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Characteristic Graph vs Benzenoid Graph

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ABSTRACT

A characteristic graph is a tree representative of its corresponding benzenoid (cyclic) graph. It may contain necessary information of several properties of benzenoids. The PI-index of benzenoids and their characteristic graphs are compared by correlating it to a structural property (π-electron energy) of the benzenoids using MLR analysis. PI index being applicable to both trees and cyclic graphs, yielded required results for benzenoid and their characteristic graph.

1. Introduction

Topological indices are a numerical representation of a chemical graph, which is obtained by imposing certain conditions on atoms, vertices, or both. The first application of these indices in the studies of structure-properties relationship (QSPR) was proposed by Weiner. Since then, for many years, more than one hundred topological indices were introduced which has enabled to characterize the physicochemical properties of most of the molecules. The most commonly used are Wiener-, Szeged -, PI, Balaban, Schultz's and Sadhana index. A characteristic graph (*or a dualistic graph*) is a tree representative of the corresponding benzenoid (cyclic) graph (*Benzenoid graphs* are graph theoretical representations of benzenoid hydrocarbons). First introduced by (Balaban *et. al.* 1976), it consists of vertices placed in the center of benzenoid rings, and edges connecting these vertices as shown in the figure 1.

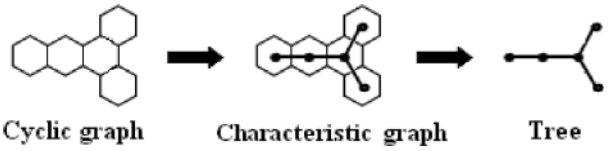

Figure 1. A benzenoid graph and its characteristic graph.

Due to different annelations of Benzenoid rings, their geometry may be represented by certain codes. Digit 0 indicates linear annelation (angle of 180º in the characteristic graph), whereas digits 1 and 2 denote kinked annelation (angles of 120° or 240° starting from one extremity of the Benzenoids, keeping the right → left direction of annelation corresponding to digits 1 and 2, respectively, and choosing among possible notations by the minimal number formed by digits 0, 1, and 2). These corresponding characteristic graphs were supposed to contain important information about the properties of the benzenoids. PI index being applicable to both trees and cycles, seems to yield desired results for benzenoid and their characteristic graph.

Statistical techniques like multiple linear regression (MLR) are the mathematical basis for the developing QSAR models. This is done by carrying out standard multi-regression calculations using multiple variables (topological indices) in a single equation. The statistical parameters like R^2 (the squared correlation coefficient), R^2_{adj} (an adjusted version of R^2), CV (coefficient of variation), F (Fischer statistic parameter) and Press R-Squared, are very useful to investigate the participation of individual topological index for modelling the QSAR models (Gupta and Kapoor 2006, Studenmund 1992). MLR is performed using NCSS software.

Comparison between the PI indices of benzenoids as well as their characteristic graphs are done by correlating it to a structural property (π-electron energy (Balaban *et al.* 2011, Singh *et. al.* 2006)) of the benzenoids using MLR analysis. The *Hückel's π-electron energy*, denoted by E_π, of

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any benzenoid graph is the total energy of the corresponding molecule obtained by the sum of the eigen values of adjacency matrix of the benzenoid graph. It is also given by the expression:

$$E_\pi = n + \frac{m}{3} \quad (1)$$

where, n = number of vertices and m = number of edges in a benzenoid graph.

3. PI Index

In the year 2000 (Khadikar, Karmarkar and Agrawal 2001, Khadikar *et. al.* 2006), Khadikar introduced an index, called *Padmakar Ivan index* (PI index). Here, it is defined as:

$$PI\ (G) = \sum \left[n_{e_u}(e \mid G) + n_{e_v}(e \mid G) \right] \quad (2)$$

where, e = uv ∈ E (G); n_{eu} and n_{ev} are the number of edges closer to u and v respectively and edges equidistance from both end of the edge uv are not counted.

In (John, Khadikar and Singh 2007), derived simpler definition of PI index using the concept of orthogonal cuts (denoted as c). Here, PI(G) for bipartite *sco* graph G was derived as:

$$PI\ (G) = m(G)^2 - \sum_{s=1}^{c} m_s(G)^2 \quad (3)$$

Several analytical formulae for computing PI index of few special class of graphs were derived using equation (2) and (3). One such result was PI index of acyclic graphs (trees) (Khadikar *et. al.* 2006). For a tree G with n-vertices, it is defined as PI (G) = (n – 1)(n – 2).

4. Main Results

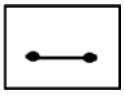
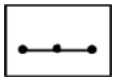
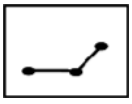
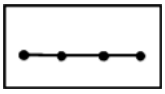
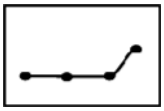
The characteristic graphs are tree equivalents of the cyclic benzenoid graphs. The question arises whether we can compare the PI indices of both of them? If yes, then we can find all the information related to a cyclic graph using that of its tree's. This is done by correlating any structural property of the given set of samples (molecular graphs) with PI index of their characteristic graphs and benzenoid graphs. If nearly same coefficient of determination (R^2) is obtained then the claim is achieved, otherwise not.

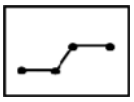
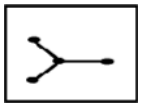
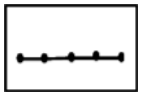
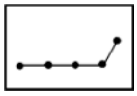
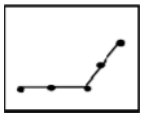
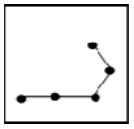
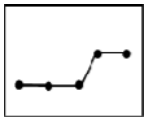
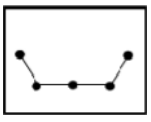
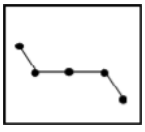
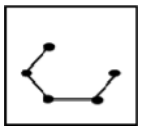
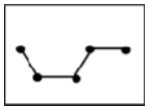
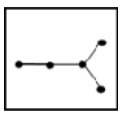
To achieve the claim, we compute the PI index of characteristic graph as well their corresponding benzenoid systems and their π-electron energy as follows:

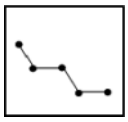
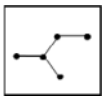
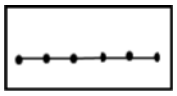
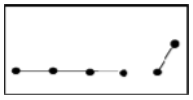
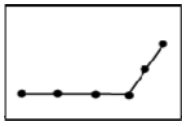
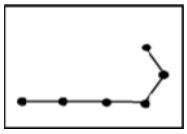
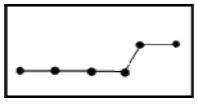
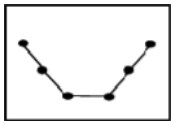
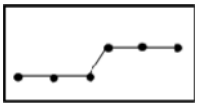
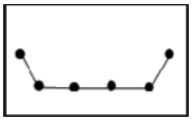
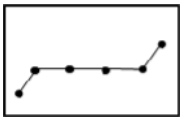
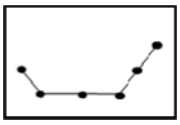
4.1 *Calculation of Huckel's π-electron energy, PI index of benzenoids, PI index of their characteristic graphs and two simple topological descriptors:*

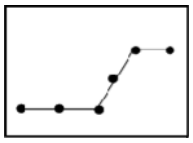
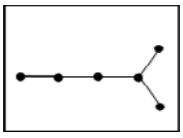
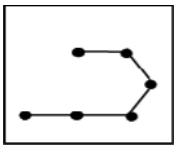
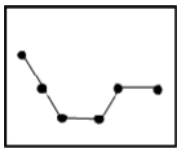
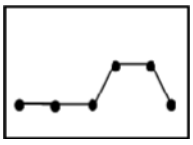
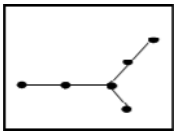
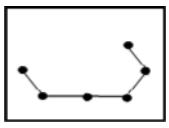
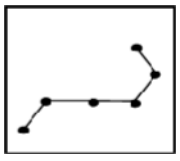
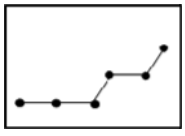
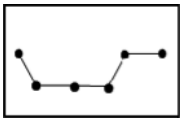
Using equations (1), (3) and (2), π-electron energies (E_π), PI of benzenoid graphs and PI of characteristic graphs of 82 benzenoid graphs (catafusenes) have been computed. The data is arranged in table 1 shown below:

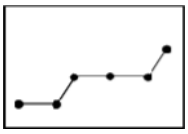
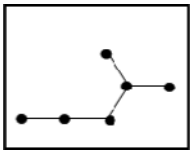
Table 1. Data for 1 – 82 characteristic graph.

S. No.	Structure	E_π	P.I.(B.G.)	P.I.(C.G.)	*h*	*n* + 1
1		13.667	96	0	2	1
2		19.334	216	2	3	2
3		19.334	218	2	3	1
4		25	384	6	4	3
5		25	388	6	4	2

6		25	390	6	4	1
7		25	390	6	4	1
8		25	390	6	4	1
9		30.667	600	12	5	4
10		30.667	606	12	5	3
11		30.667	608	12	5	3
12		30.667	610	12	5	2
13		30.667	610	12	5	2
14		30.667	610	12	5	2
15		30.667	610	12	5	2
16		30.667	612	12	5	1
17		30.667	612	12	5	1
18		30.667	610	12	5	2

19		30.667	612	12	5	1
20		30.667	612	12	5	1
21		36.333	864	20	6	5
22		36.333	872	20	6	4
23		36.333	876	20	6	4
24		36.333	878	20	6	3
25		36.333	878	20	6	3
26		36.333	880	20	6	3
27		36.333	880	20	6	3
28		36.333	878	20	6	3
29		36.333	878	20	6	3
30		36.333	880	20	6	3

31		36.333	880	20	6	2
32		36.333	878	20	6	3
33		36.333	882	20	6	2
34		36.333	882	20	6	2
35		36.333	882	20	6	2
36		36.333	880	20	6	3
37		36.333	882	20	6	2
38		36.333	882	20	6	2
39		36.333	882	20	6	2
40		36.333	882	20	6	2

41		36.333	882	20	6	1
42		36.333	882	20	6	2
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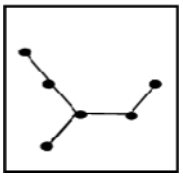
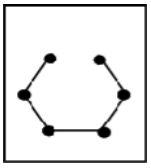
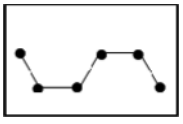
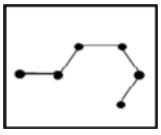
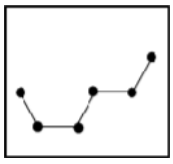
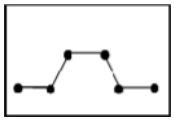
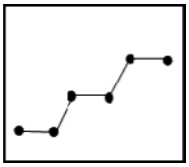
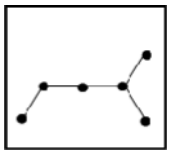
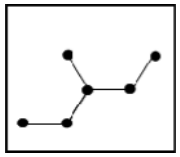
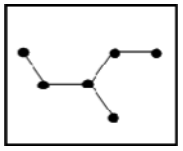
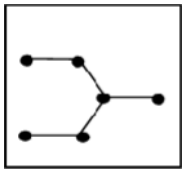
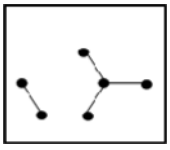
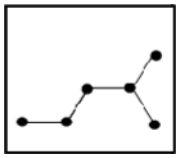
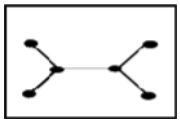
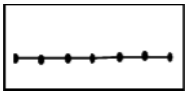
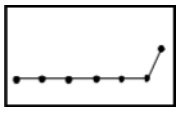
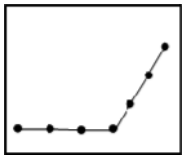
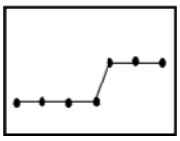
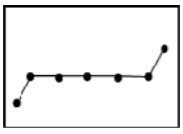
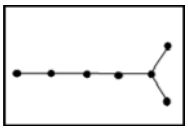
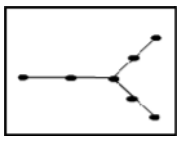
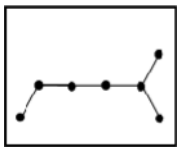
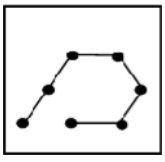
44		36.333	882	20	6	2
45		36.333	884	20	6	1
46		36.333	884	20	6	1
47		36.333	884	20	6	1
48		36.333	884	20	6	1
49		36.333	884	20	6	1
50		36.333	884	20	6	1

51		36.333	882	20	6	2
52		36.333	884	20	6	1
53		36.333	884	20	6	1
54		36.333	884	20	6	1
55		36.333	884	20	6	1
56		36.333	884	20	6	1
57		36.333	884	20	6	1
58		42	1176	30	7	6
59		42	1186	30	7	5
60		42	1194	30	7	5

61		42	1198	30	7	4
62		42	1194	30	7	4
63		42	1194	30	7	4
64		42	1200	30	7	4
65		42	1200	30	7	3
66		42	1204	30	7	2
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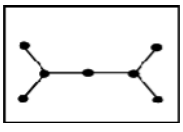
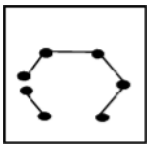
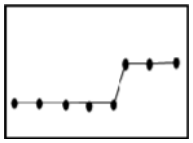
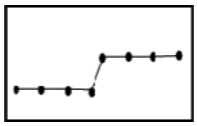
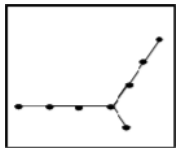
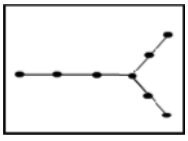
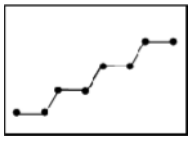
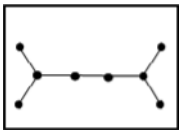
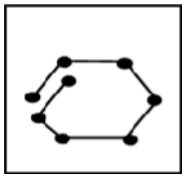
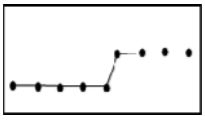
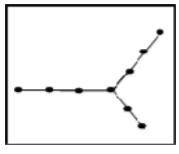
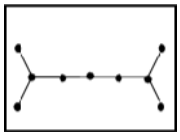
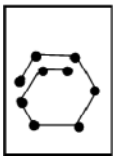
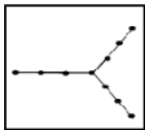
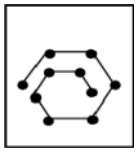
68		42	1204	30	7	2
69		42	1206	30	7	1
70		46.667	1564	42	8	5

71		46.667	1566	42	8	5
72		46.667	1566	42	8	5
73		46.667	1568	42	8	5
74		46.667	1578	42	8	1
75		46.667	1572	42	8	3
76		46.667	1578	42	8	1
77		53.3333	1982	56	9	6
78		53.3333	1986	56	9	6
79		53.3333	1988	56	9	4
80		53.3333	2000	56	9	1

81		59	2454	72	10	7
82		59	2472	72	10	1

4.2 *Correlations between π-electron energy and PI index of benzenoids and their characteristic graphs*

Using NCSS, a multiple regression analysis was performed and following results were obtained:

(i) Modeling of E_π using PI (B.G.):

$$E_\pi = 20.17057 + 1.734088E\text{-}02^* \text{ PI (B.G.)} \quad (4)$$

$$N = 82,\ R^2 = 0.9608,\ R^2_{adj} = 0.9603,\ CV = 4.361719E\text{-}02,\ F = 1958.7307$$

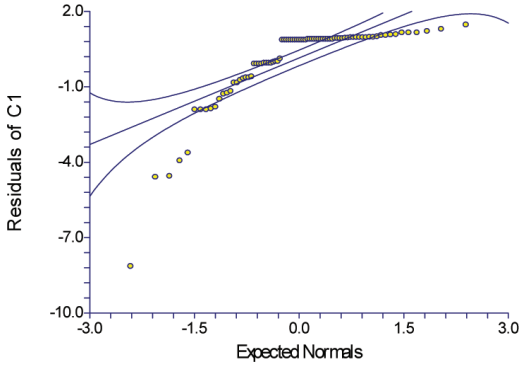


Figure 2. Normal Probability Plot of Residuals of C1

The graph in figure 2 is not completely linear which shows that the benzenoids taken are not same. They are mixture of different types of benzenoids. If their annehling were same then we would have got a linear graph.

(ii) Modeling of E_π using PI (C.G.):

$$E_\pi = 24.29913 + 0.545945^* \text{ PI (C.G.)} \quad (5)$$

$$N = 82,\ R^2 = 0.9365,\ R^2_{adj} = 0.9357,\ CV = 5.548366E\text{-}02,\ F = 1179.9257$$

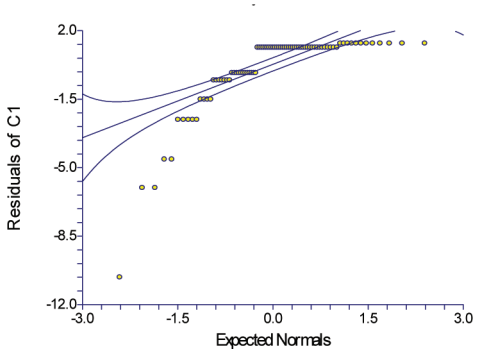


Figure 3. Normal Probability Plot of Residuals of C1

The graph in figure 3 is also not completely linear which shows that the characteristic graphs taken are not same. They are mixture of different types. If their annehling were same then we would have got a linear graph.

Conclusion

Since our objective is to examine which one of PI index is more useful for modeling E_π. For doing so we will have to examine the corresponding models in more detail and consider their regression parameters. In the reffered models (equation (4) and (5)) the statistical parameters viz R and CV are more revelent for the reason that the ratio of R / CV gives the regression quality of the model. This is called as Poglani's quality factor. Note that R is calculated from the square root of R^2. The value of such quality factor expressed as Q are found as 22.4728842 and 17.441699, indicating that the quality of the model in which we have used PI of benzenoid is greater.

The multiplication of R^2 by 100 will give us the % variance in E_π. We oberve that % in E_π using PI (B.G.) comes out to be approximately 96%, while the same using PI (C.G.) is observed to be about 94%. Clearly, we can conclude that

PI index of benzenoid is more useful for modeling E_π as compared to the PI index of characteristic graph.

Another important statistical parameter for examining the relative potential of two types of PI is to examine the values of R^2_{adj}, it will decrease if the added parameter is not favourable for the model. In the above models we observe that R^2_{adj} is of smaller for the latter model. We, therefore, conclude that if PI (B.G.) is replaced by PI (C.G.), then the addition of PI (C.G.) in place of PI (B.G.) is not favourable.

Finally, the relative potential of PI (B.G.) and PI (C.G.) is confirmed on the basis of the magnitudes of the predictive correlation. This is given by the value of Press R-Squared in NCSS software. We obtained these Press R-Squared values as Press R-Squared 0.9558 and Press R-Squared 0.9292 respectively when PI (B.G.) and PI (C.G.) are used for modelling the energy. Press R-Squared therefore finally confirm that PI (B.G.) is more useful than PI (C.G.) for modelling the energy of Benzenoids graphs.

In view of the above, we have estimated the energies of Benzenoids using the model (4) and compared it with the observed values of energies, as in table 1, in the following Table 2.

Table 2. Data for estimated and observed vales of E_π.

S. No.	E_π (from table 1)	E_π (from eq. 4)
1.	13.667	21.83529
2.	19.334	23.91620
3.	19.333	23.95088
4.	25.000	26.82946
5.	25.000	26.89883
6.	25.000	26.933511
7.	25.000	26.933511
8.	25.000	26.933511
9.	30.667	30.575028
10.	30.667	30.679073
11.	30.667	30.713755
12.	30.667	30.748436
13.	30.667	30.748436
14.	30.667	30.748436
15.	30.667	30.748436
16.	30.667	30.783118
17.	30.667	30.783118
18.	30.667	30.748506
19.	30.667	30.783118
20.	30.667	30.783118
21.	36.333	35.153020
22.	36.333	35.291817
23.	36.333	35.361108
24.	36.333	35.395862
25.	36.333	35.395862
26.	36.333	35.430544
27.	36.333	35.430544
28.	36.333	35.395862
29.	36.333	35.395862
30.	36.333	35.430544
31.	36.333	35.430544
32.	36.333	35.395862
33.	36.333	35.465156
34.	36.333	35.465156
35.	36.333	35.465156
36.	36.333	35.430544
37.	36.333	35.465156
38.	36.333	35.465156
39.	36.333	35.465156
40.	36.333	35.465156
41.	36.333	35.465156
42.	36.333	35.465156
43.	36.333	35.465156
44.	36.333	35.465156
45.	36.333	35.499907
46.	36.333	35.499907
47.	36.333	35.499907
48.	36.333	35.499907
49.	36.333	35.499907
50.	36.333	35.499907
51.	36.333	35.465226
52.	36.333	35.499907
53.	36.333	35.499907
54.	36.333	35.499907
55.	36.333	35.499907

56.	36.333	35.499907
57.	36.333	35.499907
58.	42.000	40.563444
59.	42.000	40.736853
60.	42.000	40.875580
61.	42.000	40.944944
62.	42.000	40.875580
63.	42.000	40.875580
64.	42.000	40.979626
65.	42.000	40.979626
66.	42.000	41.048989
67.	42.000	41.083671
68.	42.000	41.048989
69.	42.000	41.083671
70.	46.667	47.291706
71.	46.667	47.326388
72.	46.667	47.326388
73.	46.667	47.361069
74.	46.667	47.534478
75.	46.667	47.430433
76.	46.667	47.534478
77.	53.333	54.540194
78.	53.333	54.609555
79.	53.333	54.644239
80.	53.333	54.85233
81.	59.000	62.725089
82.	59.000	63.037225

From the graph, plotted for table 2 values, shown in figure 4 it is clear that both these values agree well with each other.

Also the value of predictive correlation coefficient comes out to be R^2 pred = 0.960570, showing good correlation.

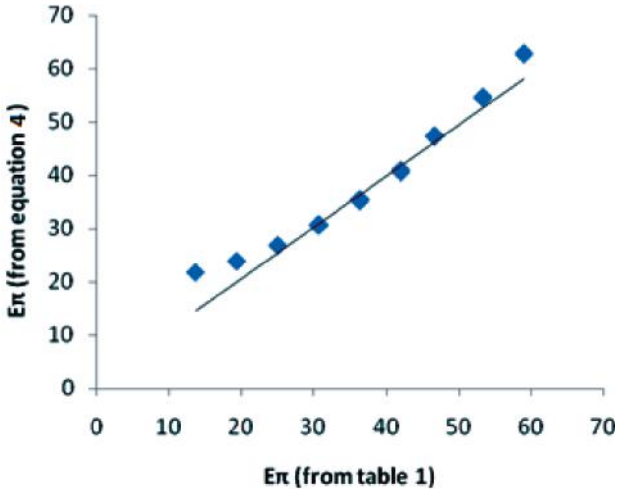


Figure 4. Plot between observed vs estimated values.

References

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