The Average Wiener Index of Trees and Chemical Trees

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Meir and Moon (*J. Combin. Theory* **1970**, 8, 99−103) reported a combinatorial formula for the average value of the distance between a pair of vertices in the class of all labeled trees with a fixed number (= n) of vertices. From this result an expression for the average Wiener index $\langle W_n \rangle^{lab}$ of labeled n-vertex trees follows immediately. We show that both the average Wiener index $\langle W_n \rangle$ of nonlabeled n-vertex trees and the average Wiener index $\langle W_n \rangle^{ch}$ of nonlabeled n-vertex chemical trees having $n \leq 20$ vertices are proportional to $\langle W_n \rangle^{1ab}$, with proportionality constants around 0.927 and 0.990, respectively. Analogous results are obtained for the Hosoya polynomial.

1. INTRODUCTION

In the numerous chemical applications of the Wiener index W (for details see the books[1,2] and recent reviews[3,4]), one usually correlates certain physicochemical or pharmacologic properties of a series of compounds with the W-values of the respective molecular graphs. If not all members of the series considered are isomers (which happens quite often), then a general difficulty is necessarily encountered,[5] because the Wiener index depends both on the structure and the size of the molecule and generally increases with the number of vertices of the molecular graph.[6] Now, if the molecular property examined is molecular size independent (e.g., proton and ^{13}C NMR chemical shifts, vibrational frequencies, photoelectron spectra), then it is not meaningful to correlate it with W. If this property is molecular size dependent, there is always a danger that the observed correlation with W is an artifact.[5]

Various remedies have been put forward to overcome this difficulty. The safest solution is to restrict the consideration to classes of isomers. If this is not possible, then usually an extra term is introduced into the correlation, which is believed to compensate for the size-dependence of W. Another way out of would be to normalize the Wiener index, i.e., to make it size-independent. This could be done by using, instead of W, the normalized Wiener index W^{norm}, defined as

$$W^{norm} = W/\langle W \rangle \tag{1}$$

where $\langle W \rangle$ is the average value of the Wiener index, with the averaging being done over a properly chosen set of (molecular) graphs. Until now, however, normalized Wiener indices have not been used, because the values of $\langle W \rangle$ were not available.

In this article we determine $\langle W \rangle$ for n-vertex trees and n-vertex chemical trees. This article is a continuation of the work,[7] in which details concerning the definition of chemical trees, Wiener index and Hosoya polynomial, and computational details can be found.

Let G be a graph on n vertices and let $d(u,v|G)$ be the distance of (the length of the shortest path between) the vertices u and v of G. Then the Wiener index[1−4] is the sum of the distances of all pairs of vertices:

$$W = W(G) = \sum_{u<v} d(u,v|G) \tag{2}$$

Denote by $d(G,k)$ the number of vertex pairs of the graph G which are at distance k. Then the Hosoya polynomial[8,9] is

$$H = H(G) = H(G,x) = \sum_{k\geq 1} d(G,k)x^k \tag{3}$$

Recall that $H'(G,1) = W(G)$.

2. TREES, LABELED TREES, CHEMICAL TREES

A tree is a connected graph without cycles. Suppose that the tree T has n vertices. If we label the vertices of T by n distinct symbols, say 1, 2, ..., n, then we get a labeled tree. In Figure 1 the two nonlabeled 4-vertex trees, together with the corresponding $12 + 4 = 16$ labeled trees[8] are depicted.

As seen from the example given in Figure 1, the number of distinct labeled trees pertaining to a nonlabeled n-vertex tree differs from case to case. (This number lies between n and $n!$) Therefore, the average value of a property of n-vertex trees will, in general, be different from the average value of the same property of n-vertex labeled trees. For instance, if π is such a property, then for nonlabeled 4-vertex trees,

$$\langle \pi \rangle = 0.5\pi(T_1) + 0.5\pi(T_2) \tag{4}$$

whereas for labeled 4-vertex trees

$$\langle \pi \rangle = 0.75\pi(T_1) + 0.25\pi(T_2) \tag{5}$$

If π is the Wiener index, $W(T_1) = 10$, $W(T_2) = 9$, then the two averages are 9.50 and 9.75, respectively.

A chemical tree is a tree in which no vertex has more than four neighbors. These represent the carbon-atom skeleton of alkanes. Both $n = 4$ trees, depicted in Figure 1, are chemical trees (representing butane and 2-methylpro-

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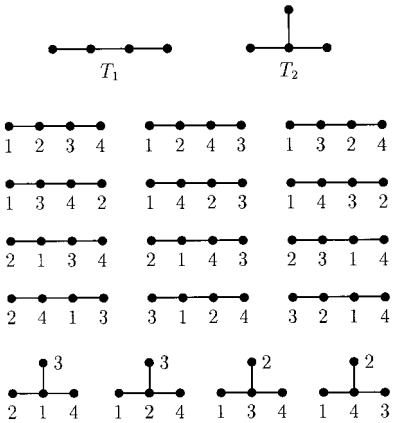

Figure 1. The two trees (T_1 and T_2) on four vertices, together with the 12 labeled trees pertaining to T_1 and the 4 labeled trees pertaining to T_2.

pane), but for larger values of n the number of chemical trees is significantly smaller than the number of all trees; for details see ref 7 and the papers quoted therein.

3. A THEOREM OF MEIR AND MOON AND ITS APPLICATIONS

In an article[10] published almost three decades ago, which apparently evaded the attention of chemical graph theoreticians, Meir and Moon reported the following remarkable result.

Let T be a random labeled tree on n vertices. Let $n(T,u,v)$ be the number of vertices in the path of T, connecting the vertices u and v. Then the probability that $n(T,u,v) = k$ is equal to

$$p(n,k) = \frac{k}{n-1}\frac{k!}{n^k}\binom{n}{k} \tag{6}$$

Clearly, $p(n, k)$ is also the probability that the distance between u and v is $k-1$. Therefore, the probability that the distance between u and v is k is equal to

$$\frac{k+1}{n-1}\frac{(k+1)!}{n^{k+1}}\binom{n}{k+1}$$

and because there are $\binom{n}{2}$ vertex pairs, the average value of $d(T,k)$ is:

$$\langle d(T,k)\rangle^{\text{lab}} = \binom{n}{2}\frac{k+1}{n-1}\frac{(k+1)!}{n^{k+1}}\binom{n}{k+1} \tag{7}$$

After simplification,

$$\langle d(T,k)\rangle^{\text{lab}} = \frac{(k+1)n!}{2n^k(n-k-1)!} \tag{8}$$

which holds for $n \geq 1$ and $k = 1, 2, \ldots, n-1$.

From eq (8) it immediately follows that

$$\langle H(T,x)\rangle^{\text{lab}} = \sum_{k=1}^{n-1}\frac{(k+1)n!}{2n^k(n-k-1)!}x^k \tag{9}$$

Table 1. The Average Wiener Index of n-Vertex Labeled Trees, Calculated According to eq 10[a]

n	$\langle W_n\rangle^{\text{lab}}$	$\langle W_n\rangle^{\text{as}}$	$\langle W_n\rangle^{\text{as}}/\langle W_n\rangle^{\text{lab}}$
4	9.75	20.05	2.06
5	18.88	35.03	1.86
6	31.94	55.26	1.73
7	49.44	81.24	1.64
8	71.84	113.44	1.58
9	99.56	152.28	1.53
10	133.01	198.17	1.49
11	172.57	251.48	1.46
12	218.60	312.60	1.43
13	271.44	381.85	1.41
14	331.44	459.57	1.40
15	398.90	546.08	1.37
16	474.15	641.70	1.35
17	557.46	746.71	1.34
18	649.14	861.41	1.33
19	749.47	986.08	1.32
20	858.72	1121.00	1.31
...	...	...	...
100	56049.80	62665.71	1.12
...	...	...	...
1000	19151606.46	19816636.49	1.03

[a] Meir and Moon showed[10] that for $n \to \infty$ the expected value of the number of vertices in a path of a labeled tree is asymptotically equal to $\sqrt{\pi n/2}$; consequently, the average Wiener index increases asymptotically as $\langle W_n\rangle^{\text{as}} = \sqrt{\pi/8}\, n^{5/2}$; for the first few values of n the agreement $\langle W_n\rangle^{\text{lab}}$ and $\langle W_n\rangle^{\text{as}}$ is quite poor.

and, because $W(T) = \sum_k kd(T,k)$,

$$\langle W_n\rangle^{\text{lab}} = \sum_{k=1}^{n-1}\frac{k(k+1)n!}{2n^k(n-k-1)!} \tag{10}$$

Thus the average of the Wiener index of labeled trees is easily calculated (by means of eq (10); its numerical values for n up to 20 are given in Table 1.

As special cases of eq 8 we point out:

$$\langle d(T,1)\rangle^{\text{lab}} = n-1$$

$$\langle d(T,2)\rangle^{\text{lab}} = \frac{3(n-1)(n-2)}{2n}$$

$$\langle d(T,3)\rangle^{\text{lab}} = \frac{2(n-1)(n-2)(n-3)}{n^2}$$

$$\vdots$$

$$\langle d(T,n-1)\rangle^{\text{lab}} = \frac{n!}{2n^{n-2}} \tag{11}$$

4. NUMERICAL WORK: AVERAGE WIENER INDICES AND HOSOYA POLYNOMIALS FOR NONLABELED TREES AND CHEMICAL TREES

Although the Meir−Moon formula (eq 6) and its consequences, eqs 8 and 10, are beautiful combinatorial results, they are not what is needed in chemical graph theory. Formulas 6 through 10 pertain to labeled graphs, whereas in chemical (and other) applications we are interested in nonlabeled graphs. As explained and exemplified above, averages over labeled and nonlabeled graphs may differ significantly.

Table 2. Average Wiener Indices $\langle W_n \rangle$ and $\langle W_n \rangle^{ch}$ of n-Vertex Nonlabeled Trees and Chemical Trees, Respectively, and the Ratios $C_n = \langle W_n \rangle / \langle W_n \rangle^{lab}$ and $C_n^{ch} = \langle W_n \rangle^{ch} / \langle W_n \rangle^{lab}$, Respectively[a]

n	N_n	$\langle W_n \rangle$	C_n	N_n^{ch}	$\langle W_n \rangle^{ch}$	C_n^{ch}
4	2	9.50	0.9744	2	9.50	0.9744
5	3	18.00	0.9534	3	18.00	0.9534
6	6	30.00	0.9391	5	31.00	0.9706
7	11	46.18	0.9341	9	48.00	0.9709
8	23	66.65	0.9278	18	69.56	0.9683
9	47	92.17	0.9258	35	96.69	0.9712
10	106	123.03	0.9250	75	129.52	0.9738
11	235	159.54	0.9245	159	168.25	0.9750
12	551	202.12	0.9246	355	213.62	0.9772
13	1301	251.07	0.9249	802	265.66	0.9787
14	3159	306.68	0.9253	1858	324.97	0.9805
15	7741	369.26	0.9257	4347	391.73	0.9820
16	19320	439.09	0.9261	10359	466.33	0.9835
17	48629	516.43	0.9264	24894	549.00	0.9848
18	123867	601.56	0.9267	60523	640.12	0.9861
19	317955	694.71	0.9270	148284	739.90	0.9872
20	823065	796.14	0.9271	366319	848.67	0.9882

[a] The values of $\langle W_n \rangle^{lab}$ are given in Table 1. N_n and N_n^{ch} are the counts of n-vertex trees and chemical trees, respectively.

In view of this we determined numerically the average Wiener index and the average Hosoya polynomial for trees and for chemical trees with n vertices ($4 \leq n \leq 20$). This required the construction of all n-vertex trees and the calculation of their respective graph invariants. Pertinent details are outlined elsewhere.[7]

The results obtained for the average Wiener index are given in Table 2, whereas the analogous results for the coefficients of the Hosoya polynomials are given in Table 3.

5. DISCUSSION

The most remarkable feature seen in Table 2 is the fact that the ratios between the average Wiener numbers of labeled and nonlabeled trees, that is the proportionality coefficients C_n and C_n^{ch}, are practically independent of n and with increasing n rapidly became equal to 0.927 and 0.990, respectively. The practical importance of this finding is that $\langle W_n \rangle$ and (surprisingly!) also $\langle W_n \rangle^{ch}$ can be estimated quite accurately by use of the average W-value of labeled trees, which, in turn, are calculated by means of the simple combinatorial formula, eq 10. In particular, reliable approximate values for $\langle W_n \rangle$ and $\langle W_n \rangle^{ch}$ can be obtained for any value of n, without the need of extensive numerical calculations:

$$\langle W_n \rangle \approx 0.927 \sum_{k=1}^{n-1} \frac{k(k+1)n!}{2n^k (n-k-1)!} \qquad (12)$$

$$\langle W_n \rangle^{ch} \approx 0.990 \sum_{k=1}^{n-1} \frac{k(k+1)n!}{2n^k (n-k-1)!} \qquad (13)$$

The case of the average Hosoya polynomial is quite different. As seen from Table 3, its coefficients are by no means proportional to the corresponding values for labeled trees. Moreover, $\langle d(T,k) \rangle$ and $\langle d(T,k) \rangle^{ch}$ are sometimes smaller and sometimes greater than $\langle d(T,k) \rangle^{lab}$. The coefficients of the average Hosoya polynomials are unimodal, with maximum at $k = 2$, i.e.,

$$\langle d(T,1) \rangle < \langle d(T,2) \rangle > \langle d(T,3) \rangle > \langle d(T,4) \rangle > \ldots > \langle d(T,n-1) \rangle$$

and

$$\langle d(T,1) \rangle^{ch} < \langle d(T,2) \rangle^{ch} > \langle d(T,3) \rangle^{ch} > \langle d(T,4) \rangle^{ch} > \ldots > \langle d(T,n-1) \rangle^{ch}$$

The general trend is that for fixed n the coefficients $\gamma_{n,k}$ and $\gamma_{n,k}^{ch}$ (defined in the legend of Table 3) are ordered in the same manner as $\langle d(T,k) \rangle$, with the exception of the last coefficients $\gamma_{n,n-1}$ and $\gamma_{n,n-1}^{ch}$.

This exception may be simply explained. Indeed, it is easy to verify that

$$\langle d(T,n-2) \rangle / \langle d(T,n-1) \rangle = \langle d(T,n-2) \rangle^{ch} / \langle d(T,n-1) \rangle^{ch} = \lceil (n+3)/2 \rceil \qquad (15)$$

where $\lceil x \rceil$ is the smallest integer not less than x. On the other hand, by formulas of section 3,

$$\langle d(T,n-2) \rangle^{lab} / \langle d(T,n-1) \rangle^{lab} = n - 1 \qquad (16)$$

Therefore

$$\gamma_{n,n-1}/\gamma_{n,n-2} = \gamma_{n,n-1}^{ch}/\gamma_{n,n-2}^{ch} = (n-1)/\lceil (n+3)/2 \rceil \qquad (17)$$

implying $\gamma_{n,n-1} < \gamma_{n,n-2}$; $\gamma_{n,n-1}^{ch} < \gamma_{n,n-2}^{ch}$ for $n = 4$, $\gamma_{n,n-1} = \gamma_{n,n-2}$; $\gamma_{n,n-1}^{ch} = \gamma_{n,n-2}^{ch}$ for $n = 5$, 6, and $\gamma_{n,n-1} > \gamma_{n,n-2}$; $\gamma_{n,n-1}^{ch} > \gamma_{n,n-2}^{ch}$ for $n \geq 7$.

We have calculated and tabulated the coefficients of the average Hosoya polynomials (with averaging done both for all nonlabeled trees and all chemical trees) up to $n = 20$. We deem that these data will suffice for practically all imaginable considerations in chemical graph theory.

The rationale for the application of the average Wiener indices has been outlined above. The average Hosoya polynomial has similar potential applicability, except that it can be used for normalizing a great variety of distance-based topological indices. Among them we mention the classes $W_\lambda(G)$ and ${}^kW(G)$, both of which generalize the Wiener index. These are defined as[11]

$$W_\lambda(G) = \sum_{k \geq 1} k^\lambda d(G,k)$$

and[12]

$${}^kW(G) = H^{(k)}(G,1)$$

where $H^{(k)}(G,x)$ stands for the kth derivative of the Hosoya polynomial, $k = 1, 2, 3, \ldots$; for $k = 1$, ${}^kW$ is just the usual Wiener index. For $\lambda = -2, -1, +1$, W_λ is the Harary index,[13] the reciprocal Wiener index,[14] and the usual Wiener index, respectively. For $\lambda = 2,3$, W_λ is simply related to the hyper-

Table 3. Average Coefficients $\langle d(T,k)\rangle$ and $\langle d(T,k)\rangle^{ch}$ of the Hosoya Polynomials of n-Vertex Nonlabeled Trees and Chemical Trees, Respectively, and the Ratios $\gamma_{n,k} = \langle d(T,k)\rangle/\langle d(T,k)\rangle^{lab}$ and $\gamma^{ch}_{n,k} = \langle d(T,k)\rangle^{ch}/\langle d(T,k)\rangle^{lab}$, Respectively[a]

n	k	$\langle d(T,k)\rangle$	$\gamma_{n,k}$	$\langle d(T,k)\rangle^{ch}$	$\gamma^{ch}_{n,k}$	n	k	$\langle d(T,k)\rangle$	$\gamma_{n,k}$	$\langle d(T,k)\rangle^{ch}$	$\gamma^{ch}_{n,k}$	n	k	$\langle d(T,k)\rangle$	$\gamma_{n,k}$	$\langle d(T,k)\rangle^{ch}$	$\gamma^{ch}_{n,k}$
4	1	3.000	1.000	3.000	1.000	13	1	12.000	1.000	12.000	1.000	17	10	0.637	0.473	1.042	0.773
	2	2.500	1.111	2.500	1.111		2	18.382	1.206	15.738	1.033		11	0.202	0.389	0.354	0.683
	3	0.500	0.667	0.500	0.667		3	17.046	1.092	15.878	1.016		12	0.053	0.323	0.099	0.599
5	1	4.000	1.000	4.000	1.000		4	13.852	1.025	14.026	1.037		13	0.011	0.267	0.021	0.513
	2	4.333	1.203	4.333	1.203		5	8.898	0.891	10.029	1.005		14	0.002	0.236	0.004	0.461
	3	1.333	0.694	1.333	0.694		6	4.779	0.762	5.990	0.955		15	0.000	0.207	0.000	0.404
	4	0.333	0.694	0.333	0.694		7	2.059	0.623	2.845	0.860		16	0.000	0.331	0.000	0.646
6	1	5.000	1.000	5.000	1.000		8	0.733	0.512	1.096	0.766	18	1	17.000	1.000	17.000	1.000
	2	6.167	1.233	5.400	1.080		9	0.200	0.408	0.315	0.645		2	26.802	1.182	23.081	1.018
	3	2.833	0.850	3.400	1.020		10	0.044	0.353	0.071	0.572		3	27.832	1.105	25.184	1.000
	4	0.833	0.600	1.000	0.720		11	0.006	0.295	0.010	0.478		4	26.407	1.079	25.010	1.021
	5	0.167	0.600	0.200	0.720		12	0.001	0.442	0.001	0.718		5	21.361	1.007	21.699	1.022
7	1	6.000	1.000	6.000	1.000	14	1	13.000	1.000	13.000	1.000		6	15.191	0.920	16.787	1.017
	2	8.000	1.244	6.889	1.072		2	20.065	1.200	17.203	1.029		7	9.408	0.816	11.414	0.990
	3	4.455	0.909	5.000	1.020		3	19.210	1.096	17.735	1.013		8	5.108	0.709	6.824	0.947
	4	2.000	0.762	2.444	0.932		4	16.272	1.041	16.164	1.034		9	2.414	0.603	3.546	0.886
	5	0.455	0.505	0.556	0.618		5	11.159	0.925	12.237	1.014		10	0.991	0.506	1.591	0.813
	6	0.091	0.606	0.111	0.741		6	6.456	0.803	7.855	0.977		11	0.349	0.421	0.607	0.731
8	1	7.000	1.000	7.000	1.000		7	3.087	0.672	4.157	0.905		12	0.104	0.348	0.194	0.647
	2	9.826	1.248	8.444	1.072		8	1.228	0.554	1.808	0.816		13	0.026	0.290	0.051	0.565
	3	6.478	0.987	6.833	1.042		9	0.398	0.453	0.630	0.716		14	0.005	0.243	0.010	0.491
	4	3.261	0.795	3.889	0.948		10	0.103	0.371	0.170	0.616		15	0.001	0.215	0.002	0.440
	5	1.130	0.612	1.444	0.782		11	0.021	0.319	0.035	0.542		16	0.000	0.198	0.000	0.406
	6	0.261	0.484	0.333	0.619		12	0.003	0.285	0.005	0.485		17	0.000	0.306	0.000	0.627
	7	0.043	0.565	0.056	0.723		13	0.000	0.412	0.001	0.700	19	1	18.000	1.000	18.000	1.000
9	1	8.000	1.000	8.000	1.000	15	1	14.000	1.000	14.000	1.000		2	28.490	1.179	24.553	1.016
	2	11.596	1.242	9.886	1.059		2	21.747	1.195	18.673	1.026		3	29.995	1.106	27.056	0.997
	3	8.468	1.020	8.543	1.030		3	21.356	1.100	19.586	1.009		4	29.007	1.083	27.263	1.018
	4	5.085	0.883	5.886	1.021		4	18.761	1.054	18.347	1.031		5	24.118	1.019	24.183	1.021
	5	2.043	0.665	2.600	0.846		5	13.550	0.951	14.512	1.019		6	17.759	0.940	19.275	1.020
	6	0.660	0.552	0.886	0.741		6	8.375	0.840	9.909	0.994		7	11.486	0.842	13.633	1.000
	7	0.128	0.421	0.171	0.565		7	4.338	0.714	5.682	0.935		8	6.569	0.740	8.569	0.964
	8	0.021	0.561	0.029	0.753		8	1.908	0.598	2.748	0.862		9	3.303	0.636	4.738	0.912
10	1	9.000	1.000	9.000	1.000		9	0.694	0.490	1.086	0.766		10	1.459	0.539	2.294	0.847
	2	13.292	1.232	11.320	1.048		10	0.210	0.404	0.351	0.675		11	0.561	0.451	0.959	0.772
	3	10.632	1.055	10.373	1.029		11	0.050	0.329	0.087	0.574		12	0.186	0.376	0.344	0.693
	4	7.019	0.929	7.787	1.030		12	0.009	0.288	0.017	0.513		13	0.052	0.311	0.103	0.610
	5	3.377	0.745	4.227	0.932		13	0.001	0.247	0.002	0.440		14	0.012	0.260	0.025	0.535
	6	1.255	0.593	1.693	0.800		14	0.000	0.384	0.000	0.685		15	0.002	0.218	0.005	0.461
	7	0.349	0.481	0.493	0.680	16	1	15.000	1.000	15.000	1.000		16	0.000	0.195	0.001	0.418
	8	0.066	0.404	0.093	0.571		2	23.430	1.190	20.141	1.022		17	0.000	0.173	0.000	0.371
	9	0.009	0.520	0.013	0.735		3	23.515	1.103	21.449	1.006		18	0.000	0.283	0.000	0.608
11	1	10.000	1.000	10.000	1.000		4	21.278	1.064	20.548	1.028	20	1	19.000	1.000	19.000	1.000
	2	15.013	1.224	12.811	1.044		5	16.064	0.974	16.857	1.021		2	30.179	1.176	26.024	1.014
	3	12.740	1.071	12.201	1.026		6	10.477	0.871	12.087	1.005		3	32.163	1.106	28.932	0.995
	4	9.204	0.973	9.818	1.037		7	5.821	0.753	7.420	0.960		4	31.624	1.088	29.527	1.015
	5	4.953	0.799	5.962	0.962		8	2.776	0.638	3.900	0.897		5	26.935	1.030	26.702	1.020
	6	2.170	0.661	2.887	0.879		9	1.122	0.531	1.724	0.815		6	20.442	0.957	21.835	1.021
	7	0.702	0.514	1.000	0.732		10	0.382	0.438	0.633	0.726		7	13.734	0.865	15.980	1.007
	8	0.183	0.437	0.270	0.646		11	0.107	0.360	0.189	0.635		8	8.219	0.767	10.481	0.978
	9	0.030	0.352	0.044	0.520		12	0.024	0.299	0.044	0.548		9	4.363	0.666	6.113	0.934
	10	0.004	0.503	0.006	0.743		13	0.004	0.261	0.008	0.487		10	2.053	0.570	3.157	0.876
12	1	11.000	1.000	11.000	1.000		14	0.001	0.238	0.001	0.443		11	0.851	0.481	1.429	0.808
	2	16.701	1.215	14.265	1.037		15	0.000	0.357	0.000	0.665		12	0.309	0.403	0.562	0.734
	3	14.913	1.085	14.039	1.021	17	1	16.000	1.000	16.000	1.000		13	0.097	0.336	0.189	0.655
	4	11.454	1.000	11.879	1.036		2	25.115	1.186	21.612	1.020		14	0.026	0.280	0.054	0.578
	5	6.831	0.852	7.949	0.991		3	25.670	1.104	23.314	1.003		15	0.006	0.234	0.013	0.506
	6	3.325	0.711	4.304	0.920		4	23.832	1.072	22.774	1.025		16	0.001	0.199	0.002	0.442
	7	1.281	0.575	1.814	0.814		5	18.671	0.992	19.254	1.022		17	0.000	0.177	0.000	0.399
	8	0.388	0.465	0.583	0.698		6	12.761	0.898	14.389	1.012		18	0.000	0.165	0.000	0.372
	9	0.091	0.391	0.141	0.607		7	7.513	0.786	9.334	0.977		19	0.000	0.262	0.000	0.588
	10	0.015	0.341	0.023	0.530		8	3.844	0.676	5.264	0.925						
	11	0.002	0.469	0.003	0.728		9	1.688	0.568	2.539	0.853						

[a] $\langle d(T,k)\rangle^{lab}$ is given by eq 8.

Wiener[15] and the Tratch−Stankevich−Zefirov index,[16] respectively. All these topological indices, and several others, can be normalized by means of the coefficients of the average Hosoya polynomial $\langle H(G,x)\rangle^{ch}$.

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