ARS MATHEMATICA CONTEMPORANEA

Also available at http://amc-journal.eu
ISSN 1855-3966 (printed ed.) ISSN 1855-3974 (electronic edn.)
ARS MATHEMATICA CONTEMPORANEA 11 (2016) 425–435

Resonance graphs of fullerenes

Niko Tratnik, Petra Žigert Pleteršek

Abstract: A fullerene G is a 3-regular plane graph consisting only of pentagonal and hexagonal faces. The resonance graph $R(G)$ of G reflects the structure of its perfect matchings. The Zhang-Zhang polynomial of a fullerene is a counting polynomial of resonant structures called Clar covers. The cube polynomial is a counting polynomial of induced hypercubes in a graph.

In the present paper we show that the resonance graph of every fullerene is bipartite and each connected component has girth 4 or is a path. Also, the equivalence of the Zhang-Zhang polynomial of a fullerene and the cube polynomial of its resonance graph is established. Furthermore, it is shown that every subgraph of the resonance graph isomorphic to a hypercube is an induced subgraph in the resonance graph. For benzenoid systems and tubulenes each connected component of the resonance graph is the covering graph of a distributive lattice; for fullerenes this is not true, as we show with an example.

Keywords: Fullerene, resonance graph, Zhang-Zhang polynomial, cube polynomial, Kekulé structure, perfect matching, distributive lattice, median graph.

Math. Subj. Class.: 92E10, 05C31, 05C70, 06D99

ARS MATHEMATICA CONTEMPORANEA

Also available at http://amc-journal.eu
ISSN 1855-3966 (printed ed.) ISSN 1855-3974 (electronic edn.)
ARS MATHEMATICA CONTEMPORANEA 11 (2016) 425–435

Resonančni grafi fulerenov

Niko Tratnik, Petra Žigert Pleteršek

Povzetek: Fuleren G je 3-regularen ravninski graf, sestavljen samo iz petkotniških in šestkotniških lic. Resonančni graf $R(G)$ grafa G odraža strukturo njegovih popolnih prirejanj. Zhang-Zhangov polinom fulerena je preštevalni polinom (rodovna funkcija) resonančnih struktur, imenovanih Clarovi krovi. Kockovni polinom je preštevalni polinom induciranih hiperkock v grafu.

V tem članku pokažemo, da je resonančni graf vsakega fulerena dvodelen in da ima vsaka njegova povezana komponenta ožino 4 ali pa je pot. Prav tako dokažemo ekvivalenco Zhang-Zhangovega polinoma fulerena in kockovnega polinoma njegovega resonančnega grafa. Pokažemo tudi, da je vsak podgraf resonančnega grafa izomorfen hiperkocki v induciranem podgrafu resonančnega grafa. Pri benzenoidnih sistemih in tubulenih je vsaka povezana komponenta resonančnega grafa krovni graf distributivne mreže; za fulerene to ne drži, kot pokaže primer.

Ključne besede: Fuleren, resonančni graf, Zhang-Zhangov polinom, kockovni polinom, kekuléjska struktura, popolno prirejanje, distributivna mreža, medianski graf.

Math. Subj. Class.: 05C50, 05B20