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Mathematical-Chemical Investigation of some Straight-Chained Alkanes

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ABSTRACT. Mathematical-chemical investigation of some straight-chained alkanes was carried out within the scope of the quasi-ANB-matrices method. Two correlation equations of "structure- properties" type were constructed. The correlations are satisfactory. *© 2011 Bull. Georg. Natl. Acad. Sci.*

Key words: *straight-chained alkanes, quasi-ANB-matrix, correlation equations.*

Mathematical chemistry often operates with contiguity matrices of molecular graphs and their various modifications and ANB-matrix falls into this type [1-2].

The diagonal elements of ANB-matrix represent atomic numbers of the chemical elements, nondiagonal elements – the multiplicities of the chemical bonds. For arbitrary XYV molecule ANB-matrix has the form:

$$\begin{Vmatrix} Zx & \Delta xy & \Delta xv \\ \Delta xy & Zy & \Delta yv \\ \Delta xy & \Delta yv & Zv \end{Vmatrix} \qquad (1)$$

where: Zx, Zy, Zv are atomic numbers of X , Y , V chemical elements; Äxy, Äxv, Äyv 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-matrix – quasi-ANB-matrix (AÑB) was elaborated. Its diagonal elements are the sums of the atomic numbers of those chemical whase elements contain the structural fragments of the molecule. Nondiagonal elements are the multiplicities of the chemical bonds between these structural fragments.

Straight-chained alkanes [3] ere investigated within the scope of the AÑB matrices method.

The simplest model was elaborated for them:

$$X - Y \qquad (2)$$

Table

$\lg(\Delta_{A\tilde{N}B})$, – $\varepsilon^{calc}_{LOMO}$ and $I_1^{\exp}$, for straight-chained alkanes

Alkane	$\lg(\Delta_{A\tilde{N}B})$	$\varepsilon^{calc}_{LOMO}$, eV	$I_1^{\exp}$, eV
C_2H_6	1.90	12.21	11.76
C_3H_8	2.18	11.22	11.21
C_4H1_0	2.35	10.72	10.80
C_5H_{12}	2.47	10.55	10.55
C_6H_{14}	2.57	10.41	10.43
C_7H_{10}	2.64	10.33	10.35
C_8H_{18}	2.71	10.25	10.24
*C_9H_{20}	2.77	(10.22)	(10.22)
$C_{10}H_{22}$	2.82	10.19	10.19
**$C_{11}H_{24}$	2.86	(9.95)	(9.97)

* The data for C_9H_{20} and $C_{11}H_{24}$ were calculated on the basis of the correlation equations (4) and (5).

where: X = CH_3, Y = CH_3, C_2H_5, C_3H_7, . . .

The corresponding AÑB -matrix has the form:

$$\begin{Vmatrix} Zx & 1 \\ 1 & Zy \end{Vmatrix} \qquad (3)$$

The data of $\lg(\Delta_{A\tilde{N}B})$, $-\varepsilon_{LOMO}^{calc}$ and $I_1^{\exp}$, the first ionization potential for the compounds [3] are represented in the Table.

Two correlation equations were constructed on computer:

$$-\varepsilon = -2.18\lg(\Delta_{A\tilde{N}B}) + 16.08 \qquad (4)$$

$$I_1 = -1.78\lg(\Delta_{A\tilde{N}B}) + 15.06 \qquad (5)$$

The correlation coefficient r is respectively equal to: 0.966; 0.987. Thus, in accordance with Jaffe's criterion [4], correlations are satisfactory.

არაორგანული ქიმია

ზოგიერთი ნორმალურჯაჭვიანი ალკანის მათემატიკურ-ქიმიური გამოკვლევა

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