

Molecules with Analogous Conducting Connections

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According to the Source and Sink Potential (SSP) model, for a chosen two-vertex-connection, a molecule is a conductor or an insulator, at the Fermi-level. Of particular interest are two classes of graphs that have analogous vertex pairs, that is the molecule shows the same behaviour for any two-vertex-connection. The first consists of the uniform-core graphs, corresponding to insulation at the Fermi-level for all two-vertex-connections and the second class, the nuciferous graphs, which are Fermi-level conducting devices with no non-bonding orbital, independent of the two-vertex-connection. The latter class has the additional property that the graphs are insulators for all one vertex connections. The criteria depend solely on the nullity of the adjacency matrix of the graph and of its vertex-deleted subgraphs. A graph G in the first class reaches the minimum allowed value for the nullity relative to that of G when the connecting vertices are deleted, for all pairs of distinct connecting vertices of G . In the second, the nullity reaches one, the maximum possible, when any vertex is deleted.