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## The isolated-pentagon rule and nice substructures in fullerenes\*

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**Abstract:** After fullerenes were discovered, Kroto in 1987 proposed first the isolated-pentagon rule (IPR): the most stable fullerenes are those in which no two pentagons share an edge, that is, each pentagon is completely surrounded by hexagons. To now the structures of the synthesized and isolated (neutral) fullerenes meet this rule. The IPR can be justified from local strain in geometry and  $\pi$ -electronic resonance energy of fullerenes. If two pentagons abut in a fullerene, a 8-circuit along the perimeter of the pentalene (a pair of abutting pentagons) occurs. This paper confirms that such a 8-circuit is always a conjugated cycle of the fullerene in a graph-theoretical approach. Since conjugated circuits of length 8 destabilize the molecule in conjugated circuit theory, this result gives a basis for the IPR in  $\pi$ -electronic resonance. We also prove that each 6-circuit (hexagon) and each 10-circuit along the perimeter of a pair of abutting hexagons are conjugated. Two such types of conjugated circuit satisfy the  $(4n + 2)$ -rule, and thus stabilise the molecule.

**Keywords:** Fullerene, patch, stability, isolated pentagon rule, Kekulé structure, conjugated cycle, cyclic edge-cut.

Math. Subj. Class.: 05C70, 05C10, 92E10

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## Pravilo izoliranega petkotnika in lepe podstrukture v fulerenih\*

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**Povzetek:** Po odkritju fulerenov je Kroto leta 1987 prvi predlagal pravilo izoliranega petkotnika (IPR): najstabilnejši fulereni so tisti, v katerih si nobena dva petkotnika ne delita povezave, tj. vsak petkotnik je obdan izključno s šestkotniki. Do sedaj so strukture sintetiziranih in izoliranih (nevtralnih) fulerenov izpolnjevale to pravilo. Pravilo IPR se da opravičiti na podlagi lokalnega seva v geometriji in  $\pi$ -elektronske resonančne energije fulerenov. Če sta dva petkotnika v fulerenu sopostavljena, nastane cikel dolžine 8 vzdolž roba pentalena (para sopostavljenih petkotnikov). Ta članek potrjuje, da takšen 8-cikel vselej predstavlja konjugirani cikel fulerena v smislu teorije grafov. Ker konjugirani cikli dolžine 8 po teoriji konjugiranih ciklov destabilizirajo molekulo, ta rezultat daje osnovo za veljavnost pravila IPR v  $\pi$ -elektronski resonanci. Dokažemo tudi, da sta vsak 6-cikel (šestkotnik) in vsak 10-cikel vzdolž roba dveh sopostavljenih šestkotnikov konjugirana. Ti dve vrsti konjugiranih ciklov zadoščata  $(4n+2)$ -pravilu in posledično stabilizirata molekulo.

**Ključne besede:** Fuleren, obliž, stabilnost, pravilo izoliranega petkotnika, Kekuléjeva struktura, konjugiran cikel, ciklični povezavni rez.

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