Computing some topological indices of Nanotubes

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Abstract- Let G = (V,E) be a graph, where V(G) is a non-empty set of vertices and E(G) is a set of edges. The degree of a vertex u Є V(G) is the number of vertices joining to u and denoted by du.In this paper hyper Zagreb indices and augmented Zagreb indices for HAC5C6C7[p,q] and TUC4C6C8[p,q] nanotubes are investigated.

Index Terms- Topological index,hyper Zagreb index,augmented Zagreb index, HAC5C6C7[p,q] nanotube,TUC4C6C8[p,q] nanotube.

I. INTRODUCTION

A graph is a pair G = (V,E) of a sets satisfying E ⊆ |V|2 ; thus the elements of E are 2-element subsets of V. A molecular graph is constructed by representing each atom of a molecule by a vertex and bonds between atoms by edges.The degree of a vertex v, dv(G) or dv is the number of edges incident v. A topological index is a map from the set chemical compounds represented by molecular graphs to the set of real numbers[1].Carbon nanotubes are cylindrical carbon molecules with novel properties which makes them potentially useful in wide variety of applications[2].Carbon nanotubes are single sheets of graphite rolled into cylinders. The Wiener index (W) is the oldest and widely used topological index. It is based on the vertex distances of the respective molecular graph and is defined as , W(G) = 2 ∑s=uv ∈ E(G)(dv + dv) 2 ,where (u,v) is any ordered pair of vertices in G and d(u,v) is the u-v geodesic [3,4].Zagreb indices belong among the oldest and most studied molecular descriptors and found noteworthy applications in chemistry. In literature there are many papers whose title contain either index or Zagreb indices, such as augmented general, modified, reformulated multiplicative, variable, Zagreb indices, Zagreb co-indices and Zagreb eccentricity index[5-12].

The hyper Zagreb index is defined as [13], HM(G) = ∑s=uv ∈ E(G)((dv + dv) 2) = ∑uw ∈ E (G)(du + dv) 2 and The augmented Zagreb index of a graph G is defined as

AZI(G) = ∑uw ∈ E(G)((du/dv + dv/du) 2)

Where E(G) is the edge set and du,dv are the degrees of vertices u and v in G respectively [14,15].In this study our notation is standard and taken from standard books of graph theory.In this paper hyper Zagreb indices and augmented Zagreb indices for HAC5C6C7[p,q] and TUC4C6C8[p,q] nanotubes are studied.

II. RESULTS AND DISCUSSION

2.1 hyper Zagreb index and augmented Zagreb index for HAC5C6C7[p,q] nanotubes

We use the notations in which p is the number of pentagons in one row, the three first rows of vertices and edges are repeated alternately, the number of these repetitions is denoted by q. The HAC5C6C7[p,q] nanotube is a C5C6C7 net and constructed by alternating C5,C6 and C7 giving a trivalent decoration[16].The 2-D lattice of HAC5C6C7[p,q] with p = 4, and q = 2 is shown in fig.(1). From fig.(1) one can see that the number of vertices and edges in this case are |V(G)| = 16pq and |E(G)| = 24pq – 2p.

There are two subsets E1(G) and E2(G).

<table>
<thead>
<tr>
<th>du,dv where uv ∈ E(G)</th>
<th>total number of edges</th>
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<tbody>
<tr>
<td>E1 = [2,3]</td>
<td>8p</td>
</tr>
<tr>
<td>E2 = [3,3]</td>
<td>24pq - 10p</td>
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The hyper Zagreb index,

HM(G) = ∑s=uv ∈ E(G)((dv + dv) 2) = ∑uw ∈ E (G)(du + dv) 2 = 8p(25 + 36) = 864pq - 160p

The augmented Zagreb index,

AZI(G) = ∑uv ∈ E(G)((du/dv + dv/du) 2) = 8(25 + 36) = 864pq - 160p

2.2 hyper Zagreb index and augmented Zagreb index for TUC4C6C8[p,q] nanotubes

The C4C6C8 net is a trivalent decoration made by altering C4, C6 and C8. It can cover either a cylinder or torus. For TUC4C6C8[p,q] nanotube, we denote the number of squares in first row by p and the three first rows of vertices and edges
repeated alternately ,the repetition by q. The 2-D graph of lattice $C_4C_6C_8[3,4]$ is shown in fig.(2). It is seen from figure (2),

$$HM(G) = \sum_{u,v \in E(G)} (dv + dv)^2$$
$$= \sum_{u,v \notin e_1, 16} + \sum_{u,v \notin e_2, 25} + \sum_{u,v \notin e_3, 36}$$
$$= 16(2q+4) + 25(4p+4q-8) + 36(9pq-8q-5p+4)$$
$$= 324pq-80p-156q+8.$$ and augmented Zagreb index
$$AZI(G) = \sum_{u,v \notin e_1, 8} + \sum_{u,v \notin e_2, 8} + \sum_{u,v \notin e_3, 11.391}$$
$$= 8(2q+4) + 8(4p+4q-8) + 11.391(9pq-8q-5p+4)$$

III. CONCLUSION

Topological indices are designed basically by transforming a molecular graph into a number[6]. We compute a new distance based hyper Zagreb index and augmented Zagreb index for $HAC_5C_6C_7[p,q]$ and $TUC_4C_6C_8[p,q]$ nanotubes.

REFERENCES


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