Computing the Clar number of fulleren graphs

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A \((3,6)\)-fullerene \(G\) is a plane cubic graph whose faces are only triangles and hexagons. It follows from Euler’s formula that the number of triangles is four. A matching of a graph \(G\) is a set of pair-wise disjoint edges \(M\) of \(G\), and a perfect matching or Kekulé structure is a matching \(M\) covering all vertices of \(G\). A cycle of \(G\) is \(M\)-alternating if its edges appear alternately in and off \(M\). Let \(F_n\) be a fullerene graph with \(n\) vertices. A set \(H\) of disjoint hexagons of \(F_n\) is called a resonant pattern -(or sextet pattern)- if \(F_n\) has a perfect matching \(M\) such that each hexagon in \(H\) is \(M\) alternating. The maximum cardinality of all sextet patterns of \(F_n\) is the Clar number of \(F_n\). The aim of this study is to study the Kekulé structure and the Clar number of \((3,6)\)-fullerenes. We also compute the Clar number of some infinite family of fullerenes.

Keywords:
Kekulé structure; sextet pattern; Clar number; fullerene graphs

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