Supporting Information


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Figure S1. The IR spectrum for 1.

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E-mail address: gcguo@fjirsm.ac.cn (G.-C. Guo).
Figure S2. The PXRD patterns for 1.
Colourless 1

![Diagram of Colourless 1 with bond lengths](image)

Black 1

![Diagram of Black 1 with bond lengths](image)

Figure S3. Bond lengths of [MV]$^{2+}$ of Colourless 1 and Black 1.
Yellowish 1

Figure S4. The total and partial DOS of title complex.
Table S1. The intermolecular distances (Å) between inorganic component, organic component and lattice water molecules.

<table>
<thead>
<tr>
<th></th>
<th>C...O</th>
<th>N...Cl</th>
<th>C...Cl</th>
<th>O...Cl</th>
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<tbody>
<tr>
<td><strong>Colourless 1</strong></td>
<td>C1...O1W 3.236  C9...O1W 2.881</td>
<td>N3...Cl11 3.318</td>
<td>C18...Cl1 3.410  C9...Cl3 3.336  C4...Cl4 3.368  C5...Cl4 3.412  C7...Cl4 3.438  C19...Cl5 3.446  C21...Cl10 3.438  C16...Cl12 3.390  C19...Cl12 3.372</td>
<td>O1W...Cl8 3.193  O2W...Cl8 3.262</td>
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<tr>
<td><strong>Yellowish 1</strong></td>
<td>C1...O1W 3.214  C9...O1W 3.013</td>
<td>N3...Cl11 3.350</td>
<td>C18...Cl1 3.403  C9...Cl3 3.299  C4...Cl4 3.367  C5...Cl4 3.396  C7...Cl4 3.440  C19...Cl5 3.447  C21...Cl10 3.420  C16...Cl12 3.405  C19...Cl12 3.394</td>
<td>O1W...Cl8 3.233  O2W...Cl8 3.260</td>
</tr>
<tr>
<td><strong>Black 1</strong></td>
<td>C1...O1W 3.196  C9...O1W 3.006</td>
<td>N3...Cl11 3.341</td>
<td>C18...Cl1 3.425  C9...Cl3 3.295  C4...Cl4 3.357  C5...Cl4 3.394  C7...Cl4 3.449  C19...Cl5 3.454  C21...Cl10 3.443  C16...Cl12 3.389  C19...Cl12 3.388</td>
<td>O1W...Cl8 3.262  O2W...Cl8 3.231</td>
</tr>
</tbody>
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