Abstract

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Network analysis using a novel highly discriminating topological index

When characterizing networks structurally, the discriminating ability of a topological measure (or also called index) is crucial. This relates to investigate its discrimination power (or also called uniqueness or degeneracy) that indicates how meaningful the given measure can distinguish nonisomorphic networks. In terms of biological and chemical graph analysis, a highly discriminative measure is desirable because it then has the ability to detect minor structural changes within the given network.

In this article, the discriminating ability of a new super index based on Shell-matrices and polynomials is tested using (real) atomic and synthetic structures. As a result, the new descriptor can distinguish all graphs uniquely. We emphasize that some molecular descriptors which are embedded in the super index have already shown excellent correlating ability with alkanes properties.

In view of the fact that most of the existing topological graph measures are degenerated, the new super index seems to be a good starting point for performing further studies in the context of network analysis. In the future, we also intent to use other sets of networks, for instance molecular graphs, to further examine the index and its meaning. In particular, we emphasize that only those indices which possess low computational complexity do have the potential to be applied for analyzing complex systems properly.