Further Considerations about the Structure of n-Propyle Alcohol by Electron Diffraction

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The experimental results showed that the molecule of n-propyle alcohol possesses a trans-configuration.1 In this paper further theoretical models are calculated for this configuration. The atomic distances considered for the calculation are given in the following table:

<table>
<thead>
<tr>
<th>Atomic distance in Å</th>
<th>Model Nr.</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1C2</td>
<td>1.56 1.54 1.53 1.52 1.52 1.56 1.54 1.53</td>
</tr>
<tr>
<td>C2C3</td>
<td>1.54 1.52 1.51 1.52 1.51 1.50 1.54 1.52 1.51</td>
</tr>
<tr>
<td>C30</td>
<td>1.42 1.42 1.42 1.42 1.42 1.42 1.41 1.41 1.41</td>
</tr>
<tr>
<td></td>
<td>10 11 12 13 14 15 16 17 18</td>
</tr>
<tr>
<td>C1C2</td>
<td>1.52 1.52 1.52 1.56 1.56 1.56 1.55 1.55 1.55</td>
</tr>
<tr>
<td>C2C3</td>
<td>1.52 1.51 1.50 1.56 1.55 1.54 1.55 1.54 1.53</td>
</tr>
<tr>
<td>C30</td>
<td>1.41 1.41 1.41 1.40 1.40 1.40 1.40 1.40 1.40</td>
</tr>
<tr>
<td></td>
<td>19 20 21 22 23 24 25 26 27</td>
</tr>
<tr>
<td>C1C2</td>
<td>1.54 1.54 1.54 1.53 1.53 1.53 1.52 1.52 1.52</td>
</tr>
<tr>
<td>C2C3</td>
<td>1.54 1.53 1.52 1.53 1.52 1.51 1.52 1.51 1.50</td>
</tr>
<tr>
<td>C30</td>
<td>1.40 1.40 1.40 1.40 1.40 1.40 1.40 1.40 1.40</td>
</tr>
</tbody>
</table>

Table 1. Atomic distances in theoretical models.

All these 27 models have the following common values:

\[
\begin{align*}
\text{CH} &= 1.09 \, \text{Å}, \\
\text{OH} &= 0.937 \, \text{Å}, \\
\angle \text{COH} &= 109° 28' 16''
\end{align*}
\]

A second group of 27 models were calculated with the same parameters mentioned above. They differ only from the above 27 models in the value of the angle \( \angle \text{C3OH} \). A third group of 27 models were also calculated with variable parameters for CH, OH and the angle \( \angle \text{C3OH} \) depending on the angle \( \angle \text{C3OH} \) being 105° 56' instead of 102°.

It has been found that the theoretical models with the \( \angle \text{C3OH} = 105° 56' \) have in general \( Q \)-values higher than their corresponding ones with an angle \( \angle \text{C3OH} = 102° \). Therefore the value 105° 56' for the angle \( \angle \text{C3OH} \) is more probable. The deviation of this value from that given by Smyth may be due to the fact that the periods which depend on the angle \( \angle \text{C3OH} \) form a greater percentage of the scattering power that the value for the angle \( \angle \text{C3OH} \) agrees with that obtained by Smyth.

To obtain more accurate values for the atomic distances and angles of valency, other theoretical models with variable parameters for CH, OH and the angle \( \angle \text{C3OH} \) must be calculated. Also other molecules similar to that of n-Propyle Alcohol but with more periods depending on the angle \( \angle \text{C3OH} \) must be investigated.

Results and Discussion

The theoretical \( X \)-values were obtained for each of the above mentioned models. The value of \( Q \) was calculated for each model. These values were found to lie between 31 and 107. The best model with \( Q = 31 \) is to be considered. This model has the following values for the atomic distances and angles of valency:

\[
\begin{align*}
\text{C1C2} &= 1.55 \, \text{Å}, \\
\text{C2C3} &= 1.55 \, \text{Å}, \\
\text{C30} &= 1.40 \, \text{Å}, \\
\text{CH} &= 1.09 \, \text{Å}, \\
\text{OH} &= 0.937 \, \text{Å}, \\
\angle \text{C3C3} &= \angle \text{HCH} = 109° 28' 16''
\end{align*}
\]

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1 NOUR EL DIN ABD EL AZIZ and F. ROGWOSKI, Z. Naturforschg. 19 b, 967 [1964].