

A Note on Fowler–Manolopoulos Predictor of Fullerene Stability

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Abstract

Fowler–Manolopoulos criterion, that is defined as the second moment of the hexagon neighbor signature, is one of the most powerful predictors for fullerene stability. In this note, we present a relationship between Fowler–Manolopoulos predictor and another hexagonal parameter, which could give Fowler–Manolopoulos predictor a graphical explanation. This result can be regarded as an understanding of Fowler–Manolopoulos criterion.

1 Introduction

A fullerene C_n is a polyhedral carbon cage with n atoms arranged in 12 pentagonal and $\frac{n}{2} - 10$ hexagonal rings. The stability issues of the fullerene isomers are concerned in a plenty of literatures [1–3]. Using the topological invariants based on chemical graph is one of the basic approaches to predict the fullerene stability. [4].

Very early it became clear that the fullerene stability is related to the pentagon structure in the corresponding graphs. The celebrated isolated-pentagon rule (IPR) is proposed by Kroto and Schmalz et al [4, 5]. This rule successfully gives a criterion of fullerene stability. Both the stable structures with 60 and 70 carbon atoms, i.e. $C_{60}(I_h)$ and $C_{70}(D_{5h})$, are the unique IPR-satisfying fullerenes among 1812 and 8149 possible

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structures, respectively. The rule still works for the fullerene isomers with more than 70 atoms. However the number of IPR isomers increases rather rapidly with the number of carbon atoms, and the IPR rule does not have discriminating power among such isomers. Hence some other graph-theoretical invariants have been proposed as predictors of fullerene stability [6–10]. The Fowler–Manolopoulos predictor is one of them [6], which shows a strong correlation with the fullerene stability [7, 8].

In this note, we present a relationship between Fowler–Manolopoulos predictor [6] and another hexagonal parameter [11], which gives this predictor a graphical explanation. This result would be helpful in further understanding Fowler–Manolopoulos criterion for IPR isomers.

2 Hexagonal indices for predicting the stability of fullerene

Raghavachari defines the neighbor index of each hexagon in a fullerene as the number of other hexagons to which it is adjacent [12]. Every fullerene isomer can be characterized by a signature of the form $(h_0, h_1, h_2, h_3, h_4, h_5, h_6)$, where h_k is the number of hexagons with neighbor index k . In an isolated-pentagon fullerene, every hexagon is adjacent to a minimum of three others. We can therefore write the hexagon neighbor index signature of an isolated-pentagon fullerene as (h_3, h_4, h_5, h_6) .

Fowler and Manolopoulos introduce the standard deviation σ_h of the hexagon neighbor index distribution as a predictor of fullerene stability [6]. That is

$$\sigma_h = \sqrt{\langle k^2 \rangle - \langle k \rangle^2},$$

where

$$\langle k \rangle = \frac{\sum_{k=0}^6 k h_k}{\sum_{k=0}^6 h_k}$$

and

$$\langle k^2 \rangle = \frac{\sum_{k=0}^6 k^2 h_k}{\sum_{k=0}^6 h_k}.$$

The sum of the entries in the hexagon neighbor index signature $\sum_{k=0}^6 h_k$ is simply the total number of hexagons, which is $\frac{n}{2} - 10$ in any fullerene C_n . Hence in some literatures [7, 8], the σ_h is also used in the form of the second moment of the hexagon neighbor signature

$$H = \sum_{k=0}^6 k^2 h_k.$$

In the IPR case,

$$H = \sum_{k=3}^6 k^2 h_k.$$

The hexagon indices u , v and w , are introduced and discussed in [11]. The u and v enumerate, respectively, the number of edges common to two hexagons and the number of vertices common to three hexagons. The parameter w counts the number of pairs of nonadjacent hexagon edges shared with two other hexagons. Figure 1 helps in the understanding of those indices. Thus, v and w complement each other by counting the two possible arrangements of three contiguous hexagons.

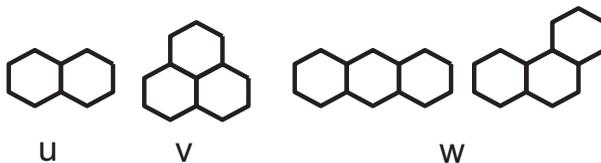


Figure 1: Substructures that contribute to the u , v and w counts

Lemma 2.1. *For the isolated-pentagon fullerenes, the parameters u and v are only dependent on n , the number of atoms, and there are*

$$u = \frac{3}{2}n - 60, \quad v = n - 60.$$

Proof. For an isolated-pentagon isomer with n atoms, there are exactly two types of edges. One is those fusing hexagon to hexagon, and the other is those fusing hexagon to pentagon. Note that there are 5×12 of these latter case. This leads to $u = \frac{3}{2}n - 60$. In the similar way, we have $v = n - 60$. □

3 The Main Result

Theorem 3.1. *For the isolated-pentagon fullerenes, one has*

$$H = \sum_{k=3}^6 k^2 h_k = 2u + 6v + 2w = 2w + 9n - 480.$$

Proof. Denote the numbers of u, v, w structures produced by every hexagon face as a signature of the form (s_u, s_v, s_w) . This index signature is counted for hexagon faces with different number k as follows. Note here that there are two possible configurations for $k = 4$.

- Hexagon with $k = 3$, the signature $(s_u, s_v, s_w) = (3, 0, 3)$, referring to Figure 2(a).
- Hexagon with $k = 4$, the signature $(s_u, s_v, s_w) = (4, 2, 4)$, referring to Figure 2(b) and 2(c).
- Hexagon with $k = 5$, the signature $(s_u, s_v, s_w) = (5, 4, 6)$, referring to Figure 2(d).
- Hexagon with $k = 6$, the signature $(s_u, s_v, s_w) = (6, 6, 9)$, referring to Figure 2(e).

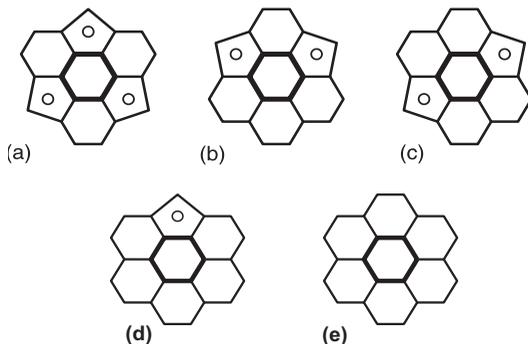


Figure 2: the structures of hexagon face and its neighbors

To sum the signatures over all the hexagon faces, one should note that every u structure is counted 2 times, every v structure is counted 3 times, and every w structure is counted just once. Hence

$$3h_3 + 4h_4 + 5h_5 + 6h_6 = 2u,$$

$$2h_4 + 4h_5 + 6h_6 = 3v,$$

$$3h_3 + 4h_4 + 6h_5 + 9h_6 = w.$$

Then

$$2u + 6v + 2w = 9h_3 + 15h_4 + 25h_5 + 36h_6 = H.$$

According to the Lemma 2.1, $u = \frac{3}{2}n - 60$ and $v = n - 60$ for all isolated-pentagon fullerenes with n atoms. Hence Fowler–Manolopoulos predictor has the following even simpler form

$$H = 2w + 9n - 480.$$

□

Remark 1: For isolated-pentagon fullerenes, the original form of Fowler–Manolopoulos predictor σ_h can be expressed in term of n and w . From the proof of theorem 3.1, we have $\sum_{k=3}^6 kh_k = 2u = 3n - 120$, hence

$$\sigma_h = \sqrt{\langle k^2 \rangle - \langle k \rangle^2} = \sqrt{\frac{4w + 18n - 960}{n - 20} - \left(\frac{6n - 240}{n - 20}\right)^2}.$$

Remark 2: In this note, only IPR case is discussed. Our results hold for all isolated-pentagon fullerenes. However, it is not clear so far that the relations between H, σ_h and pentagon and/or hexagon indices in the general fullerenes where some pentagons are adjacent to each other. This is an interesting problem for future research.

Acknowledgments

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