Structural Indices of Graphs

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Abstract

In this talk we consider some results and open problems from the Chemical Graph Theory, mainly concerning structural indices/properties.
The Atom Bond Connectivity index, also known as ABC index was defined by Estrada [4] with relation to the energy of formation of alkanes. It was quickly recognized that this index reflects important structural properties of graphs in general. The ABC index was extensively studied in the last three years, from the point of view of chemical graph theory [5, 6], and in general graphs [1]. It was also compared to other structural indices of graphs [2]. Das derives multiple results with implications to the minimum/maximum ABC-index on graphs. With relation to trees, it is known that among all the trees of the same number of vertices, the maximum ABC index is attained for the *star graph*. However, it is not known which tree(s) minimize(s) the ABC index. The problem seems to be hard. It is partially addressed in many sources [5, 1, 6], but remains open.
We further investigate the trees that minimize the ABC index. Our investigations are limited to *chemical trees*, i.e. trees in which the maximum vertex degrees is 4. The chemical trees were introduced to reflect the structure of the carbon chains and the molecules based on them. Our approach is algorithmic. We identify certain types of edges (chemical bonds) that are important and occur frequently in chemical trees. Further, we study how the removal of a certain edge, the introduction of certain edge or the contraction of certain edge affect the ABC-index of the tree. We pay particular attention to the examples of minimal ABC index chemical trees provided by Dimitrov [3].
This is joint work with Laura Huntington.
Keywords: structural graph theory, chemical graph theory, trees

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