Chemical Graph Theory - Part I

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VESNA ANDOVA, Ss. Cyril and Methodius University, Northern Macedonia
On Three Constructions of Nanotori

There are three different approaches for constructing nanotori in the literature: one with three parameters suggested by Altshuler, another with four parameters used mostly in chemistry and physics, and one with three parameters used in computer science (known as generalized honeycomb tori).

Altshuler showed that his method gives all non-isomorphic nanotori, but this was not known for the other two constructions. We show that these three approaches are equivalent and give explicit formulas that convert parameters of one construction into the parameters of the other two constructions.

JACK GRAVER, Syracuse University, USA
The Clar - Fries Mystery

Given a fullerene, the maximum number of benzene rings over all Kekule structures is the Fries number; the maximum number of pairwise disjoint benzene rings over all Kekule structures is the Clar number. Graver and Hartung constructed a fullerene family where the benzene rings giving the Clar number could not be a subset of the Fries faces. Fowler and Myrvold developed a program for computing the Clar number directly and discovered many fullerenes in which this discrepancy occurred. Comparing constructions developed for Clar chains and Fries chains by Hartung and Fenton enables us to shed light on this mystery.

ELIZABETH HARTUNG, Massachusetts College of Liberal Arts, USA
Resonance Structures and Aromaticity in Capped Carbon Nanotubes

A fullerene is a 3-regular plane graph with only hexagonal and pentagonal faces, and models a pure carbon molecule. Nanotubes are a class of fullerenes that are cylindrical in shape and extremely useful in applications. The Clar number of a fullerene is a parameter related to its aromaticity and stability. In this talk, we partition nanotubes into two classes, those with relatively small and with relatively large Clar numbers. We describe the double bond structures, or perfect matchings, capable of forming in these two classes. This is joint work with Jack Graver (Syracuse University) and Aaron Williams (Williams College).

PETRA ŽIGERT PLETERŠEK, University of Maribor, Slovenia
Topological indices of unsaturated hydrocarbons

Hydrocarbons are modeled with simple graphs but in the case of unsaturated hydrocarbons with multiple bonds the corresponding graphs should be multigraphs. There is some ambiguity in modeling such graphs, and consequently in the calculation of certain topological indices. We introduce a model of edge-weighted graphs where distances in a graph are defined in three different ways using the topological distance, the relative topological distance and the relative distance (actual lengths of bonds). The regression analysis on the obtained weighted Wiener indices is performed and gives a good model for the prediction of boiling points of alkenes and alkadienes.

DONG YE, Middle Tennessee State University, USA
Resonance graphs on perfect matchings

Let G be a graph on a surface, and $\mathcal{F}$ is a set of faces bounded by even cycles. The resonance graph of G with respect to $\mathcal{F}$, denoted by $R(G;\mathcal{F})$, is a graph such that its vertex set is the set of all perfect matchings of G and two vertices M_1 and M_2

are adjacent if and only if the symmetric difference $M_1 \oplus M_2$ is a cycle bounding some face in $\mathcal{F}$. In this talk, we will focus on resonance graphs for graphs on surfaces. This talk is based on joint work with Niko Tratnik.