Supporting information

Table A1. Overview of all existing and seven energetically feasible hypothetical clathrasil structures with six-rings as largest accessible opening.

<table>
<thead>
<tr>
<th>Structure</th>
<th>Code</th>
<th>Packing a</th>
<th>Status</th>
<th>Tiling type c</th>
<th>ΔHf [kJ/mol SiO2] d</th>
<th>Density [kg/m³]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Afghanite</td>
<td>AFG</td>
<td>(4^6^6)(4^6^6)</td>
<td>Existing</td>
<td>ST</td>
<td>12.9</td>
<td>1791</td>
</tr>
<tr>
<td>AlPO4-16</td>
<td>AST</td>
<td>(4^6^6^1^2^1)(4^6^1)</td>
<td>Existing</td>
<td>ST</td>
<td>15.8</td>
<td>1750</td>
</tr>
<tr>
<td>Dodecasil 1H</td>
<td>DOH</td>
<td>(5^1^2^6^6)(4^5^6^8)(5^1^2^6^6)</td>
<td>Existing</td>
<td>ST</td>
<td>13.4</td>
<td>1780</td>
</tr>
<tr>
<td>Franzinite</td>
<td>FRA</td>
<td>(4^6^6^1^1^1)(4^6^1)(4^6^6)</td>
<td>Existing</td>
<td>ST</td>
<td>13.2</td>
<td>1747</td>
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<tr>
<td>Giuseppettite</td>
<td>GIU</td>
<td>(4^6^6^1^1^1)(4^6^1)(4^6^6)</td>
<td>Existing</td>
<td>ST</td>
<td>12.9</td>
<td>1789</td>
</tr>
<tr>
<td>Liottite</td>
<td>LIO</td>
<td>(4^6^6^1^1^1)(4^6^6^1^1)(4^6^6)</td>
<td>Existing</td>
<td>ST</td>
<td>13.7</td>
<td>1743</td>
</tr>
<tr>
<td>Losod</td>
<td>LOS</td>
<td>(4^6^6)(4^6^6^1^1^1)</td>
<td>Existing</td>
<td>ST</td>
<td>13.1</td>
<td>1785</td>
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<tr>
<td>Linde Type N</td>
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<td>(4^6^6^1^1^1)(4^6^6^8^8)(4^6^6^8^8)(4^6^6^8^8)(4^6^6^8^8)</td>
<td>Existing</td>
<td>ST</td>
<td>14.7</td>
<td>1707</td>
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<tr>
<td>Marinellite</td>
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<td>(4^6^6^1^1^1)(4^6^6)(4^6^6)</td>
<td>Existing</td>
<td>ST</td>
<td>13.0</td>
<td>1786</td>
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<tr>
<td>Melanophlogite</td>
<td>MEP</td>
<td>(5^1^2^6^6^6)(5^1^2^6^6^6)</td>
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<td>ST</td>
<td>12.0</td>
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<td>MCM-61</td>
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<td>(6^1^1^2^6^6^6)(4^6^6^6^1^1)(4^6^6^6^1^1)</td>
<td>Existing</td>
<td>NST</td>
<td>11.8</td>
<td>1858</td>
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<tr>
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<td>MTN</td>
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<td>ST</td>
<td>14.9</td>
<td>1795</td>
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<td>NON</td>
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<td>Existing</td>
<td>NST</td>
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<td>ST</td>
<td>12.2</td>
<td>1824</td>
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<td>ST</td>
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<td>1793</td>
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<tr>
<td>Sodalite</td>
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<td>ST</td>
<td>12.9</td>
<td>1777</td>
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<tr>
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<td>UOZ</td>
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<td>1951</td>
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<tr>
<td>-</td>
<td>Dt2_106</td>
<td>(4^6^6^1^1^1)(4^6^6^6^8)(4^6^6^6^8)</td>
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<td>ST</td>
<td>13.0</td>
<td>1782</td>
</tr>
<tr>
<td>-</td>
<td>Dt2_113</td>
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<tr>
<td>-</td>
<td>Dt3_898</td>
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<td>Hypothetical</td>
<td>ST</td>
<td>13.3</td>
<td>1766</td>
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</tbody>
</table>

a Each cage type has its own description in between the brackets and the ratio between the different cage types is given by the superscripts outside the brackets. In between brackets the ring types (normal text) and their occurrence (superscript) in a cage type are given.

b The eight-ring in these structures are so-called internal eight-rings, i.e., it is not possible to access the crystals via these rings.

c An explanation of tiling type can be found in results and discussion.

d The heat of formation is given relative to that of quartz, being -12417.6 kJ/mol SiO₂. See Computational methodology section for calculation details.
Table A2. Overview of the tile volumes of the cages of all existing and hypothetical ST clathrasils.

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<th>Existing clathrasils</th>
<th>Hypothetical clathrasils</th>
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<td>Cage</td>
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<td>AFG</td>
<td>(4(^6))</td>
</tr>
<tr>
<td>AFG</td>
<td>(4(^6))</td>
</tr>
<tr>
<td>AST</td>
<td>(4(^6))</td>
</tr>
<tr>
<td>AST</td>
<td>(4(^6))</td>
</tr>
<tr>
<td>DOH</td>
<td>(5(^12)(^6))</td>
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<tr>
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<td>(5(^12))</td>
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<tr>
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<tr>
<td>FRA</td>
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</table>