Electronic Supplementary Information

Water channels and zipper structures in Schiff base-like Cu(II) and Ni(II) mononuclear complexes

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\textbf{Figure S1:} Crystal packing of 1·CHCl₃ view along the stacking direction
Figure S2: Crystal packing of 1·CHCl₃, side view
Figure S3: Crystal packing of 1·H₂O view along the stacking direction
Figure S4: Crystal packing of 1·H₂O, side view

Figure S5: Crystal packing of 1·xsolv view along the stacking direction
Figure S6: Crystal packing of 1·xsolv, side view
Figure S7: Crystal packing of 2·MeOH view along the stacking direction
Figure S8: Crystal packing of 2·MeOH, side view
Figure S9: Crystal packing of H$_2$L$_4$ view along the stacking direction
Figure S10: Crystal packing of H$_2$L$_1$, side view
Table S1: Inclination of the planar complexes with the stacking direction (vertical in the above ‘side-view’ figures); stacking distance calculated as the distance between the metal and the planes calculated through the above and below complexes within the stack; twist angles as a measure of the rotation between the pairs of complexes as depicted in Figure X of the main article (Figure repeated below this table).

<table>
<thead>
<tr>
<th></th>
<th>Inclination (°)</th>
<th>Stacking distance (Å)</th>
<th>Twist angles (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1•CHCl₃</td>
<td>75.71(3)</td>
<td>3.229 and 3.513</td>
<td>-92.0</td>
</tr>
<tr>
<td>1•H₂O</td>
<td>57.27(2)</td>
<td>3.312 and 3.440</td>
<td>-97.7</td>
</tr>
<tr>
<td>1•xsolv</td>
<td>71.66(2)</td>
<td>3.299 and 3.334</td>
<td>-89.4</td>
</tr>
<tr>
<td>2•MeOH</td>
<td>70.52(3)</td>
<td>3.317 and 3.405</td>
<td>-91.7</td>
</tr>
<tr>
<td>3</td>
<td>79.40</td>
<td>3.275 and 3.353</td>
<td>180</td>
</tr>
</tbody>
</table>

All planes are calculated though all non-hydrogen atoms of the complexes.

Fig. S11: Superposition of adjacent complexes from within a stack. Superposed by pair fitting of the central metal atoms and the primary coordination sphere of both molecules (10 pairs). Left, top view showing the similar orientation; Right, side view showing the intermolecular distance. Carbon atoms are drawn in magenta for 1•2H₂O, in cyan for 1•xsolv, in green for 1•CHCl₃ and in yellow for 2•MeOH.

Figure S12: Superposition of adjacent molecules from within a stack, carbon atoms are drawn in purple for H₂L₁ and, in green for 1•CHCl₃ (as above), left, top view and right, side view.
Figure S13. UV-Vis spectra of 1 in different solvents. The absorption maximum in the visible region shifts from 550 nm (CHCl$_3$) to 574 nm (DMSO) and 595 nm.
**Figure S14.** UV-Vis spectra of 2 in different solvents. The absorption maximum in the visible region is in the 510 – 520 nm region (shoulder) for all three solvents.

**Figure S15.** Photograph of the solution of the complexes 1 and 2 in CHCl₃, DMSO and pyridine.