Applications of Graph Theory To Chemistry I

(Org: **Patrick Fowler** (University of Sheffield))

PATRICK FOWLER, University of Sheffield

Currents in molecules

Two applications of graph theory to determination of electron flow in molecules are presented. Ballistic currents, driven through a molecule by a potential difference, are described in terms of a transmission function based on characteristic polynomials of the molecular graph and three vertex-deleted subgraphs. Ring currents, flowing in closed loops within a molecule and driven by an applied magnetic field, are described in terms of nodal characteristics of adjacency eigenvectors of the molecular graph.

CRAIG LARSON, Virginia Commonwealth University

Conjecturing with GrInvIn

GrInvIn is a program for investigating graphs. The program is open-source, easily extendable, easy-to-use and can enhance student's mathematical investigations at many levels. The author will discuss examples of using GrInvIn in an introductory proofs course, and in guiding a masters thesis on bounds for the domination number in benzenoids. Finally, we have added a new conjecturing heuristic - with the aim of improving the conjecturing power of future iterations of GrInvIn.

MILAN RANDIC, National Institute of Chemistry, Ljubljana, Slovenia

Graph Theoretical Models of Ring Currents in Conjugated Hydrocarbons

We outline a graph-theoretical approach to calculation of ring currents in polycyclic hydrocarbons. The K Kekulé valence structures (perfect matchings) are compared pairwise to give the K(K-1) sets of conjugated circuits, which are then oriented according to length. The number of appearances in conjugated circuits of each arc gives the bond (edge) current intensity and direction. The result is a purely combinatorial model for the currents associated in chemistry with aromaticity of e.g., benzenoids.

IRENE SCIRIHA, University of Malta

Interlacing and Omni-Conduction in Single Molecules

Conduction in single molecules is explored by considering singular subgraphs of the molecular graph. The Interlacing Theorem determines fluctuations in the spectrum of a graph when a vertex is deleted, illuminating the concept of electric transmission. A molecular device where conduction occurs independently of placement of terminals is an omni-conductor. Sufficient conditions for conduction are presented, enabling the classification of conducting and insulating molecular graphs.