Graph Theory with Applications in Chemistry II
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JACK E GRAVER, Syracuse University
The Fries Structures of a fullerene

Given a fullerene, consider the Kekulé structure that gives its Fries number. The edges of this Kekulé structure that do not belong to a benzene ring turn out to be the union of the edges of the Clar chains of two distinct Clar structures. The Fries and Clar numbers will be given by the same Kekulé structure when one of these Clar structures is the one giving the Clar number. We explore the conditions under which this will occur when the paired pentagons are widely separated.

ELIZABETH HARTUNG, Massachusetts College of Liberal Arts
The Clar Structures of a Fullerene

A fullerene is a 3-regular plane graph consisting of only pentagonal and hexagonal faces. The $Fries$ and $Clar$ number of a fullerene are two related parameters, and the Clar number is less understood. We introduce the $Clar\ Structure$ of a fullerene, a decomposition designed to compute the Clar number for classes of fullerenes. We also settle an open question with a counterexample: we prove that the Clar and Fries number of a fullerene cannot always be obtained with the same Kekulé structure.

DOUGLAS J KLEIN, Texas A&M University at Galveston
Substitution-reaction posets in chemistry

Substitution-reaction posets represent a chemical reaction placing substituents at different locations of a molecular skeleton. Mathematically, we let G be a permutation group acting on the members of a finite set S representing substitution positions and define a partial ordering of orbits of subsets of S. Chemically, poset members represent substitutional isomers, and the associated Hasse diagram a substitution-reaction network. This self dual, ranked poset has unique maximum and minimum elements and coincidence of three metrics: splinoid fitting, cluster expansion; and flow-network methods. Chemical examples include a 13-member poset for benzene, and a 210-member poset for polychlorinated biphenyls.

CRAIG E LARSON, Virginia Commonwealth University
Eigenvalues of Saturated Hydrocarbons

We propose a simplified Hückel-type molecular-orbital (MO) model for the valence electrons of saturated hydrocarbons and consider the consequent eigenvalue spectrum. We obtain a first foundational result, which every chemist "knows", namely that: alkanes are stable, with half their (Hückel-type MO) eigenvalues positive and half negative.

NICO VAN CLEEMPUT, Ghent University
Spherical Tilings by Congruent Quadrangles

A spherical tiling is an edge-to-edge partition of the unit sphere into spherical polygons. Each spherical polygon is called a tile. If all tiles are congruent, then it follows from Euler's formula that those tiles are either 3-, 4- or 5-gons. Polyhedra and tilings are of perennial interest in Chemistry.

In 2002, Ueno and Agaoka completed the classification of spherical tilings by congruent triangles. Recently, Akama and Sakano completed the classification of spherical tilings by congruent daggers and kites.

We will explain the planned approach to classify the remaining spherical tilings by congruent quadrangles and present some first results.