

[Croatica Chemica Acta](#)

Volume 77, Issue 3, October 2004, Pages 501-508

Document Type: Conference Paper

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Valence connectivity versus Randić, Zagreb and modified Zagreb index: A linear algorithm to check discriminative properties of indices in acyclic molecular graphs
[Vukičević, D.](#)^a [Graovac, A.](#)^{b c}
^a Department of Mathematics, Faculty of Science, University of Split, Nikole Tesle 12, HR-21000 Split, Croatia^b Department of Chemistry, Faculty of Science, University of Split, Nikole Tesle 12, HR-21000 Split, Croatia^c Ruder Bošković Inst., P.O. Box 180, HR-10002 Zagreb, Croatia**Abstract**

Valence connectivity in molecular graphs is described by 10-tuples μ_{ij} where μ_{ij} denotes the number of edges connecting vertices of valences i and j . A shorter description is provided by 4-tuples containing the number of vertices and values of Randić, Zagreb and modified Zagreb indices. Surprisingly, these two descriptions are in one-to-one correspondence for all acyclic molecules of practical interest, i.e., for all those having no more than 100 atoms. This result was achieved by developing an efficient algorithm that is linear in the number of 10-tuples.

Author Keywords


Acyclic molecular graphs; Topological indices; Valence connectivity

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