Abstract

In quantum chemistry, the physico–chemical properties of chemical compounds are often modeled by means of molecular–graph–based structure–descriptors, which are also referred to as topological indices. One of the most widely known topological descriptors is Wiener index. It is named after chemist Harold Wiener who introduced in the year 1947. It is defined by the sum of the distances between all (ordered) pairs of vertices of G. In this paper, we find the Wiener index of degree splitting of some aliphatic and aromatic hydrocarbons and classify its characterization using MATLAB.

References

Wiener Index of Degree Splitting Graph of some Hydrocarbons

- Ponraj R and Somasundaram S, On the degree splitting graph of a graph, NATL ACAD,SCI LETT, 27(7 & 8) (2004), 275-278.
- Slavko Radenković S and Ivan Gutman, Relation between Wiener index and spectral radius, Kragujevac J. Sci. 30 (2008) 57-64
- Wiener H, Structural determination of paraffin boiling points- J. Am chem. Soc. 6 (1947) 17-20
- http://mathworld.wolfram.com/WienerIndex

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