Graph Theory at Work in Carbon Chemistry

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Message from the Guest Editors

Carbon allotropes are basically distinguished by the way in which carbon atoms are linked to each other, forming different types of networks (graphs) of carbon atoms. Different structures are builds with sp2-hybridized carbon atoms like PAHs, graphite, nanotubes, nanocones, nanohorns, and fullerenes. In these chemical systems, each node has degree 3, the basic hexagonal rings are connected with other similar rings in various topological ways, and in some cases, with the introduction of some pentagonal rings. By topology, the number of 5-rings is limited to 12......

This issue is devoted to the contemporary applications of chemical graph theory tools in modeling the carbon-based molecular structures and the investigations of topological molecular descriptors and their qualities.

Keywords

- Topological properties of low dimensional systems
- Topological symmetry
- Generalized Stone–Wales transformations
- Defective graphs
- Topological descriptors
- Bounds of topological descriptors

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Special Issue

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Message from the Editor-in-Chief

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