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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 $HAC_5C_6C_7$ [p,q] and $TUC_4C_6C_8$[p,q] nanotubes are investigated.

Index Terms- Topological index,hyper Zagreb index,augmented Zagreb index, $HAC_5C_6C_7$[p,q] nanotube,$TUC_4C_6C_8$[p,q] nanotube.

I. INTRODUCTION

A graph is a pair G = (V,E) of a sets satisfying $E \subseteq |V|^2$; thus the elements of E are 2-element subsets of V. A molecular graph is constucted by representing each atom of a molecule by a vertex and bonds between atoms by edges.The degree of a vertex v, d_v(G) or d_v 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) $=\frac{1}{2}\sum_{(u,v)} d(u,v)$,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) = $\sum_{e=uv \in E(G)} (dv+dv)^2$ and The augmented Zagreb index of a graph G is defined as

AZI(G) = $\sum_{uv \in E(G)} \left(\frac{dudv}{du+dv-2}\right)^3$

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 $HAC_5C_6C_7$[p,q] and $TUC_4C_6C_8$[p,q] nanotubes are studied.

II. RESULTS AND DISCUSSION

2.1 hyper Zagreb index and augmented Zagreb index for $HAC_5C_6C_7$[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 $HAC_5C_6C_7$[p,q] nanotube is a $C_5C_6C_7$ net and constructed by alternating C_5,C_6 and C_7 giving a trivalent decoration[16].The 2-D lattice of $HAC_5C_6C_7$[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 E_1(G) and E_2(G).

du,dv where uv Є E(G)	total number of edges
E_1 = [2,3]	8p
E_2 = [3,3]	24pq-10p

The hyper Zagreb index ,

HM(G) = $\sum_{e=uv \in E(G)} (dv+dv)^2$

= $\sum_{uv \in E_1} 25 + \sum_{uv \in E_2} 36$

= (8p) 25 + 36 (24pq – 10p)

= 864 pq-160p

The augmented Zagreb index,

AZI(G) = $\sum_{uv \in (E)} \left(\frac{dudv}{du+dv-2}\right)^3$

= $\sum_{uv \in E_1} 8p + \sum_{uv \in E_2} (24pq-10p)$

= 8(8p)+ 11.391(24pq-10p).

2.2 hyper Zagreb index and augmented Zagreb index for $TUC_4C_6C_8$[p,q] nanotubes

The $C_4C_6C_8$ net is a trivalent decoration made by altering C_4, C_6 and C_8.It can cover either a cylinder or torus.For $TUC_4C_6C_8$[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),

(du,dv) where uv Є (G)	total number of edges
e_1= [2,2]	2q+4
e_2= [2,3]	4p+4q-8
e_3= [3,3]	9pq-8q-5p+4

hyper Zagreb index for $TUC_4C_6C_8$[p,q],

$$HM(G) = \sum_{e=uv\in E(G)} (dv + dv)^2$$

$$= \sum_{u\,v\,\in\,e_1} 16 + \sum_{u\,v\,\in\,e_2} 25 + \sum_{u\,v\,\in\,e_3} 36$$

$$= 16(2q+4) + 25(4p+4q-8)+36(9pq-8q—5p+4)$$

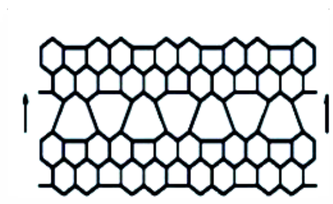
$$= 324\,pq-80\,p-156\,q+8.$$

and augmented Zagreb index

$$AZI(G) = \sum_{u\,v\,\in\,E(G)} \left(\frac{dudv}{du+dv-2}\right)^3$$

$$= \sum_{u\,v\,\in\,e_1} 8 + \sum_{u\,v\,\in\,e_2} 8 + \sum_{u\,v\,\in\,e_3} 11.391$$

$$= 8(2q+4) + 8(4p+4q-8) + 11.391(9\,pq-8\,q-5\,p+4)$$



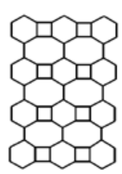


Fig.(1) 2-D lattice of $HAC_5C_6C_7$[p,q] with p=4,q=2.
Fig.(2) 2-D graph of lattice $TUC_4C_6C_8$[3,4]

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.

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