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# Mathematical-Chemical Investigation of some Carboxylic Acids

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**ABSTRACT. Some carboxylic acids Mathematical-chemical investigation was carried out within the scope of quasi-ANB-matrices method. Three correlation equations were constructed and investigated. Correlations are satisfactory. Shannon's information entropies were calculated for these acids.** *© 2016 Bull. Georg. Natl. Acad. Sci.*

**Key words:** carboxylic acids, quasi-ANB-matrix, correlation equation, information entropy.

Mathematical Chemistry is modern branch of theoretical chemistry. With application of categories of higher mathematics (groups, graphs, matrices and etc) it solves the classical problem of chemistry – correlation between the structure of compound and its static and dynamic (chemical transformations) properties. Graphs theory plays very important role in mathematical chemistry [1]. Contiguity matrices of molecular graphs and their modifications are widely used in mathematical chemistry for investigation of molecules and their transformations and ANB-matrix falls into this type [2-3].

The diagonal elements of ANB-matrix are the atomic numbers of the chemical elements, nondiagonal elements are the multiplicities of the chemical bonds.

For arbitrary XYV molecule, the ANB-matrix has the form:

$$\begin{Vmatrix} Z_X & \Delta_{XY} & \Delta_{XV} \\ \Delta_{XY} & Z_Y & \Delta_{YV} \\ \Delta_{XV} & \Delta_{YV} & Z_V \end{Vmatrix}$$

where: $Z_X$, $Z_Y$ and $Z_V$ are atomic numbers of X, Y, V chemical elements; $\Delta_{XY}$, $\Delta_{XV}$, $\Delta_{YV}$ are the multiplicities of X~Y, X~V, Y~V chemical bonds.

For large molecules calculations are very labour-consuming. Thus, the modernized form of ANB-matrix – quasi-ANB-matrix ( $A\tilde{N}B$ ) was elaborated. Its diagonal elements are the sums of the atomic numbers of those chemical elements, which the structural fragments of the molecule contain; nondiagonal elements represent multiplicities of the chemical bonds between the structural fragments. Thus, $A\tilde{N}B$ -ma-

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**Table. lg($\Delta_{A\tilde{N}B}$),$T_{boil.}$, $d_4^{20}$, $S_{298}^0$ and $H_S$ for carboxylic acids**

| Carboxylic acids | lg($\Delta_{A\tilde{N}B}$) | $T_{boil.}$, $^0$C | $d_4^{20}$ | $S_{298}^0$, cal/(mole·K) | $H_S$ |
|---|---|---|---|---|---|
| $CH_3COOH$ | 2.31 | 118.1 | 1.049 | 38.20 | 1.5000 |
| $C_2H_5COOH$ | 2.56 | 141.1 | 0.992 | (40.80) | 1.4360 |
| $C_3H_7COOH$ | 2.76 | 163.5 | 0.959 | 54.1 | 1.370 |
| $C_4H_9COOH$ | 2.88 | 187.0 | 0.942 | 62.1 | 1.3319 |
| $C_5H_{11}COOH$ | 2.96 | 205.0 | 0.929 | (67.4) | 1.2955 |

trix is constructed on the basis of the molecular model. Decimal logarithm of the value of the determinant of $A\tilde{N}B$ -matrix is effective topologic index for construction of the correlation equations of „structure-properties" type.

Carboxylic acids were investigated within the scope of $A\tilde{N}B$ -matrices method. The simplest model was elaborated for them:

$$R-Y$$

where: $R \equiv CH_3, C_2H_5, C_3H_7 \ldots$; $Y \equiv COOH$.

Corresponding $A\tilde{N}B$ -matrix has the form:

$$\begin{Vmatrix} Z_X & 1 \\ 1 & Z_Y \end{Vmatrix}$$

In the table the values of lg($\Delta_{A\tilde{N}B}$), $T_{boil.}$, $d_4^{20}$ [4], $S_{298}^0$ [5] and $H_S$ are represented for these acids.

Three correlation equations were constructed on computer:

$$T_{boil.} = 1.597 \cdot \lg(\Delta_{A\tilde{N}B}) - 267.7$$

$$d_4^{20} = -0.157 \cdot \lg(\Delta_{A\tilde{N}B}) + 1.394$$

$$S_{298}^0 = 66.7 \cdot \lg(\Delta_{A\tilde{N}B}) - 130.0$$

The correlations coefficient ***r*** is respectively equal to 0,981; 0,980; 0,983. Thus, in accordance with Jaffe's criterion [6], correlations are satisfactory. The values of $S_{298}^0$ for $C_2H_5COOH$ and $C_5H_{11}COOH$ are calculated theoretically, on the basis of corresponding correlation equation.

Shannon's information entropy is calculated by formula [7]:

$$H_S = -\sum p_i \log_2 p_i$$

where: $\mathbf{p_i}$ is the ability of some event (for example, to „choose" **c**-atom in the molecule).

For this acids the values of $\mathbf{H_S}$ were calculated and they are represented in the Table.

*ორგანული და არაორგანული ქიმია*

# ზოგიერთი კარბონმჟავას მათემატიკურ-ქიმიური გამოკვლევა

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