ON THE DETOUR INDEX OF A CHAIN OF C_{20} FULLERENES

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In this paper, we give a method for calculating the detour index of a chain of fullerenes.

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1. Introduction

A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods, and chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena [1]. The various topological indices of molecular graphs in chemical graph theory are non-empirical numerical quantities for the structure and the branching pattern of the molecule. This theory had an important effect on the development of the chemical sciences. Nowadays hundreds of researchers work in this area producing thousands articles annually. In fact, a topological index is a single unique number characteristic of the molecular graph and is mathematically known as the graph invariant. Usage of topological indices in biology and chemistry began in 1947 when chemist H. Wiener [2] introduced Wiener index to demonstrate correlations between physicochemical properties of organic compounds and the index of their molecular graphs. The detour index of a molecular graph has been introduced by Amic and Trinajstic [3] and by John [4], which is a graph invariant and is an analogue of the well-known Wiener index, defined as $D(G)=\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}r_{ij}$, where G is a simple and connected graph with vertex-set $V(G)=\{v_1,v_2,\cdots,v_n\}$, and r_{ij} denotes the length of the longest path between vertices (atoms) v_i and v_j of G. The detour index is equivalent with the Wiener index in acyclic structures, however, is different in cyclic structures. The detour index $D(G)$ is useful in QSPR studies if it is combined with the Wiener index [5]. However, the application of detour index is problematic, because the construction of an efficient algorithm to compute the detour index would

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be equivalent to the solution of the famous NP-complete problem.

In this paper, we give a method to compute the detour index of of a chain of C_{20} fullerenes.

2. Main results and discussion

Let G_1 and G_2 be two simple and connected graphs with disjoint vertex sets. For given vertices $u \in V(G_1)$ and $v \in V(G_2)$, a chain graph of G_1 and G_2 is the graph obtained by joining u and v by a new edge uv, denoted by $G_1 \square_{u,v} G_2$ or simply $G_1 \square G_2$, see Figure 1. The chain graph of $G_1, G_2, \cdots, G_k$ is $G_1 \square G_2 \square \cdots \square G_k$, and we use simply of the notation G^k if $G_1 = G_2 = \cdots = G_k = G$.

In 2010, M. Ghorbani and M. A. Hosseinzadeh [6]computed the Wiener index of a chain of graphs. Here, we give a method to compute the Harary index of a chain of C_{20} fullerenes.

Lemma 1. The detour index of fullerene C_{20} is $D(C_{20}) = 35200$.

Proof. It can be computed that $D_G(u) = \sum_{v \in V(C_{20})} r(u,v) = \sum_{j=1}^{20} r_{ij} = 0 + 19 \times 8 + 18 \times 11 = 350$

for every vertex u in $V(C_{20})$. By the definition of detour index and the symmetry, we have $D(C_{20}) = 3500$.

Lemma 2. The detour index of a chain $G_1 \square G_2$ of graphs G_1 and G_2 is

$$D(G_1 \square G_2) = D(G_1) + D(G_2) + |V(G_2)| D_{G_1}(u) + |V(G_1)| D_{G_2}(v) + |V(G_1)||V(G_2)|$$

where $D_G(u) = \sum_{v \in V(G)} r(u,v)$ and $r(u,v)$ denotes the length of the longest path between vertices u and v of G.

Proof.

$$\begin{aligned} D(G_1 \square G_2) &= \frac{1}{2} \sum_{x \in V(G_1 \square G_2)} \sum_{y \in V(G_1 \square G_2)} r(x,y) = \frac{1}{2} \sum_{x \in V(G_1)} \sum_{y \in V(G_1)} r(x,y) + \frac{1}{2} \sum_{x \in V(G_2)} \sum_{y \in V(G_2)} r(x,y) \\ &+ \sum_{x \in V(G_1)} \sum_{y \in V(G_2)} r(x,y) = D(G_1) + D(G_2) + \sum_{x \in V(G_1)} \sum_{y \in V(G_2)} [r(x,u) + 1 + r(v,y)] \\ &= D(G_1) + D(G_2) + |V(G_2)| D_{G_1}(u) + |V(G_1)| D_{G_2}(v) + |V(G_1)||V(G_2)| \end{aligned}$$

Theorem 3. Let $G = C_{20}^2 = C_{20} \square C_{20}$ be the chain graph of two fullerenes C_{20}. Then the detour index of G is $D(C_{20}^2) = 21400$.

Proof. From Lemmas 1 and 2, we have $D_{C_{20}}(u) = 350$ and

$$D(C_{20}^2) = D(C_{20} \square C_{20}) = 2D(C_{20}) + 20D_{C_{20}}(u) + 20D_{C_{20}}(v) + 20\times 20 = 21400.$$

Theorem 4. Let $G = C_{20}^k$ be the chain graph of k fullerenes C_{20}, depicted in Figure 2. Then the detour index of G is $D(C_{20}^k) = \frac{3800}{3}k^3 + 3400k^2 - \frac{3500}{3}k$.

Proof. From Lemmas 1 and 2, we have

$$\begin{aligned} D(C_{20}^k) &= D(C_{20}^{k-1}) + D(C_{20}) + 20D_{C_{20}^{k-1}}(u) + 20(k-1)D_{C_{20}}(v) + 20\times 20(k-1) \\ &= D(C_{20}^{k-1}) + 3500 + 20D_{C_{20}^{k-1}}(u) + 20(k-1)\times 350 + 20\times 20(k-1) \\ &= D(C_{20}^{k-1}) + 20D_{C_{20}^{k-1}}(u) + 7400k - 3900 \end{aligned}$$

and
$$\begin{aligned} D_{C_{20}^{k-1}}(u) &= D_{C_{20}}(u) + D_{C_{20}^{k-2}}(u) + 19\times |V(C_{20}^{k-2})| = 350 + D_{C_{20}^{k-2}}(u) + 380(k-2) \\ &= D_{C_{20}^{k-2}}(u) + 380k - 401 = D_{C_{20}^{k-3}}(u) + 380[k + (k-1)] - 401\times 2 \\ &= \cdots = D_{C_{20}}(u) + 380[k + (k-1) + \cdots + 3] - 401\times (k-2) \\ &= 190k^2 - 220k + 30 \end{aligned}$$

So,
$$\begin{aligned} D(C_{20}^k) &= D(C_{20}^{k-1}) + 20D_{C_{20}^{k-1}}(u) + 7400k - 3900 \\ &= D(C_{20}^{k-1}) + 3800k^2 + 3000k - 3300 \\ &= D(C_{20}^{k-2}) + 3800[k^2 + (k-1)^2] + 3000[k + (k-1)] - 3300\times 2 \\ &= \cdots = D(C_{20}) + 3800[k^2 + (k-1)^2 + \cdots + 2^2] + 3000[k + (k-1) + \cdots + 2] - 3300\times (k-1) \\ &= \frac{3800}{3}k^3 + 3400k^2 - \frac{3500}{3}k \end{aligned}$$

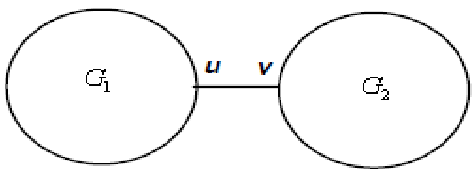

Fig. 1. A chain graph $G_1 \square G_2$ *of* G_1 *and* G_2.

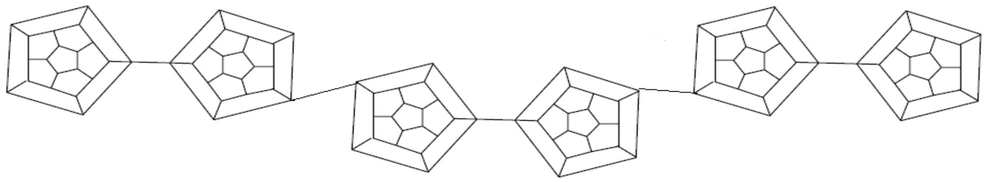

Fig. 2. The chain graph C_{20}^{6} *of* $k = 6$ *fullerenes* C_{20}.

Conclusions

The detour index of a molecular graph is an analogue of the well-known Wiener index in chemical graph theory. However, the construction of an efficient algorithm to compute the detour index is equivalent to the solution of the famous NP-complete problem. Here, we obtain an efficient method to compute the detour index of of a chain of C_{20} fullerenes.

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