Computation of the Sadhana (Sd) Index of Linear Phenylenes and Corresponding Hexagonal Sequences

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(*Received: June 2, 2009*)

ABSTRACT

The Sadhana index (Sd) is a newly introduced cyclic index. Efficient formulae for calculating the Sd (Sadhana) index of linear phenylenes are given and a simple relation is established between the Sd index of phenylenes and of the corresponding hexagonal sequences.

Keywords: Sd index, PI index, phenylenes, hexagonal chain.

1. INTRODUCTION

It is well established that structural information of molecule is precisely represented by a molecular graph [1]. Such a molecular graph is obtained by deleting all the carbon hydrogen as well as hetero-hydrogen bond from the molecular structure. In molecular graph the atoms are called vertices and are usually denoted by a dot '**.**', while the bonds are called edges, and are represented by a small line '_'. No distinction is made among single, double, triple, and aromatic bond and also among constituting atoms. A molecular graph has provided the chemist with a versatile parameter called topological index. The topological

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index is a numerical representation of the molecule, usually obtained by imposing certain conditions on atoms, vertices, or both. A plethora of topological indices are reported is the literature [2-6]. The first, oldest and widely used topological index is the Wiener (W) index [7]. Such a proliferation is still going on and is becoming counterproductive.

As stated above, the first, oldest and even today widely used molecular descriptor is the Wiener number [7], which was then renamed as Wiener index by Hosoya [8]. The Wiener index is principally advocated in the year 1947 for acyclic compounds (trees) and it remained unattended for 25 years. It was in 1972 that Hosoya [8] described its calculation using the distance matrix.

In 1994 Gutman introduced another W-like topological index which he called Szeged index, abbreviated as Sz [9]. It is worth mentioning that no name was given to the index introduced by Gutman in 1994. It was in 1995 that Gutman and Khadikar named this index as Szeged index and abbreviated as Sz [10]. Since Sz and W indices of acyclic graphs coincide, Khadikar to remove this lacuna, proposed another index in 2000, which he named Padmakar-Ivan index and abbreviated as PI [11-15]. The PI index of acyclic and cyclic graphs differs. However, the main interest of proposing a topological index for cyclic graph alone remained unresolved. Consequently, once again, in the year 2002 Khadikar proposed yet another index which he named Sadhana index and abbreviated as the Sd index[16]. At that time no mathematical definition was given to this index.

It is interesting to mention that Sz, PI and Sd indices are W-like indices having similar decrementing power. The ways in which these indices are proposed clearly indicate that there is one-to-one correlation among these four indices. Also, there is close correspondence in defining these indices as well. The Wiener index counts the number of vertices on both sides of an edge; the Szeged index makes account of number of vertices closer to both the ends of an edge; the PI index on the other hand sum up the number of edges on both the ends of an edge, and finally, Sadhana index sum up the number of edges on both the sides on an elementary cuts.

In the existing literature there are numerous reports on applications of the Wiener index; more than 100 applications of the Szeged index; and 150 cases of the PI index. Compared to these three indices, in the case of recently introduced Sadhana index lot more investigations are yet to be made.

In view of the above we have undertaken the present investigation in that by giving mathematical definition we have computed Sd index of phenylene and is the primary objective of the present study. Another objective of the present study is that phenylenes are responsible for the formation of V-phenylenic nanotubes and nanotori and the results obtained here in will be useful for solving the problems related to V-phenylenic Nanotubes and nanotori. In addition, in the present paper we provide a simple relationship between Sd index of phenylenes and of the corresponding hexagonal chains.

2. DEFINITIONS AND NOTATIONS

Let G = G(S) = (V,E) denote a connected planar graph which corresponds to the chemical structure S. V = V(G) = {1,2,…,n} denote the *vertex set* and E = E(G) = { e_1 , e_2 ,… , e_m } is the *edge set* of graph G (n = n(G), m = m(G)). The graph P = P(i, j) denote a *path* connecting the (end) vertices i, j ∈V(G). Clearly, the *length* of P, denoted by l(P), is the number of edges of graph P (l(P) = m(P)). The *distance* d(i, j) is the length of a shortest path connecting vertices i, j ∈V(G). For edge e = (i, j) ∈ E(G) let V(G; i(e)) = {k ∈ V(G)/ d(i, k) <d(j, k)} the *set* of all vertices which lie nearly to vertex i than to vertex j of G, and let n(i(e)) = n(V(G; i(e))) = / V(G; i(e))/ the *number* of this vertices.

The *Wiener index* W = W(G) was first defined for a tree G = T by the following expression:

$$W = W(T) = 1/2 * \Sigma\, d(i,j), \tag{1}$$

Where the summation going over all pairs (i, j) of vertices i, j ∈ V(G), or by

$$W = W(T) = \Sigma n(i(e)) * n(j(e)), \tag{2}$$

Where the summation going over all edges e = (i, j) ∈ E(G). The *Szeged index* Sz(G) of graph G is defined (see also equations (1),(2)) by

$$Sz(G) = \Sigma n\ (i(e)) * n(j(e)) \tag{3}$$

The right-hand side of Eq.(3), although formally identical to the right-hand side of eq.(2),differs in the interpretation of n(i(e)) and n(j(e)) . In the former case, eq.(2), they are the number of vertices of G lying on two sides of the edge e . While in case of eq.(3), if we define an edge e = (i, j), then n(i(e)) is the number of vertices closer to i than j, and n(j(e)) is the number of vertices closer to j than i ; vertices equidistant to i and j are not counted.

A graph G is called *bipartite* if the vertex set V(G) is the union of two disjoint colored vertex sets $V_b(G)$ of black and V_w (G) of white vertices such that every edge connect a black vertex with a white one. For a bipartite graph G edges e = (k,l), e' = (k',l') ∈ E(G) are called *codistant* (briefly denoted by " e *co* e' ") if d (k,k') = d(l,l') = r and d(k,l') = d(k',l) = r + 1, or vice versa (r = 0,1,2,…). Let E(G; e) ={e'∈ E(G)/ e' *co* e} denote the set of all edges e' which are codistant to edge e of graph G. If all edges e, e', e'' ∈ E(G, e) satisfy

(i) e *co* e ,
(ii) From e *co* e' follow e' *co* e, and
(iii) From e *co* e' and e' *co* e'' follow e *co* e'',

then E(G;e) is called a *strongly codistant edge set* of G. If the edge set E(G) of bipartite graph G is the union of c pair wise disjoint strongly codistant edge sets $E_1 = E_1(G)$, $E_2 = E_2(G),\ldots, E_c = E_c(G)$, graph G is called a *strongly codistant graph* (briefly: *sco* graph). For s = 1, 2,…, c let $m_s = m_s(G) = / E_s(G) / = / E_s /$ denote the edge number of E_s. The set $E_s(G)$ is called an *orthogonal cut* of *sco* graph G, and integer c = c(G) denote the number of orthogonal cuts of G.

The *Padmakar-Ivan index* PI(G) for a bipartite *SCO* graph G is defined by (s = 1, 2,…, c)

$$PI(G) = \Sigma\, m_s(G) * (m(G) - m_s(G)) \quad (4)$$

From a simple calculation follow

$$PI(G) = [m(G)]^2 - \Sigma[\, m_s(G)]^2 \quad (5)$$

The *Sadhana index* Sd(G) of a bipartite *SCO* graph G is defined (for summation index s = 1,2,…,c) by

$$Sd(G) = \Sigma\, (m(G) - m_s(G)) \quad (6)$$

For *SCO* graph G is $\Sigma\, m_s(G) = m(G)$ and with definition (6) follow immediately

$$\begin{aligned} Sd(G) &= \Sigma\, (m(G) - m_s(G)) \\ &= m(G) * c(G) - m(G) \\ &= m(G) * (c(G) - 1) \end{aligned} \quad (7)$$

For a tree G = T is every $m_s(G) = 1$, and c(T) = m(T):

$$\begin{aligned} Sd(T) &= m(T)*(c(T) - 1) \\ &= m\,(T)*(m(T) - m_s(T)) \\ &= [m\,(T)]^2 - m(T)*\, m_s(G) \\ &= [m\,(T)]^2 - c(T)*\, m_s(G) \\ &= [m\,(T)]^2 - \Sigma[\, m_s(T)]^2 \\ &= PI(T) \end{aligned}$$

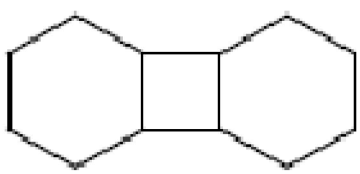
For a circuit G = C (of even length) is every $m_s(G) = 2$ (s = 1, 2,…, c(G)) and c(C) = ½*m(C), we find

$$\begin{aligned} Sd(C) &= m(C)*(c(C) - 1) \\ &= m(C)*\, (1/2*m(C) - 1) \\ &= ½*m(C)*(m(C) - 2) \\ &= ½*\{[m(C)]^2 - 2*m(C)\} \\ &= ½*\{[m(C)]^2 - (½*m(C))*(2^2)\}\} \end{aligned}$$

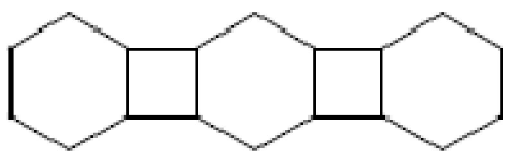
$$= ½*\{[m(C)]^2 – Σ[m_s(T)]^2 \}$$
$$= ½*PI(C)$$

3. PHENYLENES AND THEIR HEXAGONAL SQUEEZES

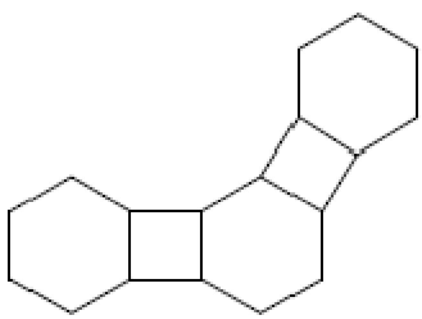
Phenylenes are a class of polycyclic non-benzenoid alternate conjugated hydrocarbons in that the carbon atoms form 6- and 4-membered cycles. Each 4-membered cycle (= square) is adjustment to two disjoined 6-membered cycles (= hexagons), and no two hexagons are adjustment. Their respective molecular graphs are also referred to as phenylenes. The number of hexagons is a phenylene is denoted by h, and then we speak about an [h] phenylene [17]. The simplest phenylene has h = 2, this is the well-known bi-phenylene (I). Starting with h = 3 here exist several isomeric [h] phenylenes. In particular there are two phenylene – a linear (II) and an angular isomer (III) – which both are known compound. Two examples of phenylenes are the system IV and V.



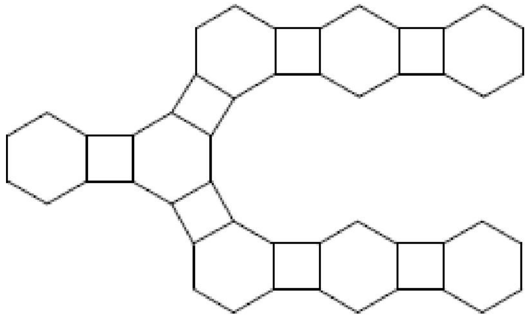
I



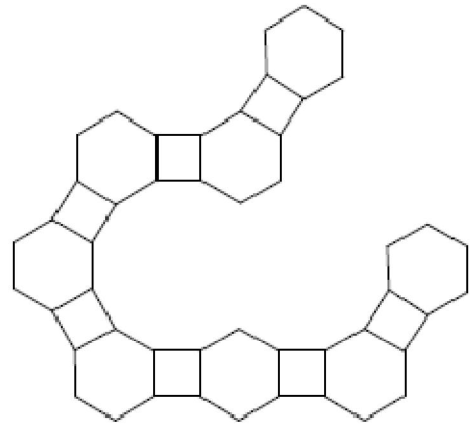
II



III



IV



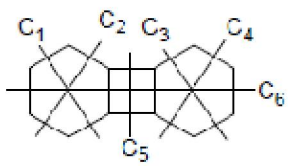
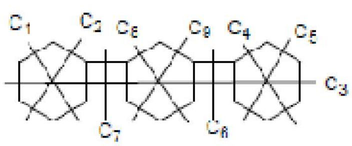
V

By eliminating, "squeezing out", the squares from a phenylene, a *cata*-condensed hexagonal system is obtained called the hexagonal squeeze of the respective phenylene. Clearly there is a one-to-one corresponding between a phenylene (PH) and its hexagonal squeeze (HS).

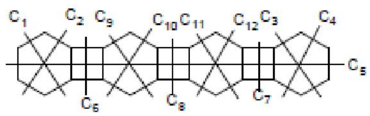
Both possess the same number (h) of hexagon. In addition a PH with to hexagons possesses h–1 squares. The number of vertices of PH and HS are 6h and 4h+2 respectively. The number of edges of PH and HS are 8h-2 and 5h+1 respectively. In the following section, we will give a formula for calculating the Sd index of PHS and establish a simple relation between the Sd index of a PH and of the corresponding HS. In doing so we will concentrate on linear phenylenes only.

4. THE SD INDEX OF PHENYLENS

By the aforementioned definition of the Sd index it is clear that the methodology of computing Sd index of phenylenes consisted of summing up the number of edges on both sides of an elementary cuts belonging to the phenylene. The results for the first four members of the phenylene are summarised below:

Phenylene	Elementary cut	Sum of the edges on both sides of elementary cut	Number of edges involved in elementary cut	Total edges
	C_1	2+10 =12	2	24
	C_2	2+10 =12	2	24
	C_3	2+10 =12	2	24
	C_4	2+10 =12	2	24
	C_5	6+6 = 12	2	24
	C_6	5+5 = 10	4	40
		Σ Sd = 70	14	PI = 160
	C_1	2+18 −20	2	40
	C_2	2+18 −20	2	40
	C_3	8+8 =16	6	96
	C_4	18+2 =20	2	40
	C_5	18+2 =20	2	40
	C_6	6+14 – 20	2	40
	C_7	14+6 – 20	2	40
	C_8	10+10 = 20	2	40
	C_9	10+10 = 20	2	40

	Σ Sd = 1+6	22	PI=418



C_1	2+26 =28	2	56
C_2	2+26 =28	2	56
C_3	2+26 =28	2	56
C_4	2+26 = 28	2	56
C_5	11+11=22	8	176
C_6	6+22 =28	2	56
C_7	22+6 =28	2	56
C_8	14+14 =28	2	56
C_9	10+18 =28	2	56
C_{10}	10+18 = 28	2	56
C_{11}	18+10 = 28	2	56
C_{12}	18+10 = 28	2	56
	Σ Sd =300	30	PI=792

Now, we can say that the sum of the edges on both sides of all elementary cut are 70, 176, 330, ---. Alternatively, this can be written as below:

$$14\times5 = 70$$
$$22\times8 = 176$$
$$30\times11 = 330$$

The number of edges in phenylenes m = 8h-2. That is, 14, 22, 30, ---- etc. corresponds to m = (8h-2). The numbers 5, 8, 11,… etc. need to be expressed is terms of h. We observe that these numbers (5, 8, 11 , … etc.) are obtained by a simple relationship i.e. (3h-1). In the present case L being 2, 3, 4 , … etc. This, Provide the following expression for the calculation of the Sd index of phenylenes.

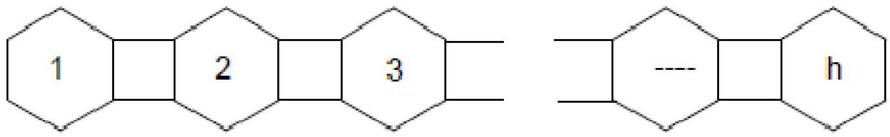
$$Sd\ (PH_2) = (3h-1)\ (8h-2)$$

Since, m = 8h-2, we have L = (m+2/8). Putting this value of h in the above expression, we have

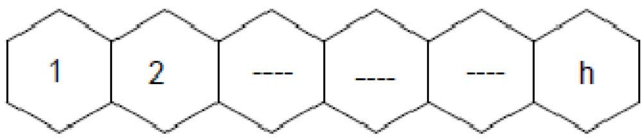
$$Sd\ (PH_2) = 1/8(3h-2)m$$

5. A RELATION OF THE SD INDEX BETWEEN PH AND HS

In the following, we establish a relationship between the Sd index of a PH and of corresponding HS. In case of linear phenylenes, the corresponding hexagonal squeezes will be linear polyacenes:



Linear phenylenes



Hexagonal squeezes of linear phenylenes

We know that the Sd index of polyacene is given by the following expression:

$$Sd(L_h = HS) = 2h\,(5h+1)$$

While the expression for the Sd index linear phenylenes is as below:

$$Sd\,(PH_h) = (3h-1)\,(8h-2)$$

In order to confirm the relationship between the Sd of PH and HS we have calculated Sd indices for the first 20 members in both the cases. These calculated values are summarized in Table 1.

The relationship between the Sd indices of PH and HS can be established in two ways: (i) by correlating their respective Sd indices and (ii) by estimating multiple factor γ, such that we can derive.

$$Sd\,(PH) = \gamma\,(HS)$$

By regression the Sd indices PH on the corresponding Sd indices of HS, gave the following expression:

$$Sd(PH) = (2.3168\,)\,HS + 66.759$$

This is further established by plotting a graph between Sd of PH and HS (Fig.1). The $R^2 = 0.9999$ indicates that there is close linearity between them.

REFERENCES

1. M. V. Diudea., M.S. Florescu. and P.V. Khadikar, Molecular Topology and Its Applications, EFICON, Bucharest, EICON Press, Backrest (2006).
2. R. Todeschini and V. Cosonni, Handbook of Molecular Descriptors Wiley-VCH Weinheim (2000).
3. N. Trinajstic, Chemical Graph Theory, CRC Press Boca Raton Fl (1992).
4. M. Karelson, Molecular Descriptors in QSAR/QSPR, Wiley New York (2000).
5. J. Devillers and A. T. Balaban, Topological Indices and Related Descriptors in QSAR And QSPR, Gordon & Breach Williston VT (2000).
6. N. Trinajstic, Chemical Graph Theory, CRC Press Boca Raton Fl , Vol. 1 and 2 (1983).
7. H .Wiener, Structural Determination of Paraffin Boiling Points. J. Amer. Chem. Soc. 69 (1947) 17-20.
8. H. Hosoya, Topological Index and Thermodynamic Properties .I. Empirical Rules on the Boiling Point of Saturated Hydrocarbons. Bull. Chem. Soc. Jpn. 45 (1972) 3415-3421.
9. I. Gutman, Wiener Index of Trees and its Extension to Cyclic, Graph Theory Notes New York. 27(1994) 9-15.
10. P. V. Khadikar, N.V. Deshpande., P.P. Kale., A. Dobrynin., I. Gutman and G. Domotor, The Szeged Index and an Analogy with the Wiener Index, J. Chem. Inf. Comput. Sci. 35(1995) 545-550.
11. P. V. Khadikar, On a Novel Structural Descriptor PI, Nat. Acad. Sci. Let. 23 (2000) 113-118.
12. P. V. Khadikar, S. Karmarkar and V.K. Agrawal, A Novel PI Index and its Applications to QSPR/QSAR Studies, J. Chem. Inf. Comput. Sci. 41(2001) 934-949.
13. P. V. Khadikar, S. Karmarkar and R.G. Verma, On Estimation of PI Index of Polyacenes, Acta. Chem. Slov. 49 (2002) 715- 771.
14. P. V. Khadikar, P.P. Kale, N.V. Deshpande, S. Karmarkar and V.K. Agrawal., Novel PI Indices of Hexagonal Chains, J. Math. Chem. 29 (2001) 143-150.
15. P. V. Khadikar, M.V. Diudea, J. Singh, P.E. John, A. Shrivastava, S. Singh, S. Karmarkar, M. Lakhwani and P.Thakur, Use of PI Index In Computer-Aided Designing of Bioactive Compounds, Curr. Bioact.Comp. 2 (2006) 19- 56.
16. P. V. Khadikar, V.K. Agrawal and S. Karmarkar. Prediction of Lipophilicity of Polyacenes Using Quantitative Structure-Activity Relationships. Bioorg. Med. Chem. 10(2002) 3499- 35071.
17. I. Gutman, P. Petkovic and P.V. Khadikar, Bound for the Total π-Electron Energy of Phenylene, Rev. Roum. De Chimie. 41 (1996) 637-643.

Table 1. Sd indices of PH and HS for the first 20 members of each of the series.

h	Sd(PH)	Sd(HS)	Sd (PH/ HS)
1	12	12	1.0000
2	70	44	1.5909
3	176	96	1.8333
4	330	168	1.9643
5	532	260	2.0462
6	782	327	2.3914
7	1080	504	2.1429
8	1426	656	2.1738
9	1820	828	2.1981
10	2262	1020	2.2176
11	2752	1232	2.2338
12	3290	1464	2.2473
13	3876	1716	2.2587
14	4510	1988	2.2686
15	5192	2280	2.2772
16	5922	2592	2.2847
17	6700	2924	2.0452
18	7526	3276	2.3083
19	8400	3648	2.3026
20	9322	4040	2.3074
21	10292	4452	2.3118

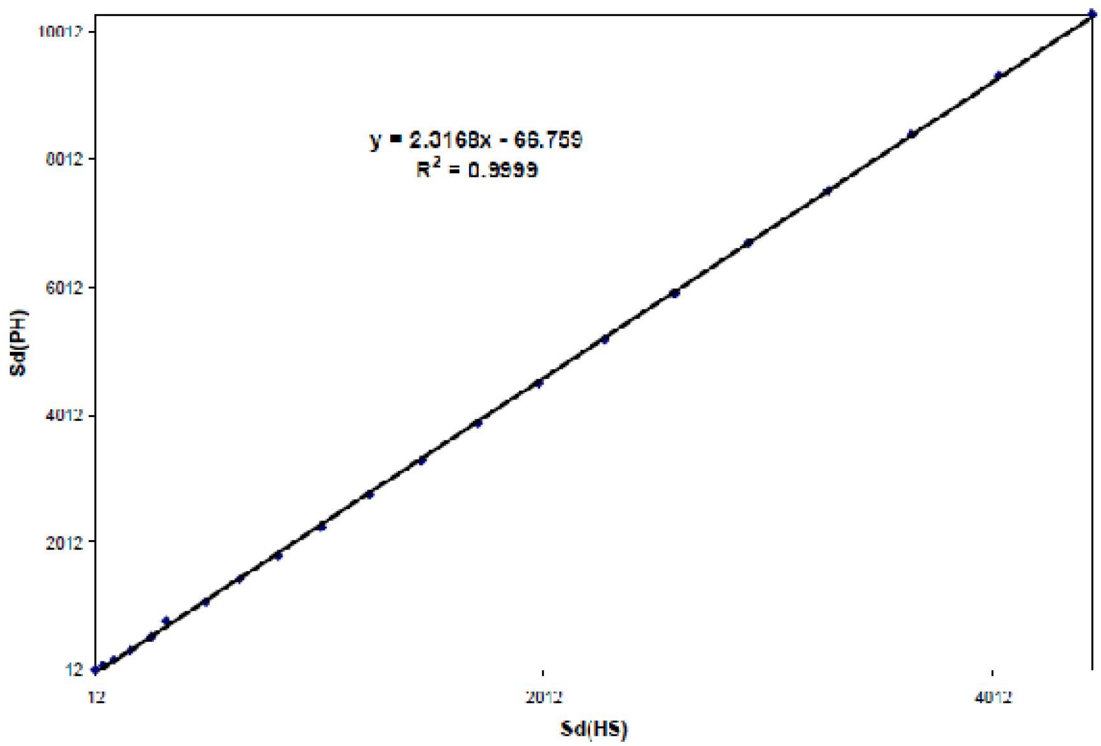


Figure 1. Correlation of Sd (HS) with Sd(PH)