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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.