Electronic Supplementary Information (ESI) for

Structural Diversity, Luminescence, and Photocatalytic Properties of Six Coordination Polymers Based on Designed Bifunctional 2-(1-imidazol-yl)terephthalic Acid

Xiutang Zhang,* a,b Liming Fan, a,b Weiliu Fan, b Bin Li, a Guangzeng Liu, a Xinzheng Liu a and Xian Zhao* b

a Advanced Material Institute of Research, College of Chemistry and Chemical Engineering, Qilu Normal University, Jinan, 250013, China.
b State Key Laboratory of Crystal Materials, Shandong University, Jinan 250100, China.

E-mail: xiutangzhang@163.com; xianzhao@sdu.edu.cn.

ESI

Figure S1. Various 2-position modified H₂TPA derivatives.

Figure S2. The MS data of the obtained H₂TPA.
Figure S3. The IR spectras of complexes 1-6.

Figure S4. The 2-fold interpenetrated framework of 1.
Figure S5. The 2D $\{6^3\}$–heb sheet of 4.

Figure S6. The 3D supramolecular structure of 4.
Figure S7. PXRD patterns of 1-6. Dark: calculated from the X-ray single-crystal data; Red: observed for the as-synthesized solids.

Figure S8. TGA curves for complexes 1–6.
Figure S9. The CIE PXRD patterns of 1 (a), 3 (b), 5 (c), and 6 (d).

Figure S10. UV-Vis absorption spectra of the MB solutions degraded without catalyst under UV irradiation at different time intervals.

Figure S11. Recycling test on complex 1 for MB photodegradation.
Figure S12. Recycling test on complex 3 for MB photodegradation.

Figure S13. Recycling test on complex 5 for MB photodegradation.

Figure S14. Recycling test on complex 6 for MB photodegradation.
### Table S1 Selected bond lengths (Å) and angles (°) for 1, and 3–6.

<table>
<thead>
<tr>
<th>Complex</th>
<th>Bond or Angle</th>
<th>Length/Angle</th>
</tr>
</thead>
<tbody>
<tr>
<td>O(2B)-Zn(1)</td>
<td>2.01(7)</td>
<td>Zn(1)-N(N2)</td>
</tr>
<tr>
<td>Zn(1)-O(2A)</td>
<td>1.90(8)</td>
<td>Zn(1)-O(4)</td>
</tr>
<tr>
<td>O(2A)-Zn(1)-N(2)</td>
<td>140.9(17)</td>
<td>N(2)-Zn(1)-O(4)</td>
</tr>
<tr>
<td>Ni(2)-Zn(1)-O(2B)</td>
<td>147.8(17)</td>
<td>O(2B)-Zn(1)-N(3)</td>
</tr>
<tr>
<td>O(2A)-Zn(1)-O(4)</td>
<td>105.2(2)</td>
<td>O(2A)-Zn(1)-O(3)</td>
</tr>
</tbody>
</table>

**Symmetry codes:**
- #1: 
  - x, y, z
- #2: 
  - x-1, y, z
- #3: 
  - x, y, z
- #4: 
  - x, y+1, z
- #5: 
  - x+y, z

**Complex 3**
- N(1)-Zn(1) | 2.038(3) | N(3)-Zn(1) |
- O(2)^4-Zn(1)-O(3)^4 | 130.90(15) | O(3)^4-Zn(1)-N(3) |
- O(2)^4-Zn(1)-N(3) | 100.33(15) | O(2)^4-Zn(1)-N(1) |

**Symmetry codes:**
- #3: 
  - x+1, y, z
- #4: 
  - x+y, z

**Complex 4**
- N(1)-Ni(1) | 2.0382(17) | Ni(1)-O(3)^2 |
- Ni(3)-Ni(1) | 2.0726(17) | Ni(1)-O(5) |
- Ni(1)-Ni(1)-O(3)^4 | 91.14(7) | O(3)^4-Ni(1)-O(5) |
- Ni(1)-Ni(1)-N(3) | 92.58(7) | N(3)-Ni(1)-O(5) |
- O(3)^4-Ni(1)-N(3) | 174.52(7) | N(1)-Ni(1)-O(7) |
- Ni(1)-Ni(1)-O(5) | 89.89(7) | Ni(1)-Ni(1)-O(7) |

**Symmetry code:**
- #2: 
  - x, y+3/2, z

**Complex 5**
- Zn(1)-O(1) | 1.917(2) | Zn(1)-O(3)^4 |
- O(1)-Zn(1) | 126.16(11) | O(3)^4-Zn(1)-N(1) |
- O(1)-Zn(1)-N(1) | 116.26(10) | O(1)-Zn(1)-N(3)^2 |

**Symmetry codes:**
- #1: 
  - x, y-1/2, z
- #2: 
  - x+1, -y+1, -z+1

**Complex 6**
- Cd(1)-N(1)^4 | 2.233(2) | Cd(1)-O(5) |
- Cd(1)-N(3) | 2.245(2) | Cd(1)-O(2)^3 |
- Ni(1)^2-Cd(1)-O(5) | 90.47(9) | Ni(1)^2-Cd(1)-O(4) |
- Ni(1)^2-Cd(1)-O(4) | 95.87(9) | Ni(3)-Cd(1)-O(4) |
- Ni(1)^2-Cd(1)-O(2)^3 | 86.01(8) | O(5)-Cd(1)-O(4) |
- N(3)-Cd(1)-O(2)^3 | 97.93(8) | O(2)^2-Cd(1)-O(4) |
- O(5)-Cd(1)-O(2)^3 | 125.99(9) | N(1)^2-Cd(1)-O(6) |

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