)-O(1)</td>
<td>2.125(6)</td>
</tr>
<tr>
<td>Ni(1)-N(2)#2</td>
<td>2.114(7)</td>
<td>Ni(1)-O(2)</td>
<td>2.152(6)</td>
</tr>
<tr>
<td>O(5)#2-Ni(1)-N(4)</td>
<td>92.8(3)</td>
<td>O(5)#2-Ni(1)-N(1)</td>
<td>99.3(3)</td>
</tr>
<tr>
<td>N(4)-Ni(1)-N(1)</td>
<td>89.8(3)</td>
<td>O(5)#2-Ni(1)-O(1)</td>
<td>102.0(3)</td>
</tr>
<tr>
<td>N(4)-Ni(1)-O(1)</td>
<td>164.4(3)</td>
<td>N(1)-Ni(1)-O(1)</td>
<td>92.2(3)</td>
</tr>
<tr>
<td>O(5)#2-Ni(1)-N(2)#1</td>
<td>85.5(3)</td>
<td>N(4)-Ni(1)-N(2)#1</td>
<td>88.0(3)</td>
</tr>
<tr>
<td>N(1)-Ni(1)-N(2)#1</td>
<td>174.8(3)</td>
<td>O(1)-Ni(1)-N(2)#1</td>
<td>88.6(3)</td>
</tr>
<tr>
<td>O(5)#2-Ni(1)-O(2)</td>
<td>161.5(2)</td>
<td>N(4)-Ni(1)-O(2)</td>
<td>103.2(3)</td>
</tr>
<tr>
<td>N(1)-Ni(1)-O(2)</td>
<td>90.0(3)</td>
<td>O(1)-Ni(1)-O(2)</td>
<td>61.3(2)</td>
</tr>
<tr>
<td>N(2)#1-Ni(1)-O(1)</td>
<td>88.6(3)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry codes: 1: #1: 1+x, 1+y, 1+z; 2: #1: 1+x, 1+y, 1+z; 3: #1: -1+x, 1+y, -1+z; 
4: #2: -2-x, 2-y, -1-z; 5: #1: x, y, 1+z; #2: 2+x, y, -1+z; 6: #1: -y-1, x-y, +z+1/3; #2: -2-x, -x+y, -z-2/3.