On Leap Hyper-Zagreb Indices of Some Nanostructures

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Abstract

In recent years, higher order topological indices have gained enormous importance because of their greater correlation with many chemical properties. One among them is leap hyper-Zagreb index which is based on both distance and degree. In this paper, we compute the expressions for first and second leap hyper-Zagreb indices of some nanostructures.

Keywords − *degree, distance, nanostructure, leap hyper-Zagreb index.*
AMS Classification − *05C07, 05C12, 05C90.*

I. INTRODUCTION

Let $G = (V, E)$ be a finite, undirected, connected graph without loops and multiple edges. The *k-neighbourhood* [23] of a vertex $v \in V(G)$ is denoted and defined by $N_k(v/G) = \{u \in V(G): d(u, v) = k\}$ in which $d(u, v)$ is a distance between the vertices u and v in G. The *k-distance degree of a vertex* $v \in V(G)$ is denoted and defined by $d_k(v/G) = |N_k(v/G)|$. Also, we denote $N_G(v)$ by $N_1(v/G)$ and $d_G(v)$ by $d_1(v/G)$. The *degree of an edge* $e = uv$ in G is denoted by $d_1(e/G)$ (or $d_G(e)$) is defined by $d_1(e/G) = d_1(u/G) + d_1(v/G) - 2$. If all the vertices of G have same degree equal to $r \in Z^+$, then G is called an r - regular graph. For undefined graph terminology and notations, refer [11] and [17].

In chemical graph theory and in mathematical chemistry, a molecular graph or chemical graph is representation of structural formula of a chemical compound in terms of graph theory. A molecular graph is a graph whose vertices correspond to the atoms of the chemical compound and edges to the chemical bonds. Chemical graph theory is a branch of mathematical chemistry which has an important role and also effective on the development of the chemical sciences. A single number that can be used to characterize the properties of a molecule is called a topological index of that graph. There are numerous molecular descriptors, which are also referred to as topological indices, see [10], have found some applications in theoretical chemistry, especially in QSPR/QSAR research. There are innumerable topological indices defined in the literature. Wiener index [24], Zagreb indices [10], F-index [1, 9], connectivity index (or Randić index) [6] are few of them. Very recently, indices such as Sanskruti index [12], second order first Zagreb index [4] are introduced. Higher order topological indices have advanced chemical applications in QSPR/QSAR study. The authors in these papers [4,5,9,13,15,20,21,22] have calculated various topological indices for some of the nanostructures. Many topological indices are there for various nanostructures such as armchair polyhex nanotube, armchair polyhex nanotorus, V-phenylenic nanotube, V-phenylenic nanotorus, H-tetracenic nanotube, V-tetracenic nanotube and tetracenic nanotorus could be found in [2,3,7,8,15,20]. In [19], Naji et al. has introduced leap Zagreb indices. Basavanagoud et al. in [5], has computed leap Zagreb indices of some transformation graphs.

Recently, Kulli in [18], has introduced leap hyper-Zagreb indices. The first leap hyper-Zagreb index and second leap hyper-Zagreb index are given by

$HLM_1(G) = \sum_{uv \in E(G)} (d_2(u/G) + d_2(v/G))^2$ and $HLM_2(G) = \sum_{uv \in E(G)} (d_2(u/G)d_2(v/G))^2$, respectively.

In this paper, we compute expressions for first and second leap hyper-Zagreb indices for some nanostructures.

II. ORDER AND SIZE OF SOME NANOSTRUCTURES

TABLE 1
Order And Size Of Nanostructures

Sl. No.	Graph	Order	Size

1	Armchair polyhex nanotube $TUAC_6[2p,q]$	$2pq$	$3pq-2p$
2	Armchair polyhex nanotorus $TUAC_6[p,q]$	$2pq$	$3pq$
3	V-Phenylenic nanotube $VPHX[p,q]$	$6pq$	$9pq-p$
4	V-Phenylenic nanotorus $VPHY[p,q]$	$6pq$	$9pq$
5	V-Tetracenic nanotube G[p,q]	$18pq$	$27pq-4p$
6	H-Tetracenic nanotube G[p,q]	$18pq$	$27pq-2q$
7	Tetracenic nanotorus G[p,q]	$18pq$	$27pq$

For convenience purpose, we use the names A, B, C, D, E, F, H for the molecular graphs of armchair polyhex nanotube, armchair polyhex nanotorus, V-phenylenic nanotube, V-phenylenic nanotorus, V-tetracenic nanotube, H-tetracenic nanotube, tetracenic nanotorus, respectively.

III. LEAP HYPER-ZAGREB INDICES OF SOME NANOSTRUCTURES

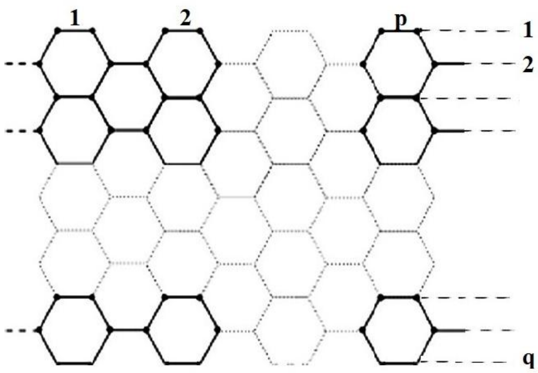

Fig. 1 (A) armchair polyhex nanotube

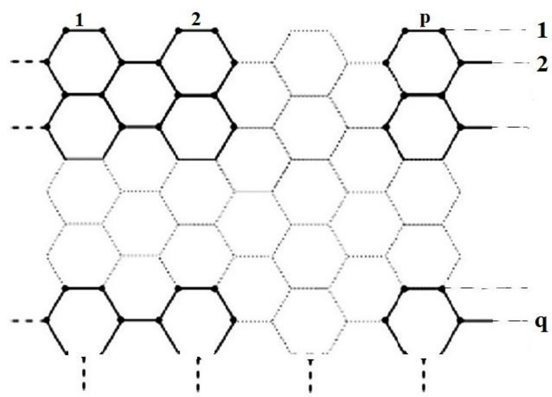

Fig. 2 (B) armchair polyhex nanotorus

TABLE 2
EDGE SET PARTITION OF GRAPH A. HERE $uv \in E(A)$.

No. of edges	$d_2(u/A)$	$d_2(v/A)$
$2p$	3	3
$4p$	3	5
$2p$	5	5
$4p$	5	6
$3pq-14p$	6	6

Theorem 3.1. *If A is an armchair polyhex nanotube $TUAC_6[2p,q]$, where $p(>1)$ is number of cycles in a row and $q(>1)$ is number of stages, then*

(i) $HLM_1(A) = 432pq - 1004p$,

(ii) $HLM_2(A) = 3888pq - 12232p$.

Proof. The graph $A = TUAC_6[2p,q]$ has $2pq$ vertices and $3pq-2p$ edges. Using the definitions of first and second leap hyper-Zagreb indices and edge set partition of the graph A given in Table 2 we get,

$$HLM_1(A) = \sum_{uv\in E(A)} [d_2(u/A) + d_2(v/A)]^2$$
$$= (3+3)^2(2p) + (3+5)^2(4p) + (5+5)^2(2p) + (5+6)^2(4p) + (6+6)^2(3pq-14p)$$
$$= 432pq - 1004p.$$

$$HLM_2(A) = \sum_{uv\in E(A)} [d_2(u/A)d_2(v/A)]^2$$
$$= (3\cdot 3)^2(2p) + (3\cdot 5)^2(4p) + (5\cdot 5)^2(2p) + (5\cdot 6)^2(4p) + (6\cdot 6)^2(3pq-14p)$$
$$= 3888pq - 12232p.$$

□

TABLE 3
EDGE SET PARTITION OF GRAPH B. HERE $uv \in E(B)$

No. of edges	$d_2(u/B)$	$d_2(v/B)$
$3pq$	6	6

Theorem 3.2. *If B is an armchair polyhex nanotorus $TUAC_6[p,q]$, where $p(>1)$ is number of cycles in a row and $q(>1)$ is number of rows, then*

(i) $HLM_1(B) = 432pq$,

(ii) $HLM_2(B) = 3888pq$.

Proof. The graph $B = TUAC_6[p,q]$ has $2pq$ vertices and $3pq$ edges. Using the definitions of first and second leap hyper-Zagreb indices and edge set partition of the graph B given in Table 3 we get,

$$HLM_1(B) = \sum_{uv\in E(B)} [d_2(u/B) + d_2(v/B)]^2$$
$$= (6+6)^2(3pq)$$
$$= 432pq.$$

$$HLM_2(B) = \sum_{uv\in E(B)} [d_2(u/B)d_2(v/B)]^2$$
$$= (6\cdot 6)^2(3pq)$$
$$=3888pq.$$

□

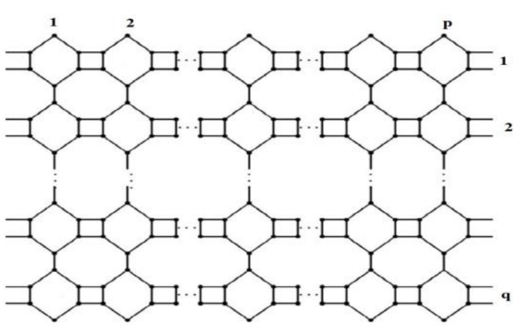

Fig. 3 (C) V-phenylenic nanotube

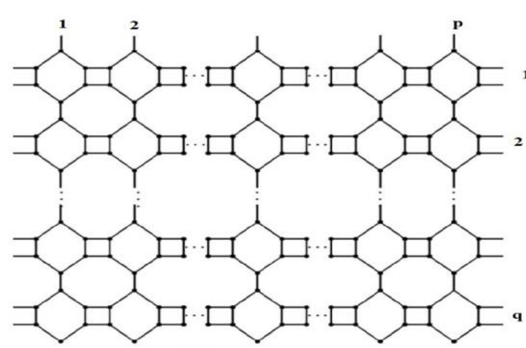

Fig. 4 (D) V-phenylenic nanotorus

TABLE 4
EDGE SET PARTITION OF GRAPH C. HERE $uv \in E(C)$

No. of edges	$d_2(u/C)$	$d_2(v/C)$
$6p$	4	4
$4p$	4	5

$2p(2q-3)$	5	5
$4p(q-1)$	5	6
$p(q-1)$	6	6

Theorem 3.3. *If C is a V-phenylenic nanotube $VPHX[p,q]$, where $p(>1)$ is number of cycles in a row and $q(>1)$ is number of rows, then*

(i) $HLM_1(C) = 1028pq - 520p$,

(ii) $HLM_2(C) = 7396pq - 4896p$.

Proof. The graph $C = VPHX[p,q]$ has $6pq$ vertices and $9pq - p$ edges. The definition of first and second leap hyper-Zagreb indices and edge set partition of the graph C given in Table 4 gives,

$$HLM_1(C) = \sum_{uv\in E(C)} [d_2(u/C)+d_2(v/C)]^2$$
$$= (4+4)^2(6p) + (4+5)^2(4p) + (5+5)^2[2p(2q-3)] + (5+6)^2[4p(q-1)] + (6+6)^2[p(q-1)]$$
$$= 1028pq - 520p.$$

$$HLM_2(C) = \sum_{uv\in E(C)} [d_2(u/C)d_2(v/C)]^2$$
$$= (4\cdot 4)^2(6p) + (4\cdot 5)^2(4p) + (5\cdot 5)^2[2p(2q-3)] + (5\cdot 6)^2[4p(q-1)] + (6\cdot 6)^2[p(q-1)]$$
$$= 7396pq - 4896p.$$

□

TABLE 5
EDGE SET PARTITION OF GRAPH D. HERE $uv \in E(D)$

No. of edges	$d_2(u)$	$d_2(v)$
$4pq$	5	5
$4pq$	5	6
pq	6	6

Theorem 3.4. *If D is a V-phenylenic nanotorus $VPHY[p,q]$, where $p(>1)$ is number of cycles in a row and $q(>1)$ is number of rows, then*

(i) $HLM_1(D) = 1028pq$,

(ii) $HLM_2(D) = 7396pq$.

Proof. The graph $D = VPHY[p,q]$ has $6pq$ vertices and $9pq$ edges. Using the definition of first and second leap hyper-Zagreb indices and edge set partition of the graph D given in Table 5 we get,

$$HLM_1(D) = \sum_{uv\in E(D)} [d_2(u/D)+d_2(v/D)]^2$$
$$= (5+5)^2(4pq) + (5+6)^2(4pq) + (6+6)^2(pq)$$
$$= 1028pq.$$

$$HLM_2(D) = \sum_{uv\in E(D)} [d_2(u/D)d_2(v/D)]^2$$
$$= (5\cdot 5)^2(4pq) + (5\cdot 6)^2(4pq) + (6\cdot 6)^2(pq)$$
$$= 7396pq.$$

□

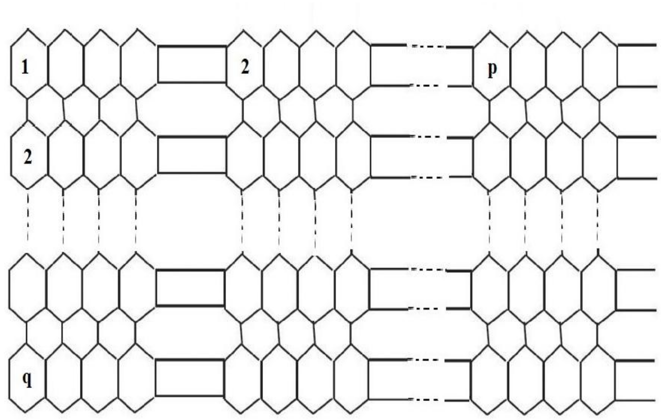

Fig. 5 (E) V-tetracenic nanotube

TABLE 6
EDGE SET PARTITION OF GRAPH E. HERE $uv \in E(E)$

No. of edges	$d_2(u/E)$	$d_2(v/E)$
$18p$	4	4
$4p$	4	5
$6p$	4	6
$4p$	5	6
$9p(3q-4)$	6	6

Theorem 3.5. *If E is a V-tetracenic nanotube $G[p,q]$, where $p(>1)$ is number of cycles in a row and $q(>1)$ is number of rows, then*

(i) $HLM_1(E) = 3888pq - 2624p$,

(ii) $HLM_2(E) = 34992pq - 33392p$.

Proof. The graph $E = G[p,q]$ has $18pq$ vertices and $27pq - 4p$ edges. Using the definition of first and second leap hyper-Zagreb indices and edge set partition of the graph E given in Table 6 we get,

$$HLM_1(E) = \sum_{uv \in E(E)} [d_2(u/E) + d_2(v/E)]^2$$
$$= (4+4)^2(18p) + (4+5)^2(4p) + (4+6)^2(6p) + (5+6)^2(4p) + (6+6)^2[9p(3q-4)]$$
$$= 3888pq - 2624p.$$

$$HLM_2(E) = \sum_{uv \in E(E)} [d_2(u/E) d_2(v/E)]^2$$
$$= (4 \cdot 4)^2(18p) + (4 \cdot 5)^2(4p) + (4 \cdot 6)^2(6p) + (5 \cdot 6)^2(4p) + (6 \cdot 6)^2[9p(3q-4)]$$
$$= 34992pq - 33392p.$$

□

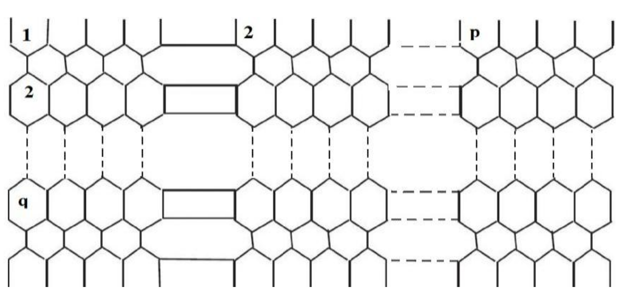

Fig. 6 (F) H-tetracenic nanotube

TABLE 7
EDGE SET PARTITION OF GRAPH F. HERE $uv \in E(F)$.

No. of edges	$d_2(u/F)$	$d_2(v/F)$
pq	3	3
$2pq$	3	5
$3pq$	5	5
$2pq$	5	6
$19pq-2q$	6	6

Theorem 3.6. *If F is a H-tetracenic nanotube $G[p,q]$,, where $p(>1)$ is number of cycles in a row and $q(>1)$ is is number of rows, then*

(i) $HLM_1(F) = 3442pq - 288q$,

(ii) $HLM_2(F) = 28830pq - 2592q$.

Proof. The graph $F = G[p,q]$ has $18pq$ vertices and $27pq - 2q$ edges. Using the definition of first and second leap hyper-Zagreb indices and edge set partition of the graph F given in Table 7 we get,

$$HLM_1(F) = \sum_{uv\in E(F)} [d_2(u/F)+d_2(v/F)]^2$$
$$= (3+3)^2(pq) + (3+5)^2(2pq) + (5+5)^2(3pq) + (5+6)^2(2pq) + (6+6)^2[(19pq-2q)]$$
$$= 3442pq - 288q.$$

$$HLM_2(F) = \sum_{uv\in E(F)} [d_2(u/F)d_2(v/F)]^2$$
$$= (3\cdot 3)^2(pq) + (3\cdot 5)^2(2pq) + (5\cdot 5)^2(3pq) + (5\cdot 6)^2(2pq) + (6\cdot 6)^2[(19pq-2q)]$$
$$= 28830pq - 2592q.$$

□

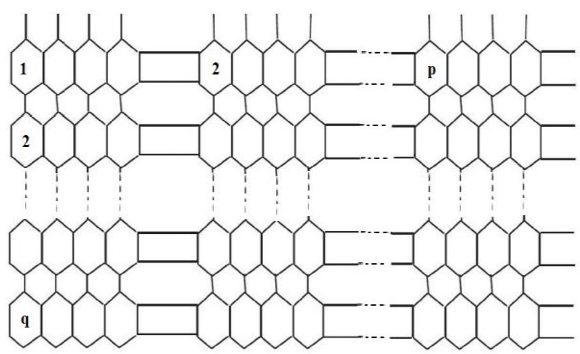

Fig. 7 (H) tetracenic nanotorus

TABLE 8
EDGE SET PARTITION OF GRAPH H. HERE $uv \in E(H)$

No. of edges	$d_2(u/H)$	$d_2(v/H)$
$4pq$	5	5
$4pq$	5	6
$19pq$	6	6

Theorem 3.7. *If H is a tetracenic nanotorus $G[p,q]$, where $p(>1)$ is number of cycles in a row and $q(>1)$ is number of rows, then*

(i) $HLM_1(H) = 3620pq$,

(ii) $HLM_2(H) = 30724pq$.

Proof. The graph $H = G[p,q]$ has $18pq$ vertices and $27pq$ edges. Using the definition of first and second leap hyper-Zagreb indices and edge set partition of the graph H given in Table 8 we get,

$$HLM_1(H) = \sum_{uv\in E(H)} [d_2(u/H) + d_2(v/H)]^2$$
$$= (5\cdot 5)^2(4pq) + (5\cdot 6)^2(4pq) + (6\cdot 6)^2(19pq)$$
$$= 3620pq.$$

$$HLM_2(H) = \sum_{uv\in E(H)} [d_2(u/H)d_2(v/H)]^2$$
$$= (5\cdot 5)^2(4pq) + (5\cdot 6)^2(4pq) + (6\cdot 6)^2(19pq)$$
$$= 30724pq.$$

□

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