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A NOTE ON IPR FULLERENES

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Omega polynomial $\Omega(G,x)$, was recently proposed by M. V. Diudea. It was defined on the ground of "opposite edge strips" *ops*. The Sadhana polynomial $Sd(G,x)$ can also be calculated by ops counting. In this paper we compute some relations between Sadhana index and Omega polynomial of IPR fullerene graphs.

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1. Introduction

Nano-era was started by discovery of a stable cluster of C_{60} fullerene and carbon nanotubes.[1-3] It opened a new gate for the science and technology at nanometer scale with wide implications in the human activities. After the discovery of carbon nanotubes, the question about the possible existence of nanotubular forms of other elements was addressed by scientists and they tried to obtain inorganic nanostructures.[4-6] Mathematical calculations are absolutely necessary to explore important concepts in chemistry. Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is an important tool for studying molecular structures. This theory had an important effect on the development of the chemical sciences.

Let $G(V,E)$ be a connected graph, with the vertex set $V(G)$ and edge set $E(G)$. Two edges $e = uv$ and $f = xy$ of G are called *codistant e co f* if they obey the following relation:[7,8]

$$d(v,x) = d(v,y) + 1 = d(u,x) + 1 = d(u,y).$$

Relation *co* is reflexive, that is, *e co e* holds for any edge *e* of *G*; it is also symmetric, if *e co f* then *f co e*. In general, relation *co* is not transitive, an example showing this fact is the complete bipartite graph $K_{2,n}$. If "*co*" is also transitive, thus an equivalence relation, then *G* is called a *co-graph* and the set of edges $C(e) := \{f \in E(G);\ f\ co\ e\}$ is called an *orthogonal cut oc* of G, $E(G)$ being the union of disjoint orthogonal cuts: $E(G) = C_1 \cup C_2 \cup \ldots \cup C_k$, $C_i \cap C_j = \varnothing, i \neq j$. Klavžar[9] has shown that relation *co* is a theta Djoković-Winkler relation.[10,11]

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Let $e = uv$ and $f = xy$ be two edges of G which are *opposite* or topologically parallel and denote this relation by e *op* f. A set of opposite edges, within the same face/ring, eventually forming a strip of adjacent faces/rings, is called an *opposite* edge *strip ops*, which is a quasi-ortogonal cut *qoc* (*i.e.*, the transitivity relation is not necessarily obeyed). Note that *co* relation is defined in the whole graph while *op* is defined only in a face/ring. The length of *ops* is maximal irrespective of the starting edge. Let m_s be the number of *ops* strips of length s. The Omega polynomial is defined as[12,13]

$$\Omega(x) = \sum_s m_s . x^s .$$

The first derivative (in x=1) equals the number of edges in the graph

$$\Omega'(1) = \sum_s m_s \cdot s = e = |E(G)| .$$

The Sadhana index $Sd(G)$ was defined by Khadikar *et al.*[14,15] as

$$Sd(G) = \sum_s m_s (|E(G)| - s) ,$$

where m_s is the number of strips of length s. The Sadhana polynomial $Sd(G,x)$ was defined by Ashrafi *et al.*[16] as

$$Sd(x) = \sum_s m_s \cdot x^{|E(G)|-s} .$$

Clearly, the Sadhana polynomial can be derived from the definition of Omega polynomial by replacing the exponent s by $|E(G)|$-s. Then the Sadhana index will be the first derivative of $Sd(x)$ evaluated at x=1. Here our notations are standard and mainly taken from [17 - 31].

2. Main results

In this section we compute some relations between Omega and Sadhana polynomials. An isolated pentagon rule fullerene is a fullerene in which none of its pentagons make contact with each other. We name it IPR fullerene.

Theorem 1. Let F be a fullerene. Then, $\Omega'(0) = 0$ if and only if F be an IPR fullerene.

Proof. Let $\Omega'(0) = 0$. This implies the multiplicity of x in definition of Omega polynomial is zero. Since every hexagonal face has 3 strips of length 2, thus none of the pentagons make contact with each other. Conversely, if F be an IPR fullerene, then the length of every strip is greater than 2. Hence, $\Omega'(0) = \lambda_1 x + \lambda_2 x^2 + ...\big|_{x=0} = 0$.

Lemma 2. Let G be a graph on n vertices, m edges and α be number of its *qoc* strips. Then

$$\alpha = \frac{Sd(G)}{m} + 1 . \tag{1}$$

Proof. By using definition of Sadhana index we have:

$$Sd(G) = \sum_s m_s (|E(G)| - s) = \sum_s m_s |E(G)| - \sum_s m_s \cdot s = (\alpha - 1)m .$$

Corollary 3. Let F_1 and F_2 be fullerenes of order n. Then

$$Sd(F_1) \le Sd(F_2) \Leftrightarrow \alpha(F_1) \le \alpha(F_2).$$

Proof. Since $Sd(G) = (\alpha - 1)m$ the proof is straightforward.

Theorem 4. Suppose *F* be an IPR fullerene, then

$$Sd(G) \le m(m-2)/2.$$

Proof. For every *qoc* strip *C* of *F*, |*C*| ≥ 2. Since $2\alpha \le m$, thus $\frac{Sd(G)}{m} + 1 \le m/2$ and so $Sd(G) \le m(m-2)/2.$

Theorem 5. Let *F* be a fullerene graph. Then

$$Sd(F) \ge (2 + \Omega'(0))m.$$

Proof. Let *r* and *s* be the number of *qoc* strips of length 1 and 2, respectively. Clearly $r = \Omega'(0)$ and since every hexagonal face has at least 3 *qoc* strips of length 2, thus $\alpha \ge 3 + \Omega'(0)$. By using equation (1) the proof is completed.

Conjecture. Among all of fullerenes *F* on *n* vertices the IPR fullerene has the minimum value of *Sd*(*F*).

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