Chiral silicate zeolites

Chaim Dryzun, Yitzchak Mastai, Ayelet Shvalb and David Avnir

1 Institute of Chemistry and the Lise Meitner Minerva Center for Computational Quantum Chemistry, The Hebrew University of Jerusalem, Jerusalem 91904, Israel; 2 Department of Chemistry, Bar-Ilan University, Ramat Gan 52900, Israel

Supplementary Information

1. Error estimation

Detailed chirality analysis of all of the building blocks of Goosecreekite are provided in Table 1S, which is discussed in the main text. We also provide the error estimations in the values of the symmetry/chirality measures, following the methodology, which is described in detail in ref. 2. It is based on the uncertainty in the atoms location, which originates from the (limited) number of reflections, and from the thermal factor. There are two situations: When the symmetry distortion is large ($S>>0$; highly chiral) one gets a new corrected $S$ and an error bar with limits, $S_{\text{max}}$ and $S_{\text{min}}$, which are not equally spaced around the corrected $S$, and which depend on the accuracy level chosen by the user. When the symmetry measure is very close to zero (very low chirality level), $S_{\text{min}}$ must be zero, because the lower limit is the (fully) symmetric (achiral) object. In this case the corrected value of $S$ will be zero, with an upper bound, $S_{\text{max}} = S_{\text{bound}}$. Note that the corrected value will be always somewhat smaller than the original value, as in the case just discussed.

2. The nearest achiral structure

A useful feature of the CCM approach is that it can also display how does the nearest achiral structure looks like. That structure has no chemical meaning; it is a mathematical construct that helps visualize the distance from achirality. Fig. 1S shows these hypothetical structures for a number of Goosecreekite's (GOO) building blocks.
Figure 1S. The nearest achiral objects of Goosecreekite's building blocks. Left: The original structures. Right: The mathematical constructs which are the nearest achiral structures. (a) The highly chiral AU (the mirror plane is perpendicular to the plane of the paper). (b) The Al(1)Si$_4$ (S=2.05; the mirror plane is near the plane of the paper). (c) The most chiral SBU=8 (S=3.08; the mirror plane is the plane of the paper).

3. Heat of dissolution of histidine

The heat of dissolution of the enantiomers of histidine in pure water is shown in Fig. 2S. Very low energy liberations have been recorded for both, near the limit of instrument sensitivity.
Fig. 2S. Heats of dissolution of D-histidine (red) compared to L-histidine injection of pure water (black).

4. References for Table 1 of the main text

<table>
<thead>
<tr>
<th></th>
<th>Zeolite</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Goosecreekite (GOO)</td>
<td>1</td>
</tr>
<tr>
<td>2.</td>
<td>Nabesite (NAB)</td>
<td>3</td>
</tr>
<tr>
<td>3.</td>
<td>Bikitaite (BIK)</td>
<td>4</td>
</tr>
<tr>
<td>4.</td>
<td>Gismondine (GIS)</td>
<td>5</td>
</tr>
<tr>
<td>5.</td>
<td>Franzinite (FRA)</td>
<td>6</td>
</tr>
<tr>
<td>6.</td>
<td>Epistilbite (EPI)</td>
<td>7</td>
</tr>
<tr>
<td>7.</td>
<td>Amicite (GIS)</td>
<td>8</td>
</tr>
<tr>
<td>8.</td>
<td>Laumontite (LAU)</td>
<td>9</td>
</tr>
<tr>
<td>9.</td>
<td>Edingtonite 10 (EDI)</td>
<td>10</td>
</tr>
<tr>
<td>10.</td>
<td>RUB 23</td>
<td>11</td>
</tr>
</tbody>
</table>
### 11. SSZ-55 (ATS)  
### 12. H-ZSM-5 (MFI)  
### 13. Zeolite N (EDI)  
### 14. Zeolite F (EDI)  
### 15. ZSM – 23 (MTT)  
### 16. GUS 1 (GON)  
### 17. LTQ (BPH)  
### 18. LTA (LTA)  
### 19. ZYT 6 (CHA)  
### 20. ERS 12  
### 21. RUB 10 (RUT)

#### References for the Supplementary Material


