ON THE ESTIMATION OF PI INDEX OF POLYACENES[#]

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[#]This paper is dedicated to Professor Ivan Gutman, teacher, inspirer, friend, and proprietor of graph theory and topology.

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Abstract

General formulae are obtained for the PI (Padmakar-Ivan) index of polyacenes. The PI is a newly proposed molecular-graph-distance-based structural descriptor. By means of this result it was possible, for the first time, to examine relative correlation potential of Wiener (W)-, Szeged (Sz)- first-order connectivity ($^1\chi$), and PI indices in developing Quantitative Structure-Property Relationships (QSPRs) of polyacenes in that hydrophobicity of polyacenes is used as the correlating property.

Introduction

A topological index is a numerical quantity derived in an unambiguous manner from the structural graph of a molecule.[1–5] It is a number extracted by a well defined algorithm from a graphical representation of a molecule. There is good reason to believe that often our difficulties in attributing a meaning to this number lie under deeper chemical theories and higher level languages and not from esoteric approaches to its definition. These indices are graph invariants which usually reflect molecular size, shape, branching, and heterogenicity.[4,5]

Wiener originally defined[6] his index (W) on trees and studied its use for correlations of physicochemical properties of alkanes, alcohols, amines, and their analogous compounds.[7,8]

The original definition[6] of Wiener index (W) was given in terms of edge weights. In an arbitrary tree, every edge is a bridge, that is, after deletion of the edge; the graph is no more connected. The weight of an edge is taken to be the product of the number of vertices in the two connected components. This number also equals the

number of all shortest paths in the tree, which go through the edge. Therefore, the usual generalization to the Wiener Index (*W*) on arbitrary graphs is defined to be the same of all distances in a graph.

Another natural generalization was previously put forward by Gutman[9,10] and called the Szeged index, abbreviated as *Sz*. Now, the weights of edges are taken to be the product of the numbers of vertices closed to the two ends of the edge. For reasons to introduce Szeged index, and for its basic properties, uses see reference.[11–60]

Wiener index (*W*) is the first, oldest, and widely used topological index. Even to day it is widely used in chemistry.[11–60] The Szeged index (*Sz*) is considered as a modification of Wiener index (*W*) to cyclic graphs.[11] For trees (acyclic graphs) Wiener and Szeged indices coincide. Comparatively little is known on the applications of Szeged index in chemistry.

For the reason of the coincidence of Wiener and Szeged indices in case of trees (acyclic graphs), we have very recently introduced another Szeged / Wiener-like topological index and named it Padmakar-Ivan index, and abbreviated as PI.[61–66] Unlike Szeged index (*Sz*), *PI* index is different for trees as well as for cyclic graphs, and not much is known about the applicability of *PI* index in chemistry.

In our earlier publications[61–66] we have defined *PI* index and discussed some of its characteristics and applicability in developing quantitative structure-property-activity (QSPR/QSAR) relationships and observed that *PI* index is quite useful in this respect. In addition, we have made comparative study of *PI* index with several other topological indices including *W, Sz*, and connectivity indices ($^{m}\chi^{R}$) and observed that *PI* index in some cases gives better results.[40,67] There we have used physicochemical property and biological activity of *n*-alkanes, cycloalkanes, alcohols, polychlorinated biphenyls, and monosubstituted nitrobenzene. However, we have not included benzenoid hydrocarbons in such studies. The present communication is, therefore, an extension of such study to benzenoid systems, in that we discuss the methods for the calculation of *PI* index for polyacenes. The other objective of our present study is to compare *W, Sz,* and *PI* indices of polyacenes. Finally, we will make an attempt to use *PI* index for modeling

hydrophobicity (log*P*) of polyacenes, thus attempting QSPR/QSAR for this interesting class of benzenoid hydrocarbons. The results as discussed below show that we are quite successful in this respect.

Results and Discussion

Linear Polyacenes

Linear polyacenes (Figure 1) are the most thoroughly investigated homologous series of conjugated molecules (benzenoid systems). A plethora of theoretical work exists devoted to these systems.[68–80] However, nothing is known regarding different methods of calculating *PI* index of polyacenes and their applicability in QSPR/QSAR studies. For QSPR/ QSAR study we need methods for efficient calculations of *PI* index. Below we present such methods. However, we first repeat in brief, the general definition of *PI* index.

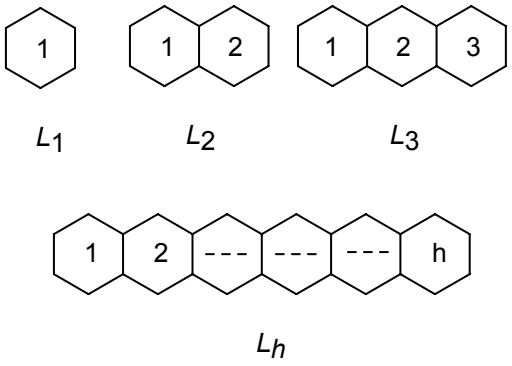

Fig. 1. Polyacene molecules

Definition of PI Index

Let *G* be a molecular graph, the vertex and edge sets of which are represented by *V(G)* and *E(G)* respectively. If *e* is an edge of *G*, connecting vertices *u* and *v* then we write *e* = *uv*. The number of vertices of *G* is denoted by |*G*|.

The distance between a pair of vertices *u, w* of *G* is denoted by *d(u,w|G)*.

We define for *e* = *uv*, two quantities $\eta_{eu}(e|G)$ and $\eta_{ev}(e|G)$. $\eta_{eu}(e|G)$ is the number of edges lying closer to the vertex *u* than the vertex *v*, and $\eta_{ev}(e|G)$ is the number of edges lying closer to the vertex *v* than the vertex *u*. Edges equidistant from

both ends of the edge *uv* are not counted (taken into account), then the *PI* index is defined as:[61–66]

$$PI = \sum_{e} [\ \eta_{eu}(e|G) + \eta_{ev}(e|G)\ ] \qquad (1)$$

The summation goes over all the edges of *G*.

The PI Index of Polyacenes

As stated earlier, in order to be able to undertake studies on the applicability of *PI* index of polyacenes, we need method(s) of its efficient calculation. In the following sections we present such methods for the calculation of PI index of polyacenes for the first time.

It is well known that polyacenes are linearly para-annelated benzenoids, which possesses transitional symmetry (Figure 1). Chemistry of polyacenes is still very much of interest to synthetic chemists, environmental chemists, cancer research chemists, structural chemists, etc.[73–80] We believe that now *PI* index will be of better value for such diversified studies.

The hexagonal chain whose *h* hexagons are arranged in a linear manner is denoted by L_h; the respective benzenoid hydrocarbons form the linear homologous series (benzene, naphthalene, anthracene, etc.) Note that the number of hexagons in the hexagonal chain *C* is denoted by *h*. Thus, we have $C_1 = L_1$, $C_2 = L_2$, $C_3 = L_3$, ..., and so on. The structure of polyacene (L_h) is shown in Fig.1.

From the definition of *PI* index (equation 1) and from the molecular graph of polyacene molecules (Figures 2 and 3), we observed that for any edge like a_ib_i, a_ib_{i+1}, c_id_i, d_ic_{i+1}, i = 1,2,3,….,n, we have:

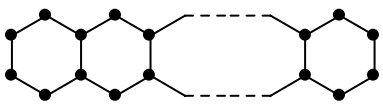

Fig. 2. Molecular graph (G_h) of polyacenes

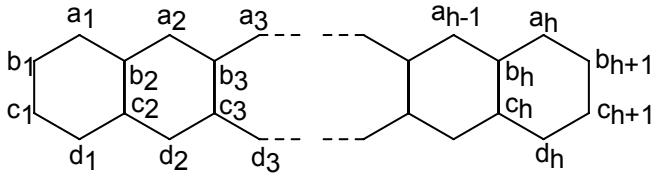

Fig. 3. Case of polyacenes used for the estimation of *PI* index

$$\eta_1(e) = |E_1| = 5_i - 3 \quad (2)$$

and $$\eta_2(e) = |E_2| = 5h - (5_i - 2) \quad (3)$$

Thus giving,

$$\eta_1(e) + n_2(e) = |E_1| + |E_2| = 5h - 1 \quad (4)$$

Similarly, for any edge like b_ic_i, i = 1,2,3,….., h+1, we have:

$$\eta_1(e) + n_2(e) = |E_1| = |E_2| = 4h \quad (5)$$

Hence, PI index of he polyacene will be given by:

$$PI(L_h) = 4h\,(5h - 1) + 4h(h + 1) = 24\,h^2 \quad (6)$$

Recall that L_h has 2 (2h + 1) = n vertices. In view of this $PI(L_h)$ in terms of vertices n is given by the following expression:

$$PI\,(L_h) = 3/2\,(n-2)^2 \quad (7)$$

The PI indicates so calculated for the first 20 polycaenes are given in Table 1.

A Case when Calculation of PI Index for Polyacene is Easy

Now consider Figure 4B, in that edges e_o, e_1, e_2, e_5 …., e_r are called vertical edges of the polyacenes and are represented by V_E, while those denoted by e_i' and e_i'' (i = 0,1,2,3,….,n) are called non-vertical edges (NV_E) of polyacenes. The sum of the vertical and non-vertical edges is denoted by m, such that $V_E + NV_E$ = m. The number of hexagons and edges in polyacenes are denoted by h and m respectively.

The lines crossing the vertical and non-vertical edges (Figure 4C) are called elementary cuts and play a distinguish role in the theory of benzenoid system.

The elementary cuts for the vertical edges (e_o, e_1, e_2,...., e_r) is presented by C_o. The elementary cuts of non-vertical edge for the ith hexagon is represented by C_i' and C_i'' respectively in Figure 4C.

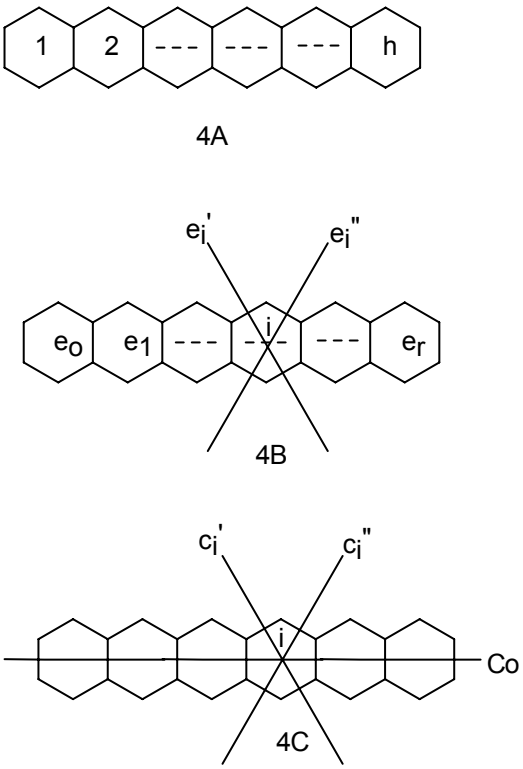

Fig. 4. Used for proposing alternative method of estimation *PI* index of polyacenes

The values of *h, n,* V_E, NV_E and *m* for the first twenty members of the polyacene series are given in Table 1. The *PI* values estimated from Equation (1) are given in Table 2. The *PI* values calculated from equations (6) and (7) are also found to be the same.

Now, a critical examination of the calculation *PI* index using equation (1) indicates that in terms of V_E, NV_E and *m* the estimation of *PI* index is still easy and consists of the following two terms:

(1) $(V_E) \,.\, (NV_E)$, and

(2) (m-2) . NV_E

Thus giving:

$$PI = (V_E) \,.\, (NV_E) + (m\text{-}2)\, NV_E \qquad (8)$$

Say for example, for the polyacenes L_1 (i.e.,benzene, V_E =2,NV_E = 4. Therefore, $m = V_E + NV_E = 6$.

Therefore, equation (8) gives *PI* Index for L_1 as:

$$PI\ (L_1) = (2 \times 4) + (6 - 2)\ 4 = 8 + 16 = 24 \qquad (9)$$

which comes out to be the same when *PI* index for L_1 is calculated from equations (1), (6) and (7).

Table 1. Calculated values of *PI* index for polyacenes using equation 1 and the log*P* values of polyacene molecules.

S. No.	*L*	*n*	Names of abbreviated polyacenes	*PI*	Log*P*
1	1	6	L_1	24	2.202
2	2	10	L_2	96	3.396
3	3	14	L_3	216	4.590
4	4	18	L_4	384	5.784
5	5	22	L_5	600	6.978
6	6	26	L_6	864	8.172
7	7	30	L_7	1172	9.366
8	8	34	L_8	1536	10.560
9	9	38	L_9	1922	11.754
10	10	42	L_{10}	2400	12.948
11	11	46	L_{11}	2904	14.142
12	12	50	L_{12}	3456	15.336
13	13	54	L_{13}	4056	16.530
14	14	58	L_{14}	4704	17.724
15	15	62	L_{15}	5400	18.918
16	16	66	L_{16}	6144	20.112
17	17	70	L_{17}	6936	21.306
18	18	74	L_{18}	7776	22.500
19	19	78	L_{19}	8664	23.694
20	20	82	L_{20}	9600	24.880

Table 2. Data needed for alternative method for the calculation of PI index of polyacenes

Polyacenes	L	n	NV_E	V_E	NV_E+V_E	PI from eqs. 8, 13 & 14
L_1	1	6	4	2	6	24
L_2	2	10	8	3	11	96
L_3	3	14	12	4	16	216
L_4	4	18	16	5	21	384
L_5	5	22	20	6	26	600
L_6	6	26	24	7	31	864
L_7	7	30	28	8	36	1176
L_8	8	34	32	9	41	1536
L_9	9	38	36	10	46	1949
L_{10}	10	42	40	11	51	2400
L_{11}	11	46	42	12	56	2904
L_{12}	12	50	48	13	61	3456
L_{13}	13	54	52	14	66	4056
L_{14}	14	58	56	15	71	4704
L_{15}	15	62	60	16	76	5400
L_{16}	16	66	64	17	81	6144
L_{17}	17	70	68	18	86	6936
L_{18}	18	74	72	19	91	7776
L_{19}	19	78	76	20	96	8664
L_{20}	20	82	80	21	101	9600

Similarly, we can calculate *PI* indices for the set of 20 polyacene molecules from their respective values of V_E, NE_V and again found to be the same as presented in Table 1 (Table 2).

A Case when Estimation of PI is Still Easier

A perusal of Table 2 shows that:

$$V_E = h + 1 \tag{10}$$

and $$NV_E = 4h \tag{11}$$

So that,

$$m = 4L + h + 1 = 5h + 1 \tag{12}$$

Substituting the values of V_E, NE_V, and m in equation (8) we get the following:

$$PI = (V_E)(NV_E) + (m - 2)\,NV_E \quad (13)$$

$$= 4h(h + 1) + \{(5h + 1 - 2)\,4h\}$$

$$= 4h(h + 1) + 4L(5h - 1)$$

$$= 4h\{h + 1 + 5h - 1\}$$

$$= 4h(6h)$$

$$= 24h^2 \quad (14)$$

Thus, the estimation of *PI* index of polyacenes is made still easier by equation (13).

Comparison of W, Sz, and PI Indices of Polyacenes

It will be interesting to study relatedness among *W, Sz,* and *PI* indices of polyacenes. Such a study will provide us a way to predict their relative correlation potential in developing QSPR/QSAR relationships.

As stated above the expression for estimating *PI* index (equation 6) is:

$PI\,(L_h) = 24\,h^2$

The corresponding expressions for estimating *W* and *Sz* are as under:[77,78]

$$W(L_h) = 1/3\,(16h^3 + 36h^2 + 26h + 3) \quad (15)$$

$$Sz(L_h) = 1/3\,(44h^3 + 72h^2 + 43h + 3) \quad (16)$$

From the aforementioned equations (15) and (16) we observed that *Sz* index for linear polyacenes have a similar cubic polynomial dependence on molecular size as that of *W* index, but *PI* has not. Furthermore, the coefficient involved in these equations (15) and (16) are much higher than in the equation (6). In fact the coefficients of *h* terms are largest for equation (16). This indicates that the numerical value of *Sz* will be the largest among the three topological indices under present investigation. The order of the magnitudes of *W, Sz,* and *PI* indices follow the following sequence:

$$Sz(L_h) > W(L_h) > PI(L_h) \quad (17)$$

The values of *Sz, W* and *PI* indices for the first 20-polyacene molecules are presented in Table 3. The best account of the relatedness of *W, Sz* and *PI* of polyacenes

could be made by subjecting the data in Table 3 to regression analysis. First step in such a study is to obtain correlation matrix. Such a matrix obtained in the present study is presented in Table 4. The regression analysis gives regression parameters as well as quality of relatedness.[81–85] The quality parameters are presented in Table 4.

Table 3. *W, Sz, PI* and ${}^1\chi$ indices of polyacenes

Polyacenes	*W*	*Sz*	*PI*	${}^1\chi$
L_1	27	54	24	3.000
L_2	109	243	96	4.967
L_3	279	640	216	6.933
L_4	569	1381	384	8.899
L_5	1011	2506	600	10.866
L_6	1637	4119	864	12.832
L_7	2479	6308	1176	14.798
L_8	3569	9161	1536	16.765
L_9	4939	12766	1944	18.731
L_{10}	6621	17211	2400	20.697
L_{11}	86457	22584	2904	21.663
L_{12}	11049	28933	3456	24.630
L_{13}	13859	36466	4056	26.596
L_{14}	17109	45151	4704	28.562
L_{15}	20831	55116	5400	30.529
L_{16}	25057	66449	6144	32.495
L_{17}	29819	292230	6936	34.641
L_{18}	35149	93571	7770	36.428
L_{19}	41079	109536	8664	38.394
L_{20}	47641	127221	9600	40.360

Table 4. Correlation matrix for investigating relatedness among *W, Sz*, and *PI* indices of poylacenes

	W	*Sz*	*PI*
W	1.0000		
Sz	0.9999	1.0000	
PI	0.9887	0.9885	1.0000

Proposed regression expressions:

$$PI\ (L_h) = 0.1672\ (\pm\ 0.0053)\ W\ (L_h) + 1075.3313$$

$$PI\ (L_h) = 0.0625\ (\pm\ 0.0020)\ Sz\ (L_h) + 1096.6398$$

Quality of aforementioned correlations:

Correlation	*Se*	*R*	*F*	*P*	*Q*
PI – W	724.1565	0.9887	1001.679	0.000E+00	0.0014
PI – Sz	731.8385	0.9885	980.280	0.000E+00	0.0014

A perusal of Table 4 shows that *W, Sz* and *PI* are highly linearly correlated; *Sz* correlates with *W* slightly more than *PI* index; while the correlation of *PI* index with *W* and *Sz* is similar. The corresponding relatedness of *PI* with *W* and *Sz* is given by the following regression expressions:

$$PI\ (L_h) = 0.1672\ W\ (L_h) + 1075.3313 \qquad (18)$$

and

$$PI\ (L_h) = 0.0625\ Sz\ (L_h) + 1096.6398 \qquad (19)$$

The corresponding qualities viz., standard error of estimation (*Se*), correlation coefficient (*R*), F-ratio, and probability values also indicates similar relatedness between *PI-W* and *PI-Sz* (Table 4).

It is worth recording that in addition to high relatedness, a particular index will be preferred over the other index in that fewer efforts are made for its estimation. Therefore, compared to both *W* and *Sz, PI* index is better as it is given by $4h^2$ only. Thus, least efforts are required for its calculation.

From the aforementioned results and discussion we can conclude that correlation potential of *W, Sz,* and *PI* indices are similar. Also that, like *W* and *Sz, PI* index also takes care of size, shape and branching. The size-shape dependence of *W* and *Sz* is well established[86-88]. But, as discussed below we observe that *PI* index contains hither to unknown structural features, which dominates over size and shape. This makes *PI* index to give better results than *W* and *Sz* in some cases.[61]

Modeling of Hydrophobicity of Polyacenes Using W, Sz, and PI Indices

It is well established that hydrophobic interaction in biosystems can be modelled by log*P* i.e. logarithm of partition coefficient (*P*) between octanol-water or in some other suitable organic solvent / water partitioning systems.[81–92] Modeling of log*P* with molecular descriptors (topological indices) has two-fold advantage, first log*P* is considered as a physicochemical property and secondly it can also be used to represent physiological activity of organic compound acting as drugs.

The log*P* values[89–92] for the first 20 polyacene molecules are presented in Table 5. In addition to *W, Sz* and *PI* indices we have also chosen $^1\chi$-index[67] because it is most widely used topological index in QSPR and QSAR studies. That is now, we are considering relative ability of *W, Sz, PI,* and $^1\chi$ indices for modeling, monitoring, estimating log*P* of polyacenes. These $^1\chi$ values are presented in Table 3.

Table 5. Correlation matrix for investigation relatedness among *W, Sz, PI,* and $^1\chi$ and their correlation with log*P* of polyacene molecule

	Log*P*	*W*	*Sz*	$^1\chi$	*PI*
Log*P*	1.0000				
W	0.9264	1.0000			
Sz	0.9258	0.9999	1.0000		
$^1\chi$	0.9999	0.9273	0.9267	1.0000	
PI	0.9707	0.9887	0.9885	0.9713	1.0000

Proposed regression expressions for modeling log*P* of polyacene molecules using *W, Sz,* $^1\chi$, and *PI* indices.

$$\log P = 2.9087 \times 10^{-4} (\pm 2.4652 \times 10^{-5})\, W + 9.171;$$

$$\log P = 1.088 \times 10^{-4} (\pm 9.2641 \times 10^{-6})\, Sz + 9.211;$$

$$\log P = 0.6070 (\pm 1.7450 \times 10^{-3})\, {}^1\chi + 0.1240;$$

$$\log P = 1.8027 \times 10^{-3} (\pm 9.3062 \times 10^{-5})\, PI + 6.9680.$$

Quality of aforementioned correlations:

Correlating parameter	*Se*	*R*	*F*	*P*	*Q*
W	3.3800	0.9260	139.215	3.099×10^{-11}	0.2740
Sz	3.3940	0.9260	137.867	3.406×10^{-11}	0.2728
$^1\chi$	0.1240	1.0000	120842.000	0.00E+0	8.0645
PI	2.1570	0.9710	375.224	0.000E+0	0.4502

We have first obtained correlation matrix for the parameters *W, Sz, PI,* $^1\chi$ and log*P* (Table 5). This correlation matrix indicates that compared to both *W* and *Sz, PI*-index is a better topological index for modeling log*P* of polyacene molecules. However, $^1\chi$ is the most appropriate index for this purpose. That is, correlation potential of *PI* index in modeling log*P* is inferior to $^1\chi$ but superior than *W* and *Sz*. Whether this is the case with other properties / activities is a problem for further investigation. Attempts in this direction are under way and the results will be published soon.

In order to obtain better insight into the problem of modeling log*P* with *W, Sz, PI,* $^1\chi$ we have subjected the data to regression analysis and obtained corresponding regression parameters i.e., the values of *Se, R, F, P* and *Q* (Table 5). Here, *Q* is the quality factor[93,95] obtained from the ratio of correlation coefficient (*R*), and standard error of estimation (*Se*) (*Q* = *R*/*Se*). The advantage of using *Q* is that it takes accounts of *R* and *Se* simultaneously. The quality factor Q is directly proportional to *R* and inversely proportional to *Se*. Hence, larger the value of *R*, smaller the *Se*, higher will be *Q*, and the better will be the proposed correlation.

The data presented in Table 5 indicates that correlation potential of *W* and *Sz* in modeling log*P* of polyacene molecules is similar. The *PI* index, is slightly more efficient than *W* and *Sz* for this purpose and that $^1\chi$ is the most appropriate index among *W, Sz, PI* and $^1\chi$ for modeling log*P*. *Q*-values show that $^1\chi$ is almost two-fold better index than *PI*, and that the relative potential of the topological indices in modeling log*P* follow the following sequence.

$$^1\chi(L_h) > PI(L_h) > W(L_h) \approx Sz(L_h) \qquad (20)$$

Once again we state that shape-size dependence of *W* and *Sz* is well established. Inspite of high collinearity among *W, Sz,* and *PI*, the *PI* index is found better than both *W* and *Sz*. The *Q*-value of 0.4502 compared to ≈ 0.2746 or 0.2728 indicates that in addition to size and shape, the *PI* index contain some other hither to unknown structural feature, which dominates over shape and size. As stated earlier the study in this direction is underway and results will be published soon.

In order to investigate probable unknown parameter(s) hidden in PI index we considered the polynomials for logP = f(L) and logP = f($^1\chi$). From the data presented in Table 5 we have:

$$\log P = 1.8022 \times 10^{-3} (\pm 9.3062 \times 10^{-5}) PI + 6.9680 \quad (21)$$

and, $$\log P = 0.6070 (\pm 1.7450 \times 10^{-3}) \, ^1\chi + 0.1240 \quad (22)$$

The first order connectivity index ($^1\chi$) conveys more information about the number of atoms in a molecule. Therefore, according to equation (22) it is the atomic contribution, which accounts for the exhibition of logP. Similarly, according to equation (21), the PI index is directly related to logP. While the defination of PI index (= 24 h^2, equation 6) shows that PI is directly related to number of cycles (h) present in the polyacene molecule. Hence, the unknown parameter hidden in PI index is the cyclicity. That is, in additive to first, shape, branching, the PI index also accounts for cyclicity, thus, hither to unknown structural feature contain in PI index is the cyclicity which domination over shape and size.

Conclusions

The aforementioned results and discussion lead us to the following conclusions:

(1) The estimation of *PI* index for polyacene molecules is much simpler than the estimation of *W* and *Sz*;

(2) Both *W* and *Sz* are cubic polynomials while *PI* index is not;

(3) Coefficient of h parameters in the corresponding expressions proposes the following order of magnitudes of *W, Sz*, and *PI.*

$Sz(L_h) > W(L_h) > PI(L_h)$;

(4) High collinearity among *W, Sz,* and *PI* indicates their similar correlation potential in proposing QSPR/QSAR models, and also their similar dependence on shape and size;

(5) High quality of correlation of log*P* with *PI*, compared to both *W* and *Sz*, indicates that in addition to size and shape, the *PI* index depends upon some hither to unknown structural feature which dominates over shape and size.

Experimental

For the calculation of PI index the molecular structures are transformed into their molecular graphs in that atoms (vertices) are depicted by dots and bonds (edges) by small lines.

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Povzetek

Prikazane so splošne formule za PI (Padmakar-Ivan) indekse poliacenov. PI je na novo predlagan strukturni descriptor molekularne strukturne formule in razdalj. Na osnovi prikazanih rezultatov je možno primerjati uporabnost Wienerjevih (W)-, Szegedovih (Sz)-povezav prve vrste ($^1\chi$) in PI indeksov v razvijanju QSPR poliacenov, pri čemer kot korelacijsko lastnost uporabimo hidrofobnost.