Electric Supplemental Information for:

**Coexistence of Interconnected and Interweaved Double Helixes in an Octamolybdate-based Compound: Synthesis, Structure, and Photocatalytic Properties†**

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**Table S1** Summarization of known double helical compounds based on POMs towards a specific disposition in I and/or II types.

<table>
<thead>
<tr>
<th>Compounds and structures</th>
<th>types</th>
<th>References</th>
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<tbody>
<tr>
<td>[Cu₂Mo₂O₈(4,4-bpy)]ₙ·3nH₂O</td>
<td>I</td>
<td><em>Lu et al.</em> <em>Chem. Commun.</em> 2002, 152–153</td>
</tr>
<tr>
<td>[NH₄][Mo₂O₄Gd(H₂O)₆(L-CH₂OH)₂]·4H₂O</td>
<td>I</td>
<td><em>Lu et al.</em> <em>Chem. Commun.</em> 2003, 1284–1285</td>
</tr>
<tr>
<td>{A[Mo₂²⁺ⅢLnⅢ(H₂O)₆(C₄H₂O₆)₂]·4H₂O}ₙ</td>
<td>I</td>
<td><em>Lu et al.</em> <em>Dalton Trans.</em> 2003, 3192–3198</td>
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<tr>
<td>Structure</td>
<td>Reference</td>
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<tr>
<td><img src="image3" alt="Structure 3" /></td>
<td>Yan et al. <em>Dalton Trans.</em> 2013, 42, 7803–7809</td>
<td></td>
</tr>
<tr>
<td><img src="image4" alt="Structure 4" /></td>
<td>Yan et al. <em>Chem. Asian J.</em> 2013, 8, 2254–2261</td>
<td></td>
</tr>
</tbody>
</table>

1. \([\text{Ni(phen)}H_2O][\text{V}_2O_6]\)
2. \([(\text{C}_6\text{H}_5\text{NO}_2)\text{Ln(H}_2\text{O})_3][\text{H}_2\text{W}_{12}\text{O}_{40}]\cdot\text{nH}_2\text{O}\)
3. \(\text{Na}[\text{Ag}_6(\text{pyttz})(\text{H}_2\text{O})][\text{PMo}_{12}\text{O}_{40}]\)
4. \(\text{K}[\text{Ag}_{14}(\text{pyttz})_4(\text{H}_2\text{O})_4][\text{HSiW}_{12}\text{O}_{40}]\cdot\text{H}_2\text{O}\)
5. \(\text{K}[\text{Ag}_{14}(\text{pyttz})_4(\text{H}_2\text{O})_2][\text{PW}_{12}\text{O}_{40}]_2\cdot(\text{OH})\cdot\text{5H}_2\text{O}\)
6. \([\text{Co(bimb)}\text{V}_2\text{O}_6]\)
<table>
<thead>
<tr>
<th>Complex</th>
<th>Reference</th>
</tr>
</thead>
</table>
| $[(\text{CH}_3)_2\text{NH}_2]_4[V_{10}\text{O}_{10}(\text{H}_2\text{O})_2(\text{OH})_4(\text{PO}_4)_3]\cdot4\text{H}_2\text{O}$ | Haushalter and Zubieta et al.  
*Science*  
1993, 259, 1596-1599 |
| $\text{KH}_2[(\text{C}_3\text{H}_6\text{NO}_2)_4(\text{H}_2\text{O})\text{Cu}_3][\text{BW}_{12}\text{O}_{40}]\cdot5\text{H}_2\text{O}$ | Wang and Su et al.  
*Angew. Chem. Int. Ed.*  
2005, 44, 1–5 |
| $(\text{bpy})[\text{Zn}(4,4\text{-bpy})_2]_2[\text{H}_4\text{ClV}_{16}\text{O}_{38}]\cdot6\text{H}_2\text{O}$ and $(\text{bpy})[\text{Co}(4,4\text{-bpy})_2]_2[\text{H}_4\text{ClV}_{16}\text{O}_{38}]\cdot6\text{H}_2\text{O}$ | Peng et al.  
*J.Mol.Struct.*  
827, (2007), 50–55 |
| $[\text{Cu}^{\text{II}}(\text{L})_2(\text{H}_2\text{O})_2][\text{Cu}^{\text{I}}_2(\text{L})_2]_2\text{PMo}_{12}\text{O}_{40}$ | Wang and Su et al.  
*Chem. Commun.*  
2007, 4245–4247 |
| $[\text{Cu}(\text{H}_2\text{O})_2]\text{H}_2[\text{Cu}(\text{dap})_4(\text{H}_2\text{O})_2(\alpha\text{-B-GeW}_{9}\text{O}_{34})_2]$ | Yang et al.  
*Chem. Commun.*  
2008, 570–572 |
| $[\text{Co}(\text{H}_2\text{O})_6][\text{C}_3\text{H}_6\text{N}]_4[\text{CoW}_{12}\text{O}_{40}]\text{NO}_3\cdot3\text{H}_2\text{O}$ | Ali et al.  
*Polyhedron*  
2014, 68, 265–271 |
Fig. S1. View of the helical channels in I: (a) the channels formed by a pair of interweaved right- and left-handed helical chains and (b) the channels formed by a pair of interconnected right- and left-handed helical chains.

Fig. S2. Detailed view of the $\pi \cdots \pi$ interactions in the inorganic-organic supramolecular layer.
Fig. S3. The 3D topology of the network for 1. Color code: {β-Mo$_8$O$_{26}$}, purple; {Cu(H$_2$O)$_{N_2}$O$_3$} octahedron, green.

Fig. S4. IR spectrum of 1.

Fig. S5 Output of a calculated powder X-ray patterns by POWDER CELL.