

DECIMAL LOGARITHM OF THE DETERMINANT OF
AND-MATRIX-AS EFFECTIVE TOPOLOGIC INDEX

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The contiguity matrices of molecular graphs and their various modifications are effectively used for algebraic-chemical characteristics of molecules and their transformations [1].

The diagonal elements of ANB-matrix represent the atomic numbers of chemical elements, whereas nondiagonal ones-multiplicities of chemical bonds [2]. For arbitrary ABC molecule ANB - matrix has a form:

$$ABC \begin{vmatrix} Z_A & \Delta_{AB} & \Delta_{AC} \\ \Delta_{AB} & Z_B & \Delta_{BC} \\ \Delta_{AC} & \Delta_{BC} & Z_C \end{vmatrix},$$

where Z_A , Z_B , Z_C are atomic numbers of chemical elements A , B , C ; Δ_{AB} , Δ_{AC} , Δ_{BC} represent the multiplicities of chemical bonds between A and B , A and C , B and C .

It was established that $\lg(\Delta_{ANB})$ (the decimal logarithm of the determinant of ANB-matrix) is effective topologic index and "structure-properties" type correlation equations can be constructed on its basis [3]:

$$P = a \lg(\Delta_{ANB}) + b$$

where P -is definite physical-chemical property of chemical substance, a and b are rational numbers.

R e f e r e n c e s

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