Synthesis, structures, surface photovoltage and luminescent properties of two new nickel(II) carboxyphosphonates with a 3D framework structure
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Supplementary Materials

Fig. S1 The simulated XRD pattern of compound 1 (down) and experimental powder XRD pattern of compound 1 (up)

Fig. S2 The simulated XRD pattern of compound 2 (down) and experimental powder XRD pattern of compound 2 (up)
Fig. S3 The IR spectrum of compound 1.
**Fig. S4** The IR spectrum of compound 2.

**Fig. S5** The TG curve of compound 1.
Fig. S6 The TG curve of compound 2.
**Fig. S7** The X-ray powder diffraction pattern of the final product in the thermal decomposition for compound **1**.

The final product is Ni$_2$P$_2$O$_7$ (JCPDS 01–074–1604).

**Fig. S8** The X-ray powder diffraction pattern of the final product in the thermal decomposition for compound **2**.

The final product is Ni$_2$P$_2$O$_7$ (JCPDS 01–074–1604).
Fig. S9 Solid–state emission spectrum of 4,4′-bipy at room temperature.

Fig. S10 Solid–state emission spectrum of H$_2$L at room temperature.

Table S1 Selected bond angles (°) for compounds 1 and 2
<table>
<thead>
<tr>
<th>Compound</th>
<th>Bond</th>
<th>Angle</th>
<th>Bond</th>
<th>Angle</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>O(4)–Ni(1)–O(1)</td>
<td>91.18(13)</td>
<td>O(9)–Ni(2)–O(10)#3</td>
<td>90.67(14)</td>
</tr>
<tr>
<td></td>
<td>O(4)–Ni(1)–O(3)#1</td>
<td>178.45(13)</td>
<td>O(2)–Ni(2)–O(10)</td>
<td>87.69(12)</td>
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</tbody>
</table>
Symmetry transformations used to generate equivalent atoms: #1 \(-x + 1/2, -y + 3/2, -z\); #2 \(-x + 1/2, y - 1/2, -z + 1/2\); #3 \(-x + 1/2, -y + 1/2, -z\); #4 \(-x + 1/2, y + 1/2, -z + 1/2\) for 1; #1 \(-x + 1/2, y + 1/2, -z + 1/2\); #2 \(-x, y, -z + 1/2\); #3 \(-x + 1/2, y - 1/2, -z + 1/2\) for 2.

<table>
<thead>
<tr>
<th>O(8)#2–Ni(2)–N(3)</th>
<th>95.9</th>
<th>P(2)–O(4)–Ni(1)</th>
<th>114.5(3)</th>
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<tbody>
<tr>
<td>N(3)#2–Ni(2)–N(3)</td>
<td>179.75(10)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\(^a\) Symmetry transformations used to generate equivalent atoms: #1 \(-x + 1/2, -y + 3/2, -z\); #2 \(-x + 1/2, y - 1/2, -z + 1/2\); #3 \(-x + 1/2, -y + 1/2, -z\); #4 \(-x + 1/2, y + 1/2, -z + 1/2\) for 1; #1 \(-x + 1/2, y + 1/2, -z + 1/2\); #2 \(-x, y, -z + 1/2\); #3 \(-x + 1/2, y - 1/2, -z + 1/2\) for 2.