High-Silica, Heulandite-Type Zeolites Prepared by Direct Synthesis and Topotactic Condensation

Joel E. Schmidt\textsuperscript{a}, Dan Xie\textsuperscript{b} and Mark E. Davis\textsuperscript{a*}

\textsuperscript{a}Chemical Engineering, California Institute of Technology, Pasadena, CA 91125, USA. Email: mdavis@cheme.caltech.edu
\textsuperscript{b}Chevron Energy Technology Company, Richmond, CA 94802, USA.

Deconvolution of CIT-8 $^{29}\text{Si}$ MAS NMR.

\begin{table}[h]
\begin{tabular}{|c|c|c|}
\hline
Peak location & Normalized Area & Coordination \\
\hline
-113.78 & 1.00 & Si(OSi)$_4$ \\
\hline
-108.24 & 0.54 & Si(OAl)(OSi)$_3$ \\
\hline
-102.68 & 0.15 & Si(OAl)(OSi)$_3$ \\
\hline
\end{tabular}
\end{table}

The Si/Al ratio was found to be 9.8.
Deconvolution of the CIT-8 \(^{29}\)Si MAS NMR including a \(\text{Si(Al)}_2\text{(OSi)}_2\) resonance that was found to be insignificant

<table>
<thead>
<tr>
<th>Peak location</th>
<th>Normalized Area</th>
<th>Coordination</th>
</tr>
</thead>
<tbody>
<tr>
<td>-113.78</td>
<td>1.00</td>
<td>(\text{Si(OSi)}_4)</td>
</tr>
<tr>
<td>-108.23</td>
<td>0.545</td>
<td>(\text{Si(Al)(OSi)}_3)</td>
</tr>
<tr>
<td>-102.63</td>
<td>0.147</td>
<td>(\text{Si(Al)(OSi)}_3)</td>
</tr>
<tr>
<td>-96.644</td>
<td>0.007</td>
<td>(\text{Si(Al)}_2\text{(OSi)}_2)</td>
</tr>
</tbody>
</table>

The Si/Al ratio was found to be 9.8.
Silanol Calculation

There are 5 crystallographic unique T sites in HEU. T-2 atoms are the only ones exposed to the surface of the layer. The multiplicity of the 5 unique T atoms are:

- $T_1 = 8$
- $T_2 = 8$
- $T_3 = 8$
- $T_4 = 8$
- $T_5 = 4$

So, ideally, there are $\frac{T_2}{(T_1+T_2+T_3+T_4+T_5)} = \frac{8}{36} = 22.22\%$ silicon atoms as silanols.