

Expected values of some molecular descriptors in random phenylene chain

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Strong connections between the chemical characteristics of chemical compounds, materials and drugs and their topological structures have been proved by lots of previous research. For instance, they get the connections in melting point and boiling point. The chemical indices from these molecular topological structures turn out to be favorable for chemists, material and medical scientists, when they try to get the relevant chemical reactivity, biological activity and physical features. As a result, the shortage of the experiments can be covered and made up, if we conduct the study of the topological indices on the molecular structures. A special class of conjugated hydrocarbons known as phenylenes, which is composed of a special arrangement of six- and four-membered rings. In particular, any two six-membered rings (hexagons) are not adjacent, and every four-membered ring(square) is adjacent to a pair of nonadjacent hexagons. If each hexagon of phenylene is adjacent only to two squares, then the obtained chain is called the phenylene chain. The main object of this talk is to determine the expected values of the sum-connectivity, harmonic, and symmetric division, variable inverse sum degree and general Randic indices for this class of conjugated hydrocarbons. The comparisons between the expected values of these indices with respect to the random phenylene chains have been determined explicitly. The graphical illustrations have been given in terms of the differences between the expected values of these indices

Keywords: phenylene chain, sum-connectivity, harmonic, and symmetric division, variable inverse sum degree and general Randic indices, expected values, comparisons.