CYCLICALLY DOMINATION POLYNOMIAL OF MOLECULAR GRAPH OF SOME NANOTUBES

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A domination polynomial of a molecular graph is important in computing domination number. This number is most important for mathematical- Chemistry scientists. In this paper, we define new polynomials called "*cyclically* domination", and then we will determined this polynomial for some molecular graph of V- Phenylenic and TUC4C8(S) nanotubes . Some open questions also included.

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1. Introduction

Graph polynomials are invariants of graphs (i.e. functions of graphs that are invariant with respect to graph isomorphism); they are usually polynomials in one or two variables with integer coefficients. Graph polynomials can be interpreted as ordinary generating functions for the coefficient sequences which count in most cases certain subgraphs. Some polynomials (e.g. the chromatic polynomial) are defined by their values. Important examples of graph polynomials are chromatic polynomial, independence polynomial, matching polynomial, Tutte polynomial, reliability polynomial, characteristic polynomial, subgraph polynomial, clique polynomial, forest polynomial, Padmakar-Ivan polynomial, Omega polynomial. For definition of these polynomials see [1- 5],[9,11,13].

Now we define a new polynomial called *"cyclically domination polynomial"*. At first we define a multi-cyclically graph. Let $G = (V,E)$ be a simple connected finite the graph. We say that G is a *multi-cyclically graph* if and only if $V(G)$ separated to $A_1,A_2, . . . ,A_s$, where A_j is the cycle C_n. Also $A_1,A_2, . . . ,A_s$, are the cyclically-partitions of G. Although we may identify a graph G with its set of vertices, in cases where we need to be explicit we write $V(G)$ to denote the vertex set of G. Now assume that $G = (V,E)$ be a multi-cyclically graph of finite order m and with cyclically-partitions $A_1,A_2, . . . ,A_s$.

A subset D of the vertices of a graph G is called a *domination set* provided each vertex of $V \setminus D$ is adjacent to a member of D. The domination set with cardinality f is called f-set, and family of f–sets denote by $F(G)$.

The domination number of G, denoted by $\gamma(G)$, is the cardinality of a smallest domination set in G. Suppose that every A_j have same share, say k, where $\gamma(C_n)< k < n$, on every domination set in G. By this terminologies cyclically domination polynomial of multi-cyclically graph G (by the cyclically partitions $A_1,A_2, . . . ,A_s$), which show by $P(G, k)$, is equal to:

$$P(G, k) = \Sigma\, d(G, k)x^i, \quad where : i = ksn;$$

where $d(G, k) = jd(G, k)j$ and $d(G, k)$ is the family of i - sets of G, which every A_j . have same share, say k, $\gamma(C_n)< k < n$, in every i- sets in G.
In series of papers, Diudea, et.al. [6,8] investigated the structure and omega polynomial of some nanotubes and nanotori. Also in [10] the authors computed a new cyclic index of some molecular graphs. In this paper we continue this work to compute the cyclically domination polynomial of V -Phenylenic and $TUC4C8(S)$ nanotubes, see Figures 3 and 4. Throughout of this paper, our notation is standard.They are appearing as in the same way as in [12, 14]. We encourage the readers to consult [15- 19] for background materials as well as basic.

2. Main results and discussion

In this section, the cyclically domination polynomial of V-Phenylenic and TUC4C8(S) nanotubes. Following M.V. Diudea [7], we denote a molecular graph of V-Phenylenic nanotube by $G = V\,PHX[4n, 2m]$ or $C_4C_6C_8(m, n)$. We also denote a molecular graph of $TUC_4C_8(S)$ nanotubes by $H = C_4C_8(m, n)$.

In the following theorem we compute the cyclically domination polynomial of G and H, Figures 3,4.

Theorem 1. Suppose that G and H are two molecular graphs of $C_4C_6C_8(m, n)$ and $C_4C_8(m, n)$ nanotubes , respectively. Then with the above notations we have:
i) $P(G, k) = 4m.x^{2m}n+24mn.x^{3mn}+60mn.x^{4mn}+56mn.x^{5mn}+28mn.x^{6mn}+8mn.x^{7mn}+x^{8mn}$.

ii) $P(H, k) = 2x^{2mn} +6mn.x^{3mn} +33mn.x^{4mn} +38mn.x^{5mn} +28mn.x^{6mn} +8mn.x^{7mn} +x^{8mn}$.

Proof. To compute the cyclically domination polynomial of G and H, it is enough to calculate $d(G, k)$ and $d(H, k)$ (for every k as defined in the cyclically domination polynomial. We first consider the molecular graph G. To prove of $P(G, k)$, obviously G separated to Hexagons, and cardinality of a smallest domination set in a hexagon is equal to 2. So $k \in \{2, 3, 4, 5, 6, 7, 8\}$ and $i = kmn$. Hence with simple computations we have: It is known that molecular graph $C_4C_6C_8(m, n)$ has m rows of cycle C_8 and in every arbitrary octagons, we have four different case for each C_8 in a row, so there exist $4m$ domination set of size $2mn$, thus $d(G, 2) = 22m$.(see fig 1)

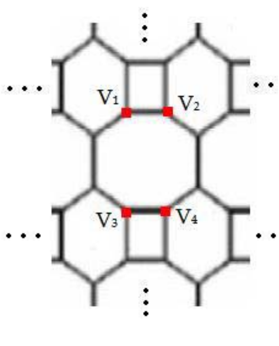

Fig. 1.The subgraph C_8 in the Molecular Graph of V-Phenylenic Nanotube, four case for choice distinct domination set: (v_1, v_3),(v_1, v_4),(v_2, v_3),(v_2, v_4).

Similarly:

$d(G, 3) = [c(4, 1).c(6, 1)]_{mn} = 24_{mn}$;
$d(G, 4) = [c(4, 1).c(6, 2)]_{mn} = 60_{mn}$;
$d(G, 5) = [c(8, 5)]_{mn} = 56_{mn}$;
$d(G, 6) = [c(8, 6)]_{mn} = 28_{mn}$;
$d(G, 7) = [c(8, 7)]_{mn} = 8_{mn}$;
$d(G, 8) = [c(8, 8)]_{mn} = 1_{mn} = 1$.

Hence we obtain the following domination polynomial for V-Phenylenic Nanotube.
$P(G, k) = 4_{m}.x^{2m}n+24_{mn}.x^{3mn}+60_{mn}.x^{4mn}+56_{mn}.x^{5mn}+28_{mn}.x^{6mn}+8_{mn}.x^{7mn}+x^{8mn}$.
and the proof of (i) is completed.

Now we consider the molecular graph $H = C_4C_8(m, n)$. Similarly H separated to octagons as labeled columns in Figure 2, and cardinality of a smallest domination set in a octagon is equal to 3. So $k \in \{2, 3, 4, 5, 6, 7, 8\}$ and also $i = kmn$. Hence again with simple calculationswe can get the followings:
Since for selected of minimum number domination vertex in C_8, is sufficient that to consider two vertices incident on one of the diagonals of C_8, we have two different domination set, thus $d(H, 2) = 2$. (see fig 2).

Similarly:

$d(H, 3) = [c(2, 2).c(6, 1)]_{mn} = 6_{mn}$;
$d(H, 4) = [c(2, 2).c(6, 2) + c(2, 1).c(3, 1).c(2, 2) + c(2, 1).c(3, 1).c(2, 1)]_{mn} = [15 + 6 + 12]_{mn} =$
33_{mn};
$d(H, 5) = [c(2, 2).c(6, 3) + c(2, 1).c(3, 2).c(3, 2)]_{mn} = 38_{mn}$;
$d(H, 6) = [c(8, 6)]_{mn} = 28_{mn}$;
$d(H, 7) = [c(8, 7)]_{mn} = 8_{mn}$;
$d(H, 8) = [c(8, 8)]_{mn} = 1_{mn} = 1$.
Thus, by these equalities we have:
$P(H, k) = 2x^{2mn} +6_{mn}.x^{3mn} +33_{mn}.x^{4mn} +38_{mn}.x^{5mn} +28_{mn}.x^{6mn} +8_{mn}.x^{7mn} +x^{8mn}$.

Thus the results now follows and the proof of theorem 1 is complete.

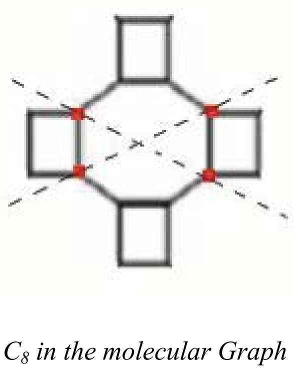

Fig.2. The subgraph C_8 in the molecular Graph of $TUC_4C_8(S)$ Nanotube.

3. Some open questions

Question 1. Let $P(x)$ be an arbitrary polynomial with positive integers coefficients.

Is there any multi-cyclically graph G by Multi-cyclically polynomial $P(G, k)$, such that $P(G, k) = P(x)$?

Question 2. Is there any multi-cyclically graph G with multi-cyclically polynomial $P(G, k)$, in which $P'(G, k)|_{x=1} = \gamma(G)$?

Question 3 . Suppose that G_1 and G_2 are two Multi-cyclically graphs with multicyclically polynomials $P(G_1, k)$, $P(G_2, k)$,respectively. Let $H = G_1 * G_2$ denote the joint of two graphs. What can say about the relationship between $P(G_1, k)$,

$P(G_2, k)$ and $P(H, k)$?

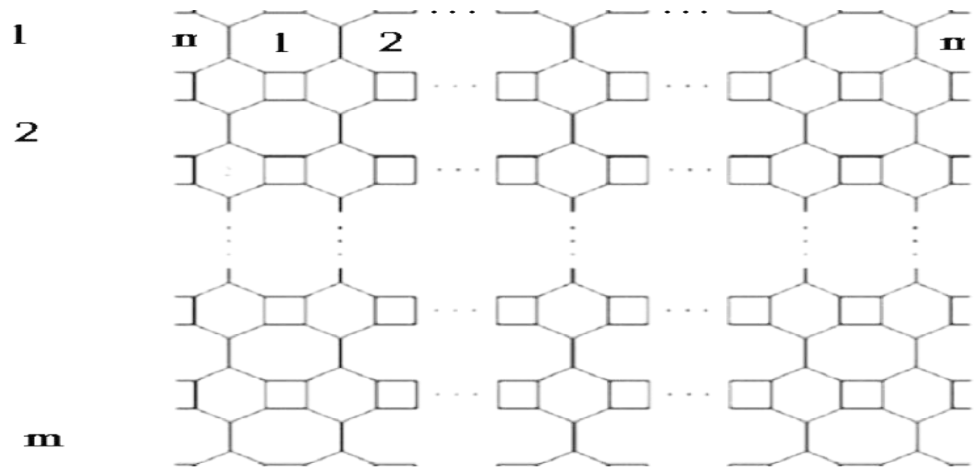

Fig. 3.The Molecular Graph of V-Phenylenic Nanotube or $C_4C_6C_8(m, n)$

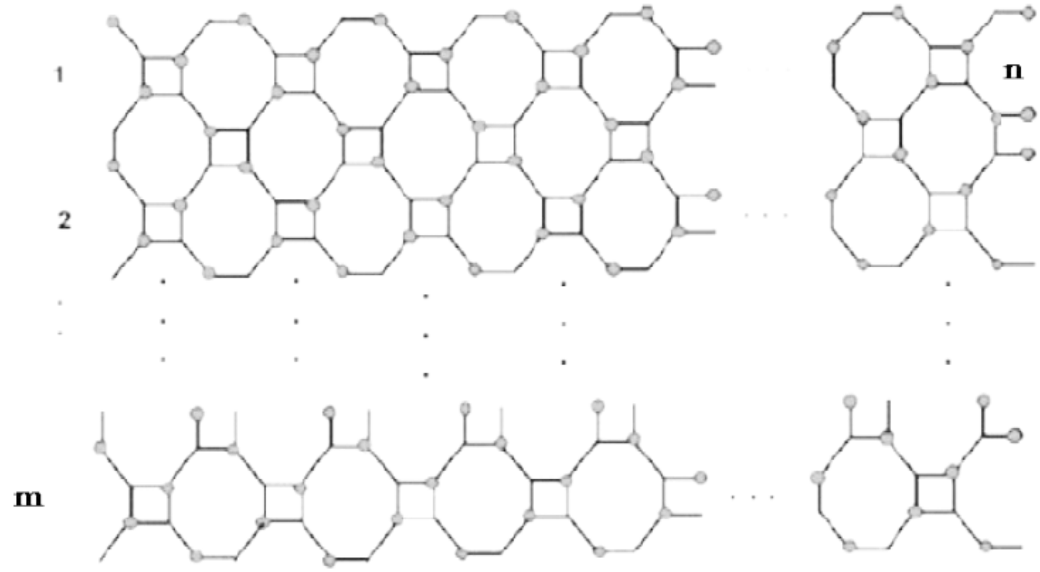

Fig.4. The Molecular Graph of $TUC_4C_8(S)$ Nanotube or $C_4C_8(m, n)$

4. Conclusions

In this paper we define a polynomial which has applied in mathematical chemistry , called “"*cyclically* domination". In the paper, we will determined this polynomial for some molecular graph of V-Phenylenic and TUC4C8(S) nanotubes.

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