Chemical Graph Theory - Part II

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PATRICK W. FOWLER, University of Sheffield, UK

The Chemical Significance of Graph Energy

Energy is a well-defined physical quantity with discrepant definitions in the mathematical chemistry of π systems. In an extensive mathematical literature, graph energy, $E_{\mathrm{G}}(G)$, is the sum of absolute values of adjacency eigenvalues of graph G. This is a tractable but imperfect mimic of the physical Hückel energy, $E_\pi(G,N)$, a quantity that depends on both G, the molecular graph of the conjugated carbon framework, and the π electron count, N. Discrepancies between $E_{\mathrm{G}}(G)$ and $E_\pi(G,N)$ can be arbitrarily large, but we reconcile the two definitions with a natural connection to the chemical concept of bond number.

IRENE SCIRIHA, University of Malta, Malta

The conductivity of the connected sum of root graphs with a common nullspace

Two connected root–graphs, H_1 and H_2, with isomorphic subgraphs $H_1 - z_1$ and $H_2 - z_2$, are glued together to form their connected-sum Z. If their μ–eigenspace is generated by vector $\mathbf{y}$ for some eigenvalue μ of their 0-1-adjacency matrix, then the μ-multiplicity of Z is shown to depend on the μ–type of z_1 and z_2 in the root–graphs. A sufficient condition for the uniqueness of $H_1(\simeq H_2)$, for a given $\mathbf{y}$, when constructed from $H_1 - z_1$, is also established. The SSP model for ballistic conduction in a pi-molecule predicts that 5 out of the 11 feasible MEDs can be Z.

JELENA SEDLAR, University of Split, Croatia

Two types of indices and their extremal trees

We introduce the ordering of tree graphs so that the star S_n is minimal and the path P_n is maximal graph. Topological indices are of Wiener or anti-Wiener type, if they are increasing or decreasing functions with respect to the introduced ordering. If an index is of Wiener type S_n is minimal and P_n is maximal tree, for anti-Wiener type the reverse holds. We introduce a simple criterion to establish if a topological index is of Wiener or anti-Wiener type and apply our result to several generalizations of Wiener index.

RISTE ŠKREKOVSKI, University of Ljubljana, Slovenia

On 12-regular nut graphs

A nut graph is a simple graph whose adjacency matrix is singular with 1-dimensional kernel and corresponding eigenvector with no zero elements. For each $d \in \{3,4,\ldots,11\}$ are known all values n for which there exists a d-regular nut graph of order n. In the talk, we consider all values n for which there exists a 12-regular nut graph of order n. (This is a joint work Nino Bašić and Martin Knor.)

DRAGAN STEVANOVIĆ, Mathematical Institute of the Serbian Academy of Sciences and Arts, Serbia

On Hosoya's dormants and sprouts

Study of cospectral graphs is a traditional topic of spectral graph theory. Haruo Hosoya recently drew attention to a particular aspect of constructing cospectral graphs using coalescences: that cospectral graphs can be constructed by attaching multiple copies of the same rooted graph in different ways to subsets of vertices of an underlying graph. We address expectations and questions raised in Hosoya's papers, and present an explicit formula for the characteristic polynomial of such multiple

coalescences, establishing a necessary and sufficient condition for their cospectrality in the case when the attached rooted graph may be arbitrary.

(Joint work with Salem Al-Yakoob.)