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ON DISTANCE-BASED TOPOLOGICAL INDICES OF $HC_5C_7[4p,8]$ NANOTUBES

ALI REZA ASHRAFI•, HAMID SAATI AND MODJTABA GHORBANI
Institute of Nanoscience and Nanotechnology, University of Kashan, Kashan 87317-51167, I. R. Iran

Let G be a connected graph, $n_u(e)$ is the number of vertices of G lying closer to u and $n_v(e)$ is the number of vertices of G lying closer to v. Then the Szeged index of G is defined as the sum of $n_u(e)n_v(e)$, over edges of G.. The PI index of G is a Szeged-like topological index defined as the sum of $[m_u(e)+ m_v(e)]$, where $m_u(e)$ is the number of edges of G lying closer to u than to v, $m_v(e)$ is the number of edges of G lying closer to v than to u and summation goes over all edges of G. In this paper, the PI and Szeged indices of a $HC_5C_7[4p,8]$ nanotube are computed for the first time.

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1. Introduction

Carbon nanotubes are molecular-scale tubes of graphitic carbon with outstanding properties. They are among the stiffest and strongest fibres known, and have remarkable electronic properties and many other unique characteristics. For these reasons they have attracted huge academic and industrial interest, with thousands of papers on nanotubes being published every year. Commercial applications have been rather slow to develop, however, primarily because of the high production costs of the best quality nanotubes.

A major part of the current research in mathematical chemistry, chemical graph theory and quantitative structure-activity-property relationship studies involves topological indices.[1] Topological indices (TIs) are numerical graph invariants that quantitatively characterize molecular structure.

The problem of distances in graph continues to focus the attention of scientist both as theory and applications. In 1947, Harold Wiener has proposed his path number, as the total distance between all carbon atoms for correlating with the thermodynamic properties of alkanes. Numerous of its chemical applications were reported and its mathematical properties are well understood[2-5]. The Szeged index is another topological index which is introduced by Ivan Gutman.[6-8] To define the Szeged index of a graph G, we assume that e = uv is an edge connecting the vertices u and v. Suppose $M_{eu}(e|G)$ is the number of vertices of G lying closer to u and $M_{ev}(e|G)$ is the number of vertices of G lying closer to v. Edges equidistance from u and v are not taken into account. Then the Szeged index of the graph G is defined as $Sz(G) = \sum_{e=uv\in E(G)} M_{eu}(e|G)M_{ev}(e|G)$.

Khadikar and co-authors[9-13] defined a new topological index and named it Padmakar-Ivan index. They abbreviated this new topological index as PI. This newly proposed topological index does not coincide with the Wiener index for acyclic molecules. It is defined as $PI(G) = \sum_{e\in G}[n_{eu}(e|G)+ n_{ev}(e|G)]$, where $n_{eu}(e|G)$ is the number of edges of G lying closer to u than to v and $n_{ev}(e|G)$ is the number of edges of G lying closer to v than to u.

• Corresponding author. E-mail: ashrafi@kashanu..ac.ir

The most important works on the geometric structures of nanotubes, nanotori and their topological indices was done by Diudea and his co-authors.[14-20] In some research papers they computed the Wiener index of some nanotubes and nanotori. One of the present authors (ARA),[21-28] computed the PI index of some nanotube and hexagonal chains. In this paper, we continue this program to compute the Szeged and PI indices of a class of HC_5C_7 nanotubes. Our notation is standard and mainly taken from Cameron[29] and Trinajestic.[30]

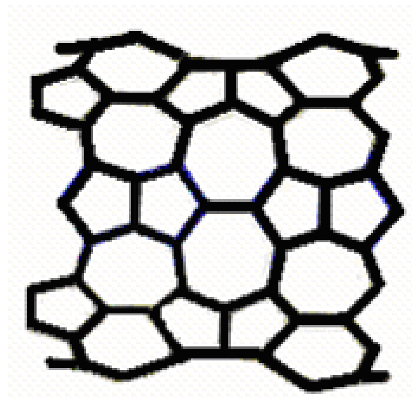

Fig. 1. A HC_5C_7 Nanotube.

2. Main results and discussion

Hexagonal systems are defined as finite connected plane graphs with no cut-vertices, in which all interior regions are mutually congruent regular hexagons. An important class of hexagonal systems are the graph representations of benzenoid hydrocarbons. More details on this important class of molecular graphs can be found in the book of Gutman and Cyvin[31] and in the references cited therein.

There are several paper related to computing the Szeged and PI indices of hexagonal systems. In this section, we consider the molecular graph of a HC_5C_7 nanotube which is not hexagonal. We first describe some notations which will be adhered to throughout. Let G be a simple molecular graph without directed or multiple. respectively. G is said to be connected if for every pair of vertices x and y there exists a path between x and y. In this paper we only consider connected graphs. The distance between a pair of vertices u and w of G is denoted by d(u,w). Suppose G is a graph, $e = xy$, $f = uv \in E(G)$ and $w \in V(G)$. Define $d(w,e) = \mathrm{Min}\{d(w,x), d(w,y)\}$. We say that e is parallel to f if $d(x,f) = d(y,f)$. In this case, we write $e \parallel f$. This relation is not necessarily symmetric or transitive. To prove the relation of parallelism is not reflexive, we consider a subgraph of T depicted by heavy lines in Figure 3. Suppose e = ab and f = cd. Then $e \parallel f$ but $b \nparallel a$. To prove $\parallel$ is not transitive, it is enough to consider the 2-dimensional lattice of a polyhex nanotorus, Figure 2. $e \parallel f$ and $f \parallel g$ but $e \nparallel g$.

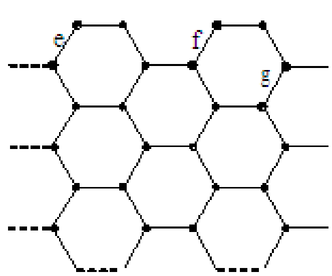

Fig. 2. The 2-Dimensional Lattice of a Polyhex Nanotorus.

In this section the Szeged and PI indices of T = $HC_5C_7[4p,8]$ nanotube are computed, where p is the number of parts of T, Figure 3.

2.1. Szeged Index of $HC_5C_7[4p,8]$

The aim of this section is computing the Szeged index of a $HC_5C_7[4p,8]$ nanotube T. To do this, we consider thirteen separate cases for an arbitrary edge e of T, Figures 3 and 4. In Table 1, some exceptional values for the vertices codistant to those of O = {σ, e_1, e_2, e_3, e_4, e_5, e_6, e_7, e_8, b_1, b_2, b_3, b_4} are computed, see Figure 3. Suppose f = uv ∈ O. In Table 1, the first number of each entry is $n_u(f)$, the second is $n_v(f)$ and the third is the number of codistant vertices from u and v.

Table 1. Some Exceptional Values of Sz(T).

p	**e_1**	**e_2**	**e_3**	**e_4**	**e_5**	**e_6**
4	48,58,22	34,67,27	82,22,24	65,43,20	91,15,22	34,60,34
5	64,74,22	45,84,31	98,30,32	81,59,20	106,22,32	50,76,34
6	80,90,22	57,98,37	114,41,37	97,75,20	80,58,22,	66,92,34
7	96,106,22	71,115,38	130,51,43	113,91,20	137,40,47	82,108,34
8	112,122,22	86,130,40	146,65,45	129,107,20	154,51,51	98,124,34
9	128,138,22	102,146,40	162,78,48	145,123,20	168,63,57	114,140,34
10	144,154,22	118,162,40	178,94,48	161,139,20	185,77,58	130,156,34
11	160,170,22	134,178,40	194,110,48	177,155,20	200,92,60	146,172,34

Table 1.(Continued)

p	**e_7**	**e_8**	**b_1**	**b_2**	**b_3**	**b_4**	**σ**
4	60,60,8	53,53,22	27,59,42	85,21,22	3,91,34	59,53,16	42,57,29
5	76,76,8	64,64,32	27,67,66	104,27,29	3,107,50	75,69,16	55,72,33
6	92,92,8	72,72,48	27,72,93	120,29,43	3,120,69	91,85,16	68,88,36
7	108,108,8	80,80,17	27,75,122	136,35,53	3,131,90	107,101,16	84,104,36
8	124,124,8	88,88,80	27,75,154	149,37,70	3,139,114	123,117,16	100,120,36
9	140,140,8	96,96,96	27,75,186	163,43,82	3,144,141	139,133,16	116,136,36
10	156,156,8	104,104,112	27,75,118	173,45,102	3,147,170	155,149,16	132,152,36
11	172,172,8	112,112,128	27,75,150	51,187,114	3,147,202	171,165,16	148,168,36

By calculations given in Table 1, we have the following:

Table 2. Some Exceptional Values of Sz(T).

P	1	2	3	4	5	6	7	8	9	10	11
Sz(T)	5452	4738	16882	28647	46312	68598	94375	125609	162116	203490	250549

One of the main results of this section is the following theorem:

Theorem 1. Suppose p ≥ 12. Then the Szeged index of a $HC_5C_7[4p,8]$ nanotube is as follows:

$$Sz(T) = \begin{cases} 9536p^3 - 16512p^2 - 3988p & \text{p is even} \\ 9536p^3 - 16384p^2 - 3508p & \text{p is odd} \end{cases}.$$

Proof. By Figure 3, there are 32 vertices between lines ω and ϖ. On the other hand, $HC_5C_7[4p,8]$ has exactly p parts similar to the region surrounded by ω and ϖ. Thus $|V(HC_5C_7[4p,8])| = 32p$. We now compute the value of $L_e = n_u(e)n_v(e)$ for an arbitrary edge e of T. Using Figure 3 and symmetries of a $HC_5C_7[4p,8]$ nanotube, one can see that it is enough to compute L_e for $e \in O$. Our main proof will consider a number of separate cases as follows:

Case 1. $L_\sigma = 256p^2 - 128p + 16$. Suppose σ = uv. By Figure 4(a) there are eight vertices codistant from u and v and so $n_u(\sigma) = n_v(\sigma) = 16p - 4$. This implies that $L_\sigma = 256p^2 - 128p + 16$.

Case 2. Assume that e_1 = uv, where u is the left side vertex of e_1, Figure 3. By Figure 4(b) there are 34 vertices codistant from u and v. On the other hand there are 16p – 4 vertices lying closer to u than to v and 16p – 30 vertices lying closer to v than to u. Thus $L_{e_1} = 256p^2 - 34p + 120$. A similar argument shows that $L_{e_2} = 256p^2 - 960p + 2016$, $L_{e_3} = 256p^2 - 320p - 21$, $L_{e_4} = 256p^2 - 768p - 1188$, $L_{e_5} = 256p^2 - 640p - 84$, $L_{e_6} = 256p^2 - 352p + 96$, $L_{e_7} = 256p^2 - 576p + 224$ and $L_{e_8} = 256p^2 - 304p + 70$.

Table 3. The Values of $n_u(e_i)$ and $n_v(e_i)$, $1 \le i \le 8$.

Edges	**e_1**	**e_2**	**e_3**	**e_4**
$n_u(e_i)$	16p-30	16p+24	16p+1	16p+18
$n_v(e_i)$	16p-4	16p-84	16p-21	16p-66
Parallel Edges	34	60	20	48
Edges	**e_5**	**e_6**	**e_7**	**e_8**
$n_u(e_i)$	16p-42	16p-16	16p-28	16p-5
$n_v(e_i)$	16p+2	16p-6	16p-8	16p-14
Parallel Edges	40	22	36	16

Case 3. Suppose b_1 = uv, where u is the upper vertex of b_1, Figure 3. By Figure 4(j) there are 32p – 150 vertices codistant from u and v. On the other hand there are 3 vertices lying closer to u than to v and 147 vertices lying closer to v than to u. Thus $L_{b_1} = 141$. If b_3 = xy then a similar argument as above shows that there are 32p – 102 vertices codistant from x and y, 27 vertices lying closer to x than to y and 75 vertices lying closer to y than to x. Thus $L_{b_3} = 2025$. We now assume that b_4 = rs, Figures 3 and 4(m). Then there are 16p – 48 vertices codistant from r and s. Also, 8p + 24 vertices are closet to r and 8p + 24 vertices are closer to s. Hence $L_{b_4} = 64p^2 + 384p + 576$. Finally, we consider b_2 = cd. To compute L_{b_2}, we consider two cases that p is odd or even. If p is odd then there are 16p – 62 codistant vertices from p and q. Also, there are 12p + 55 vertices closer to c and 4p + 7 vertices closer to d. So, $L_{b_2} = 48p^2 + 304p + 385$. If p is even then there are 16p – 58 codistant vertices from p and q, 12p + 53 vertices closer to c and 4p + 5 vertices closer to d. This implies that $L_{b_2} = 48p^2 + 272p + 265$.

Therefore, $Sz(G) = \sum_{e=uv\in E(G)} n_u(e)n_v(e) = 4p(L_\sigma + \sum_{i=1}^{8} L_{e_i} + L_{b_2}) + 2p(L_{b_1} + L_{b_3} + L_{b_4})$ and by Cases 1-3, the theorem is proved. ■

2.2. PI Index of $HC_5C_7[4p,8]$.

In this section, the PI index of the graph T = $HC_5C_7[4p,8]$ were computed. We assume that E = E(T) is the set of all edges of T and $N(e) = |E| - (m_u(e) + m_v(e))$. Then $PI(T) = |E|^2 - \sum_{e\in E} N(e)$. Hence to compute PI index of T, it is enough to compute the value of N(e), for an arbitrary edge of

T. John, Khadikar and Singh[13] introduced a method named “orthogonal cut” which is useful for computing PI index of bipartite graphs. This method is not work in our example, because T is not bipartite.

In Table 4, some exceptional values for the edges parallel to those of O are computed, Figure 3. Suppose $f = uv \in O$. In this table, each entry denotes the number of parallel edges to those of O.

Table 4. The Number of Parallel Edges to Those of Edges of O.

p	$N(e_1)$	$N(e_2)$	$N(e_3)$	$N(e_4)$	$N(e_5)$	$N(e_6)$	$N(e_7)$	$N(e_8)$	$N(b_1)$	$N(b_2)$	$N(b_3)$	$N(b_4)$	$N(\sigma)$
4	53	35	29	34	37	32	40	24	53	30	62	32	12
5	52	49	29	45	49	32	48	24	71	45	98	50	12
6	52	60	29	53	50	32	48	23	98	61	137	72	12
7	52	68	28	60	56	32	51	23	128	80	179	94	12
8	52	78	29	65	56	32	50	23	164	100	225	118	12
9	51	81	28	67	57	32	51	23	203	123	271	140	12
10	52	85	28	68	56	32	50	23	245	145	317	164	12

By calculations given in Table 4, we have the following table:

Table 5. Some Exceptional Values of Sz(T).

P	1	2	3	4	5	6	7	8	9	10
Sz(T)	1691	6736	15390	27464	43010	62412	85134	11408	141444	175040

We are ready to prove the second main results of this section.

Theorem 2. The PI index of a $HC_5C_7[4p,8]$ nanotube is computed as follows:

$$PI(T) = \begin{cases} 1794p^2 - 448p & p \text{ is even} \\ 1794p^2 - 4428p & p \text{ is odd} \end{cases}.$$

Proof. By Figure 3, there are 46 edges between lines ω and ϖ. On the other hand, $HC_5C_7[4p,8]$ has exactly p parts similar to the region surrounded by ω and ϖ. Thus $|E(HC_5C_7[4p,8])| = 46p$. We now compute the value of N(e), for an arbitrary edge e of T. Using Figure 3 and symmetries of a $HC_5C_7[4p,8]$ nanotube, one can see that it is enough to compute N(e) for $e \in O$, $O = \{\sigma, e_1, e_2, \ldots, e_8, b_1, \ldots, b_4\}$. Using Figure 5(a-m) and a similar argument as Theorem 1, one can see that $N(\sigma) = 12$, $N(e_1) = 51$, $N(e_3) = 28$, $N(e_6) = 32$, $N(e_8) = 23$, $N(b_1) = 46p - 215$ and $N(b_3) = 46p - 143$. On the other hand,

$$N(e_2) = \begin{cases} 87 & 2 \nmid p \\ 86 & 2 \mid p \end{cases}; \quad N(e_4) = \begin{cases} 69 & 2 \nmid p \\ 68 & 2 \mid p \end{cases}; \quad N(e_5) = \begin{cases} 56 & 2 \nmid p \\ 57 & 2 \mid p \end{cases}$$

$$N(e_7) = \begin{cases} 50 & 2 \nmid p \\ 51 & 2 \mid p \end{cases}; \quad N(b_2) = \begin{cases} 23p - 85 & 2 \nmid p \\ 23p - 84 & 2 \mid p \end{cases} \text{ and } N(b_2) = \begin{cases} 23p - 67 & 2 \nmid p \\ 23p - 66 & 2 \mid p \end{cases}$$

On the other hand, $PI(T) = |E|^2 - \sum_{e \in E(T)} N(e) = 2116p^2 - 4p\,(\sum_{i=1}^{8} N(e_i) + N(\sigma) + N(b_2)) - 2p(N(b_1) + N(b_3) + N(b_4))$. This completes the proof. ■

A Gap Program for Computing PI and Szeged Indices of Molecular Graphs

```
f:=function(M)
local l, ss, S, T, e, tt, dd, g, gg, ddd, gg1, g1, h, gg2, g2, uu1, v1, T1, q, h3, B3, BB, i, j, k, U1, S1,
V1, a, b, ii, jj, q1, a2;
 l:=Length(M); ss:=0; S:=[]; T:=[]; e:=[]; tt:=0; dd:=[]; g:=[]; gg:=[]; ddd:=[]; gg1:=[]; g1:=[];
h:=[]; gg2:=[]; g2:=[]; uu1:=0; v1:=0; S1:=[]; T1:=[]; q:=0; B3:=[]; h3:=[]; BB:=[];
for i in [1..l]do
for j in[i+1..l] do
if M[i][j]=1 then
Add(e,[i,j]);
fi;
od;
```

```
od;
for a in e do
for i in [1..l] do
if M[a[1]][i]>M[a[2]][i]  then
AddSet(S,i);
fi;
if M[a[1]][i]<M[a[2]][i]  then
AddSet(T,i);
fi;
od;
ss:=ss+Length(S)+Length(T);Add(dd,Length(S)+Length(T));
tt:=tt+Length(S)*Length(T);Add(ddd,Length(S)*Length(T));
T:=[];S:=[];
od;
Sort(dd);
U1:=[];V1:=[];q1:=0;
S1:=[];
T1:=[];
ii:=0;jj:=0;
for a in e do
for b in e do
AddSet(U1,M[a[1]][b[1]]);
AddSet(U1,M[a[1]][b[2]]);
AddSet(V1,M[a[2]][b[1]]);
AddSet(V1,M[a[2]][b[2]]);
if V1[1]<U1[1] then
AddSet(T1,b);
fi;
if V1[1]>U1[1] then
AddSet(S1,b);
fi;
U1:=[];V1:=[];
od;
ii:=ii+Length(S1)+Length(T1);
jj:=jj+Length(S1)*Length(T1);
Add(h,Length(e)-(Length(S1)+Length(T1)));
S1:=[];T1:=[];q1:=q1+1;
od;
Sort(h);
for i in dd do
for j in dd do
if j=i then
Add(g,j);
fi;
od;
AddSet(gg,g);g:=[];
od;
Sort(ddd);
for i in ddd do
for j in ddd do
if j=i then
Add(g1,j);
fi;
od;
AddSet(gg1,g1);g1:=[];
od;
Print("************************************************************","\n");
```

```
Print("\n"); Print("Number of edges for this Graph is: ,Length(e),"\n"); Pint("\n"); Print("\n");
Print("PI Polynomial= ");
for i in h do
for j in h do
if j=i then
Add(g2,j);
fi;
od;
AddSet(gg2,g2);g2:=[];
od;
for i in [1..Length(gg2)-1] do
Print(Length(gg2[i]),"x^");Print(Length(e)-gg2[i][1]);Print("+");
uu1:=uu1+Length(gg2[i])*(Length(e)-gg2[i][1]);
od;
a2:=Length(gg2);
Print(Length(gg2[a2]),"x^"); Print(Length(e)-gg2[a2][1],"\n"); Print("\n");Print("\n");
Print("Szeged Index=",tt,"\n"); Print("\n"); Print("\n");
Print(" PI Index is= ",ii,"\n"); Print("\n");
Print("\n");
Print("*********************************************************","\n");
return;
end;
```

To compute the PI and Szeged indices of molecular graphs, we first draw it by HeperChem.[32] Then we apply TopoCluj software of Diudea and his team[33] to compute adjacency and distance matrices of the molecular graph under consideration. We now upload A and D in our GAP program[34] to compute the PI and Szeged indices of a molecular graph. Using this program we obtain eleven exceptional cases that $1 \le p \le 11$. Our method can be applied to compute the PI and Szeged indices of nanotubes and tori presented by Diudea and his co-authors.[13-20,35,36]

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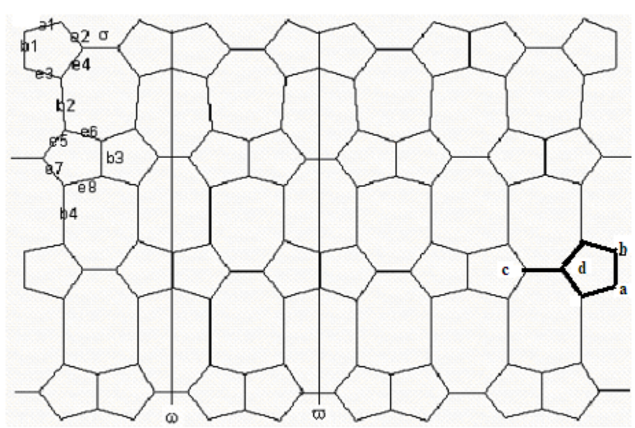

Fig. 3.The 2-Dimensional Lattice of $HC_5C_7[16,8]$ nanotube.

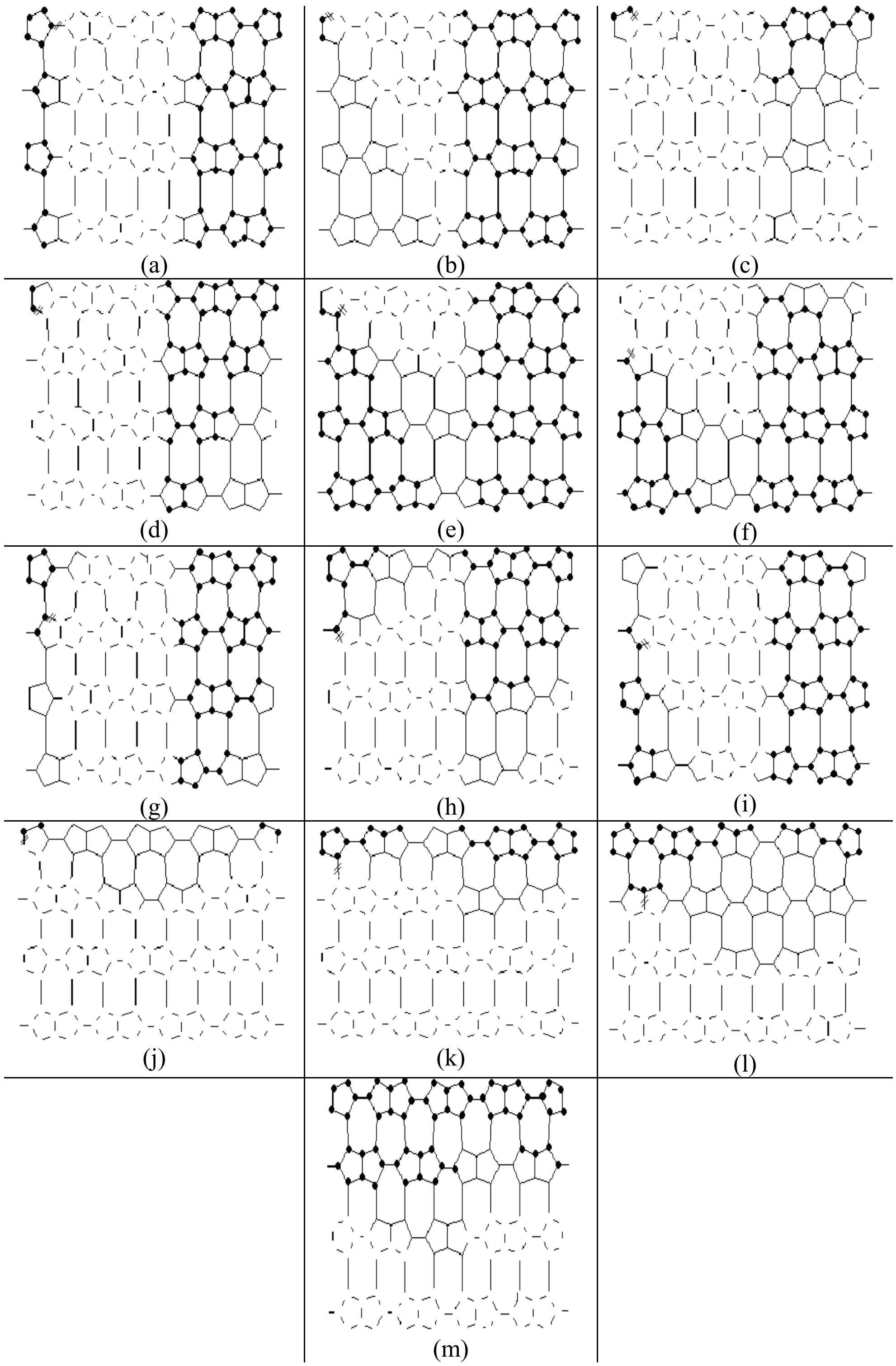

Fig. 4. Thirteen Cases of Codistant Vertices of an Edge in a HC_5C_7 Nanotube.

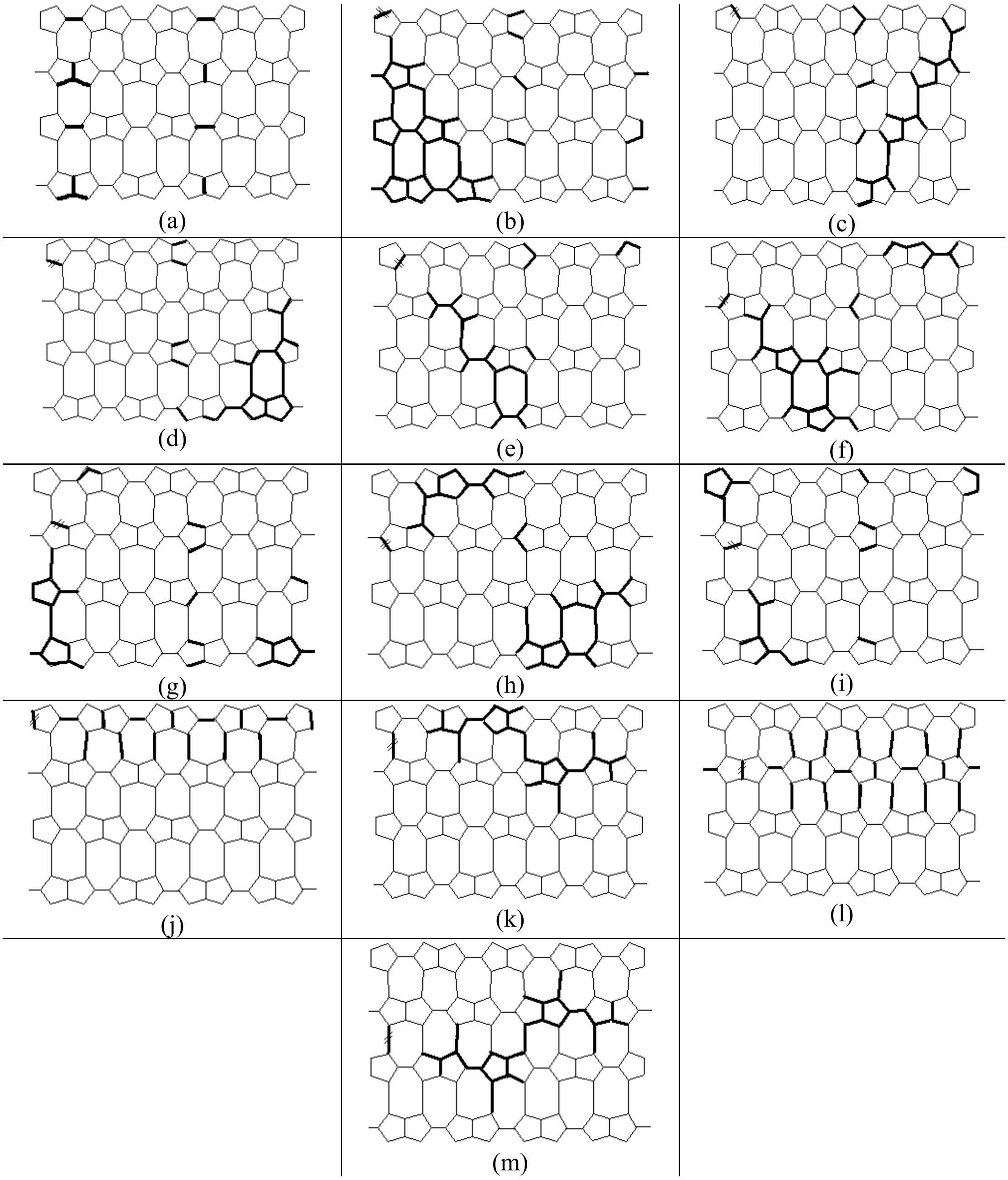

Fig. 5. Thirteen Separate Cases of Parallel Edges in a HC_5C_7 Nanotube.

References

[1] E. Cornwell, J. Chil. Chem. Soc. **51** (1), 765 (2006).
[2] H. Wiener, J. Am. Chem. Soc. **69,** 17 (1947).
[3] R. Todeschini and V. Consonni, Handbook of Molecular Descriptors, Wiley, Weinheim, 2000.
[4] D.E. Needham, I.C. Wei, P.G. Seybold, J. Am. Chem. Soc. **110,** 4186 (1988).
[5] G. Rucker and C. Rucker, J. Chem. Inf. Comput. Sci. **39,** 788 (1999).
[6] I. Gutman, Graph Theory Notes of New York **27,** 9 (1994).
[7] M. V. Diudea and I. Gutman, Croat. Chem. Acta **71** (1), 21 (1998).
[8] O. M. Minailiuc, G. Katona, M. V. Diudea, M. Strunje, A. Graovac and I. Gutman, Croat. Chem. Acta **71**(3), 473 (1998).
[9] P. V. Khadikar, Nat. Acad. Sci. Lett. **23,** 113 (2000).
[10] P. V. Khadikar; P.P. Kale; N.V. Deshpande; S. Karmarkar and V.K. Agrawal, J. Math. Chem. **29,** 143 (2001).
[11] P.V. Khadikar; S. Karmarkar, J. Chem. Inf. Comput. Sci. **41,** 934 (2001).
[12] P.V. Khadikar, S. Karmarkar and R.G. Varma, Acta Chim. Slov. **49,** 755 (2002).
[13] P. E. John, P.V. Khadikar and J. Singh, J. Math. Chem. (In press).
[14] M.V. Diudea and A. Graovac, MATCH Commun. Math. Comput. Chem. **44,** 93 (2001).
[15] M.V. Diudea, I. Silaghi-Dumitrescu and B. Parv, MATCH Commun. Math. Comput. Chem. **44,** 117 (2001).
[16] M.V. Diudea and P.E. John, MATCH Commun. Math. Comput. Chem. **44,** 103 (2001).
[17] M. V. Diudea, Bull. Chem. Soc. Jpn. **75,** 487 (2002).
[18] M. V. Diudea, MATCH Commun. Math. Comput. Chem. **45,** 109 (2002).
[19] P. E. John and M. V. Diudea, Croat. Chem. Acta **77,** 127 (2004).
[20] M.V. Diudea, M. Stefu, B. Parv and P.E. John, Croat. Chem. Acta, **77**, 111 (2004).
[21] A.R. Ashrafi and A. Loghman, MATCH Commun. Math. Comput. Chem., **55,** 447 (2006).
[22] S. Yousefi and A.R. Ashrafi, MATCH Commun. Math. Comput. Chem., **56,** 169 (2006).
[23] A.R. Ashrafi and A. Loghman, Ars Combinatoria, **80,** 193 (2006),.
[24] A.R. Ashrafi and A. Loghman, J. Comput. and Theor. Nanosci., **3**(3), 378 (2006).
[25] A.R. Ashrafi and A. Loghmam, J. Chilean Chem. Soc. **51**(3), 968 (2006).
[26] A.R. Ashrafi and F. Rezaei, MATCH Commun. Math. Comput. Chem. **57,** 243 (2007).
[27] A. R. Ashrafi and S. Yousefi, MATCH Commun. Math. Comput. Chem., **57** (2), 403 (2007).
[28] S. Yousefi and A. R. Ashrafi, J. Math. Chem. **42**(4), 1031 (2007).
[29] P.J. Cameron, Combinatorics: Topics, Techniques, Algorithms, Cambridge University Press, Cambridge, 1994.
[30] N. Trinajstic, Chemical Graph Theory, CRC Press, Boca Raton**,** FL. 1992.
[31] Gutman, I.; Cyvin, S.J. Introduction to the Theory of Benzenoid Hydrocarbons; Springer-Verlag: Berlin, 1989.
[32] HyperChem package Release 7.5 for Windows, Hypercube Inc., 1115 NW 4th Street, Gainesville, Florida 32601, U. S. A. 2002.
[33] M. V. Diudea, O. Ursu and Cs. L. Nagy, TOPOCLUJ, Babes-Bolyai University, Cluj **2002.**
[34] The GAP Team, GAP, Groups, Algorithms and Programming, Lehrstuhl De für Mathematik, RWTH, Aachen, 1995.
[35] M. V. Diudea, B. Parv and E. C. Kirby, MATCH Commun Math Comput Chem **47,** 53 (2003**)**.
[36] M. V. Diudea and E. C. Kirby, Fullerene Sci Technol **9,** 445 (2001),.