COMPUTING BIPARTITE EDGE FRUSTRATION OF SOME NANOTUBES

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The smallest number of edges that have to be deleted from a molecular graph G to obtain a bipartite spanning subgraph is called the bipartite edge frustration of G, denoted by φ(G). In this paper this number is computed for some important classes of nanotubes.

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1. Introduction

Let G = (V,E) be a simple graph, a graph without multiple edges and loops. A subgraph S of G is a graph whose set of vertices and set of edges are all subsets of G. A spanning subgraph is a subgraph that contains all the vertices of the original graph. The graph G is called bipartite if the vertex set V can be partitioned into two disjoint subsets V1 and V2 such that all edges of G have one endpoint in V1 and the other in V2. Bipartite edge frustration of a graph G, denoted by φ(G), is the minimum number of edges that need to be deleted to obtain a bipartite spanning subgraph.

It is easy to see that φ(G) is a topological index and G is bipartite if and only if φ(G) = 0. Thus φ(G) is a measure of bipartivity. It is a well-known fact that a graph G is bipartite if and only if G does not have odd cycles. Holme, Liljeros and Edling introduced the edge frustration as a measure in the context of complex network, [8].

In [5,6] Fajtlowicz claimed that the chemical stability of fullerenes is related to the minimum number of vertices/edges that need to be deleted to make a fullerene graph bipartite. We mention here that before publishing the mentioned papers of Fajtlowicz, Schmalz et al. [10] observed that the isolated pentagon fullerenes (IPR fullerenes) have the best stability. Doslic [1], presented some computational results to confirm this relationship. So it is natural to ask about relationship between the degree of non-bipartivity of nanotubes and their stability.

Throughout this paper all graphs considered are finite and simple. Our notation is standard and taken mainly from [7,9]. We encourage the reader to consult papers by Doslic [1-4] for background material and more information on the problem. Our main results are the following two theorems:

**Theorem 1.** Suppose \( E = TUC_4C_8(R)[p,q] \), Figure 1, and \( F = TUC_4C_8(S)[p,q] \), Figure 2, are \( C_4C_8 \) nanotubes in which \( p \) and \( q \) are the number of rhombs and squares in each row and column, respectively. Then \( \phi(F) = 0 \) and

\[
\phi(E) = \begin{cases} 
0 & |p| = pq \\
\frac{2}{q} & |p| = p \\
\frac{2}{p} & |p| = q 
\end{cases}
\]

**Theorem 2.** Suppose \( A = HC_5C_7[r,t] \), \( B = VC_5C_7[r,t] \), \( C = SC_5C_7[r,t] \) and \( D = HAC_5C_7[r,t] \) are \( C_5C_7 \) nanotubes, where \( 2r \) is the number of pentagons in each period and \( t \) is the number of periods, Figures 3-7. Then \( \phi(B) = \phi(C) = \phi(D) = 2rt \) and we have:

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\[\varphi(A) = \begin{cases} 
2rt - \frac{r}{2} & \text{if } 2k + 1 = \frac{r}{2}\\ 
2rt - \frac{r}{2} + 1 & \text{if } 2k = \frac{r}{2} \end{cases}\]

We encourage the reader to consult papers by Diudea and his co-author for some background material as well as basic computational methods on mathematical properties of nanomaterials, [11-13].

2. Results and discussion

In this section the edge frustration number of five infinite class of nanotubes containing TUC4C8(R)[p,q], TUC6C8(S)[p,q], HC5C7[r,t], VC5C7[r,t], SC5C7[r,t] and HAC5C7[r,t] are computed. At first, we compute \(\varphi(TUC4C8(R))\), Figure 1. If \(p\) is even then obviously the molecular graph of TUC4C8(R)[p,q] is bipartite and so \(\varphi(TUC4C8(R)) = 0\). Suppose \(p\) is odd. Then \(E\) has a cycle of length \(3p\) and so it is not bipartite. We notice that the subgraph \(H\) constructed from \(G\) by deleting edges \(e_1, \ldots, e_q\), Figure 1, is biparetite. This implies that \(\varphi(TUC4C8(R)) \leq q\). On the other hand, it is clear that we cannot find less that \(q\) edges such that the graph constructed from \(G\) by deleting them, is bipartite. Thus \(\varphi(TUC4C8(R)) = q\).

![Fig. 1. The 2-dimensional Lattice of TUC4C8(R)[p,q].](image)

In Figure 2, a 2-colouring of the graph TUC6C8(S)[p,q] is presented and so \(\varphi(TUC6C8(S)) = 0\).
We now consider the \( \text{HC}_3C_7[r,t] \) nanotube constructed from \( t \) copies of the graph \( L \) depicted in Figure 3. Obviously \( r \) is even. We first consider the case that \( r/2 \) is even. In Figure 3, a 2-dimensional representation of this graph is depicted. In this case, the odd length cycles have exactly 5 and 7 edges. Therefore, we must delete at least one edge from each pentagon and heptagon. To compute \( \phi(\text{HC}_3C_7[r,t]) \), we must delete the common edges between all pentagon – pentagon and heptagon – heptagon of the molecular graph of \( \text{HC}_3C_7[r,t] \) nanotube. From Figure 4, one can see that there are \( rt \) edges between pentagon-pentagon and \( tr/2 + (t-1)r/2 \) edges between heptagon – heptagon of the graph. Therefore, \( \phi(\text{HC}_3C_7[r,t]) = 2rt – r/2. \)
We now assume that $r/2$ is odd. In this case there are other odd cycles of length $5r/2$. To delete these cycles, we must change our algorithm. In Figure 5, our deletion algorithm is depicted. By this figure, one can prove $\phi(\text{HC}_7^2[r,t]) = 2rt - r/2 + 1$.

**Fig. 5. The 2-Dimensional Lattice of HC$_7^2[r,t]$ when $r/2$ is Odd.**

Consider the molecular graph of VC$_7^2[r,t]$ nanotube. The only odd cycles of this graph are pentagons and heptagons. Using a similar method as in HC$_7^2[r,t]$, we delete edges between adjacent pentagons and adjacent heptagons to construct a bipartite graph. From Figure 6, one can see that $\phi(\text{VC}_7^2[r,t]) = rt + rt = 2rt$.

**Fig. 6. The 2-dimensional Lattice of VC$_7^2[r,t]$.**

Finally, we consider the molecular graph of SC$_7^2[r,t]$ and HAC$_7^2[r,t]$. These molecular graphs have exactly three types of odd cycles containing pentagons, heptagons and cycles of a lengths $j$. It is possible to choose edges $e_i's$ for deletion such that $e_i's$ are edges of pentagons and...
heptagons, see Figures 7,8. Therefore, $\phi(\text{SC}_3C_7[r,t]) = \phi(\text{HAC}_3C_7[r,t]) = 2rt$.

Fig. 7. The 2-dimensional Lattice of $\text{SC}_3C_7[r,t]$.

Fig. 8. The 2-dimensional Lattice of $\text{HAC}_3C_7[r,t]$.

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References