THERMAL DECOMPOSITION OF ALKYLCYCLOHEXANE MIXTURES

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In petroleum refining and petrochemistry fractions with different group and fractional compositions are utilized. Regularities in the thermal decomposition of individual hydrocarbons, including stock naphthenes, have been studied previously by several authors [1,2]. Relative activity of hydrocarbons in the cyclohexane series can be determined according to Ref. [1]. Let their activity be characterized by the conversion and let the cyclohexane activity be equal to unity. Then the relative activity of its homologs can be estimated as the ratio of their conversion relative to that of cyclohexane (Table 1).

Relative activity of hydrocarbon mixtures can be determined as

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$$A_{mix} = \frac{\sum_{i=1}^{n} q_i a_i}{a_0}$$  \hspace{1cm} (1)
where $g_i$ is the molar content of the i-th component in the mixture and $a_i$ is its relative activity.

The aim of the present study was to establish the dependence between the yield of the main products of thermal decomposition of naphthene mixtures and the $A$ value.

The available literature data concerning the dependence of the yield of cracking products (mainly $H_2$, $CH_4$, $C_2H_4$) on the average molecular mass of stock material are conflicting [3,4]. It is likely that such a correlation is rather rough and does not account for the structure of initial components. For example, the yields of propylene, divinyl and higher molecular dienes in petroleum cracking are considerably dependent on the hydrocarbon structure, which was confirmed by the experimental data [2].

Since the qualitative composition of fractions is often the same [5], it is of interest to carry out experiments with the thermal decomposition of a group of hydrocarbons with different ratios of components within the group.

We have examined thermal decomposition in alkylcyclohexane mixtures prepared from the main components of this homologous series, entering into the gasoline fraction (Table 1).

Table 1
Initial composition of alkylcyclohexane mixtures (mol%)

<table>
<thead>
<tr>
<th>No.</th>
<th>Components</th>
<th>Mixture 1</th>
<th>Mixture 2</th>
<th>Relative activity of hydrocarbons estimated according to Ref.[1]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Cyclohexane</td>
<td>13.86</td>
<td>6.48</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>Methylcyclohexane</td>
<td>28.14</td>
<td>12.04</td>
<td>1.34</td>
</tr>
<tr>
<td>3</td>
<td>Dimethylcyclohexanes</td>
<td>25.05</td>
<td>15.23</td>
<td>1.44</td>
</tr>
<tr>
<td>4</td>
<td>trimethyl + methyl + ethylcyclohexanes</td>
<td>18.07</td>
<td>50.31</td>
<td>1.55</td>
</tr>
<tr>
<td>5</td>
<td>Methyl + isopropyl-cyclohexanes</td>
<td>14.88</td>
<td>19.93</td>
<td>1.65</td>
</tr>
</tbody>
</table>