On Computation of Topological Descriptors for Symmetrically Configured Pentagonal Structure of Carbon Nanocones

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ABSTRACT

Nanoparticles have unique and dazzling properties that have potential applications in material science, electronics, medicine and many other fields. Carbon nanocones, also known as carbon nanohorns are carbon networks which are planar in structure and has majority of hexagonal faces along with some non-hexagonal faces, which are most commonly pentagons. Depending on the positioning of the pentagons in the structure, symmetrically and asymmetrically configured nanocones are obtained. Carbon nanocones are good replacement for carbon nanotubes and have also secured their place in fields such as electrochemical sensing or biosensing, biofuel cells, as electrode materials, supercapacitors, gas storage devices and biomedical applications. The idea of modelling a chemical structure in the form a chemical graph and quantitatively analysing the corresponding graph using topological descriptors brought breakthrough in the field of mathematics and chemistry. Topological descriptors helps in analysing a chemical structure without any experiments and it have application in wide fields of chemistry, computer science, biology, etc. A chemical graph is a simple graph in which atoms and bonds are represented by vertices and edges, respectively. The degree of a vertex $v$is the number of edges incident to it and is denoted by d_v. The maximum degree of vertex among the vertices of a graph is denoted by Δ. The concept of reverse vertex degree was introduced by V.R. Kulli, defined as $r_v = \Delta - d_v + 1$. The temperature of a vertexis defined as $t_v = \frac{d_v}{|V(G)|-d_v}$, where $|V(G)|$ is the number of vertices in graph G. Fajtlowicz defined the idea of vertex's temperature and later the temperature based topological descriptors were introduced by V.R. Kulli.

In this work, the reverse degree based topological descriptors as well as temperature descriptors for symmetrically configured pentagonal carbon nanocones were determined using the edge partition approach. The numerical and graphical comparison based on the determined analytical expressions was drawn. A comparison study in between the descriptors was also carried out.

Keywords: Carbon Nanocone, Reverse degree based descriptors, Temperature descriptors

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