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A highly correlated topological index for polyacenes

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Abstract
The most used molecular graph descriptors in establishing Quantitative structure-property relationships (QSPRS) and Quantitative structure-activity relationships (QSARS) are topological indices. Molecular descriptors are normally chosen based on their ability to give good results in statistical models. In this paper we introduce a set of five new indices (Kekule indices) K, K_1, K_2, K_3, K_4 and we establish that the Kekule index (K) has excellent correlation (r = 0.99999997250969) with log p values in case of polyacenes.

Keywords: Kekule index, Polyacenes.

INTRODUCTION

A topological index of a chemical compound is an integer, derived following a certain rule, which can be used to characterize the chemical compound. The first topological index is Wiener index introduced by Harold Wiener in 1947 to demonstrate its relation with physicochemical properties of alkanes, alcohols and amines. Ever since it is known that topological indices can be used to establish Quantitative structure - property relationships (QSPRS) and Quantitative structure - activity relationships (QSARS) in pharmacology, researchers are pursuing several investigations to find topological indices having correlation one or nearer to one with physicochemical properties of organic compounds. In this paper we introduce a new index K (Kekule index) having correlation (r = 0.99999997250969) with log p values of polyacenes.

DEFINITIONS

In this section we define five new topological indices and explain the procedure of computation.

Kekule index: The Kekule index of a graph G = (V, E) is defined as K (G) = $\sum_{e=uv\in E(G)} W(e)$ where $W(e) = |i - j|$, i, j are the degrees of the vertices u and v in G.

K_1 index: The K_1 index of a graph G = (V, E) is defined as $K_1(G) = \sqrt{\sum_{e=uv\in E(G)} W(e)}$ where $W(e) = |i - j|^2$, i, j are the degrees of the vertices u and v in G.

K_2 index: The K_2 index of a graph G = (V, E) is defined as $K_2(G) = \sum_{e=uv\in E(G)} W(e)$ where $W(v)$ = sum of the degrees of the neighboring vertices in G.

K_3 index: The K_3 index of a graph G = (V, E) is defined as $K_3(G) = \sum_{e=uv\in E(G)} W(e)$ where $W(v)$=product of the degrees of the neighboring vertices in G.

K_4 index: The K_4 index of a graph G = (V, E) is defined as $K_4(G) = \sum_{e=uv\in E(G)} W(e)$ where $W(v) = \max\{d(v,v_i)/v_i \in V(G)\}$. Where $d(v, v_i)$ is the maximum distance between v and v_i.

We compute these indices considering the chemical graph of the compound Naphthalene given below.

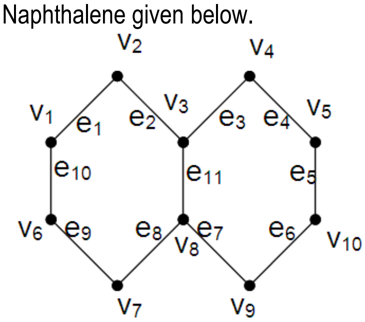

Fig 1. Graph of Naphthalene

Calculation of K index:
$W(e_1)=|2-2|=0$, $W(e_2)=|2-3|=1$, $W(e_3)=|3-2|=1$, $W(e_4)=|2-2|=0$, $W(e_5)=|2-2|=0$, $W(e_6)=|2-2|=0$,
$W(e_7)=|3-2|=1$, $W(e_8)=|3-2|=1$, $W(e_9)=|2-2|=0$, $W(e_{10})=|2-2|=0$, $W(e_{11})=|3-3|=0$
Therefore K(G)=1+1+1+1=4.
Calculation of K_1 index:
$W(e_1)=|2-2|^2=0$, $W(e_2)=|2-3|^2=1$, $W(e_3)=|3-2|^2=1$, $W(e_4)=|2-2|^2=0$, $W(e_5)=|2-2|^2=0$,
$W(e_6)=|2-2|^2=0$, $W(e_7)=|3-2|^2=1$, $W(e_8)=|3-2|^2=1$, $W(e_9)=|2-2|^2=0$, $W(e_{10})=|2-2|^2=0$,
$W(e_{11}) = |3-3|^2=0$
Therefore $K_1(G) = \sqrt{1+1+1+1} = 2$.

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Calculation of K_2 index:
$W(v_1)$= 2+2=4, $W(v_2)$= 2+3=5, $W(v_3)$= 2+3+2=7, $W(v_4)$= 3+2=5, $W(v_5)$= 2+2=4,
$W(v_6)$= 2+2=4, $W(v_7)$= 2+3=5, $W(v_8)$= 2+2+3=7, $W(v_9)$= 3+2=5, $W(v_{10})$= 2+2=4,
Therefore K_2 (G) = 4+5+7+5+4+4+5+7+5+4=50.
Calculation of K_3 index:
$W(v_1)$= 2×2=4, $W(v_2)$= 2×3=6, $W(v_3)$= $2\times 3\times 2$=12, $W(v_4)$= 3×2=6, $W(v_5)$= 2×2=4,
$W(v_6)$= 2×2=4, $W(v_7)$= 2×3=6, $W(v_8)$= $2\times 2\times 3$=12, $W(v_9)$= 3×2=6, $W(v_{10})$= 2×2=4,
Therefore K_3 (G) = 4+6+12+6+4+4+6+12+6+4=64.
Calculation of K_4 index:
W (v_1) = 5, W (v_2) = 4, W (v_3) = 3, W (v_4) = 4, W (v_5) = 5, W (v_6) = 5, W (v_7) = 4,
W (v_8) = 3, W (v_9) = 4, W (v_{10}) = 5,
Therefore K_4(G)=5+4+3+4+5+5+4+3+4+5=42.

NOTATION

The molecular graph of polyacenes is a chain of hexagons arranged linearly.
For convenience we adopt the following notation:
Let L (*a*) be the graph consisting of a hexagons in **one** row as shown in the figure below. Here *a* is a positive integer.

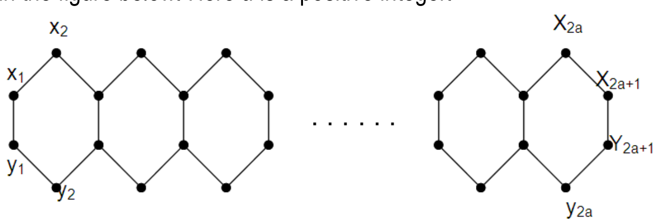

Fig 2. Graph of polyacene with *a* hexagons in 1 row

MAIN RESULTS

Throughout the paper we take

$A=\{x_1,x_2,...,x_{2a+1}\}$, $B=\{y_1,y_2,...,y_{2a+1}\}$.
$E_1=\{x_ix_{i+1}/i=1,2,...,2a\}$, $E_2=\{y_iy_{i+1}/i=1,2,...,2a\}$, $E_3=\{x_iy_i/i=1,3,...,2a+1\}$

Theorem 4.1: If L(*a*) is the chemical graph (see Figure 2) then the K index of the graph L(*a*) is K(L(*a*)) =4(*a*-1), where *a* is a positive integer.

Proof: Consider

$$K(L(a))=\sum_{e=\{x_ix_{i+1}\}\in E_1}W(e)+\sum_{e=\{y_iy_{i+1}\}\in E_2}W(e)+\sum_{e=\{x_iy_i\}\in E_3}W(e)$$

Here

$$\sum_{e=\{x_ix_{i+1}\}\in E_1}W(e)=(2a-2)1$$

(since there are 2*a*-2 edges with | *i*-*j*|=1 in E_1).

$$\sum_{e=\{y_iy_{i+1}\}\in E_2}W(e)=(2a-2)1$$

(since there are 2*a*-2 edges with | *i*-*j*|=1 in E_2).

$$\sum_{e=\{x_iy_i\}\in E_3}W(e)=0$$ (since for every edge in E_3, | *i*-*j*|=0).

Therefore $K(L(a))=2a-2+2a-2=4a-4=4(a-1)$.

Theorem 4.2: If L(*a*) is the chemical graph (see Figure 2) then the K_1 index of the graph L(*a*) is K_1(L(*a*)) =2$\sqrt{(a-1)}$, where *a* is a positive integer.

Proof: Consider

$$K_1(L(a))=\sum_{e=\{x_ix_{i+1}\}\in E_1}W(e)+\sum_{e=\{y_iy_{i+1}\}\in E_2}W(e)+\sum_{e=\{x_iy_i\}\in E_3}W(e)$$

here

$$\sum_{e=\{x_ix_{i+1}\}\in E_1}W(e)=(2a-2)1$$

(since there are 2*a*-2 edges with | *i*-*j*|^2=1 in E_1).

$$\sum_{e=\{y_iy_{i+1}\}\in E_2}W(e)=(2a-2)1$$

(since there are 2*a*-2 edges with | *i*-*j*|^2=1 in E_2).

$$\sum_{e=\{x_iy_i\}\in E_3}W(e)=0$$

(since for every edge in E_3, | *i*-*j*|^2=0).
Therefore

$$K_1(L(a))=\sqrt{2a-2+2a-2}=\sqrt{4a-4}=2\sqrt{(a-1)}$$

Theorem 4.3: If L(*a*) is the chemical graph (see Figure 2) then the K_2 index of the graph L(*a*) is K_2(L(*a*)) =26*a*-2, where *a* is a positive integer.

Proof: In the set A two vertices namely x_1 and x_{2a+1} having weight 4, two vertices namely x_2 and x_{2a} having weight 5, (*a*-2) vertices namely $x_4,x_6,x_8,...,x_{2a-2}$ having weight 6, (*a*-1) vertices namely $x_3,x_5,x_7,...,x_{2a-1}$ having weight 7.

In the set B two vertices namely y_1 and y_{2a+1} having weight 4, two vertices namely y_2 and y_{2a} having weight 5, (*a*-2) vertices namely $y_4,y_6,y_8,...,y_{2a-2}$ having weight 6, (*a*-1) vertices namely $y_3,y_5,y_7,...,y_{2a-1}$ having weight 7.
Therefore

$$K_2(L(a))=\sum_{\{x_i\}\in A}W(x_i)+\sum_{\{y_i\}\in B}W(y_i)$$

Here

$$\sum_{\{x_i\}\in A}W(x_i)=2(4)+2(5)+(a-2)6+(a-1)7$$

$$\sum_{\{y_i\}\in B}W(y_i)=2(4)+2(5)+(a-2)6+(a-1)7$$

Therefore

$$K_2(L(a))=2(4)+2(5)+(a-2)6+(a-1)7+2(4)+2(5)+(a-2)6+(a-1)7=26a-2\cdot$$

Theorem 4.4: If L(*a*) is the chemical graph (see Figure 2) then the K_3 index of the graph L(*a*) is K_3(L(*a*)) = 24 when *a* = 1= 42*a*-20, where *a*>1 is a positive integer.

Proof: In the set A two vertices namely x_1 and x_{2a+1} having weight 4, two vertices namely x_2 and x_{2a} having weight 6, (*a*-2) vertices namely $x_4, x_6, x_8, \ldots, x_{2a-2}$ having weight 9, (*a*-1) vertices namely $x_3, x_5, x_7, \ldots, x_{2a-1}$ having weight 12.

In the set B two vertices namely y_1 and y_{2a+1} having weight 4, two vertices namely y_2 and y_{2a} having weight 6, (*a*-2) vertices namely $y_4, y_6, y_8, \ldots, y_{2a-2}$ having weight 9, (*a*-1) vertices namely $y_3, y_5, y_7, \ldots, y_{2a-1}$ having weight 12.

Therefore

$K_3(L(a)) = \sum_{\{x_i\}\in A} W(x_i) + \sum_{\{y_i\}\in B} W(y_i)$

Here

$$\sum_{\{x_i\}\in A} W(x_i) = 2(4) + 2(6) + (a-2)9 + (a-1)12$$

$$\sum_{\{y_i\}\in B} W(y_i) = 2(4) + 2(6) + (a-2)9 + (a-1)12$$

Therefore

$$K_3(L(a)) = 2(4) + 2(6) + (a-2)9 + (a-1)12 + 2(4) + 2(6) + (a-2)9 + (a-1)12 = 42a - 20.$$

Theorem 4.5: If L(*a*) is the chemical graph (see Figure 2) then the K_4 index of the graph L(*a*) is $K_4(L(a))$ = 18 when *a* = 1= $6a^2+8a+2$, where *a*>1 is a positive integer.

Proof: We know $K_4(G) = \sum_{v\in V(G)} W(v)$

$K_4(L(a)) = \sum_{\{x_i\}\in A} W(x_i) + \sum_{\{y_i\}\in B} W(y_i)$ Here

$$\sum_{\{x_i\}\in A} W(x_i) = 2\left[(2a+1) + (2a) + (2a-1) + \ldots + (2a-(a-2))\right] + (2a-(a-1))$$

$$\sum_{\{y_i\}\in B} W(y_i) = 2\left[(2a+1) + (2a) + (2a-1) + \ldots + (2a-(a-2))\right] + (2a-(a-1))$$

Therefore

$$K_4(L(a)) = 2\left[(2a+1) + (2a) + (2a-1) + \ldots + (2a-(a-2))\right] + (2a-(a-1)) + 2\left[(2a+1) + (2a) + (2a-1) + \ldots + (2a-(a-2))\right] + (2a-(a-1))$$

$$= 2\left[2(a)(2a) - 2(2+3+\ldots+(a-2))\right] + 2(a+1)$$

$$= 2\left[4a^2 - (a-2)(a-1) + 2\right] + (2a+2)$$

$$= 6a^2 + 8a + 2.$$

Remark 4.6: K_1, K_2, K_3 can be represented in terms of K as follows:

$K_1 = \sqrt{K},\ K_2 = \frac{26}{4}K + 24,\ K_3 = \frac{42}{4}K + 22$ (where $a \neq 1$ in K_3)

COMPARISON OF RESULTS

In this section we compute the correlation of log p with K, K_1, K_3 and K_4 considering the first 20 compounds of polyacenes (L(*a*), *a*=1 to 20)

The values of K, K_1, K_2, K_3, K_4 and log p for these compounds are tabulated below (Table 1).

Table 1.

No	K	K_1	K_2	K_3	K_4	log p
1	0	0	24	24	18	2.202
2	4	2	50	64	42	3.396
3	8	2.828	76	106	80	4.590
4	12	3.464	102	148	13	5.784
5	16	4	128	190	192	6.978
6	20	4.472	154	232	266	8.172
7	24	4.8989	180	274	352	9.366
8	28	5.2915	206	316	450	10.560
9	32	5.657	232	358	560	11.754
10	36	6	258	400	682	12.948
11	40	6.3245	284	442	816	14.142
12	44	6.6332	310	484	962	15.336
13	48	6.928	336	526	1120	16.530
14	52	7.211	362	568	1290	17.724
15	56	7.4833	388	610	1472	18.918
16	60	7.7459	414	652	1666	20.112
17	64	8	440	694	1872	21.306
18	68	8.2642	466	736	2090	22.500
19	72	8.4852	492	778	2320	23.694
20	76	8.7178	518	820	2562	24.880

Following are correlation coefficients of log p with K, K_1, K_3 and K_4

Table 2.

r	log p
K	0.99999997250969
K_1	0.96545941249478
K_3	0.99999854115530
K_4	0.97445287313308

CONCLUSIONS

From the table it is clear that K is highly correlated with log p compared to other indices. In [10] we observed that among W, PI, Sz, Sh and Fr indices of polyacenes, Sh7 is highly correlated with log p with the value of r = 0.9996. However our new index K has better correlation 0.99999997250969 (almost one) than Sh index and this is more suitable for QSAR/QSPR studies. The regression equation between log p and K is log p = 2.20268571428571 + 0.29847142857143 K and the graphs of log p and predicted log p are given below.

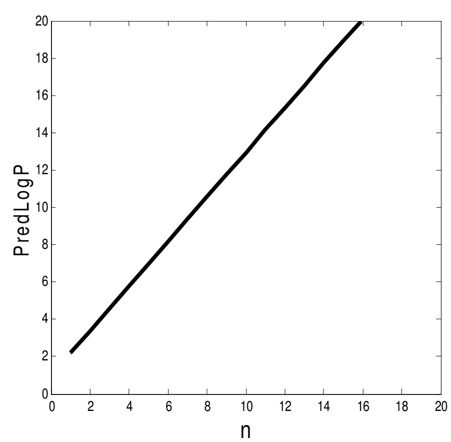

Fig 3 (a). Graph of predicted log p

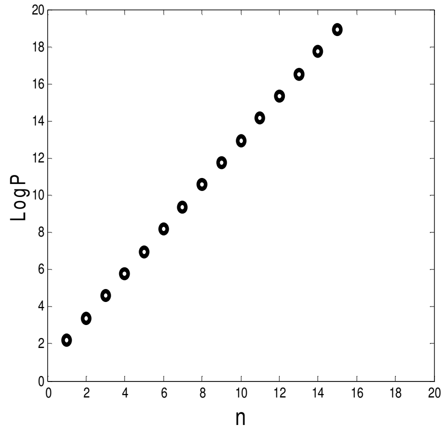

Fig 3 (b). Graph of log p

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REFERENCES

[1] Ali Reza Ashrafi, Amir Loghman, 2006. PI index of some Benzenoid graphs, *Journal of Chilean Chemical Society,* 51(3)(2006), 968-970.

[2] Damir Verkicevic, Nenod Trinajstic, 2004. Wiener index of Benzenoid graphs, *Bulletin of Chemists and Technologists of Macedonia*, 23(2),113-129.

[3] Gutman I,1999. Graph Theory Notes, Newyork, 27,9-15.

[4] Mojtaba Shamsipur, Bahram Hemmateenejad, Morteza Akhond, 2004. Highly Correlating Distance/Connectivity-Based Topological Indices, *Bull. Korean Chem. Soc.* Vol.25, No.2, 253-259.

[5] Prabhakara Rao N, Lavanya Lakshmi K, 2008. On the computation of PI,Sz and S indices of tetragonal systems, *Acta Ciencia Indica*, Vol.XXXIV M, No.4,1753-1766.

[6] Prabhakara Rao N, Lavanya Lakshmi K, Laxmi Prasanna A, 2007. On the Wiener index of product Of Path graphs, proceedings of national conference on discrete mathematics and its applications, NCDMA, Thiagarajar college of engineering, Madurai, p(30)-p(37).

[7] Prabhakara Rao N, Lavanya Lakshmi K, Laxmi Prasanna A, 2007.On the Wiener index of Penta chains, proceedings of national conference on discrete mathematics and its applications, NCDMA, Thiagarajar college of engineering, Madurai.

[8] Prabhakara Rao N, Lavanya Lakshmi K, 2008. On PI index of multiple phenylenes, *International journal of combinatorial Graph theory and applications,* Vol.1, No.2, pp.117-124.

[9] Prabhakara Rao N, Lavanya Lakshmi K, 2009. On Sz index of multiple phenylenes, *International Journal of Computational Cognition*, Vol.7, No.3, pp.44-49.

[10] Prabhakara Rao N, Lavanya Lakshmi K, 2010. On a svd based topological index for polyacenes,*International journal of computational cognition,* Vol.8, No.4, pp.60-63.

[11] Lavanya Lakshmi K, On Wiener index of multiple phenylenes, *International journal of combinatorial Graph theory and applications,* Vol.2, No.1, pp.57-62.

[12] Lavanya Lakshmi K, 1947. On Fr indices of phenylenes, International journal of computational cognition, Vol.8, No.3, pp.44-46, september-2010.Wiener H, Structural Determination of Paraffin boiling points, *Journal of American Society,* 69,17-20.