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Mathematical-Chemical Investigation of some Straight-Chained Alkyl Mono-Halides

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ABSTRACT. Mathematical-chemical investigation of some straight-chained alkyl monohalides was carried out within the scope of the pseudo-ANB-matrices method. Six correlation equations of "structure-properties" type were constructed. Correlations are satisfactory. © *2011 Bull. Georg. Natl. Acad. Sci.*

Key words: *alkyl monohalides, pseudo-ANB-matrix, correlation equation.*

Contiguity matrices of molecular graphs and their various modifications are widely used in mathematical chemistry for investigation of molecules and their transformations and ANB-matrix falls into this type [1-2].

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

$$\begin{Vmatrix} Zx & \Delta xy & \Delta xv \\ \Delta xy & Zy & \Delta yv \\ \Delta xv & \Delta yv & Zv \end{Vmatrix},$$

where Zx, Zy, Zv are atomic numbers of X,Y,V chemical elements; Δxy, Δxv,Δyv 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 – pseudo – ANB – matrix $(\overline{ANB})$ was elaborated. Its diagonal elements are the atomic numbers of chemical elements and the sums of the atomic numbers of those chemical elements, which the structural fragments of the molecular contain. Nondiagonal elements are the multiplicities of the chemical bonds between the structural fragments.

Straight-chained alkyl monohalides [3] were investigated within the scope of $\overline{ANB}$ - matrices method. The simplest model was elaborated for them:

$$R - X,$$

where X = CI, Br, I.

Corresponding $\overline{ANB}$ - matrices have the form:

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

In the Table the data of $\lg(\Delta_{\overline{ANB}})$, $T_{boil.}$, and d_4^{20} [3] are represented for these compounds.

The correlation equations were constructed on computer.

For alkyl chlorides:

$$T_{boil.} = 243.67^{\lg(\Delta_{\overline{ANB}})} - 576.68$$

$$d_4^{20} = -0.0244^{\lg(\Delta_{\overline{ANB}})} + 0.9529$$

For alkyl bromides:

$$T_{boil.} = 232.89^{\lg(\Delta_{\overline{ANB}})} - 597.47$$

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Table

$lg(\Delta_{\overline{ANB}})$, T_{boil}, and d_4^{20} for straight-chained alkyl monohalides

R	Chloride			Bromide			Iodide		
	$lg(\Delta_{\overline{ANB}})$	$T_{boil.}$, C°	d_4^{20}	$lg(\Delta_{\overline{ANB}})$	T_{boil}, C°	d_4^{20}	$lg(\Delta_{\overline{ANB}})$	T_{boi}, C°	d_4^{20}
CH_3	2.18	-24	-	2.50	5	-	2.68	43	2.279
C_2H_5	2.46	12.5	-	2.77	38	1.446	2.95	72	1.933
C_3H_7	2.63	47	0.890	2.94	71	1.333	3.12	102	1.747
C_4H_9	2.75	78.5	0.884	3.06	102	1.276	3.24	130	1.617
C_5H_{11}	2.84	108	0.883	3.16	130	1.223	3.34	157	1.517
C_6H_{13}	2.92	134	0.882	3.23	156	1.173	3.41	180	1.441
C_7H_{25}	2.99	160	0.880	3.30	180	-	3.48	204	1.401
C_8H_{17}	3.04	185	0.879	3.36	202	-	3.54	225.5	-

$$d_4^{20} = -0.5648^{lg(\Delta_{\overline{ANB}})} + 3.0015$$

For alkyl iodides:

$$T_{boil.} = 214.95^{lg(\Delta_{\overline{ANB}})} - 552.95$$

$$d_4^{20} = -1.1063^{lg(\Delta_{\overline{ANB}})} - 5.2168$$

The correlation coefficient r is respectively equal to: 0.978; 0.973; 0.979; 0.998; 0.976; 0.998. Thus, in accordance with Jaffe's criterion [4], correlations are good.

ორგანული და არაორგანული ქიმია

ზოგიერთი ნორმალურჯაჭვიანი მონოჰალოგენალკანის მათემატიკურ-ქიმიური გამოკვლევა

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REFERENCES

1. *M. Gverdtsiteli, G. Gamziani, I. Gverdtsiteli* (1996), The Contiguity Matrices of Molecular Graphs and their Modifications. Tbilisi.
2. *K. Kupatadze, T. Lobzhanidze, M. Gverdtsiteli* (2007), Algebraic-Chemical Investigation of some Organic Molecules and their Transformations. Tbilisi.
3. *R. Morrison, P. Boyd* (1970), Organic Chemistry. Boston.
4. *M. Gverdtsiteli* (1982), Fizikur-organuli kimia [Physical Organic Chemistry]. Tbilisi (in Georgian).

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