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Ionization energy of nanostructures using the reciprocal randić index

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Topological indices are constant of graph, used to study quantitative structure activity relationship (QSAR) and quantitative structure Properties relationship (QSPR). In addition to mathematics, graph theory is used in physics, chemistry, pharmacology, genetics, and also some other sciences. These indices are widely used to illustrate the relationship between molecular structure and physical and chemical properties. This study aims to obtain a simple model based on graph theory to predict the Ionization Energy of phenacenes with chemical formula $C_{4n+2}H_{2n+4}$. Therefore, we first calculated the Reciprocal

Randić Index for the family. Reciprocal Randić index, $RR(G)$ is defined by $RR(G) = \sum_{ij \in E} \sqrt{d_i d_j} / \sum_{ij \in E} \sqrt{d_i}$. The Ionization Energy of phenacenes was calculated using Gaussian 09 software and the experimental data of references were compared with those mentioned in valid papers. The prediction of Ionization Energy about a very high accuracy through reciprocal Randić index, with $R^2=0.9873$. The prediction is given by: $E_{ionization} = 0.0002(RR)^2 - 0.0425(RR) + 8.787$.

Biography

Ali Asghar Khakpoor received his B. Sc. in Applied Physics from Esfahan University, Iran, M. Sc. degree in Solid state Physics from the Esfahan University in Iran and ph.d in Nano Physics at Material and Energy Research Center (MERC) in Iran. He is currently a assistant professor in Islamic Azad University- Central Tehran Branch (IAUCTB). He is a member of the Iranian Crystallography Association (ICA) and Iranian Physics Society (IPS). He has a project in TiO2 thin film as a self cleaning material and have several project in nano structures. He is interested to nano physics, thin films, quantum mechanic and mathematical physic. He has co-authored 2 books and approximately and has published over 36 publications on various aspects of atomic physics, TiO2 thin film and nano-science. He is also a lecturer at since 1993 in Iran, teaching different subject in Physics.

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