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Highly Correlated Wiener Polarity Index -A Model to Predict Log p

I.Pothuraju
Department of Mathematics
Bapatla Engineering College, Bapatla, Andhra Pradesh, India.
im_praju@yahoo.com

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Abstract: *Wiener polarity index of a more generalized graph of chemical graphs of polyacenes and phenylenes is computed and the results are used to design a model for predicting log p values of polyacenes. The multiple regression with two descriptors gives improved models with correlation coefficient 0.999999980642502.*

Keywords: *Wiener polarity index, QSAR/QSPR model, Benzenoid graph.*

1. INTRODUCTION

Quantitative structure – Activity and Structure – property relationships (QSAR/QSPR) are used chemometric methods to study how a given biological activity or a physiochemical property varies as a function of topological descriptors describing the chemical structure of the molecules. With these studies it is possible to replace costly and time taking biological tests or experiments of a given physiochemical property with models involving topological descriptors. In 2002 P.V.Khadikar [1] designed a model to predict Lipophilicity of polyacenes with topological indices PI and Sd indices. Quiet recently A.Behmarami [2] obtained new bounds for Wiener polarity index of a class of graphs. In this paper we have considered the popular topological indices Wiener polarity index, Wiener index, Szeged index, PI index , first Zagreb index , second Zagreb index , Randic index, Sadhna index and using linear and multiple (taking two descriptors) regressions we present models of highest accuracy to predict log p.

2. PRELIMINARIES

In this section we list definitions and theorems that are required for the paper.

Definition 2.1. [4]: The wiener polarity index of a graph G= (V, E) is defined as the number of unordered pairs of vertices (u, v) of G such that the shortest distance d_G(u, v) between u and v is 3 i.e. $Wp(G) = \left| \left\{ (u,v) \,/\, d_G(u,v) = 3, u,v \in V \right\} \right|$.

Definition2.2. **[**3]: The wiener index of a graph G= (V, E) is defined as $W(G) = \frac{1}{2}\sum_{u \in V}\sum_{v \in V} d_G(u,v)$, where d_G(u, v) is the length of the shortest path connecting u and v in G.

Definition2.3.[6]: The Szeged index of a graph G is defined as

$Sz(G) = \sum_{e=(u,v)\in E(G)} N_u(e \setminus G)\ N_v(e \setminus G)$, where $N_u(e \setminus G)$ is the number of

vertices of G lying closure to u and $N_v(e \setminus G)$ is the number of vertices of G lying closure to v and vertices equidistance from u and v are not taken into account.

Definition 2.4.[1]: The PI index of a graph G is defined as

$PI(G) = \sum_{e=(u,v)\in E(G)} [n_{eu}(e \setminus G) + n_{ev}(e \setminus G)]$, the summation goes over all the edges of G.

For e= {u, v}, $n_{eu}(e \setminus G)$ is the number of edges lying closure to u than the vertex v. Edges at the equidistant from both ends of the edge e = {u, v} are not counted.

Definition2.5. [5]: The first Zagreb index is defined as $Zb_1(G) = \sum_{u\in V(G)} (d(u))^2$, where d (u) is the degree of vertex.

Definition2.6.[5]: The second Zagreb index is defined as $Zb_2(G) = \sum_{e=\{u,v\}\in E(G)} d(u)\, d(v)$, where d(u) is the degree of the vertex and d(u).d(v) is the weight of edge {u, v}.

Definition2.7.[1]: The Randic index of a graph G is defined as $\chi(G) = \sum_{u,v\in E(G)} \frac{1}{\sqrt{d_u d_v}}$,

d_u(or d_v) denote the degree of vertex u (or v).

Now we state theorems which are already proved and useful in our model. In the following theorems L_a is the chemical graph of polyacenes with 'a' benzenoids. (See Fig 3)

Theorem2.8.[1]: The wiener index of L_a is W (L_a) = $\frac{1}{3}$ ($16a^3 + 36a^2 + 26a + 3$).

Theorem2.9.[1]: The Szeged index of L_a is Sz (L_a) = $\frac{1}{3}$ ($44a^3 + 72a^2 + 43a + 3$).

Theorem2.10.[1]: The PI index of L_a is PI (L_a) = $24a^2$.

Theorem2.11.[7]: The first Zagreb index of L_a is $Zb_1(L_a)$ = 26a-2.

Theorem2.12. [7]: The second Zagreb index of L_a is $Zb_2(L_a)$ = 33a-9.

Theorem2.13. [1]: The Randic index of L_a is $\chi(L_a) = 3 + \frac{a-1}{3} + \frac{4a-4}{\sqrt{6}}$.

Theorem2.14.[1]: The Sadhna index of L_a is Sd (L_a) = 2a (5a+1)

NOTATION:

Throughout the paper we denote the graph consisting of 'n' benzenoid (6 cycle) segments each of length 'a',with 4 cycle segment of length k in between two 6 cycle segments by G(a,k,n) and the graph is shown below.

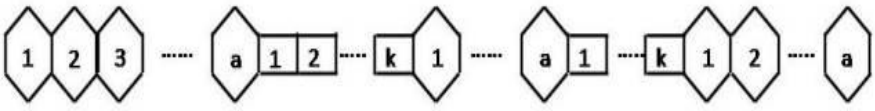

Figure 1

Taking a=1 and k=1, we get the graph G (1, 1, n), the chemical graph of linear phenylenes as shown below.

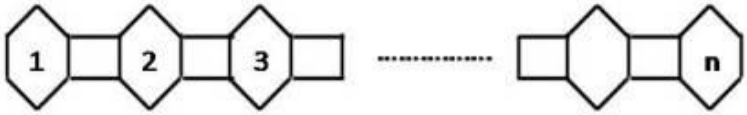

Figure 2

Taking k=0 and n=1 in G (a, k, n), we get the chemical graph of linear polyacenes consisting of 'a' benzenoids (graph L_a) as shown below.

Figure 3

3. RESULTS

Theorem3.1: The Wiener polarity index (Wp) of the graph G (a, k, n) is 9an+4kn-4k-6.

Proof:

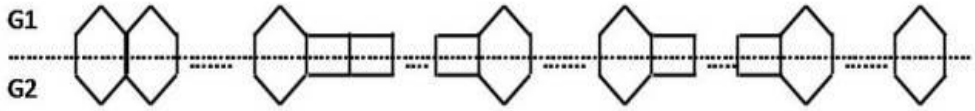

Figure 4

Let G1 be the upper half of the graph and let G2 be the lower half of the graph G (a, k, n) as shown above. To compute the number of unordered pairs of vertices with shortest distance 3,

we have to compute i) The number of unordered pairs of vertices {u, v}; u, v are both in G1

ii) The number of unordered pairs of vertices {u, v}; u,v are both in G2

iii) The number of unordered pairs of vertices{u,v};one in G1 and another in G2.

i) As G1 is a path graph with n(2a+1)+(n-1)(k-1)=2an+kn-k+1 vertices, the number of unordered pairs of vertices with shortest distance 3 = 2an+kn-k+1-3=2an+kn-k-2.

ii) Considering G2 in a similar way as above, the number of unordered pairs of vertices with shortest distance 3 = 2an+kn-k+1-3 = 2an+kn-k-2.

iii) To compute the number of unordered pairs {u,v}of vertices with shortest distance 3 such that one vertex in G1 , another vertex in G2 we label the vertices in G1 for convenience as follows.

Label vertices in the upper half of i^{th} (i=1 to n) segment of 6-cycles (Benzenoids) as $b_{i,1};b_{i,2};\ldots\ldots\ldots\ldots;b_{i,2a+1}$.

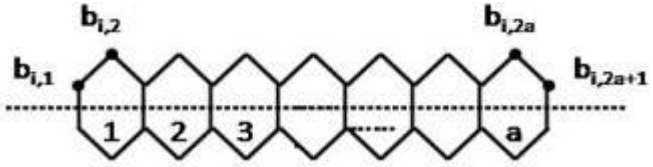

Figure 5

Label vertices in the upper half of i^{th} (i=1 to n) segment of 4-cycles as $p_{i,1};p_{i,2};\ldots\ldots\ldots\ldots;p_{i,k-1}$.

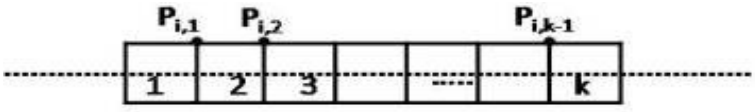

Figure 6

With the above notation, for each vertex u in G1, we list out the number of unordered pairs of vertices {u,v},v in G2 with shortest distance 3 in the following table.

Table 1:

Vertex u in G1	**The no. of unordered pairs {u,v},v Є G2**	**Component in Wp index**
$b_{1,1}$	1	1
$b_{1,2}$	2	2
$b_{1,i}$ (i= 3,5,…..,2a+1)	2 for each i	2a
$b_{1,i}$ (i=4,6,……..,2a)	3 for each i	3(a-1)
$b_{n,2a+1}$	1	1
$b_{n,2a}$	2	2
$b_{n,i}$ (i=1,3,…,2a-1)	2 for each i	2a
$b_{n,i}$ (i=2,4,…,2a-2)	3 for each i	3(a-1)
$b_{l,m}$ (l=2,3,…..,n-1 ; m=1,3,….. ,2a+1)	2 for each pair l,m	2(a+1)(n-2)
$b_{l,m}$ (l=2,3,…..,n-1 ; m=2,4,….. ,2a)	3 for each pair l,m	3a(n-2)
$P_{l,m}$ (l=1,2,…..,n-1 ; m=1,2,….. ,k-1)	2 for each pair l,m	2(k-1)(n-1)

Thus the number of unordered pairs of vertices with shortest distance 3 in this case is = 5an+2kn-2k-2 (sum of last column in the above table 1).

Hence the Wiener polarity index = (2an+kn-k-2) + (2an+kn-k-2) + (5an+2kn-2k-2) =9an+4kn-4k-6.

From the above theorem we can deduce the Wiener polarity index of linear phenylenes and linear polyacenes.

Corollary3.2: The Wiener polarity index of the graph G (1, k, n) is 4kn+9n-4k-6.

Corollary3.3: The Wiener polarity index of the chemical graph G (1, 1, n) of linear phenylenes is 13n-10.

Corollary3.4: The Wiener polarity index of the chemical graph G (a, 0, 1) (same as L_a) of linear polyacenes is 9a-6.

4. CORRELATION BETWEEN LOGP AND KNOWN TOPOLOGICAL INDICES

In this section we obtain the model to calculate log p of polyacenes using linear and multiple regressions. We consider first 20 compounds of polyacenes and the values of topological indices of these compounds are obtained by corresponding formulas mentioned in section2 and section3. The values obtained are tabulated in the following table:

Table 2: Topological indices of polyacenes

Polyacenes	**log p**	**Wp**	**W**	**Sz**	**PI**	**Zb_1**	**Zb_2**	**X**	**Sd**
L_1	2.202	3	27	54	24	24	24	3.000	12
L_2	3.396	12	109	243	96	50	57	4.967	44
L_3	4.590	21	279	656	216	76	90	6.933	96

L_4	5.784	30	569	1381	384	102	123	8.899	168
L_5	6.978	39	1011	2506	600	128	156	10.866	260
L_6	8.172	48	1637	4119	864	154	189	12.832	372
L_7	9.366	57	2479	6308	1176	180	222	14.798	504
L_8	10.560	66	3569	9161	1536	206	255	16.765	656
L_9	11.754	75	4939	12766	1944	232	288	18.731	828
L_{10}	12.948	84	6621	17211	2400	258	321	20.697	1020
L_{11}	14.142	93	8647	22584	2904	284	354	21.663	1232
L_{12}	15.336	102	11049	28973	3456	310	387	24.630	1464
L_{13}	16.530	111	13859	36466	4056	336	420	26.596	1716
L_{14}	17.724	120	17109	45151	4704	362	453	28.562	1988
L_{15}	18.918	129	20831	55116	5400	388	486	30.529	2280
L_{16}	20.112	138	25057	66449	6144	414	519	32.495	2592
L_{17}	21.306	147	29819	79238	6936	440	552	34.641	2924
L_{18}	22.500	156	35149	93571	7776	466	585	36.428	3276
L_{19}	23.694	165	41079	109536	8664	492	618	38.394	3648
L_{20}	24.880	174	47641	127221	9600	518	651	40.360	4040

The correlation coefficients between log p and topological indices (mentioned in the above table) are obtained, and it is observed that log p values are highly correlated with each of Wiener polarity index, first Zagreb index, second Zagreb index and Randic indices with correlation coefficient 0.999999972509691 (in each case) and the corresponding linear regression equations are

log p =1.80472381+0.132653968 Wp.
log p =1.100637363+0.045918681 Zb_1.
log p =1.334405195+0.036178355 Zb_2.
log p =0.381192301+0.607164471 χ.

To improve the strength of the model we have used multiple regression taking two indices from the above table. It is observed that log p has highest correlation coefficient 0.999999980642502 (better than linear regression case) with each of the pairs 1)Wiener polarity index and Szeged index 2)Randic index and Szeged index 3)first Zagreb index and Szeged index 4)second Zagreb index and Szeged index.

The corresponding regression equations are

log p = 1.803188477 - 6.029E-08 Sz +0.132695797 Wp.
log p = 0.379208093 - 6.029E-08 Sz+0.607355225 χ.
log p = 1.098880014 - 6.029E-08 Sz+0.045933161 Zb_1.
log p = 1.332721559 - 6.029E-08 Sz+0.036189763 Zb_2.

5. CONCLUSIONS

Introducing Wiener polarity index in the design of the model, we conclude among the topological indices we considered

(i).Wiener polarity index is better than Szeged index, Wiener index, PI index and Sd index.
(ii).The combination of Wiener polarity index with Szeged index improves the correlation coefficient in multiple regression and thus provides a model with greater accuracy to predict log p values.

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REFERENCES

[1] Padmakar V. Khadikar, et al., "Prediction of Lipophilicity of Polyacenes Using Quantitative Structure-Activity Relationships," Biorganic and medical chemistry, vol. 10, pp. 3499-3507, 2002.
[2] Behmaram.A And Yousefi−Azari.H., "Further Results on Wiener Polarity Index of Graphs," Iranian Journal of Mathematical Chemistry, Vol. 2, pp. 67−70, September2011
[3] Wiener.h, "Structural determination of paraffin boiling points", J Am Chem soc 69 (1), pp 17-20, 1947.
[4] Bolian Liu, Huoquan Hou, Yufei Huang, "On the wiener polarity index of trees with maximum degree or given number of leaves," Computers and Mathematics with applications, vol. 60, pp. 2053-2057, 2010.
[5] Ante.Milicevic, Sonja n, "On variable Zagreb indices," Croatica Chemica Acta, CC AC AA77 (1–2), pp. 97-101, 2004.
[6] Shouzhong Wang, Bolian Liu, "A method of calculating the Edge-Szeged index if Hexagonal Chain," Match Commun Math Comput Chem, vol. 68, pp. 91-96, 2012.
[7] Tomislav Doslic, "On Discriminative of Zagreb indices," IJMC, vol. 3, 2012.

AUTHORS BIOGRAPHY

He is working as Assistant professor in Department of Mathematics, Bapatla Engineering College. He has two years of teaching experience. He did M.Sc(Mathematics) in Bapatla Engineering College. He obtained MBA from Pydah College,Andhra University. He completed his B.Sc(M.P.C) in Bapatla College of Arts & Science. He has a zeal to invent new findings in Mathematics.