საქართველოს მეცნიერებათა ეროვნული აკადემიის მოამბე, ტ. 10, №1, 2016
BULLETIN OF THE GEORGIAN NATIONAL ACADEMY OF SCIENCES, vol. 10, no. 1, 2016

Organic Chemistry

Mathematical-Chemical Investigation of some Straight-Chained Monohydric Alcohols

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ABSTRACT. Mathematical-chemical investigation of some straight-chained monohydric alcohols was carried out within the scope of ANB-and quasi-ANB-matrices methods. Four correlation equations of „structure-properties" type were constructed. Two correlations are good, two – satisfactory.

Key words: monohydric alcohols, ANB- and quasi-ANB-matrices, correlation equation

Contiguity matrices of molecular graphs and their various modifications are widely used in mathematical chemistry for investigation of molecules (chemical statics) and their transformations (chemical dynamics) and ANB- and quasi-ANB-matrices ($A\tilde{N}B$) fall into their type [1,2].

The diagonal elements of ANB-matrix represent atomic numbers of the chemical elements, which the molecule contains. 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; Δ_{XY}, Δ_{XV}, Δ_{YV} are the multiplicities of X~Y, X~V, Y~V chemical bonds.

For large molecules the calculations on the basis of ANB-matrices are rather labour-consuming, thus the modernized form of ANB-matrices – quasi-ANB-matrix ($A\tilde{N}B$) was elaborated. Its diagonal elements are the atomic numbers of chemical elements, which some structural fragments of the molecule contain; nondiagonal elements are the multiplicities of the chemical bonds between the structural fragments. Thus, $A\tilde{N}B$ -matrices are constructed on the basis of molecular models.

Straight-chained monohydric alcohols were investigated within the scope of ANB- and $A\tilde{N}B$ -matrices methods. The simplest model was elaborated for these alcohols:

$$R - X,$$

where $R = CH_3, C_2H_5, C_3H_7 \ldots$ $X = OH$.

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

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

In the Table the data $\lg(\Delta_{ANB})$, $\lg(\Delta_{A\tilde{N}B})$, $T_{boil.}$ and S^0_{298} are represented for some straight-chained monohydric alcohols [3].

Table. $\lg(D_{ANB})$, $\lg(\Delta_{A\tilde{N}B})$, $T_{boil.}$ and S^0_{298} for straight-chained monohydric alcohols

alcohol	$\lg(\Delta_{ANB})$	$\lg(\Delta_{A\tilde{N}B})$	$T_{boil.}$, ^0C	S^0_{298}, eu
CH_3OH	1.30	1.90	64.72	57.29
C_2H_5OH	1.87	2.18	78.32	67.54
C_3H_7OH	2.44	2.35	97.17	77.59
C_4H_9OH	3.01	2.47	117.7	86.90

Four correlation equations were constructed on computer:

$$T_{boil.} = 34.51 \cdot \lg(\Delta_{ANB}) + 13.77$$

$$S^0_{298} = 16.91 \cdot \lg(\Delta_{ANB}) + 35.92$$

$$T_{boil.} = 135.86 \cdot \lg(\Delta_{A\tilde{N}B}) - 217.9$$

$$S^0_{298} = 66.76 \cdot \lg(\Delta_{A\tilde{N}B}) - 78.01$$

The correlations coefficient ***r*** is respectively equal to 0.992; 0.993; 0.982; 0.984. Thus, in accordance with Jaffe's criterion [4], the first two correlations are good, the third and fourth – satisfactory.

Thus, $\lg(\Delta_{ANB})$ and $\lg(\Delta_{A\tilde{N}B})$ are effective topological indexes for construction of correlation equation „structure-properties" type.

ორგანული ქიმია

ზოგიერთი ნორმალურჯაჭვიანი ერთატომიანი სპირტის მათემატიკურ-ქიმიური გამოკვლევა

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ი. ჯავახიშვილის სახელობის თბილისის სახელმწიფო უნივერსიტეტი

(წარმოდგენილია აკადემიის წევრის შ. სამსონიას მიერ)

ჩატარებულია ზოგიერთი ნორმალურჯაჭვიანი ერთატომიანი სპირტის მათემატიკურ-ქიმიური გამოკვლევა ანბ- და კვაზი-ანბ-მატრიცების მეთოდის გამოყენებით. აგებულია ,,აღნაგობა-თვისებების" ტიპის ოთხი კორელაციური განტოლება. გამოთვლებმა აჩვენა, რომ პირველი ორი კორელაცია კარგია, ბოლო ორი – დამაკმაყოფილებელი.

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Received January, 2016