Electronic Supporting Information

A dual-synthon in pyridinium chloride: formation of ladder-like and columnar motifs through hydrogen bonds and cation-π interactions

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### Table S1. Distances and angles of intermolecular hydrogen bonds in the crystal 1b.

<table>
<thead>
<tr>
<th>D-H···A(^a) (Å)</th>
<th>D···A (Å)</th>
<th>H···A (Å)</th>
<th>〈DHA (deg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>N2(^i) - H2(^i)···Cl(^i)</td>
<td>3.087(5)</td>
<td>2.218</td>
<td>169.48</td>
</tr>
<tr>
<td>C5-H1···Cl1</td>
<td>3.547(6)</td>
<td>2.726</td>
<td>145.1</td>
</tr>
<tr>
<td>C15-H15···Cl11</td>
<td>3.673(5)</td>
<td>2.804</td>
<td>152.52</td>
</tr>
<tr>
<td>N1-H1···Cl2</td>
<td>3.032(4)</td>
<td>2.201</td>
<td>157.04</td>
</tr>
<tr>
<td>C1(^ii) - H1(^ii)···Cl2</td>
<td>3.488(6)</td>
<td>2.789</td>
<td>136.28</td>
</tr>
<tr>
<td>C19(^i) - H19(^i)···Cl2</td>
<td>3.543(6)</td>
<td>2.637</td>
<td>159.82</td>
</tr>
<tr>
<td>C15(^i) - H15(^i)···Cl11</td>
<td>3.673(5)</td>
<td>2.804</td>
<td>152.52</td>
</tr>
<tr>
<td>C1-H1···Cl2(^ii)</td>
<td>3.488(6)</td>
<td>2.789</td>
<td>136.28</td>
</tr>
<tr>
<td>N1(^ii) - H1(^ii)···Cl2(^ii)</td>
<td>3.032(4)</td>
<td>2.201</td>
<td>157.04</td>
</tr>
<tr>
<td>N2-H1···Cl1(^i)</td>
<td>3.087(5)</td>
<td>2.218</td>
<td>169.48</td>
</tr>
</tbody>
</table>

\(^a\)Symmetry transformations used to generate equivalent atoms:
(i) -X+1,Y+1,Z+2; (ii) -X+2,Y+1,Z+2

### Table S2. Distances and angles of intermolecular hydrogen bonds in the crystal 1c.

<table>
<thead>
<tr>
<th>D-H···A(^a) (Å)</th>
<th>D···A (Å)</th>
<th>H···A (Å)</th>
<th>〈DHA (deg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>N2(^i) - H2(^i)···Cl(^i)</td>
<td>3.027(5)</td>
<td>2.235</td>
<td>149.69</td>
</tr>
<tr>
<td>C5-H5···Cl(^i)</td>
<td>3.416(7)</td>
<td>2.778</td>
<td>125.43</td>
</tr>
<tr>
<td>C15(^i) - H15(^i)···Cl11(^ii)</td>
<td>3.380(8)</td>
<td>2.643</td>
<td>134.82</td>
</tr>
<tr>
<td>N1-H1···Cl2(^iv)</td>
<td>3.076(5)</td>
<td>2.241</td>
<td>158.37</td>
</tr>
<tr>
<td>C12-H12···Cl2(^iv)</td>
<td>3.587(8)</td>
<td>2.673</td>
<td>161.71</td>
</tr>
<tr>
<td>N2(^i) - H2(^i)···Cl1(^i)</td>
<td>3.027(5)</td>
<td>2.235</td>
<td>149.69</td>
</tr>
<tr>
<td>C15-H15···Cl(^i)</td>
<td>3.380(8)</td>
<td>2.643</td>
<td>134.82</td>
</tr>
<tr>
<td>N12-H12···Cl2(^v)</td>
<td>3.076(5)</td>
<td>2.241</td>
<td>158.37</td>
</tr>
<tr>
<td>C19(^i) - H19(^i)···Cl2(^v)</td>
<td>3.599(8)</td>
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<tr>
<td>C1-H1···Cl2(^r)</td>
<td>3.587(8)</td>
<td>2.673</td>
<td>161.71</td>
</tr>
</tbody>
</table>

\(^a\)Symmetry transformations used to generate equivalent atoms:
(i) X+2,Y,Z; (ii) -X+3,Y+1,Z; (iii) -X+1,Y,-Z; (iv) X+1,Y,Z; (v) -X+2,Y+1,-Z
Table S3. Results of CSD search for styrylpyridinium chloride.

<table>
<thead>
<tr>
<th>Refcode</th>
<th>R</th>
<th>H2O(equiv)</th>
<th>Type</th>
<th>Column type</th>
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</thead>
<tbody>
<tr>
<td>EQOSOT1)</td>
<td>H</td>
<td>3</td>
<td>close to III</td>
<td>head-to-tail</td>
</tr>
<tr>
<td>EQOTAG1)</td>
<td>4-CF3</td>
<td>3</td>
<td>close to III</td>
<td>head-to-tail</td>
</tr>
<tr>
<td>EQOTEK1)</td>
<td>3,5-diCl</td>
<td>0</td>
<td>IV</td>
<td>head-to-head</td>
</tr>
<tr>
<td>EQOTIO1)</td>
<td>perfluoro</td>
<td>0</td>
<td>close to IV</td>
<td>head-to-head</td>
</tr>
<tr>
<td>EQOTUA1)</td>
<td>4-F</td>
<td>3</td>
<td>close to III</td>
<td>head-to-tail</td>
</tr>
<tr>
<td>EQOVEM1)</td>
<td>4-Cl</td>
<td>2</td>
<td>close to III</td>
<td>head-to-tail</td>
</tr>
<tr>
<td>EQOVOW1)</td>
<td>4-Br</td>
<td>2</td>
<td>III</td>
<td>head-to-tail</td>
</tr>
<tr>
<td>EQOWAJ1)</td>
<td>4-I</td>
<td>2</td>
<td>III</td>
<td>head-to-tail</td>
</tr>
<tr>
<td>EQOWIR1)</td>
<td>4-MeO</td>
<td>2.67+(0.33HCl)</td>
<td>close to III</td>
<td>head-to-tail</td>
</tr>
<tr>
<td>UYAPIU2)</td>
<td>H</td>
<td>2</td>
<td>III</td>
<td>head-to-tail</td>
</tr>
<tr>
<td>YINTUL3)</td>
<td>Naphthyl</td>
<td>3</td>
<td>III</td>
<td>head-to-tail</td>
</tr>
</tbody>
</table>

References

Fig. S1. Thermogravimetric analysis of 1b.

Fig. S2. Thermogravimetric analysis of 1c.
Fig. S3  Crystal structure of 2. (a) Top view of the packing structure. The 2D sheet motif contains dual-synthons, A and B. (b) Side view of the column with a head-to-head arrangement
Fig. S4  Crystal structure of 3. (a) Top view of the packing structure. The 2D sheet motif contains dual-synthons A and B. (b) Side view of the column with a head-to-tail arrangement.
Fig. S5  Crystal structure of 4. (a) Top view of the packing structure. The 2D sheet motif contains dual-synthons A and B. (b) Side view of the column with a head-to-tail arrangement.

Fig. S6  Hydrogen bonds of a chloride ion of 4
Fig. S7  Crystal structure of 5. (a) Top view of the packing structure. The 2D sheet motif contains dual-synthons A and B. (b) Side view of the column with a head-to-tail arrangement.