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Fullerene patches I

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Abstract

Large carbon molecules, discovered at the end of the last century, are called fullerenes. The most famous of these, C_{60} has the structure of the soccer ball: the seams represent chemical bonds and the points where three seams come together represent the carbon atoms. We use the term *fullerene* to represent all mathematically possible structures for the chemical fullerenes: trivalent plane graphs with only hexagonal and pentagonal faces. A simple consequence of Euler's formula is that each fullerene has exactly 12 pentagonal faces; the only restriction on the number of hexagonal faces is that it not be 1. The chemical motivation for this paper is to answer the question: When is it possible to alter a fullerene by changing the structure inside a region of the fullerene bounded by a simple closed circuit? Such a region or patch is said to be ambiguous if alterations may be made to its interior without disturbing the structure of the fullerene outside of the region. In this paper, we show that, relative to the minimum distance between pentagonal faces, there are no small ambiguous patches.

Keywords: Fullerenes, fullerene patches, ambiguous patches, graphite patches.

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Fullerenska krpičja I

Povzetek

Velike ogljikove molekule, odkrite ob koncu prejšnjega stoletja, se imenujejo fulereni. Najbolj poznani od teh, C₆₀ ima strukturo nogometne žoge: šivi predstavljajo kemične vezi, točke, kjer se združijo trije šivi, pa ogljikove atome. Tukaj izraz *fuleren* uporabimo za predstavitev vseh matematično mogočih struktur za kemijske fulerene: ravninske grafe stopnje tri s šestkotnimi in petkotnimi lici. Enostavna posledica Eulerjeve formule je, da ima vsak fuleren natanko 12 petkotnih lic; edina omejitev glede števila šestkotnih lic je, da le-to ni enako ena. Kemijska motivacija za ta članek je iskanje odgovora na vprašanje: Kdaj je mogoče spremeniti fuleren s spremembo strukture znotraj nekega območja fulerena, omejenega z neko enostavno sklenjeno krivuljo? Za tako območje pravimo, da je *dvoumno*, če lahko spremenimo njegovo notranjost ne da bi zmotili strukturo fulerena zunaj območja. V tem članku

pokažemo, da glede na minimalno razdaljo med petkotnimi lici ni majhnih dvoumnih območij.

Ključne besede: Fulereni, fullerenska krpičja, dvoumna krpičja, grafitna krpičja.