# Metal-organic frameworks based on naphthalene-1,5-diyldioxy-di-acetate: Structures, topologies, photoluminescence and photocatalytic properties

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## Table S1 Selected bond lengths (Å) and angles (º) for complexes 1-5

<table>
<thead>
<tr>
<th>Complex 1</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mn(1)-O(1)</td>
<td>2.098(2)</td>
<td>Mn(1)-O(5)</td>
<td>2.250(2)</td>
</tr>
<tr>
<td>Mn(2)-O(6)</td>
<td>2.227(2)</td>
<td>Mn(2)-O(5)</td>
<td>2.196(2)</td>
</tr>
<tr>
<td>O(3)-Mn(1)-O(5)</td>
<td>89.25(6)</td>
<td>O(5)-Mn(1)-O(5)#1</td>
<td>180.00(7)</td>
</tr>
<tr>
<td>O(1)-Mn(1)-O(5)</td>
<td>89.42(7)</td>
<td>O(7)#2-Mn(2)-O(6)</td>
<td>82.56(7)</td>
</tr>
<tr>
<td>O(5)#2-Mn(2)-O(6)</td>
<td>171.01(7)</td>
<td>O(5)-Mn(2)-O(6)</td>
<td>89.00(7)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Complex 2</th>
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</tr>
</thead>
<tbody>
<tr>
<td>Cd(1)-O(8)</td>
<td>2.251(2)</td>
<td>Cd(1)-O(2)</td>
<td>2.624(3)</td>
</tr>
<tr>
<td>Cd(1)-O(1)</td>
<td>2.287(3)</td>
<td>Cd(1)-O(7)</td>
<td>2.337(2)</td>
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<tr>
<td>O(1)-Cd(1)-O(7)</td>
<td>167.67(10)</td>
<td>O(1)-Cd(1)-O(2)</td>
<td>52.83(9)</td>
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<tr>
<td>O(8)-Cd(1)-O(2)</td>
<td>80.38(9)</td>
<td>O(7)-Cd(1)-O(2)</td>
<td>138.91(9)</td>
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<table>
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<tr>
<th>Complex 3</th>
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</thead>
<tbody>
<tr>
<td>Pb(2) - O(5)</td>
<td>2.479(4)</td>
<td>Pb(2) - O(1)</td>
<td>2.737(6)</td>
</tr>
<tr>
<td>Pb(1)-O(2)</td>
<td>2.555(4)</td>
<td>Pb(3)-O(7)</td>
<td>2.629(7)</td>
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<tr>
<td>O(2)-Pb(2)-O(1)</td>
<td>48.78(13)</td>
<td>O(7)-Pb(3)-O(1)</td>
<td>154.7(2)</td>
</tr>
<tr>
<td>Bond</td>
<td>Distance (Å)</td>
<td>Bond</td>
<td>Distance (Å)</td>
</tr>
<tr>
<td>-----------------------</td>
<td>--------------</td>
<td>-----------------------</td>
<td>--------------</td>
</tr>
<tr>
<td>O(2)-Pb(3)-O(7)</td>
<td>128.6(2)</td>
<td>O(4)-Pb(1)-O(7)</td>
<td>71.02(17)</td>
</tr>
</tbody>
</table>

**Complex 4**

- Cd(1)-N(1) 2.4161(2)
- Cd(1)-O(2) 2.3300(2)
- N(1)#3-Cd(1)-N(1) 68.80(8)
- O(3)-Cd(1)-O(2)#3 83.19(5)
- O(3)-Cd(1)-O(2) 100.70(5)

**Complex 5**

- Cd(2)-N(2) 2.320(8)
- Cd(1)-O(11) 2.343(6)
- Cd(1)-O(12) 2.244(6)
- Cd(3)-O(5) 2.621(7)
- Cd(3)-O(13)#4 2.176(6)

Symmetry transformations used to generate equivalent atoms:

- #1 -x+2,-y+1,-z+1
- #2 -x+1,-y,-z+1
- #3 -x+2,y,-z+3/2
- #4 -x+1,-y,-z+1
- #5 x,y+1,z

(a)
Fig. S1 Infinite Mn-O-Mn rods constructed by vertex-sharing \( \{\text{MnO}_6\} \) octahedra in complex 1. Ball-and-stick (a) and polyhedral representation (b); 3D framework of complex 1, in which each Mn-O-Mn rod is connected to six neighboring rods (c) (H atoms and C, N atoms of DMF omitted for clarity).
Fig. S2 Temperature dependence of $\chi_M^{-1}$ for complex 1, the red solid line corresponds to the Curie–Weiss fit (a); $\chi_M$ and $\chi_M T$ vs T plots (b).
Fig. S3 Infinite Cd-O-Cd rods constructed by vertex-sharing \{CdO\_7\} pentagonal bipyramids in complex 2 (a); 2D framework of complex 2, in which each rod is connected to two neighboring rods (b) (H atoms omitted for clarity).
Fig. S4 Infinite Pb-O-Pb rods constructed by edge-sharing \{PbO_6\} polyhedra in complex 3 (a); 3D framework of complex 3, in which each Pb-O-Pb rod is connected to four neighboring rods (b) (H atoms and C, N atoms of DMF omitted for clarity).
Fig. S5 Infinite Cd-O-C-OCd rods along c axis in complex 4 (a); the ladder SBU with the carboxylate C atoms at the vertices (b); 3D framework of complex 4, in which each
ladder SBU is connected to four neighboring ladder SBUs through the vertices of C atoms linked together by the \(-\text{CH}_2\text{-O-C}_{10}\text{H}_6\text{-O-CH}_2\) moities of \(L^2\) \(c\); Schematic illustrating the sra topology of complex 4 \(d\) (H atoms, C and H atoms of phen omitted for clarity).
Fig. S6 Infinite rods along \(a\) axis, which is constructed by \(\{\text{CdN}_2\text{O}_4\}\) polyhedra and edge-sharing \(\{\text{CdO}_6\}\) octahedra in complex 5, ball-and-stick (a) and polyhedral representation (b); 3D framework of complex 5, in which each rod is connected to six neighboring rods (c) (H atoms, C and H atoms of 2,2’-bpy omitted for clarity).
Fig.S7 The PXRD patterns of complexes 1 (a), 2 (b), 3 (c), 4 (d) and 5 (e).

(a)
Fig. S8 Thermogravimetric carves of complexes 1 (a), 2 (b), 3 (c), 4 (d) and 5 (e).
**Fig. S9** UV-vis absorption spectra at room temperature for the free organic ligands and complexes 1-5.

**Fig. S10** Solid-state emission spectra at room temperature for the free $\text{H}_2\text{L}$, phen,
2,2’-bpy and complexes 2-5.

**Fig. S11** The diffuse reflectance spectra of the pure ligands H$_2$L, phen, 2,2’-bpy and complexes 1-5 in Kubelka–Munk units. F(R) is the Kubelka–Munk function, where

\[ F(R) = \frac{(1-R)^2}{2R} \]

\( R \) is the experimentally observed reflectance.

The formula for the calculation of band gap is as follows:

\[
\text{Band Gap energy} = \frac{hc}{\lambda} = \frac{1240}{\lambda} \text{ eV}
\]

\( h = \) planks constant = \( 6.626 \times 10^{-34} \) Joules \( \cdot \) sec

\( c = \) Speed of light = \( 3.0 \times 10^8 \) meter/sec

\( \lambda = \) cut off wavelength (nm)

where 1eV = \( 1.6 \times 10^{-19} \) Joules (conversion factor)
λ, the cut off wavelength, is obtained according to the diffuse reflectance spectrum \{F(R)\} vs. wavelength, \(F(R) = (1-R)^2/2R\), \(R\) is the experimentally observed reflectance.

Fig. S12 The apparatus for photocatalysis
Fig. S13 Changes in $C_t/C_0$ plot of MO solutions ($1.5 \times 10^{-5}$ mol·L$^{-1}$) versus reaction time in the absence and presence of 25 mg free organic ligands (a) or complexes 2–5 (b).