Bul. Ştiinţ. Univ. Baia Mare, Ser. B,
Matematică-Informatică, Vol. XVIII(2002), Nr. 2, 153 - 158

GRAPH MODELLING OF CHEMICAL STRUCTURES

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Abstract. In this paper we describe a mathematical model for representing chemical structures containing multiple bonds, heteroatoms and benzenoid hidrocarbons, using recently developed methods for calculating the weighted electronic distance, w.e.d. We also illustrate the power of w.e.d. in differentiating the chemical bonds according to the context in which they are found in the molecule. For the chemical structures showed here we calculate the ZEP and RZ topological indices using the weighted electronic connectivity matrix, CEP, introduced by the first author in [1].

MSC: 94C15
Key words: molecular graph, weighted electronic distance, topological index, weighted electronic connectivity matrix, correlation