

*Organic Chemistry*

## Algebraic-Chemical Investigation of the Correlation “Structure-Properties” for Alkyl Halides within the Scope of Quasi-ANB-Matrices Method

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**ABSTRACT.** The correlation equations “structure-boiling point” were constructed for alkyl halides within the scope of quasi-ANB-matrices method. According to Japphe’s criterion, the correlations are satisfactory. © 2007 Bull. Georg. Natl. Acad. Sci.

**Key words:** alkyl halides, quasi-ANB-matrices, correlation.

A quasi-ANB-matrix ( $\tilde{ANB}$ ) falls into the type of modified contiguity matrices of molecular graphs [1-3].  $\tilde{ANB}$ -matrices can be constructed on the basis of mo-

lecular models. Their diagonal elements are the sums of the atomic numbers of the chemical elements contained in the molecular structural fragments (such fragments are considered to be quasi-atoms). Nondiagonal elements are

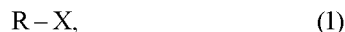
Table

Data on boiling point (Bp) for some alkyl halides

Alkyl halide (R)	bp ( $^{\circ}$ C)	Alkyl halide (R)	bp ( $^{\circ}$ C)
CH <sub>3</sub> F	-78.4	CH <sub>3</sub> Cl	-23.8
C <sub>2</sub> H <sub>5</sub> F	-37.7	C <sub>2</sub> H <sub>5</sub> Cl	13.1
C <sub>3</sub> H <sub>7</sub> F	-2.5	C <sub>3</sub> H <sub>7</sub> Cl	46.6
C <sub>4</sub> H <sub>9</sub> F	32	C <sub>4</sub> H <sub>9</sub> Cl	28.4
C <sub>5</sub> H <sub>11</sub> F	62	C <sub>5</sub> H <sub>11</sub> Cl	108.2
CH <sub>3</sub> Br	3.6	CH <sub>3</sub> I	42.5
C <sub>2</sub> H <sub>5</sub> Br	38.4	C <sub>2</sub> H <sub>5</sub> I	72
C <sub>3</sub> H <sub>7</sub> Br	70.8	C <sub>3</sub> H <sub>7</sub> I	102
C <sub>4</sub> H <sub>9</sub> Br	101	C <sub>4</sub> H <sub>9</sub> I	130
C <sub>5</sub> H <sub>11</sub> Br	129.6	C <sub>5</sub> H <sub>11</sub> I	155

the multiplicities of chemical bonds.

Alkyl halides were investigated in terms of the quasi- $\tilde{ANB}$ -matrices method. The simplest model was constructed for these molecules:



where R is an alkyl radical, X – halogen. The corresponding  $\tilde{ANB}$ -matrix has the form:

$$\begin{vmatrix} Z_R & 1 \\ 1 & Z_X \end{vmatrix}, \quad (2)$$

where  $Z_R$  is the sum of atomic numbers of the elements which the R alkyl radical contains;  $Z_X$  is the atomic number of the corresponding halogen.

The Table contains the data on boiling points (bp) for some alkyl halides [4].

The correlation equations  $bp \sim \lg(\Delta_{\tilde{ANB}})$  were constructed on computer for alkyl fluorides, alkyl chlorides, alkyl bromides and alkyl iodides and they are given below:

$$bp=209.56 \lg(\Delta_{\tilde{ANB}})-476.55 \quad (3)$$

$$bp=200.00 \lg(\Delta_{\tilde{ANB}})-459.80 \quad (4)$$

$$bp=190.91 \lg(\Delta_{\tilde{ANB}})-476.68 \quad (5)$$

$$bp=170.45 \lg(\Delta_{\tilde{ANB}})-414.30 \quad (6)$$

The correlation coefficients  $r$  respectively equal 0.981; 0.986; 0.983; 0.988. Thus, according to Japphe's criterion, the correlations are satisfactory [5].

## ორგანული ქიმია

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