Chemical Graph Theory - Part III

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NINO BAŠIĆ, University of Primorska, Slovenia

Pentagonal Clusters in Fullerenes

IPR-fullerenes form an important and well-studied family of fullerenes. In 2017, the Pentagonal Incidence Partition (PIP) was introduced which generalises this concept. All possible partitions of the number 12 were characterised, for which a fullerene with a prescribed PIP exists. In this sense, IPR-fullerenes can be described as fullerenes F with $\mathrm{PIP}(F) = (1, 1, \ldots, 1)$. We further generalise this notion and introduce the Pentagonal Patch Partition (PPP). We show which PPPs are admissible.

TOMISLAV DOŠLIĆ, University of Zagreb, Croatia

Nice subgraphs of fullerene graphs with prescribed components

Let G be a graph with a perfect matching. A subgraph H of G is nice if $G - V(H)$ still has a perfect matching. In a chemical context, nice subgraphs of molecular graphs serve as mathematical models of addition patterns in the corresponding molecules such that the rest of the molecule still has a resonant structure. In this contribution we consider classical and generalized fullerene graphs and look for nice subgraphs with prescribed components such as, e.g., stars and odd cycles. We also report some computational results for small fullerenes and list some open problems.

TOMAŽ PISANSKI, University of Ljubljana, Slovenia

Flat benzenoid complexes

Benzenoids form an important family of chemical graphs. Several other families, such as coronenes, helicenes, tubulenes, etc. that generalize benzenoids play an important role in theoretical chemistry. This talk introduces flat benzenoid complexes as a language in which all these generalizations may be expressed. Roughly speaking a flat benzenoid complex is a structure that is locally benzenoid. We present a basic theory of flat benzenoid complexes. A special emphasis will be on catacondensed flat benzenoid complexes having the property that all vertices belong to the boundary of the complex. This is work in progress with Patrick Fowler and Nino Bašić.

LAVANYA SELVAGANESH, Indian Institute of Technology (BHU), India

Bounds Of The Symmetric Division Deg Index For Graphs With Cyclomatic Number At Most 2 And With A Perfect Matching

The Symmetric division deg (SDD) index is a well-established valuable index in the analysis of quantitative structure-property and structure-activity relationship for molecular graphs. Introduced by Vukicevic and Gasperov in 2010, the SDD index was shown to have the best correlation ability for predicting the total surface area of polychlorobiphenyls. In this talk, we will study the range of SDD-index for graphs with the cyclomatic number at most 2, that is, trees, unicyclic and bicyclic graphs. In particular, we compute the bounds for the SDD-index of these graphs, which admit a perfect matching and identify the graphs that attain these bounds.

DAMIR VUKIČEVIĆ, University of Split, Croatia

Vukicevic, Boskovic: Adriatic graphs - mathematical properties and applications to correct NIST database

Let F be a family of graphs. Adriatic graph A(F) is a graph which vertices are ordered pairs of graphs in F that have the same number of vertices. Two vertices (G_1, G_2) and (H_1, H_2) are adjacent if: there is a non-pendant vertex v_i in graph G_i which all neighbors except one are leaves, i =1,2; v_1 and v_2 have the same degrees; and graph obtained by replacing one pendant

vertex of v_i by path of length two is isomorphic to H_i, i=1,2. Mathematical properties of these graphs and their application in chemistry will be discussed.