

Mathematical modeling in chemistry and resonance graphs

Abstract

Hydrocarbon molecules can be modeled with molecular graphs in a simple way - the carbon atoms are the vertices of a graph and the edges are the C-C bonds. We will show that the resonance graph of a molecular graph, which reflects the interaction between the Kekulé structures of aromatic hydrocarbon molecules, is a daisy cube, if the molecules considered can be modeled with the so called kinky benzenoid systems, i.e. catacondensed benzenoid systems without linear hexagons. Daisy cubes have been recently introduced as the isometric subgraphs of n -cubes Q_n , induced with intervals between the maximal elements of a poset $(V(Q_n), \leq)$ and the vertex $0^n \in V(Q_n)$.