

Mathematical-Chemical Investigation of some Derivatives of Bis(1H-indolo-5-yl)Methane

Nunu Tsetsadze

Faculty of Chemical Technologies and Metallurgy, Georgian Technical University, Tbilisi, Georgia

(Presented by Academy Member Shota Samsoniya)

Mathematical-chemical investigation of some derivatives of Bis(1H-indolo-5-yl)Methane was carried out within the scope of the quasi-ANB-matrices method. 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 (\overline{ANB}) was elaborated. Its diagonal elements are the sums of the atomic numbers of those chemicals whose elements contain the structural fragments of the molecule. Non-diagonal elements are the multiplicities of the chemical bonds between these structural fragments. One correlation equation of “structure-properties” type was constructed. The correlation is good. © 2021 Bull. Georg. Natl. Acad. Sci.

Bis(1H-indolo-5-yl) Methane, quasi-ANB-matrices, correlation equation

Mathematical chemistry often operates with contiguity matrices of molecular graphs and their various modifications and ANB-matrix falls into this type [1-4].

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:

$$\begin{pmatrix} Z_x & \Delta_{xy} & \Delta_{xv} \\ \Delta_{xy} & Z_y & \Delta_{yv} \\ \Delta_{xy} & \Delta_{yv} & Z_v \end{pmatrix}, \quad (1)$$

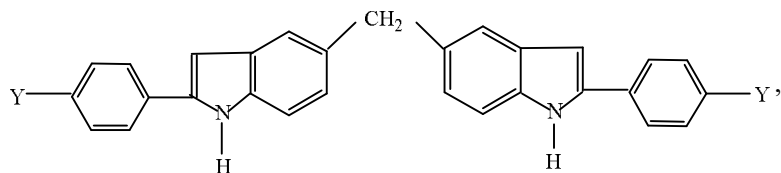
where: Z_x, Z_y, Z_v are atomic numbers of X, Y, V chemical elements; $\Delta_{xy}, \Delta_{xv}, \Delta_{yv}$ are the multiplicities of $X \sim Y, X \sim V, Y \sim V$ chemical bonds.

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 (\overline{ANB}) was elaborated. Its diagonal elements are the sums of the atomic numbers of those chemicals whose elements contain the structural fragments of the

molecule. Non-diagonal elements are the multiplicities of the chemical bonds between these structural fragments.

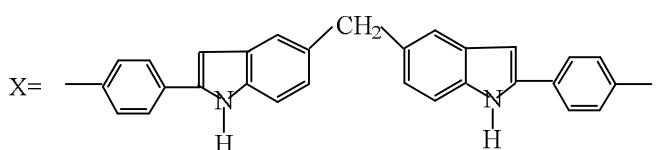
Bis(1H-indolo-5-yl) Methane [5] are investigated within the scope of (\widetilde{ANB}) matrices method.

Research substances can be described as follows:



where $Y = \text{NO}_2, \text{Br}, \text{I}$.

X is the main structural fragment of the molecule:



The simplest model was elaborated for them:



The corresponding (\widetilde{ANB}) matrix has the form:

$$\begin{vmatrix} Z_x & 1 & 1 \\ 1 & Z_y & 0 \\ 1 & 0 & Z_y \end{vmatrix} \quad (3)$$

The data of $\lg(\Delta_{\widetilde{ANB}})$ and $T_{\text{melt.}}$ for the compounds are represented in the Table.

Table. (\widetilde{ANB}) , $T_{\text{melt.}}$ Presented for three compounds

| Y | $\lg(\Delta_{\widetilde{ANB}})$ | $T_{\text{melt.}}$ |
|---------------|---------------------------------|--------------------|
| NO_2 | 5,04 | 172 |
| Br | 5,4 | 306 |
| *I | 5,7 | (418) |

*The data for I was calculated on the basis of the correlation equation (4).

One correlation equation was constructed on computer:

$$T_{\text{melt.}} = 372 \lg(\Delta_{\widetilde{ANB}}) - 1703. \quad (4)$$

The correlation coefficient r is respectively equal to 0.99. Thus, in accordance with Jaffe's criterion [6], correlations are good.

მათემატიკური ქიმია

ზოგიერთი ბის(1H-ინდოლ-5-ილ)მეთანის წარმოებულების მათემატიკურ-ქიმიური გამოკვლევა

ნ. ცეცაძე

საქართველოს ტექნიკური უნივერსიტეტი, ქიმიური ტექნოლოგიისა და მეტალურგიის ფაკულტეტი,
თბილისი, საქართველო

(წარმოდგენილია აკადემიის წევრის შ. სამსონიას მიერ)

ჩატარებულია ზოგიერთი ბის(1H-ინდოლ-5-ილ) მეთანის წარმოებულების მათემატიკურ-ქიმიური გამოკვლევა კვაზი-რნბ-მატრიცის (რნბ) მეთოდის ფარგლებში. აგებულია „აღნაგობათვისებები“-ს ტიპის კორელაციის განტოლება. გამოთვლებმა აჩვენა, რომ ადგილი აქვს ბრწყინვალე კორელაციას.

REFERENCES

1. Gamzai G. (1990) Mathematical Chemistry, p. 95 (25-55) Tbilisi.
2. Sidamonidze N.N., Kupatadze K.T., Gverdtsiteli M.I. (2009) Teoreticheskoe issledovanie korreliatsii "strukturna-svoistva" v ramkakh metodov PNS-, kvazi-PNS i EP-matrits. *Applied Physics*, 6: 36-39 (in Russian).
3. Kupatadze K., Lobzhanidze T., Gverdtsiteli M. (2007) Algebraic-chemical investigation of some organic molecules and their transformations, p. 22. Tbilisi.
4. Samsoniya Sh., Chikvaidze I., Narimanidze N., Tsetsadze N. (2003) Synthesis of the new derivatives of Bis(1H-Indolo-5-yl)Methane. *Proceed. Georg. Acad. Sci.*, 29 (3-4): 222-224.

Received October, 2020