Iranian Journal of Mathematical Chemistry, Vol. 1, No. 1, April 2010, pp. 43 – 67

IJMC

Comparison of Topological Indices Based on Iterated 'Sum' versus 'Product' Operations

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(*Received August 1,2009*)

ABSTRACT

The Padmakar-Ivan (*PI*) index is a first-generation topological index (TI) based on *sums over all edges* between numbers of edges closer to one endpoint and numbers of edges closer to the other endpoint. Edges at equal distances from the two endpoints are ignored. An analogous definition is valid for the Wiener index *W*, with the difference that *sums* are replaced by *products*. A few other TIs are discussed, and comparisons are made between them. The best correlation is observed between indices *G* and *PI*; satisfactory correlations exist between W/n^3 and PI/n^2, where *n* denotes the number of vertices in the hydrogen-depleted graph.

Keywords: topological indices; PI index; Balaban index *J*; Wiener index *W*; *F* and *G* indices

1. INTRODUCTION ABOUT TOPOLOGICAL INDICES

Topological indices are numbers associated with molecular graphs for the purpose of allowing quantitative structure-activity/property/toxicity relationships.[1-6] In hydrogen-depleted (or hydrogen-suppressed) molecular graphs, vertices symbolize non-hydrogen atoms, and edges symbolize covalent bonds, and such graphs are the every-day formulas of organic compounds. The first topological index *W* was introduced by Harold Wiener and bears his name.[7] For trees (acyclic graphs) Wiener defined *W* as the sum of products of the numbers of vertices on the two sides of each edge. Haruo Hosoya advanced his index *Z*,

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introduced the name "topological index", and gave a simpler and more general definition for W as the half-sum of all entries in the distance matrix **D** of the hydrogen-suppressed graph.[8] In this matrix, entries d_{ij} are topological distances along the shortest paths between vertices i and j, whereas in the adjacency matrix **A** entries v are 1 for neighboring (adjacent) vertices and 0 otherwise. Row sums in the adjacency matrix are called vertex degrees v_i and row sums in the distance matrix are called distasums s_i.

The Zagreb indices M_1 and M_2 followed.[9] With the molecular connectivity χ proposed by Milan Randić,[10] topological indices began to be used for many quantitative structure-activity relationships (QSARs) in drug design and the search for new pharmaceuticals.

$$W = \Sigma_i \Sigma_j \, d_{ij} / 2 \tag{1}$$

$$\chi = \Sigma_{\text{all edges}} \, (v_i \times v_j)^{-½} \tag{2}$$

Analogues of χ were developed by Lemont B. Kier and Lowell H. Hall using products of vertex degrees for other paths than edges ij or including information on heteroatoms or multiple bonds in the valence-connectivity index χ^v. Thus, ${}^2\chi$ is the sum of reverse square roots for products of the three vertex degrees of all paths of length 2. Then ${}^1\chi = \chi$ (Randić molecular connectivity), and ${}^0\chi$ is the sum of reverse square roots of all vertex degrees.[4-6]

Both indices W and χ (including higher-order connectivity indices) increase with size and decrease with branching, just as the boiling points of alkanes.

The Schultz molecular topological index (*MTI*) is the sum of E_i elements in the row matrix consisting of v_i(A + D):[11,12]

$$MTI = \Sigma_i \, E_i \tag{3}$$

Although many more topological indices continued to be proposed, we shall discuss here only a few more indices.

(i) The average distance-based connectivity index J, known as the Balaban index, uses distasums instead of vertex degrees and is averaged by the number e of edges and by the cyclomatic number (conventional number of rings) $R = E - n + 1$, where n is the number of graph vertices. It has a lower degeneracy than all previous topological indices.[13-16] Index J increases appreciably with branching, but the very slight increase with graph size is limited asymptotically: for an infinite path its value is the number $\pi = 3.14159\ldots$ Because index J is practically normalized for graph size, it should not be used in monoparametric correlations with properties where the molecular size accounts for a significant part of the variance.

$$J = [\, E/(R + 1)] \, \Sigma_{\text{all edges}} \, (s_i \times s_j)^{-½} \tag{4}$$

(ii) For those properties where not only the "shape" but also the size of the graph influences the property/activity, two indices related to J have been developed. The first of these is index F, defined as:

$$F = E \sum_{\text{all edges}} (s_i \times s_j)^{-½} = J\,(R + 1). \quad (5)$$

This index is able to separate graph size, cyclicity, and branching.[17]

(iii) The other J-related index, called index G, is more convenient for correlations. It is defined as:[17]

$$G = [n^2E/(n + R + 1)] \sum_{\text{all edges}} (s_i \times s_j)^{-½} = n^2J\,(R + 1)/(n + R + 1)] = n^2F/(n + R + 1). \quad (6)$$

It was found that two indices that had been described previously are well correlated with index G, namely the Kier-Hall index TOTOP, and the "triplet index" $DN^2S(4)$.[18] The latter correlation is linear, whereas G and TOTOP are correlated parabolically.

(iv) Ivan Gutman defined a new topological index that he called the Szeged index (Sz) by analogy with the Wiener index for trees: one sums for each graph edge ij the products between the number of vertices n_i that lie closer to vertex i and the number of vertices n_j that lie closer to vertex j (and one ignores any vertices that are equidistant to both endpoints of an edge).[19,20] For trees $W = Sz$, but for cyclic graphs the two indices are distinct.

$$Sz = \sum_{\text{all edges}} (n_i \times n_j) \quad (7)$$

(v) Padmakar Khadikar introduced a new topological index that he called the Padmakar-Ivan (PI) index because Professor Ivan Gutman had initiated him for graph-theoretical applications.[21-51] It differs from the preceding index by the fact the iterated *'product operation'* is replaced by the *'sum operation'*:

$$PI = \sum_{\text{all edges}} (n_i + n_j) \quad (8)$$

By definition, acyclic graphs (trees) are connected graphs with no rings ($R = 0$). They have n vertices, $n - 1$ edges, and for each term (edge) in the above summation $n - 2$ vertices, hence according to eq. 8 the above summation yields for trees a constant value $PI = (n - 1)(n - 2)$, indicating complete degeneracy, therefore the PI index is meaningful only for cyclic graphs. Most of the comparisons discussed here will involve this index.

It should be mentioned that the Cluj-Ilmenau index introduced by Mircea Diudea (a professor at the Cluj University) and Peter John (a professor at the Ilmenau University) is related with the PI index, and for some graphs is equal to it. There are numerous published papers on QSAR studies using the Cluj-Ilmenau index.[52-70]

(vi) Very recently, another index called the sum-connectivity index (${}^s\chi$) was proposed by Bono Lučić, Nenad Trinajstić, and Bo Zhou,[71] following the above trend, and replacing in the Randić product-connectivity index (eq. 2) the *'product operation'* by the *'sum operation'*:

$${}^s\chi = \sum_{\text{all edges}} (v_i + v_j)^{-½} \quad (9)$$

The above authors compared indices ${}^{s}\chi$ and ${}^{1}\chi = \chi$ (Randić's index) and found that ${}^{s}\chi$ presents some interesting features, so that it may be considered as a proper TI.

(vii) To close this section, one should continue further this trend and explore similar replacements of the 'product operation' by the 'sum operation', obtaining for instance the sum-analog (${}^{s}J$) of index J, defined according to equation (10). Similarly, sum-based analogs ${}^{s}F$ and ${}^{s}G$ of indices F and G can be proposed. This will be done in a future contribution, examining properties of such indices.

$$ {}^{s}J = [E/(R+1)] \sum_{\text{all edges}} (s_i + s_j)^{-1/2} \qquad (10) $$

Finally, one must add that two recent generalizations of topological indices proposed by Estrada [72-77] and by Skvortsova, Palyulin and Zefirov [78] encompass many of the TI discussed here.

2. COMPARISON AND CORRELATIONS BETWEEN SOME THE ABOVE TOPOLOGICAL INDICES

Several authors have explored comparisons between some of the above indices for restricted classes of molecular graphs. Khadikar and coworkers investigated correlations between the Wiener index and the PI index and found that for n-alkanes with n vertices (non-branched saturated acyclic hydrocarbons C_nH_{2n+2} or n-paths) they are polynomially-correlated. We take the opportunity for correcting equation (4) in ref. 21 and to present the correct relationship valid for n-paths (eq. 11):

$$ PI = 6W/n - 3(n-1) \qquad (11) $$

Separately, when indices PI and W are applied to such alkanes (or n-paths), relationships (12) and (13) hold:

$$ PI = = (n-1)(n-2) \qquad (12) $$

$$ W = n(n^2-1)/6 \qquad (13) $$

and also recursion formulas:

$$ PI_n = PI_{n-1} + 2n \qquad (14) $$

$$ W_n = W_{n-1} + n(n+1)/2 \qquad (15) $$

For non-branched cycloalkanes with n carbon atoms (C_n-graphs) these indices are:

$$ PI = n(n-2) - n[(-1)^n - 1]/2 \qquad (16) $$

$$ W = n^3/8 - n[(-1)^n - 1]/4 \qquad (17) $$

For vapor pressures (VP) at 25 and 100ºC of 15 polychlorobiphenyl derivatives (PCBs) with 0 to 10 chlorine substituents, the W, Sz, and PI indices led to correlations with coefficients R ranging from –0.911 to –0.973. The same data for PCBs were used in investigating correlations with indices J, PI, and MTI. It was found that PI and MTI which increase with graph size (number n or vertices) are highly intercorrelated with each other (R

= 0.9985) and yield good correlation coefficients with the VP data, but as expected, the monoparametric correlation with *J* is less satisfactory.

Trinajstić and coworkers found that for 30 benzenoid hydrocarbons the sum-connectivity index ($^{s}\chi$) and the Randić product-connectivity index (χ) are correlated with each other and with the π-electronic resonance energy.[71]

In the present paper several comparisons will be made between indices *PI, W, F,* and *G*, using three sets of structures: all possible 90 connected planar chemical graphs with 4 to 6 vertices; 54 aromatic hydrocarbons with various substituents and partly hydrogenated rings; and 71 fully conjugated hydrocarbons where all carbon atoms have sp^2 hybridization.

We present in Table 1 the structures of all 90 possible planar graphs with 4, 5, and 6 vertices with vertex degrees at most 4, together with some of their topological indices. The numbers correspond to those from ref. 11, and the missing numbers are the three non-planar graphs (**27**, **83**, and **92**) that cannot represent chemical compounds where each edge corresponds to one covalent bond. Even some of the structures included in Table 1 are too strained to exist as stable compounds, e. g. the C_6 octahedral elemental carbon (**93**).

Taking into account that, according to equations (12), (13), (16), and (17) for paths and non-branched cycloalkanes, *W* is an n^3-polynomial and *PI* an n^2-polynomial, we present in Fig. 1A a plot of W/n^3 versus PI/n^2 for 88 planar graphs with 4, 5, and 6 vertices, with a modest linear correlation coefficient $R^2 = 0.7407$ (the last two graphs in Table 1 with 6 or 4 vertices of degree 4 have been omitted because they do not represent stable molecules). Taking into account that the ten acyclic graphs contribute to the curving of the plot because they have the highest W/n^3 values, whereas PI/n^2 does not vary with *n*, by omitting these ten graphs, in Fig. 1B the correlation coefficient is raised to $R^2 = 0.7527$.

We explored if there is any correlation between index PI and indices *J*, *F*, and *G*. From Figure 2 one can see that there is a satisfactory correlation with $R^2 = 0.95$ between G and *PI* for all the above 88 planar graphs with 4 – 6 vertices. For the same graphs, a modest correlation exists between *F* and *PI* ($R^2 = 0.80$) and there is practically no correlation between *J* and *PI.*

In Table 2 we present the names of 54 aromatic (partly hydrogenated and/or substituted) compounds together with some of their TIs. As seen in Fig. 3, an excellent correlation exists between indices *G* and *PI*, with $R^2 = 0.96$, and a modest correlation between F and PI ($R^2 = 0.76$). Again we investigated for the same set of 54 aromatic hydrocarbons how well W/n^3 correlates with PI/n^2 and the result is presented in Fig. 4 ($R^2 = 0.89$).

In Fig. 5 we display the structures of 71 fully conjugated polycyclic hydrocarbons with all carbon atoms having sp^2 hybridization, and their TIs are presented in Table 3. Fifteen of these structures appeared also in Table 2, and they are indicated in the column labeled T-2 of Table 3. One can see in Fig. 6 that *G* and *PI* are well correlated ($R^2 = 0.91$) whereas *F* and *PI* are less satisfactorily correlated ($R^2 = 0.55$).

3. CONCLUSIONS

The Padmakar-Ivan (*PI*) index is the first topological index related to an index described earlier and differing from it by the fact that the product operation is replaced by the sum operation. Similarly related indices are ${}^{s}\chi$ and χ. It was found that an index called *G* that is related to the Balaban index *J* correlates well with the index *PI* for three sets of mono- and polycyclic graphs numbering 90, 54, and 71 graphs. Also, there is a satisfactory correlation between the Wiener index *W* and the *PI* index when the former is divided by n^3, and the latter by n^2, where *n* denotes the number of graph vertices.

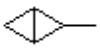
REFERENCES

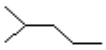
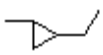
1. A. T. Balaban, O. Ivanciuc, In: J. Devillers and A.T. Balaban (editors), *Topological Indices and Related Descriptors in QSAR and QSPR*, Gordon and Breach. The Netherlands, 1999.
2. M. Karelson, *Molecular Descriptors in QSAR/QSPR*, Wiley-Interscience, New York, 2000.
3. R. Todeschini, V. Consonni, *Molecular Descriptors for Chemoinformatics*, 2nd ed., Wiley-VCH, Weinheim, 2009.
4. L. B. Kier, L. H. Hall, *Molecular Connectivity In Chemistry and Drug Research.* Academic Press, New York (1976).
5. 4. L. B. Kier, L. H. Hall, *Molecular Connectivity in Structure-Activity Analysis.* Wiley, London, 1986.
6. 4. L. B. Kier, L. H. Hall, *Molecular Structure Description: The Electrotopological State*, Academic Press, San Diego, 1999.
7. H. Wiener*, J. Am. Chem. Soc.* **1947**, *69*, 17-20, 2636-2638.
8. H. Hosoya, *Bull. Chem. Soc. Jpn.,* **1971**, *44*, 604-621.
9. I. Gutman, B. Rusčić, N. Trinajstić, C. F. Wilcox, *J. Chem. Phys.* **1975,** *62*, 3399-3409.
10. M. Randic, *J. Am. Chem. Soc.* **1975**, *97*, 6609-6615.
11. H. P. Schultz, *J. Chem. Inf. Comput. Sci.* **1989**, *29*, 227-228.
12. H. P. Schultz, E. B. Schultz, T. P. Schultz, *J. Chem. Inf. Comput. Sci.* **1990**, *30*, 27-29.
13. A. T. Balaban, *Chem. Phys. Lett.*, **1982**, *80*, 399-404.
14. A. T. Balaban, *MATCH Commun. Math. Comput. Chem*. **1986**, *21*, 115-122.
15. A. T. Balaban, O. Ivanciuc, in "*MATH/CHEM/COMP 1988*" (ed. A. Graovac). *Studies in Physical and Theoretical Chemistry,* No. 63, Elsevier, Amsterdam, 1989, pp. 193-211.
16. O. Ivanciuc, T. Ivanciuc, A. T. Balaban, *J. Chem. Inf. Comput. Sci.,* 1998, **38**, 395-401.
17. A. T. Balaban, D. Mills, V. Kodali, S. C. Basak, *SAR QSAR Environ. Res.* **2006**, *17*, 429-450.
18. P. A. Filip, T. S. Balaban, and A. T. Balaban, *J. Math. Chem.*, **1987**, *1*, 61-83.
19. I. Gutman, *Graph Theory Notes (New York)*, **1994,** *27***,** 9-13**.**
20. P. V.Khadikar, N. V. Deshpande, P. P. Kale, A. Dobrynin, I. Gutman, G. Domotor, *J. Chem. Inf. Comput. Sci.* **1995**, *35*, 547-550.

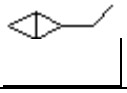
21. P. V. Khadikar, S. Karmakar, V. K. Agarwal, *J. Chem. Inf. Comput. Sci.* **2001**, 41, 934-949.
22. P. V. Khadikar, S. Singh, A. Shrivastava, *Natl. Acad. Sci. Lett. (India)* **2000**, *23*, (No. 11 & 12) 165-1128
23. P. V. Khadikar, S. Karmakar, V. K. Agrawal, *Natl. Acad. Sci. Lett. (India)* **2000**, *23*, (No. 11 & 12) 165-170.
24. P. V. Khadikar, S. Karmakar, V. K. Agrawal, *Natl. Acad. Sci. Lett. (India)* **2000**, *23*, (No. 9 & 10) 124-128.
25. M. Mandloi, A. Sikarwar, N. S. Sapre, S. Karmakar, P. V. Khadikar, *J. Chem. Inf. Comput. Sci.,* **2000**, *40*, 57-62.
26. P. V. Khadikar, *Natl. Acad. Sci. Lett.* **2000**, 23, 113-118.
27. P. V. Khadikar, P. P. Kale, N. V. Deshpande, S. Karmakar,V. K. Agrawal, *J. Math. Chem.* **2001**, *29*, 143-150.
28. P. V. Khadikar, S. Karmakar, S. Singh, A. Shrivastava, *Bioorg. Med. Chem. Lett.* **2002**, *12*, 1125-1128.
29. P. V. Khadikar, V. K. Agrawal, S. Karmakar, *Bioorg. Med. Chem.* **2002**, *10*, 3499-3507.
30. P. V. Khadikar, S. Karmakar, R. G. Varma, *Acta Chim. Slov.* **2002**, *49*, 755-771.
31. P. V. Khadikar, S. Karmakar, J. Singh, A. Shrivastava, *Bioorg. Med. Chem.* **2002**, *10*, 3163-3170.
32. P. V. Khadikar, A. Phadnis, A. Shrivastava, *Bioorg. Med. Chem.* **2002**, *10*, 1181-1188.
33. P. V. Khadikar, D. Mandloi, A. V. Bajaj, S. Joshi, *Bioorg. Med. Chem. Lett.* **2003**, *13*, 419-422.
34. P. V. Khadikar, M. Mandloi, A. V. Bajaj, S. Joshi, *Bioorg. Med. Chem. Lett.* **2003**, *13*, 419-422.
35. P. V. Khadikar, S. Joshi, A. V. Bajaj, M. Mandloi, *Bioorg. Med. Chem. Lett.* **2004**, *14*, 1187-1191.
36. P. V. Khadikar, S. Singh, M. Jaiswal, M. Mandloi, *Bioorg. Med. Chem. Lett.* **2004**, *14*, 4795-4801.
37. M. Jaiswal, P. V. Khadikar, *Bioorg. Med. Chem.* **2004**, *12*, 1731-1736.
38. M. Jaiswal, P. V. Khadikar, *Bioorg. Med. Chem.* **2004**, *12*, 1793-1798.
39. P. V. Khadikar, S. Singh, V. K. Agrawal, S. Karmakar, K. C. Mathur, *Oxidation Commun*. **2004**, *27*, 17-22.
40. P. V. Khadikar, M. V. Diudea, J. Singh, P. E. John, A. Shrivastava, S. Singh, S. Karmakar, M. Lakhwani, P. Thakur, *Curr. Bioact. Comp.* **2006**, *2*, 19-56.
41. P. E. John, P. V. Khadikar, J. Singh, *J. Math. Chem.* **2007**, *42*, 37-45.
42. P. V. Khadikar, J. Singh, M. Ingle, *J. Math. Chem.* **2007**, *42*, 433-445.
43.. A. R. Ashrafi, M. Mirzargar, *J. Indian Chem. Soc.* **2008,** *47A*, 538-341.
44. M. Mirzargar, MATCH *Commun*. *Math*. *Comput*. *Chem*. (*MATCH*) **2009**, *62*, 363-370.
45. A. Bahrami, J. Yazdani, *Digest J. Nanometer. Biostruct.* **2008**, *3*, 265-267.
46. J. Yazdani, A. Bahrami, *Digest J. Nanometer. Biostruct.* **2009**, *4*, 507-510.
47. H. Yousefi-Azari, A. R. Ashrafi, *J. Comput. Theor. Nanosci.* **2008**, *5,* 2280-2283.
48. A. R. Ashrafi, A. Loghman, *J. Comput. Theor. Nanosci.* **2008**, *5,* 1431-1434.
49. A. Iranmanesh, O. Khormali, *J. Comput. Theor. Nanosci.* **2008**, *5,* 131-139.

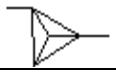
50. H. Yousefi-Azari, A. Bahrami, A. R. Ashrafi, *J. Comput. Theor. Nanosci.* **2008**, *5,* 129-130.
51. H. Deng, S. Chen, *J. Math. Chem.* **2008**, *43*, 19-25.
52. M. V. Diudea, *J. Chem. Inf. Comput. Sci.* **1996**, *36*, 833-836.
53. M. V. Diudea and M. Randić, *J. Chem. Inf. Comput. Sci.* **1997**, *37*, 1095-1100.
54. M. V. Diudea, *MATCH Commun. Math. Comput. Chem.,* **1997**, *35*, 169-183.
55. M. V. Diudea, *J. Chem. Inf. Comput. Sci.* **1997**, *37*, 300-305.
56. M. V. Diudea, B. Pârv, M. I. Topan, *J. Serb. Chem. Soc.* **1997**, *62*, 267-276.
57. M. V. Diudea, B. Parv, and I. Gutman, *J. Chem. Inf. Comput. Sci.* **1997**, *37*, 1101-1108.
58. A. A. Kiss, G. Katona, M. V. Diudea, *Coll. Sci. Papers Fac. Sci. Kragujevac*, **1997**, *19*, 95-107.
59. I. Gutman, M. V. Diudea, *J. Serb. Chem. Soc.* **1998**, *63*, 497-504.
60. M. V. Diudea, G. Katona, I. Lukovits, N. Trinajstić, *Croat. Chem. Acta*, **1998**, *71*, 459-471.
61. M. V. Diudea, *Croat. Chem. Acta,* **1999**, *72*, 835-851.
62. L. Jäntschi, G. Katona, M. V. Diudea, *MATCH Commun. Math. Comput. Chem.*, **2000**, *41*, 151-188.
63. G. Katona, G. Turcu, A. A. Kiss, O. M. Minailiuc, M. V. Diudea, *Rev. Roum. Chim.* **2001**, *46*, 137-151.
64. M. Ardelean, G. Katona, I. Hopartean, M. V. Diudea, *Studia Univ. "Babes-Bolyai"*, **2001**, *45*, 81-95.
65. A. A. Kiss, G. Turcu, M. V. Diudea, *Studia Univ. "Babes-Bolyai"*, **2001**, *45*, 99-106.
66. M. V. Diudea, O. Ursu, *Indian J. Chem.*, **2003**, *42A*, 1283-1294.
67. M. V. Diudea, *Studia Univ. "Babes-Bolyai"*, **2002,** *47*, 131-139.
68. G. Katona, M. V. Diudea, *Studia Univ. "Babes-Bolyai"*, **2003,** *48*, 41-76.
69. M. V. Diudea, *J. Math. Chem.*, 2009, *45*, 295-308.
70. M. V. Diudea, A. E. Vizitiu, D. Janežič, *Chem. Inf. Model.*, **2007**, *47*, 864-874.
71. B. Lučić, N. Trinajstić, B. Zhou, *Chem. Phys. Lett.* **2008**, *475*, 146-148.
72. E. Estrada, *Chem. Phys. Lett.* **2001**, *336*, 248-252.
73. E. Estrada, Y. Gutierrez, *MATCH Commun. Math. Comput. Chem.*, **2001**, *44*, 155-167.
74, E. Estrada, A. R. Matamala, *Chem. Phys. Lett.* **2005**, *410*, 343-347.
75. A. R. Matamala, E. Estrada, *J. Phys. Chem. A,* **2005**, *109*, 9890-9895.
76 E. Estrada, A. R. Matamala, *J. Chem. Inf. Model.* **2007**, *47*, 794-804.
77. E. Estrada, A. R. Matamala, *J. Math. Chem.* **2008**, *43*, 508-517.
78. M. I. Skvortsova, V. A. Palyulin, N. S. Zefirov, *SAR QSAR Env. Res.* **2009**, *20*, 357-377.

Table 1. Topological indices of all 90 possible *connected planar graphs* with 4–6 vertices

No.	Struct.	*R*	*n*	*W*	χ^0	χ^1	χ^2	*Sz*	*PI*	*J*	*F*	*G*
1		0	4	10	3.4142	1.9142	1.0000	10	6	1.9747	1.9747	6.3192
2		0	4	9	3.5774	1.7321	1.7321	9	6	2.3238	2.3238	7.4361
3		1	4	8	2.8284	2.0000	0.7071	16	8	2.0000	4.0000	10.6667
4		1	4	8	2.9916	1.8938	0.8165	8	11	2.1711	4.3422	11.5792
5		2	4	7	2.5689	1.9663	0.2887	9	20	2.4801	7.4402	17.0061
6		3	4	6	2.3094	2.0000	0.0000	6	24	3.0000	12.0000	24.0000
7		0	5	20	4.1213	2.4142	1.3536	20	12	2.1906	2.1906	9.1275
8		0	5	18	4.2845	2.2701	1.8021	18	12	2.5395	2.5395	10.5814
9		0	5	16	4.5000	2.0000	3.0000	16	12	3.0237	3.0237	12.5988
10		1	5	15	3.5355	2.5000	1.7678	20	20	2.0833	4.1667	14.8809
11		1	5	16	3.6987	2.3938	1.3938	28	16	2.0797	4.1593	14.8548
12		1	5	15	3.9142	2.2071	1.9142	15	18	2.3822	4.7644	17.0157
13		1	5	16	3.8618	2.3045	1.4832	16	18	2.2034	4.4069	15.7389
14		1	5	17	3.6987	2.4319	0.9856	17	18	1.9989	3.9979	14.2781
15		2	5	14	3.2760	2.4663	1.0488	24	24	2.1939	6.5818	20.5681
16		2	5	14	3.4916	2.3123	1.2458	16	28	2.3720	7.1159	22.2372
17		2	5	15	3.4392	2.3938	0.9024	19	29	2.1924	6.5771	20.5533
18		2	5	14	3.3284	2.4142	1.0000	14	24	2.2997	6.8990	21.5593

19		2	5	14	3.2760	2.4495	1.1017	36	18	2.1909	6.5727	20.5396
20		3	5	13	3.0689	2.4343	0.6898	18	40	2.4861	9.9443	27.6230
21		3	5	13	3.0165	2.4832	0.6639	29	32	2.3890	9.5560	26.5446
22		3	5	13	3.2321	2.3660	0.8660	13	33	2.5547	10.2186	28.3850
23		3	5	13	3.1213	2.3713	0.7500	19	42	2.5808	10.3232	28.6756
24		4	5	12	2.8618	2.4451	0.4082	16	48	2.8043	14.0214	35.0535
25		4	5	12	2.8094	2.4880	0.3849	24	52	2.7111	13.5554	33.8885
26		5	5	11	2.6547	2.4821	0.1667	15	60	3.1375	18.8248	42.7836
28		0	6	35	4.8284	2.9142	1.7071	35	20	2.3391	2.3391	12.0296
29		0	6	32	4.9916	2.7701	2.1825	32	20	2.6272	2.6272	13.5114
30		0	6	31	4.9916	2.8081	1.9217	31	20	2.7542	2.7542	14.1644
31		0	6	29	5.1547	2.6427	2.4880	29	20	3.1685	3.1685	16.2951
32		0	6	28	5.2071	2.5607	2.9142	28	20	2.9935	2.9935	15.3951
33		1	6	27	4.7321	2.7321	2.0000	27	27	2.3114	4.6227	20.8022
34		1	6	26	4.7845	2.6278	2.4814	26	27	2.4133	4.8266	21.7196
35		1	6	27	4.6213	2.7678	1.9142	27	27	2.2763	4.5527	20.4870
36		1	6	29	4.5689	2.8425	1.6742	29	27	2.0939	4.1878	18.8452
37		1	6	31	4.4058	2.9319	1.3660	31	27	1.8763	3.7526	16.8866
38		1	6	28	4.5689	2.8045	1.7154	28	27	2.1295	4.2589	19.1652
39		1	6	29	4.4058	2.9319	1.5629	45	26	2.0143	4.0285	18.1284

40		1	6	26	4.6213	2.7071	2.4142	42	26	2.3114	4.6229	20.8030
41		1	6	28	4.5689	2.7877	2.1574	46	26	2.1124	4.2247	19.0113
42		1	6	27	4.5689	2.8045	1.9546	44	26	2.2016	4.4032	19.8144
43		1	6	26	4.4058	2.8938	2.3896	33	29	2.1841	4.3682	19.6570
44		1	6	27	4.2426	3.0000	2.1213	54	24	2.0000	4.0000	18.0000
45		2	6	25	4.1987	2.8349	1.6052	25	34	2.1689	6.5066	26.0262
46		2	6	25	4.3618	2.7498	1.7570	29	39	2.2321	6.6962	26.7846
47		2	6	24	4.4142	2.6642	2.1642	26	38	2.3385	7.0155	28.0620
48		2	6	26	4.1463	2.9319	1.1154	34	40	2.0967	6.2902	25.1609
49		2	6	24	4.1987	2.7854	2.0148	56	30	2.1866	6.5598	26.2392
50		2	6	25	4.1463	2.8770	1.6624	55	30	2.1085	6.3254	25.3015
51		2	6	24	4.1987	2.8123	1.9886	38	35	2.2156	6.6468	26.5873
52		2	6	25	4.1463	2.8938	1.6624	37	34	2.1131	6.3393	25.3573
53		2	6	25	4.1463	2.8770	1.6941	40	35	2.0835	6.2504	25.0018
54		2	6	27	4.3094	2.8214	1.5258	35	40	2.0568	6.1705	24.6821
55		2	6	25	4.3618	2.7272	1.8588	31	40	2.2137	6.6410	26.5638
56		2	6	25	3.9831	2.9663	1.5731	59	32	2.0277	6.0832	24.3329
57		2	6	24	3.9831	2.9963	1.9797	34	40	2.0949	6.2846	25.1383
58		2	6	27	3.9831	2.9663	0.9428	27	34	1.9156	5.7467	22.9866

59		2	6	23	3.9831	2.9495	2.2564	40	38	2.1625	6.4875	25.9500
60		3	6	24	3.8868	2.9107	1.2440	48	45	2.1184	8.4736	30.5048
61		3	6	23	3.9392	2.8392	1.6064	47	45	2.2343	8.9373	32.1742
62		3	6	23	3.9392	2.8492	1.5416	43	44	2.2594	9.0376	32.5354
63		3	6	24	3.9392	2.8718	1.2285	32	52	2.1947	8.7786	31.6030
64		3	6	23	3.9916	2.7963	1.5505	30	52	2.3102	9.2410	33.2675
65		3	6	23	3.7760	2.9343	1.3338	41	49	2.2034	8.8137	31.7293
66		3	6	22	3.7760	2.9175	1.6064	34	44	2.2636	9.0544	32.5960
67		3	6	23	3.7236	2.9663	1.3277	38	48	2.1508	8.6030	30.9709
68		3	6	23	4.1547	2.7380	1.6547	23	44	2.3699	9.4795	34.1261
69		3	6	25	3.9392	2.9267	0.9659	25	44	2.1088	8.4353	30.3670
70		3	6	24	3.9916	2.8189	1.2356	34	55	2.2671	9.0685	32.6467
71		3	6	22	3.7760	2.9074	1.5981	48	41	2.2621	9.0485	32.5747
72		3	6	24	3.7760	2.9343	1.0206	30	48	2.1476	8.5903	30.9250
73		4	6	21	3.5689	2.9451	1.1700	33	54	2.4127	12.0637	39.4812
74		4	6	22	3.7321	2.8600	1.1607	40	66	2.3842	11.9212	39.0148
75		4	6	21	3.5165	2.9712	1.2961	40	64	2.3635	11.8174	38.6751
76		4	6	23	3.7321	2.8927	0.9107	31	62	2.3249	11.6243	38.0430
77		4	6	22	3.7845	2.8231	1.1696	28	61	2.4555	12.2776	40.1812
78		4	6	22	3.5689	2.9283	0.9558	34	68	2.3544	11.7722	38.5272

79		4	6	21	3.4641	3.0000	1.1547	51	54	2.3143	11.5715	37.8702
80		4	6	22	3.5689	2.9283	1.0522	49	62	2.3544	11.7722	38.5272
81		4	6	21	3.5165	2.9612	1.1440	41	56	2.3622	11.8108	38.6534
82		4	6	21	3.5165	2.9612	1.2271	54	52	2.3622	11.8108	38.6534
84		5	6	21	3.5774	2.8660	0.8943	29	75	2.6035	15.6211	46.8634
85		5	6	20	3.3618	2.9451	0.8737	38	82	2.5812	15.4874	46.4623
86		5	6	20	3.3094	2.9761	0.8110	50	64	2.5336	15.2014	45.6043
87		5	6	20	3.3094	2.9821	0.8849	49	70	2.5351	15.2106	45.6318
88		5	6	20	3.3618	2.9392	0.8960	52	70	2.5797	15.4783	46.4348
89		5	6	21	3.4142	2.9142	0.7071	34	80	2.5739	15.4433	46.3300
90		5	6	20	3.3618	2.9552	0.9234	41	70	2.5825	15.4948	46.4845
91		6	6	19	3.1547	2.9821	0.5997	48	94	2.7644	19.3507	53.5864
93		7	6	18	3.0000	3.0000	0.3750	48	120	3.0000	24.0000	61.7143

Table 2. Topological indices of 54 aromatic (partly hydrogenated and/or substituted) compounds

No.	*R*	*n*	Compound	*W*	*Sz*	*Pl*	*J*	*F*	*G*
1	3	13	Fluorene	219	420	186	1.762	24.668	70.07
2	3	14	9,10-Dihydroanthracene	279	656	216	1.682	25.230	73.26
3	3	14	Anthracene	279	656	216	1.682	25.230	73.26
4	3	14	9,10-Dihydrophenanthrene	271	632	218	1.74	26.100	75.79
5	3	14	Phenanthrene	271	632	218	1.74	26.100	75.79
6	3	14	1-Methylfluorene	267	499	214	1.786	26.790	77.79
7	3	15	2-Methylanthracene	342	782	248	1.673	26.768	79.25
8	3	15	1-Methylanthracene	334	766	248	1.714	27.424	81.19
9	3	15	2-Methylphenanthrene	334	758	250	1.722	27.552	81.57
10	3	15	1-Methylphenanthrene	326	742	250	1.763	28.208	83.51
11	3	15	9-Ethylfluorene	319	610	252	1.831	29.296	86.73
12	3	16	2-Ethylanthracene	420	923	282	1.642	27.914	84.07
13	3	16	3,6-Dimethylphenanthrene	396	872	284	1.746	29.682	89.40
14	3	16	9-Vinylanthracene	388	859	282	1.784	30.328	91.34
15	3	18	2-(tert-Butyl)anthracene	582	1211	356	1.652	31.388	97.32
16	3	18	1-Methyl-7-isopropylphenanthrene	573	1202	358	1.692	32.148	99.67
17	4	15	4H-Cyclopenta[d,e,f]phenanthrene	300	726	270	1.694	27.104	95.29
18	4	16	7,8,9,10-Tetrahydroacephenanthrene	370	863	309	1.638	27.846	99.84
19	4	16	1,2,3,6,7,8-Hexahydropyrene	362	1008	308	1.671	28.407	101.85
20	4	16	Pyrene	362	1008	308	1.671	28.407	101.85
21	4	16	Fluoranthene	364	801	304	1.677	28.509	102.22
22	4	17	1-Methylpyrene	428	1158	346	1.677	30.186	110.15
23	4	18	Benzo[a]anthracene	553	1325	388	1.512	28.728	106.50
24	4	18	Benzo[c]phenanthrene	529	1253	390	1.587	30.153	111.78
25	4	18	Triphenylene	513	1269	390	1.642	31.198	115.65
26	4	18	3-Ethylfluoranthene	515	1076	378	1.653	31.407	116.43
27	4	19	10-Methylbenz[a]anthracene	648	1516	430	1.502	30.040	112.96
28	4	19	5-Methylbenz[a]anthracene	632	1500	430	1.541	30.820	115.90
29	4	19	6-Methylbenz[a]anthracene	628	1492	430	1.552	31.040	116.72

Table 2. (Continued)

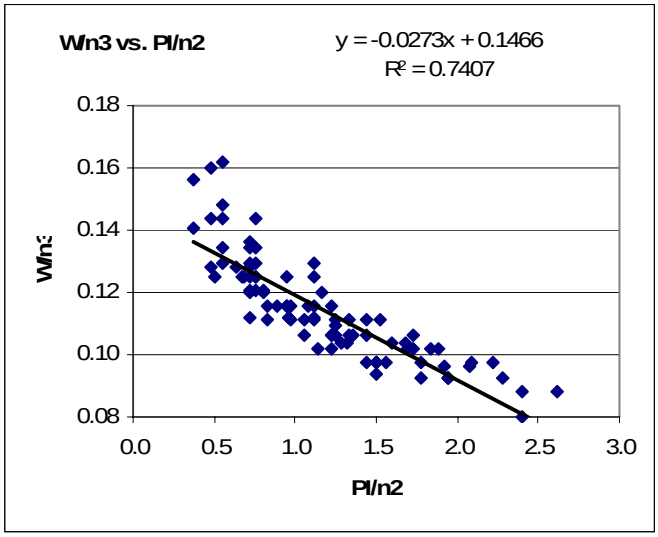
30	4	19	9-Phenylfluorene	621	1146	425	1.587	31.740	119.36
31	4	20	3,9-Dimethylbenz[a]anthracene	762	1762	474	1.480	31.080	118.40
32	4	20	9-Benzylidenefluorene	757	1321	468	1.494	31.374	119.52
33	4	20	9-Benzylfluorene	757	1321	468	1.494	31.374	119.52
34	4	20	9-p-Tolylfluorene	731	1334	468	1.557	32.697	124.56
35	4	20	n-Butylpyrene	732	1714	472	1.561	32.781	124.88
36	4	20	9-Phenylanthracene	714	1526	476	1.581	33.201	126.48
37	4	20	6-Ethylchrysene	714	1638	476	1.582	33.222	126.56
38	4	20	9-m-Tolylfluorene	718	1308	468	1.582	33.222	126.56
39	5	20	Benzo[k]fluoranthene	698	1553	495	1.453	30.513	134.12
40	5	20	Benzo[a]pyrene	680	1887	508	1.487	31.227	137.26
41	5	20	Perylene	654	1858	506	1.545	32.445	142.62
42	5	20	Benzo[e]pyrene	652	1852	508	1.553	32.613	143.35
43	5	21	3-Methylcholanthrene	804	1916	550	1.441	31.702	141.22
44	5	21	3-Methylcholanthrene	804	1916	550	1.441	31.702	141.22
45	5	21	5,6-Dihydro-4H-dibenz[a,k,l]anthracene	786	2032	558	1.469	32.318	143.96
46	5	21	10-Methylbenzo[a]pyrene	772	2094	556	1.499	32.978	146.90
47	5	22	Dibenz[a,h]anthracene	971	2354	610	1.346	30.958	139.60
48	5	22	Benzo[b]triphenylene	907	2290	610	1.449	33.327	150.28
49	5	22	7,10-Dimethylbenzo(a)pyrene	875	2335	606	1.504	34.592	155.99
50	6	22	Indeno(1,2,3-cd)pyrene	845	2211	630	1.428	32.844	166.83
51	6	22	Benzo[g,h,i]perylene	815	2571	644	1.475	33.925	172.32
52	6	24	Dibenzo[a,i]pyrene	1142	3174	758	1.336	33.400	173.77
53	6	24	Dibenzo[a,l]pyrene	1066	3023	758	1.433	35.825	186.38
54	7	24	Coronene	1002	3438	798	1.409	35.225	202.90

Table 3. Topological indices of 71 fully conjugated hydrocarbons with sp^2-hybridized carbon atoms; numbers in the column labeled T-2 correspond to compounds in Table 2.

No.	*R*	*n*	T-2	*W*	$^0\chi$	$^1\chi$	*Sz*	*PI*	*J*	*F*	*G*
1	2	10		109	6.81	4.97	243	96	1.93	5.79	44.54
2	2	12		198	8.23	5.97	360	144	1.80	5.40	51.84
3	3	14	**3**	279	9.38	6.93	656	216	1.68	6.72	73.17
4	3	14	**5**	271	9.38	6.95	632	218	1.74	6.96	75.79
5	3	18		657	12.2	8.93	1170	362	1.45	5.80	85.42
6	4	16	**20**	362	10.5	7.93	1008	308	1.67	8.35	101.79
7	4	16	**21**	364	10.5	7.95	801	304	1.68	8.40	102.40
8	4	18	**25**	513	17.1	12.8	1269	390	1.17	5.85	82.41
9	4	18		545	17.1	12.8	1301	390	1.18	5.90	83.11
10	4	18		569	11.9	8.9	1381	384	1.47	7.35	103.54
11	4	18	**23**	553	11.9	8.92	1325	388	1.51	7.55	106.36
12	4	24		1548	16.2	11.9	2736	678	1.19	5.95	118.18
13	5	20	**39**	698	13.1	9.92	1553	495	1.45	8.70	133.85
14	5	20	**40**	680	13.1	9.92	1887	508	1.49	8.94	137.54
15	5	20		676	13.1	9.93	1553	498	1.50	9.00	138.46
16	5	20		678	13.1	9.93	1524	496	1.50	9.00	138.46
17	5	20		666	13.1	9.93	1556	499	1.53	9.18	141.23
18	5	20	**41**	654	13.1	9.93	1858	506	1.55	9.30	143.08
19	5	20	**42**	652	13.1	9.93	1852	508	1.55	9.30	143.08
20	5	22		1011	14.5	10.9	2506	600	1.29	7.74	133.79
21	5	22		963	17.1	12.9	2330	612	1.30	7.80	134.83
22	5	22		897	14.5	10.9	2410	606	1.32	7.92	136.90
23	5	22		971	14.5	10.9	2454	610	1.35	8.10	140.01
24	5	22		883	14.5	10.9	2202	612	1.35	8.10	140.01
25	5	22		931	14.5	10.9	2234	612	1.37	8.22	142.09
26	5	22	**47**	971	14.5	10.9	2354	610	1.40	8.40	145.20
27	5	22		979	17.1	12.9	2378	608	1.43	8.58	148.31
28	5	22		939	14.5	10.9	2258	610	1.49	8.94	154.53
29	5	22		955	11.9	8.93	2290	610	1.54	9.24	159.72
30	5	22	**48**	907	11.9	8.95	2290	610	1.64	9.84	170.09
31	6	22		871	14.3	10.9	1899	608	1.39	9.73	162.39
32	6	22		839	14.3	10.9	2613	644	1.43	10.01	167.06
33	6	22	**51**	815	14.3	10.9	2571	644	1.48	10.36	172.90
34	6	24		1200	15.7	11.9	2713	734	1.27	8.89	165.18
35	6	24		1166	15.7	11.9	3198	756	1.30	9.10	169.08

Table 3. (Continued)

36	6	24		1160	15.7	11.9	2671	736	1.31	9.17	170.38
37	6	24		1142	15.7	11.9	3174	758	1.34	9.38	174.29
38	6	24	**52**	1142	15.7	11.9	3174	758	1.34	9.38	174.29
39	6	24		1110	15.7	11.9	3128	756	1.37	9.59	178.19
40	6	24		1082	15.7	11.9	3095	756	1.41	9.87	183.39
41	6	24		1088	15.7	11.9	2679	742	1.41	9.87	183.39
42	6	24		1068	15.7	11.9	3029	756	1.43	10.01	185.99
43	6	24	**53**	1066	15.7	11.9	3023	758	1.43	10.01	185.99
44	6	24		1062	16.4	12.4	3096	748	1.46	10.22	189.89
45	6	26		1573	17.1	12.9	3847	880	1.19	8.33	170.64
46	6	26		1453	17.1	12.9	3647	882	1.20	8.40	172.07
47	6	26		1573	17.1	12.9	3847	880	1.20	8.40	172.07
48	6	26		1605	17.1	12.9	3975	872	1.27	8.89	182.11
49	6	26		1581	14.5	10.9	3879	878	1.36	9.52	195.02
50	6	26		1589	14.5	10.9	3903	876	1.41	9.87	202.19
51	6	26		1485	14.5	10.9	3783	878	1.45	10.15	207.92
52	6	26		1333	11.9	8.93	3447	884	1.59	11.13	228.00
53	7	24	**54**	1002	15.4	11.9	3438	798	1.41	11.28	203.04
54	7	26		1305	16.8	12.9	3032	878	1.36	10.88	216.32
55	7	26		1285	16.8	12.9	4075	922	1.37	10.96	217.91
56	7	28		1674	18.2	13.9	4866	1050	1.28	10.24	223.00
57	7	28		1656	18.2	13.9	4794	1058	1.30	10.40	226.49
58	7	28		1626	18.2	13.9	4624	1056	1.32	10.56	229.97
59	7	28		1630	18.2	13.9	4661	1054	1.32	10.56	229.97
60	7	30		2383	19.66	14.83	5860	1200	1.08	8.62	204.06
61	7	30		2375	19.66	14.85	5836	1202	1.08	8.64	204.63
62	7	30		2407	14.5	10.9	5964	1194	1.34	10.72	253.89
63	8	30		2059	19.4	14.9	6287	1250	1.17	10.53	243.00
64	8	30		1931	19.4	14.9	6123	1248	1.25	11.25	259.62
65	8	30		1859	19.4	14.9	4589	1196	1.31	11.79	272.08
66	8	32		2674	20.81	15.83	7340	1404	1.07	9.65	240.96
67	8	32		2674	20.81	15.83	7340	1404	1.07	9.66	241.19
68	9	30		1791	19.1	14.9	6590	1306	1.27	12.70	285.75
69	9	34		2675	21.97	16.9	8334	1626	1.18	11.84	311.07
70	9	34		2657	21.97	16.9	8262	1634	1.20	11.95	313.96
71	9	34		2645	21.97	16.9	8146	1636	1.20	12.00	315.27



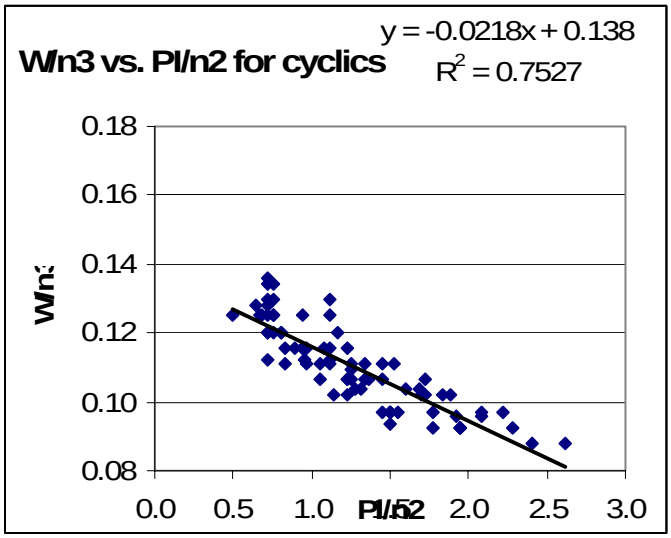


Fig. 1. Plots of W/n^3 versus PI/n^2 for connected graphs with 4, 5, and 6 vertices: A (top), set of 90 *acyclic and cyclic* planar graphs; B (bottom), set of 80 *cyclic* planar graphs from Table 1.

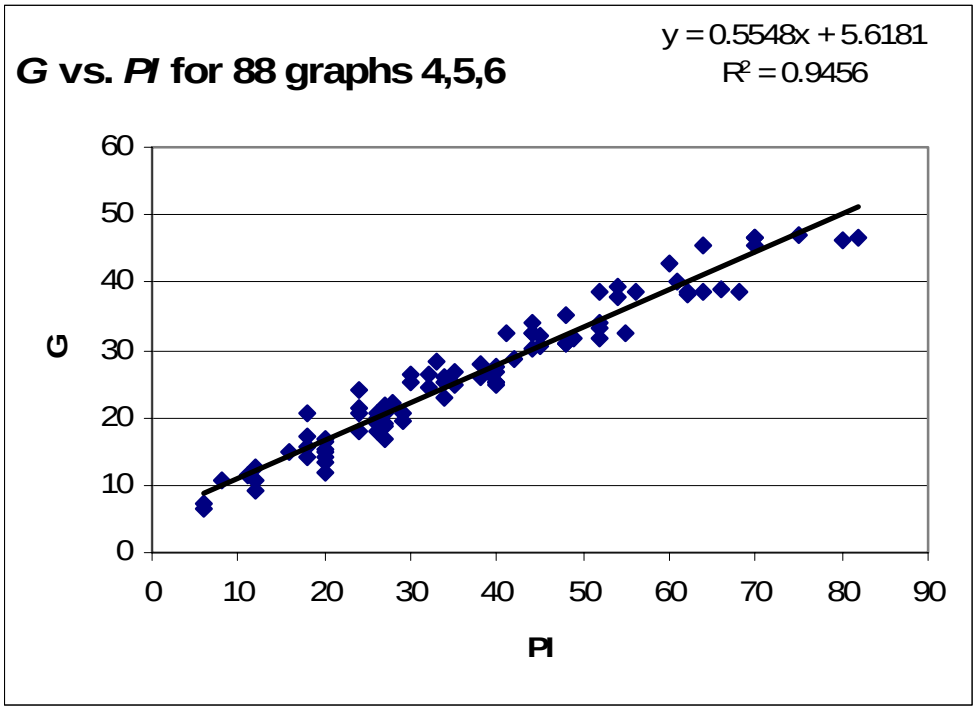


Fig. 2. Plot of index *G* versus index *PI* for 90 planar graphs with 4, 5, and 6 vertices.

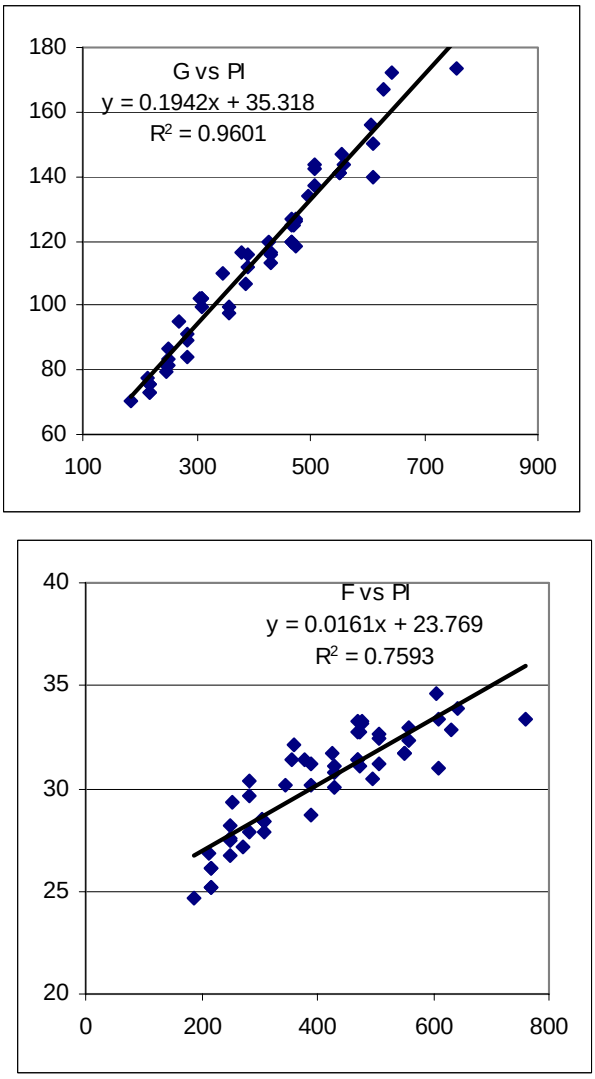


Fig. 3. Plots of *G* versus *PI* for the set of 54 hydrocarbons listed in Table 2 (top), and for the same set, *F* versus *PI* (bottom).

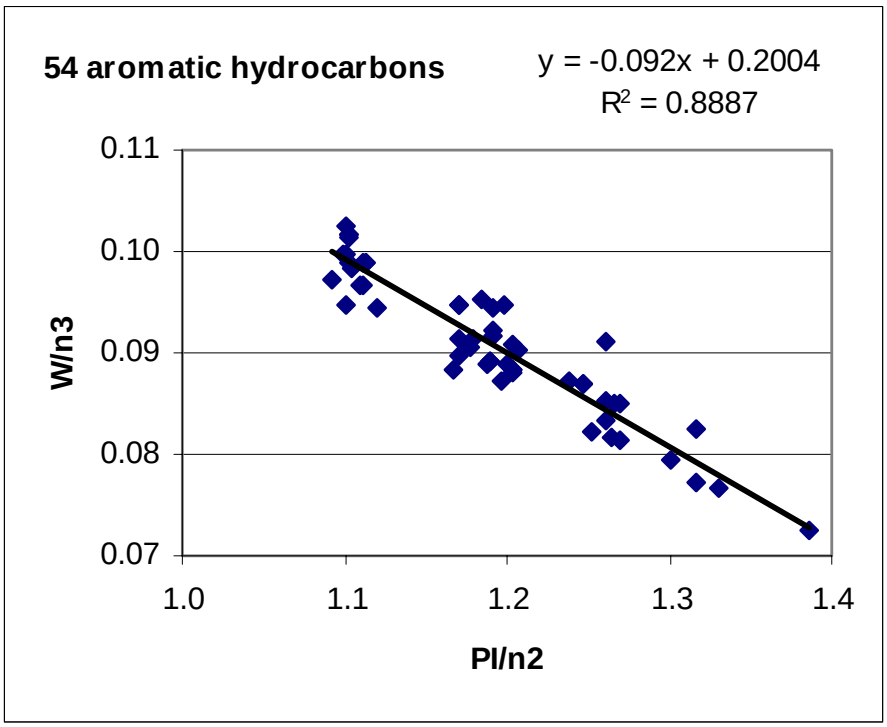
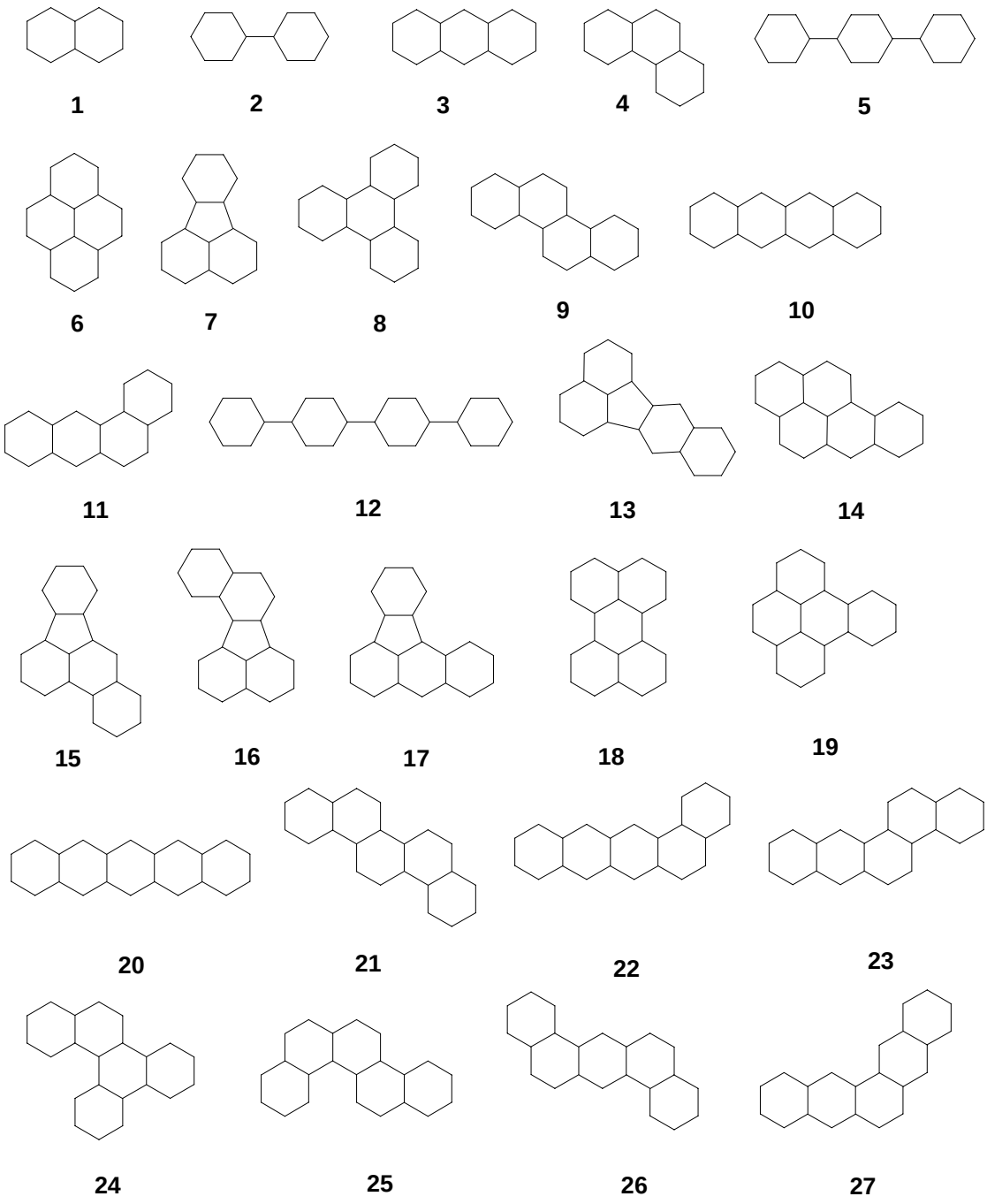


Fig. 4. Plot of W/n^3 versus PI/n^2 for the set of 54 hydrocarbons listed in Table 2.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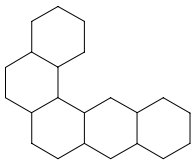

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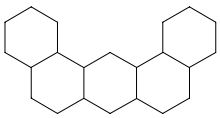

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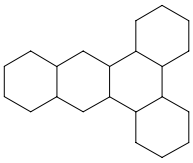

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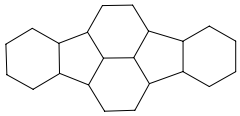

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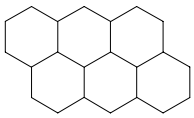

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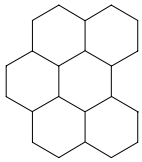

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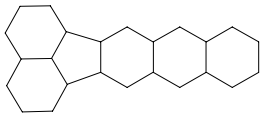

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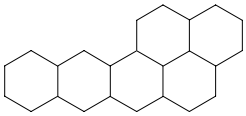

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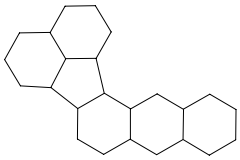

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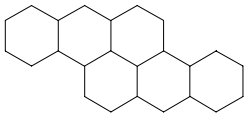

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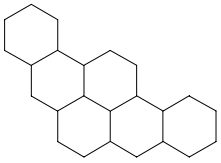

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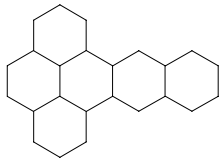

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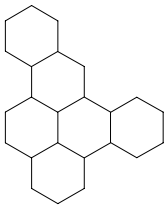

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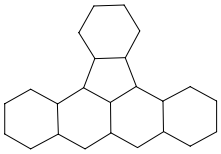

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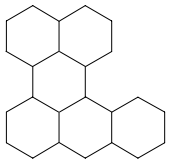

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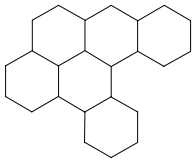

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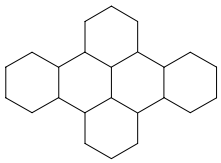

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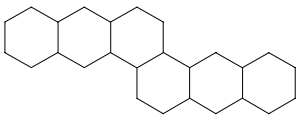

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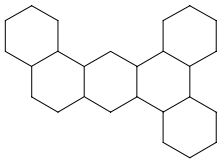

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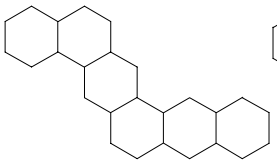

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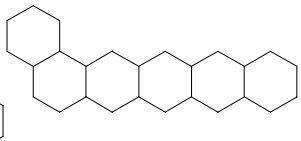

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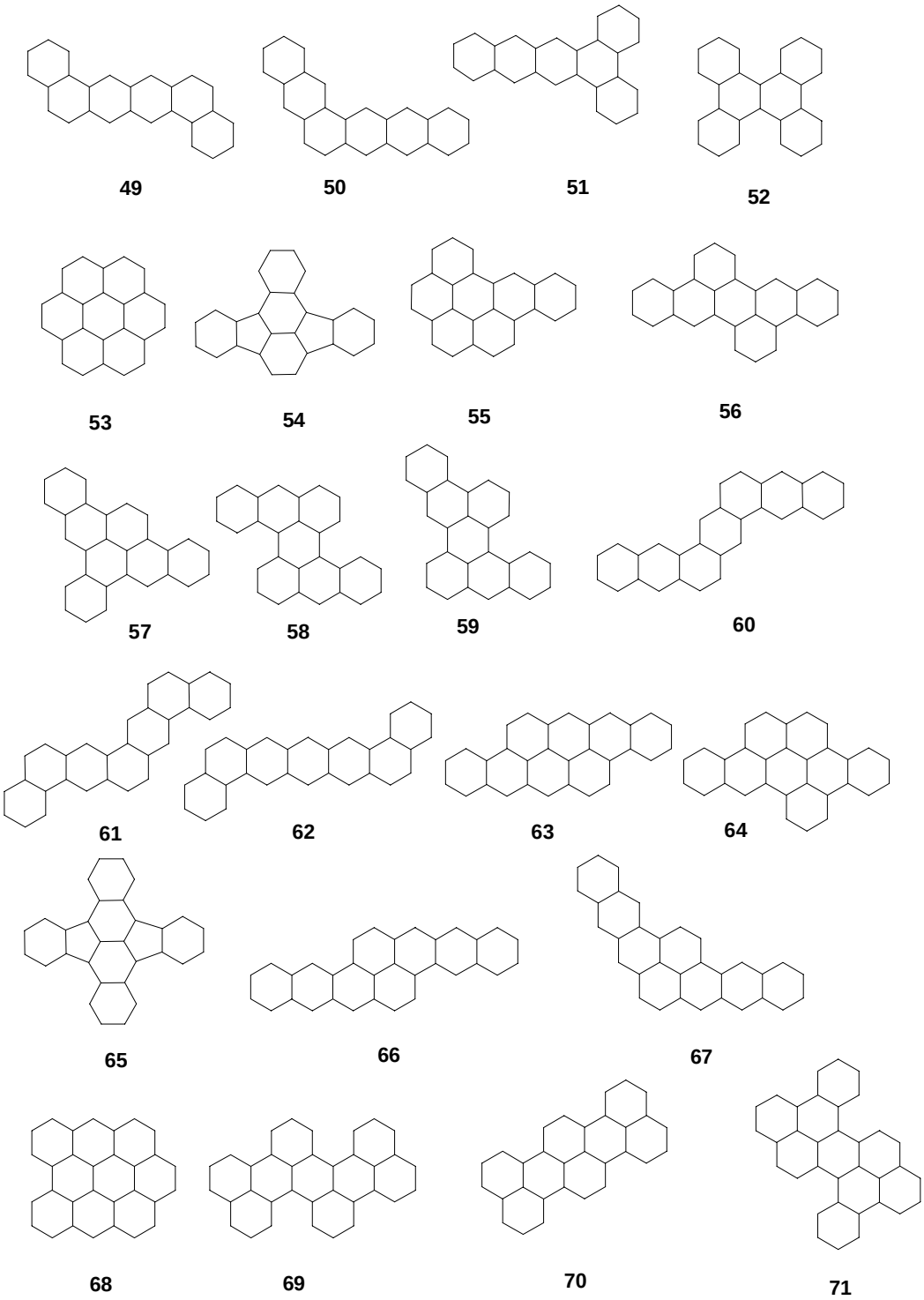

Fig. 5. Structures of 71 sp^2-hybridized fully conjugated hydrocarbons

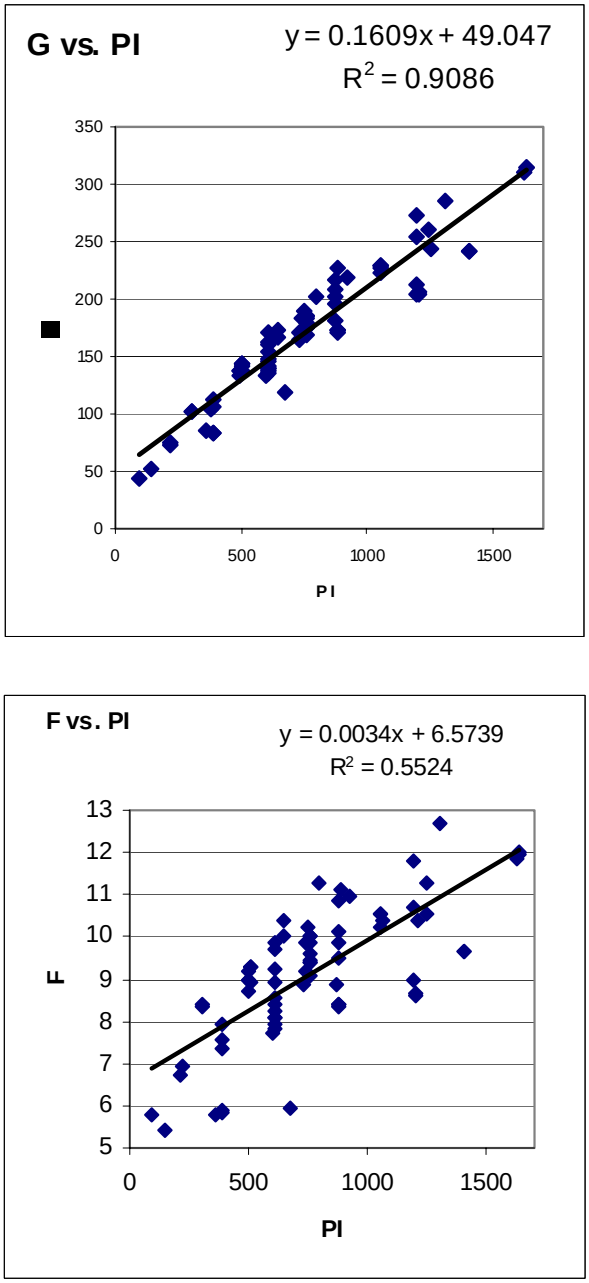

Fig. 6. Plot of *G* versus *PI* for the set of 71 sp^2-hybridized fully conjugated hydrocarbons listed in Table 3 and Fig. 5 (top); and for the same set, *F* versus *PI* (bottom).