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Eccentric connectivity index of molecular grapgs of chemical trees with application to alkynes (Article)

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Abstract

Let G = (V,E) be a simple connected **molecular** graph. The **eccentric connectivity index** ξ (G) is a distance-based **molecular** structure descriptor that was recently used for mathematical modelling of biological activities of diverse nature. In such a simple **molecular** graph, vertices represent atoms and edges represent **chemical** bonds, we denoted the sets of vertices and edges by V = V (G) and E = E(G), respectively. If d(u, v) be the notation of distance between vertices u, v ∊ V and is defined as the length of a shortest path connecting them. Then, the eccentricity **connectivity index** of a **molecular** graph Gis defined as $\xi(G) = \sum_{v\in} V(G)$ deg(v)ec(v), where deg(v) (or simply dv) is degree of a vertex v ∊ V (G), and is defined as the number of adjacent vertices with v. ec(v) is defined as the length of a maximal path connecting to another vertex of v. In this paper, we establish the general formulas for the eccentricity **connectivity index** of **molecular** graphs classes of **chemical trees** with **application** to **alkynes**.

Author keywords

Alkynes; **Chemical trees**; **Eccentric connectivity index**; Eccentricity; **Molecular** graphs

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