communications in mathematical
match
and in computer chemistry

no. 43, March 2001

ISSN 0340-6253

MATCDY (43) 7-15 (2001)

SZEGED INDICES OF HEXAGONAL CHAINS

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Received July 1999,

Abstract

The Szeged index (Sz) is a topological index based on distances between vertices of a graph. In this communication we introduce combinatorial formulas for the Szeged index (Sz) of hexagonal chains namely linear polyacenes, zig-zag fibonacenes, helicenes and polyphenylenes. In addition, we have also discussed the correlation of Sz for these benzenoid hydrocarbons with the Wiener index (W) and the results are critically discussed. It was proposed that the expresion $[T_{h+1} - 3T_h + 3T_{h-1} - T_{h-2}]$ where T is W or Sz, is a unique invariant.

Introduction

The Szeged index (Sz), introduced and named by Gutman et al [1,2], was found to be correlated with a variety of physico-chemical as well as biological properties [3-6]. Some properties of Sz are also reported[7-10]. Formulas for the calculation of Szeged index (Sz) for benzenoid hydrocarbons from the elementary cuts were reported recently [11-16]. It has also been demonstrated that in the case of trees the Sz index coincides [9] with Wiener index (W) and thus Sz is considered as the generalization of W for cyclic graphs. In the present communication,we introduce combinotorial formulas for estimating Sz for polyacenes, fibonacenes, helicenes and polyphenylenes and correlating them with their respective W

indices. The relations between the Sz and W for thes benzenoid systems are critically discussed. Based on the results we have proposed a new graph invariant.

Definition of Szeged index (Sz)

Let u and v be the vertices of a graph G, then the number of edges in a shortest path connecting them is said to be their distance and is denoted by d(u,v).

Let e=(u,v) be an edge of the graph G. Denote by $n_u=n_u(e)$ and $n_v=n_v(e)$ the number of elements of the vetex sets $\{w|d(w,u)<d(w,v)\}$ and $\{w|d(w,v)<d(w,u)\}$, respectively. In other words, $n_u(e)$ is the number of vertices of G lying closoer to one end point of the edge e (namely to the vertex u) than to its another end point (namely to the vertex v). Analogously, n_v (e) counts the vertices lying closer to v than u, then the Szeged index (Sz) is defined as

$$Sz= Sz(G) = \sum_{e} n_u(e)\, n_v(e) \qquad (1)$$

with the summation going aver all edges of the graph G.

Hexagonal chains

Frank Harary was the first to realize that hexagonal systems (or , as named by him "hexagonal animals") are very attractive objective for graph theoretical studies and he was the first to initiate series of mathematical investigations on these types of graphs [17]. A hexagonal chain is a hexagonal system with the properties that (i)it has no vertex belonging to three hexagons and (ii) it has no hexagon with more than two adjacent hexagons. Hexagonal chains are extremal in the Harary-Harborth sense:they posses a maximum number of vertices and a maximum number of edges for a given number of hexagons.

Hexagonal systems are of great importance for theoretical chemists because they are the natural graph representation of benzenoid hydrocarbons [18]. A considerable amount of research in mathematical chemistry has been devoted to hexagonal systems [17,18]. Hexagonal chains are the graph representatives of an important subclass of benzenoid molecules, namely of the so called unbranched catacondensed benzenoids.The structure of these graphs is apparently the simplest among all hexagonal systems. Therefore, it is not surprising that a great deal of mathematical and mathematico-chemical results known in the theory of hexagonal systems apply, in fact, only to hexagonal chains [19-23].

In harmony with Harary's original definition of a hexagonal animal the following notation and terminology will be used throughout this paper. The hexagonal chains considered by us include geometrical planar molecules.

The number of hexagons in a hexagonal chain C is denoted by h. All hexagonal chains with h hexagons have 4h+2 vertices and 5h+1 edges. The set of all hexagonal chains with h hexagons will be denoted by C_h .

In the present paper, we shall be mainly concerned with molecular graphs G_h, whose general formula is given by

Fig.1. G_h

Here G_o denotes an arbitrary (not necessarily benzenoid) terminal fragment to which a chain of h linearly annelated hexagons is attached.

Szeged index (Sz) for linear polyacenes (L_h)

In the simplest case when G_o is isomorphic to the path P_L i.e.when G_o consists of two mutually connected vertices, G_h reduces to the molecular graph of linear polyacenes L_h, its structure is shown in Fig. 2.

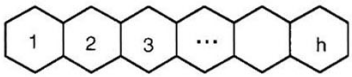

Fig. 2. The molecular graph of polyacenes (L_h)

By the definition of Szeged index (Sz) we see that Sz for L_h is given by:

$$Sz(L_h)=(h+1)(2h+1)^2+4[3(4h-1)+7(4h-5)+.....+.....+3(4h-1)]$$

$$=(h+1)(2h+1)^2+4\sum_{k=1}^{h}(4k-1)(4h-4k+3) \qquad (2)$$

Recall that,

$$\sum_{k=1}^{h} k=h(h+1)/2 \qquad (3)$$

and

$$\sum_{k=1}^{h} k^2 = h(h+1)(2h+1)/6 \qquad (4)$$

Considering the Eqns. 3 and 4 , Eq.2 gives

$$Sz(L_h) = 1/3[44h^3 + 72h^2 + 43h + 3] \qquad (5)$$

From Eq. 5 we see that for all molecular graphs of the form G_h the Szeged index (Sz) is a cubic polinomial of the number of linearly annelated hexagons.

Szeged index (Sz) for zig-zag chain (fibonacene) (F_h)

The molecular structure of the zig-zag benzenoids called fibonacence is shown in Fig. 3.

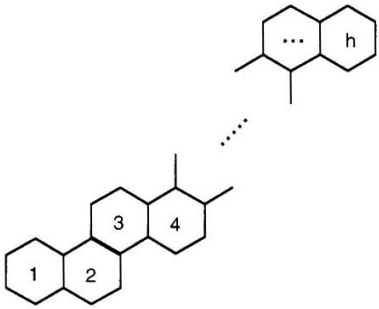

Fig. 3. The molecular graph of zig-zag fibonacenes (F_h)

The Szeged indez (Sz) for F_h (zig-zag fibonacene) is considered under two cattagories namely: (i) when h=2n and (ii) when h=2n+1.

Case I, h=2n

Consider now F_h with different types of edges as shown in Fig. 4.

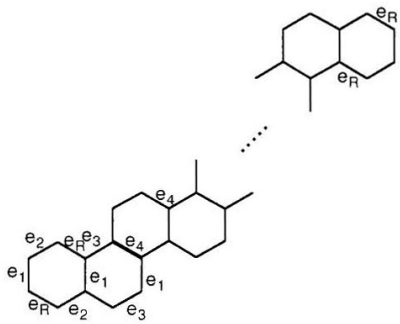

Fig. 4. The molecular graph of F_h with different types of edges.

From Fig. 4 and by the definition of Sz (Eq. 1) we find that

(i) Contribution to Sz (G_{2h}) of F_h due to edges of type e_1 is given by

$$3\sum_{k=1}^{n} (8k-3)(8n-8k+5) \tag{6}$$

(ii) Contribution to Sz(G_{2h}) of F_h due to edges of type e_2 is given by

$$2\sum_{k=1}^{n} (8k-5)(8n-8k+7) \tag{7}$$

(iii) Contribution to Sz(G_{2h}) of F_h due to edges of type e_3 is given by

$$2\sum_{k=1}^{n} (8k-1)(8n-8k+3) \tag{8}$$

(iv) Contribution to Sz(G_{2h}) of F_h due to edges of type e_4 is given by

$$3\sum_{k=1}^{n-1} (8k+1)(8n-8k+1) \tag{9}$$

(v) Contribution to Sz(G_{2h}) of F_h due to edges of type e_k is given by

$$4.3.(8n-1) \tag{10}$$

Summing the contribution to Sz due to all the edges of F_h we can obtain the Szeged index (Sz) of F_h. Thus, through long mathematical calculations we have

$$Sz(G_{2h})=1/3[320\,n^3+240\,n^2+214n-45] \quad (11)$$

Case II: h=2n+1

In this case, when h=2n+1, the contribution to $Sz(G_{2h+1})$ due to edges of the type e_1, e_2, e_3, e_4, and e_k are given by the Eqns. 12-16 respectively.

$$3\sum_{k=1}^{n} (8k-3)(8n-8k+9)+2.3(8n+3) \quad (12)$$

$$2\sum_{k=1}^{n} (8k-5)(8n-8k+11)+2.3(8n+3) \quad (13)$$

$$2\sum_{k=1}^{n} (8k-1)(8n-8k+7); \quad (14)$$

$$3\sum_{k=1}^{n} (8k+1)(8n-8k+5); \quad (15)$$

and $$(2).(3)\ (8n+3). \quad (16)$$

Once again, summing the Eqns. 12-16 and through series of mathematical calculations, we have

$$Sz(G_{2h+1})=2/3[160\,n^3+360\,n^2+347n+81] \quad (17)$$

General formula for Sz of zig-zag fibonacenes (F_h)

If now we replace n by h/2 in Eq. 11 and n by (h-1)/2 in Eq.17, we have a general expression for estimating Sz for fibonacenes which is applicable to the values of n (odd or even). In doing so we have

$$Sz(F_h)=1/3[40h^3+16\,h^2+107h-45] \quad (18)$$

Szeged index (Sz) for helicenes (H_h)

The molecular graph of helicenes (H_h) is shown in Fig. 5.

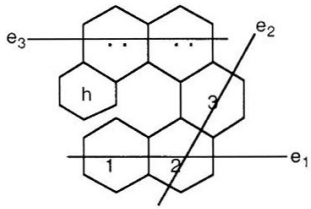

Fig. 5. Molecular graph of helicenes (H_h)

In this we will have to consider the contributiuons to $Sz(H_h)$ due to the edges of the type e_1, e_2 and e_3. Adding their contributions we obtained an expression for estimating Sz of H_h. The expression so obtained is found to be:

$$Sz(H_h)=1/3[16h^3+204\ h^2\ -157h+99] \qquad (19)$$

Szeged index for polyphenylenes

Let there be h hexagons in the polyphenylene as shown in Fig. 6.

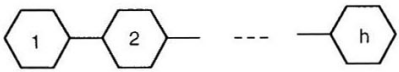

Fig. 6. Molecular graphs of polyphenylenes (G)

The Szeged index (Sz), through a series of long mathematical calculations, is found to be given by:

$$Sz=SZ(G)= \quad 6\sum_{k=1}^{h} (6k-3)(6h-6k+3)+ \sum_{k=1}^{h} 6k(6h-6k)$$

which on simplification gives

$$Sz=Sz(G)=6h(7h^2\ +2) \qquad (20)$$

Recall that here G stands for molecular graph of polyphenylenes.

Correlation between Wiener (W) and Szeged (Sz) indices of benzenoid molecules

The expressions for the estimation of Wiener indices (W) of L_h, F_h and H_h were reported earlier and are written as:

$$W(L_h)=1/3[16h^3+36\ h^2\ +26h+3]; \qquad (21)$$

$$W(F_h)=1/3[16h^3+24\ h^2\ +62h-21]; \qquad (22)$$

and $$W(H_h)=1/3[8h^3+72\ h^2\ -26h+27] \qquad (23)$$

In order to examine the correlation between the Wiener (W) and Szeged indices (Sz) of the benzonoid systems under present investigation we have designed sets of corresponding graphs, each containing 100 elements.

The Sz and W values were calculated from the respective expressions. Then, Sz indices were plotted against W indices of L_h, F_h and H_h respectively. The statistical analysis [24] indicated that they are linearly correlated as expressed by the following expression:

$$Sz=aW+b \tag{24}$$

where a and b are the statistical parametrs involved.

General observations

Note that W and Sz for the benzenoid hydrocarbons considered in the present study are cubic in h. Therefore, if we use T to represent W or Sz for such systems then we can write

$$T_h = ah^3+bh^2+ch+d] \tag{25}$$

then T_{h+1} will be

$$= T_h+3ah^3+(3a+2b)h+a+b+c \tag{26}$$

Threfore,

$$T_h = T_{h+1}+3a(h-1)^2+(3a+2b)(h+1)+a+b+c \tag{27}$$

Subtracting Eq. 27 from Eq. 26 we obtain:

$$T_{h+1}-2\,T_h + T_{h-1} = 6ah+2b \tag{28}$$

Therefore,

$$\frac{T_{h+1} + T_{h-1}}{2} - T_h = 3ah+b \tag{29}$$

Replacing h by (h-1) Eq. 28 reduces to

$$T_h - 2T_{h-1}+T_{h-2} = 6a(h-1)+2b \tag{30}$$

Subtracting Eq. 30 from Eq. 21, we get

$$T_{h+1} - 3T_h+3T_{h-1} -T_{h-2} = 6a \tag{31}$$

This means that for a given hexagonal chain of h hexagons, the expression

$$T_{h+1} - 3T_h+3T_{h-1} -T_{h-2}$$

is an invariant and its value is 6a.

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