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Topological Indices for Some New Type of Carbon Crystal

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Abstract : In QSAR/QSPR study, topological indices are used to predict the physiochemical and bioactivity of chemical compounds. A large number of such indices depend only on vertex degree of the molecular graph. In this paper, we compute few degree based topological indices for a new type of 2D Carbon Crystal prepared from 1,3,5-trihydroxy benzene and a possible 2D crystal pattern in the 4-6 carbophene family. Also, we compute the Sanskruti index for graphene and its line graph.

Keywords and phrases : Topological index; Molecular graph; Line graph; Graphene; 4-6 Carbophene family.

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Introduction : According to the IUPAC definition [21], a topological index (or molecular structure descriptor) is a numerical value associated with the chemical constitution for the correlation of chemical structure with various physical properties, chemical reactivity or biological activity. There is a strong and natural correspondence between chemical and graph theoretical notions. An atom and bond of a Molecule correspond to vertex and edge of the molecular graph. The significant correlation to topological indices and physiochemical properties of the molecules stimulate to find many topological indices based on distances between pairs of vertices and degree of a vertex. More precisely, given nonnegative numbers $\gamma(i,j)$ a vertex-degree-based topological index is expressed as

$$TI_1(G) = \sum_{1\le i\le j\le n-1} m_{ij}\gamma(i,j) \tag{1}$$

$$TI_2(G) = \prod_{1\le i\le j\le n-1} m_{ij}\mu(i,j) \tag{2}$$