

# An All-Path Version of the Wiener Index

István Lukovits

Central Research Institute of Chemistry, Hungarian Academy of Sciences,  
H-1525 Budapest, P.O. Box 17, Hungary

Received July 9, 1997<sup>®</sup>

The Wiener index  $W(G)$  has originally been defined for acyclic graphs. Therefore its extension to cycle-containing structures is not unambiguous; there are several possibilities, some of which have already been realized. In this paper, we proposed an “all-path” version of  $W$  and showed that its maximal value is equal to  $N^2(N-1)2^{N-4}$ , where  $N$  denotes the number of vertices in a graph. In contrast, the maximal values of  $W$  and its close analogues, the detour index,  $w(G)$ , and the Szeged index,  $Sz(G)$ , are polynomials of order 4 or less in terms of  $N$ , and therefore, it may be expected that the new version will discriminate cycle-containing structures more efficiently than  $W(G)$ ,  $w(G)$ , or  $Sz(G)$ .

## INTRODUCTION

The Wiener index  $W(G)$  is the sum of distances between all pairs of vertices in a graph  $G$ :

$$W(G) = \sum_{i < j} D_{ij} \quad (1)$$

where  $D_{ij}$  denotes the length of the shortest path (i.e., distance) between vertices  $i$  and  $j$ . Even though this expression of  $W(G)$  was already suggested by Wiener,<sup>1</sup> eq 1 was first written by Hosoya.<sup>2</sup> Wiener presented another formula for the computation of  $W(G)$ :

$$W(G) = \sum_e N_1 N_2 \quad (2)$$

where  $N_1$  and  $N_2$  denote the number of vertices in the two subgraphs resulting after an edge  $e$  has been deleted from  $G$ . Clearly eq 2 is valid for trees only, but the “bond-contribution” picture could be extended for cycle-containing structures, too, although much later than eq 2 was proposed.<sup>3</sup> As a matter of fact, eq 1 is already an extended version of the Wiener index and it can also be used for cycle-containing structures. It has to be noted that Rouvray suggested<sup>4</sup> another variant of the Wiener index, which is equal to  $2W(G)$ . Here we shall consider those extensions of  $W(G)$  only, which yield values identical with  $W(G)$  if  $G$  is acyclic but differ from  $W(G)$  if  $G$  is a cycle-containing graph. Various other versions of  $W(G)$  not fulfilling this restriction will not be considered here but nevertheless have to be mentioned.<sup>5–11</sup> All of these analogues can be computed by adding elements above the main diagonal of a symmetric matrix. In this sense  $W(G)$  is the “Wiener sum” of the distance matrix.<sup>12</sup> On this topic, the reader may find more details in reviews.<sup>13,14</sup>

The “detour index”<sup>15–17</sup>  $w(G)$  is closely related to  $W(G)$ : it may be obtained by replacing distance  $D_{ij}$  with the length of the *longest* path between vertices  $i$  and  $j$  in eq 1. Gutman used eq 2 to derive another extended version of  $W(G)$ , the Szeged index  $Sz(G)$ .<sup>18</sup> The “resistance-distance” version of

$W(G)$  was obtained by Klein and Randić,<sup>19</sup> by replacing each edge in  $G$  with a unit resistor. To obtain the resistance distance index,  $D_{ij}$  in eq 1 has to be replaced by the value of the resistance between vertices  $i$  and  $j$ .  $W(G)$  may also be computed by adding the reciprocals of the positive eigenvalues of the Laplacian matrix, the sum of which is equivalent to  $W(G)$  in acyclic graphs. The sum will differ from  $W(G)$  in cycle-containing structures.<sup>20</sup> It has been shown recently that the resistance index and “Laplacian–Wiener” are equivalent.<sup>21</sup>

In the present paper, we propose a graph invariant  $P(G)$ , which is an “all-path” variant of  $W(G)$ :

$$P(G) = \sum_{i < j} \sum_{\pi_{ij}} |\pi_{ij}| \quad (3)$$

where  $\pi_{ij}$  denotes a path between vertices  $i$  and  $j$  and  $|\pi_{ij}|$  denotes the length of this path. The summations have to be performed between all pairs of vertices  $i$  and  $j$  and for all paths between  $i$  and  $j$ . Clearly  $P(G)$  is a “legitimate” extension of  $W(G)$  because in all acyclic graphs between any pair of vertices there exists a single path only and therefore, by definition,  $P(T) = W(T)$ , where  $T$  denotes an acyclic graph (i.e., a tree). It will be shown that  $P(G)$  may assume higher values than any of the previously proposed variants of  $W$  and therefore may more efficiently discriminate cycle-containing structures. It has to be noted that Wilkins and Randić<sup>22</sup> have already proposed an “all-paths” approach to classify molecules, and in their approach, the numbers of paths of various length were used.

Expressions “graph” and “structural formula”, “bond” and “edge”, and “atom” and “vertex” (or “point”) will be used interchangeably, hereafter. Hydrogen-suppressed graphs will be considered only. Throughout this paper, symbols  $G_N$ ,  $K_N$ ,  $T_N$ ,  $C_N$ ,  $L_N$ , and  $S_N$  will denote graphs, complete graphs, trees, cycles, chains, and stars, respectively, and the lower index will be used to denote the number of vertices in these graphs. Readers who want to learn more about chemical graph theory may wish to consult a textbook.<sup>23</sup>

<sup>®</sup> Abstract published in *Advance ACS Abstracts*, December 15, 1997.

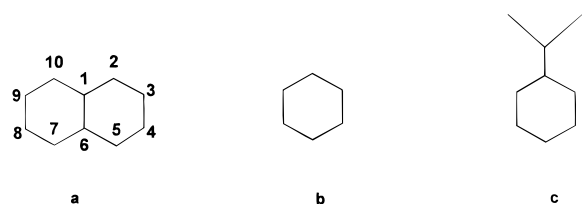


Figure 1.

SOME PROPERTIES OF  $P(G)$ 

$P(G)$  may be obtained numerically by using the same “back-track” algorithm used to calculate the detour indices.<sup>24</sup> Note that this algorithm, and also the algorithm proposed by Trinajstić et al.,<sup>25</sup> is not efficient.

To derive formulas for some cycle-containing graphs, we introduce the  $\Omega$  matrix, each entry  $\Omega_{i,j}$  of which will denote the sum of lengths of all possible paths between vertices  $i$  and  $j$ . For naphthalene (Figure 1a), the upper triangle of the  $\Omega$  matrix ( $\Omega_{i,j} = \Omega_{j,i}$ ,  $\Omega_{i,i} = 0$  for any  $i$  and  $j$ ) is listed below:

0	15	14	13	12	11	12	13	14	15
	0	15	14	13	12	22	22	22	22
		0	15	14	13	22	22	22	22
			0	15	14	22	22	22	22
				0	15	22	22	22	22
					0	15	14	13	12
						0	15	14	13
							0	15	14
								0	15
									0

The sum of these entries is equal to  $P(\text{naphthalene}) = 751$ . In full analogy to eq 1, we may write

$$P(G) = \sum_{i < j} \Omega_{i,j} \quad (4)$$

To derive a formula for simple cycles, consider the graph of cyclohexane (or benzene) depicted in Figure 1b. Between each pair of vertices there are two paths, and the sum of the length of these paths is, irrespective of the position of the vertices, six. There are  $6 \times 5/2 = 15$  pairs of vertices altogether; therefore  $P(\text{cyclohexane}) = 6 \times 15 = 90$ . These considerations can easily be extended to any cycle, and therefore, we obtain for an  $N$ -cycle  $C_N$  that

$$P(C_N) = N^2(N-1)/2 \quad (5)$$

It should be noted that a single formula was enough to obtain  $P(C_N)$ , in contrast to  $W(C_N)$ ,  $w(C_N)$ , and  $Sz(C_N)$ , where separate formulas apply for cases  $N = \text{even}$  and  $N = \text{odd}$ .<sup>26–28</sup> It has also to be noted that  $P(C_N)$ , like the formulas derived for  $W(C_N)$ ,  $w(C_N)$  and  $Sz(C_N)$ , is a third-order polynomial in terms of  $N$ .

For naphthalene (Figure 1a) observe that  $\Omega_{i,j} = 22$  for any pair of vertices located in different hexagons, whereas for pairs of vertices located in the same hexagon,  $\Omega_{i,j} = 16 - D_{i,j}$ , if the shortest path does not include two branching atoms, and  $\Omega_{i,j} = 10 + D_{i,j}$ , if the shortest path does include two branching atoms. To distinguish the various subcases we shall subdivide the graph of any fused bicyclic graph into its constituent chains, that is, subgraphs which are chains.

Naphthalene consists of three chains, the number of vertices in these are six, six, and two, respectively. By denoting the number of vertices in these chains by letters  $k$ ,  $m$ , and  $l$  ( $k$ ,  $m$ , and  $n$  will also denote the respective chains), we can express  $N$  in terms of  $k$ ,  $m$ , and  $n$ :  $N = k + m + n - 4$ . The branching vertices belong to all three chains. Therefore, any fused bicyclic graph is determined unambiguously if we list its constituting chains  $k$ ,  $m$ , and  $n$ , and for  $P(k,m,n)$ , we obtain after some elementary but lengthy algebra:

$$P(k,m,n) = 2(k-2)(m-2)(k+m+n-3) + 2(k-2)(n-2)(k+m+n-3) + 2(m-2)(n-2)(k+m+n-3) + k(k-1)(m+n-2)/2 + m(m-1)(k+n-2)/2 + n(n-1)(m+n-2)/2 + k(k-1)^2 + m(m-1)^2 + n(n-1)^2 - (k^3 - k)/6 - (m^3 - m)/6 - (n^3 - n)/6 - 2k - 2m - 2n + 6 \quad (6)$$

where the first three terms refer to “interchain contributions”, that is, for naphthalene  $2 \times 4 \times 4 \times 11 = 352 = 16 \times 22$  (observe the number of elements  $\Omega_{i,j} = 22$ , above). The remaining terms are the “intrachain” contributions; negative signs denote contributions which were taken into account two times and therefore have to be subtracted. Equation 6 may be simplified:

$$P(k,m,n) = (5k^3 + 5m^3 + 5n^3 + 15k^2m + 15km^2 + 15k^2n + 15kn^2 + 15m^2n + 15mn^2 + 36kmn - 66k^2 - 66m^2 - 66n^2 - 138km - 138kn - 138mn + 289k + 289m + 289n - 396)/6 \quad (7)$$

Again there is a single formula for even and odd  $k$ ,  $m$ , and  $n$ , unlike for  $W(G)$ ,  $w(G)$ , and  $Sz(G)$ , where four subcases had to be considered.<sup>24,28,29</sup> It was also not necessary to use the “system of linear equations” method, needed for the derivation of formulas of  $W(G)$ ,  $w(G)$ , and  $Sz(G)$ . Equation 7 may be used to find structures with a given value of  $P(G)$  and, in this way, to solve—at least numerically—the “graph reconstruction problem” for this class of structures.

It is also easy to derive formulas for cutpoint graphs, an example is shown in Figure 1c.

$$P(\text{cutpoint}) = P(C_N) + W(A) + (N_C - 1)ks_A + (N_A - 1)s_C \quad (8)$$

where  $P(C_N)$  denotes the index  $P$  of the  $N$ -cycle,  $W(A)$  is the Wiener—and therefore the “all-path”—index of the acyclic part,  $N_C$  and  $N_A$  denote the number of vertices in the cyclic and acyclic parts, respectively (the branching atom, which belongs to both systems is considered in both subgraphs),  $s_A$  and  $s_C$  is the connectedness<sup>30</sup> of the cyclic and acyclic parts, respectively, and  $k$  denotes the number of paths connecting two vertices in a cycle (i.e.,  $k = 2$ ). If the cyclic part is a simple cycle then from eq 4 it follows that at each vertex

$$s_C = N(N-1) \quad (9)$$

For the “central” vertex of a star we obtain

$$s_A = N - 1 \quad (10)$$

the lowest possible value for any  $N$ -vertex acyclic graph. Thus, for isopropylcyclohexane (Figure 1c), we obtain  $P(\text{isopropylcyclohexane}) = 90 + 9 + (5 \times 2 \times 5) + (3 \times 30) = 239$ .

### EXTREMAL VALUES OF $P(G)$

Let  $K_N$  denote the complete graph involving  $N$  points. Between any pair of vertices  $i$  and  $j$  there is a single path of length  $N - 1$  if the order of the points appearing in the path is not taken into account. If all paths containing the same points in different order would be taken into account separately, there would be  $(N - 2)!$  paths of length  $N - 1$ . However, such cases are rather rare in graphs of chemical interest, and therefore, we just consider which points appear in the path but will ignore their order, hereafter. Using the same approximation, there are  $N - 2$  paths of length  $N - 1$ ,  $(N - 2)(N - 3)/2$  paths of length  $N - 2$ , etc. There is no other graph in which the number of paths could be higher, since this would mean that there exists at least a single pair of vertices between which there are multiple bonds, and such multigraphs will not be considered in this work. Omission of any edge in  $K_N$ , will result in a graph  $G$  for which  $P(G) < P(K_N)$ , since all paths which involve this edge are missing in  $G$ . Therefore we can state our first theorem:

Theorem 1. For any  $N$ -vertex graph  $G_N$ ,  $P(K_N) > P(G_N)$ .

In  $K_N$ , for any pair of vertices  $i$  and  $j$ ,  $\Omega_{ij}$  is equal to

$$\Omega_{ij} = \sum_{k=0}^{N-2} (k+1) \begin{bmatrix} N-2 \\ k \end{bmatrix} \quad (11)$$

but

$$\begin{bmatrix} N-2 \\ k \end{bmatrix} = \begin{bmatrix} N-2 \\ N-2-k \end{bmatrix} \quad (12)$$

The factors are  $k + 1$  and  $N - 2 - k + 1$ , respectively, and their mean value is  $N/2$ . Therefore

$$\sum_{k=0}^{N-2} (k+1) \begin{bmatrix} N-2 \\ k \end{bmatrix} = (N/2) \sum_{k=0}^{N-2} \begin{bmatrix} N-2 \\ k \end{bmatrix} = N2^{N-2}/2 \quad (13)$$

and for all  $N(N-1)/2$  pairs

$$P(K_N) = N^2(N-1)2^{N-2}/4 = N^2(N-1)2^{N-4} \quad (14)$$

The maximal values of  $W(G)$  and  $w(G)$  are third-order polynomials<sup>24,28</sup> in terms of  $N$ , whereas for  $Sz(G)$ , it is a fourth-order polynomial.<sup>31</sup> Therefore it may be expected that  $P(G)$  will discriminate more efficiently cycle-containing structures than other Wiener-type indices.

To find the graph for which  $P(G)$  is minimal recall that, for all  $N$ -vertex acyclic graphs  $T_N$ , the value of  $W(T_N)$  is minimal<sup>32</sup> if  $T_N$  is a "star"  $S_N$  ( $S_N$  contains  $N - 1$  vertices of degree 1 and a single vertex of degree  $N - 1$ ). Evidently  $P(S_N) < P(T_N)$  if  $S_N \neq T_N$ . We want to show that  $P(S_N) < P(G_N)$  for any  $G_N$ . If  $G_N$  is a cycle-containing graph, then there is a spanning-tree  $T_N^{(G)}$  of  $G_N$  and clearly  $P(T_N^{(G)}) < P(G_N)$ . Therefore we can state our theorem 2:

Theorem 2.  $(N - 1)^2 = P(S_N) < P(G_N)$ .

Let's consider graph  $G_N^{(1)}$  (Figure 2). Graph  $G_N^{(1)}$  can be generated from a star  $S_N$ , by connecting two nonadjacent

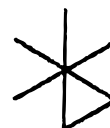


Figure 2.

Table 1. Path Numbers of Several Special Graphs

no. of vertexes	$S_N$	$L_N$	$G_N^{(1)}$	$C_N$	$K_N$
2	1	1	—	—	1
3	4	4	9	9	9
4	9	10	20	24	48
5	16	20	33	50	200
6	25	35	48	90	720
7	36	56	65	147	2352

vertices with an edge.  $G_N^{(1)}$  is a cutpoint graph consisting of a star  $S_{N-2}$  and the smallest possible cycle  $C_3$ . From eq 8 follows that cutpoint graphs containing a single  $C_3$  ring and a star (with  $N - 3$  vertices outside the cycle) have the lowest possible  $P$ -index among all  $N$ -vertex cycle-containing cutpoint graphs. Any transformation of  $G_N^{(1)}$  into another  $N$ -vertex cycle-containing graph with two (or three) side branches will increase the corresponding index  $P(G)$ . Therefore we can formulate our third theorem:

Theorem 3.  $P(G_N^{(1)}) < P(G_N^{(C)})$ , where  $G_N^{(C)}$  denotes a cycle-containing graph.

To find those integers which cannot be path numbers of any graph consider Table 1. Note that negative integers cannot be path numbers. Number zero is associated with methane and number 1 is equal to the path number of the only two-vertex tree, ethane (which happens also to be a complete graph). The minimal value of  $P(G_3)$  is 4; therefore, no three-vertex graph exists for which the path number would be equal to 2 or 3. But  $P(T_N)$  is maximal if  $T_N = L_N$ , whereas the lowest path number of cycle-containing three-vertex graphs is equal to 9. Therefore numbers 5, 6, 7, and 8 cannot be path numbers. The  $P$  index of four-vertex trees may be either 9 or 10, and the minimal path number of four-vertex cycle-containing graphs is 20. The path number of five-vertex trees is either 16, 20, or 18 (the path number of methylbutane); therefore, numbers 11, 12, 13, 14, 15, 17, and 19 cannot be path numbers. A similar procedure reveals that numbers 21, 22, and 23 also cannot be path numbers.

### EDGE DECOMPOSITION OF $P(G)$

Let us consider eq 3 and rearrange the order of summation according to increasing path lengths:

$$P(G) = \sum_{i < j} \sum_{\pi_{ij}} |\pi_{ij}| = \sum_{i < j} \left( \sum_{\pi_{ij,1}} 1 + \sum_{\pi_{ij,2}} 2 + \dots + \sum_{\pi_{ij,m}} m \right) = \sum_{i < j} \sum_k \sum_{\pi_{ij,k}} k \quad (15)$$

where  $m$  denotes the maximal path length and  $\pi_{ij,k}$  denotes a path (if any) between vertices  $i$  and  $j$  of length  $k$ . There are  $k$  edges within each path, and let  $\pi_{ij,k}^{(e)}$  denote the number of times paths  $\pi_{ij,k}$  contain edge  $e$  and  $\#(\pi_{ij,k})$  is the number of paths  $\pi_{ij,k}$ . Therefore for any path of length  $k$

$$\sum_e \pi_{ij,k}^{(e)} = k \#(\pi_{ij,k}) \quad (16)$$

where the summation has to be performed for all edges  $e$  in  $G$ . Therefore

$$\sum_{\pi_{i,j,k}} k = k\#(\pi_{i,j,k}) = \sum \pi_{i,j,h}^{(e)} \quad (17)$$

and inserting the rhs of eq 17 into eq 15 we obtain

$$P(G) = \sum_{i < j} \sum_k \sum_e \pi_{i,j,k}^{(e)} = \sum_e \sum_k \sum_{i < j} \pi_{i,j,k}^{(e)} = \sum_e P_e \quad (18)$$

where  $P_e$  denotes the "contribution" of bond  $e$  to  $P(G)$ . Equation 18 is valid for acyclic and cycle-containing graphs as well and means that  $P(G)$  can be decomposed into bond contributions.

As an example we demonstrate the calculation of the contribution of bond (1,2) of naphthalene (Figure 1a). From eq 18  $P_e$  can be obtained as

$$P_e = \sum_k \sum_{i < j} \pi_{i,j,k}^{(e)} \quad (19)$$

and

$$\begin{aligned} \sum_k \sum_{i < j} \pi_{i,j,k}^{(e)} = & \\ & 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + \\ & 2 + 2 + 2 + 2 + 2 + 2 + 2 + 2 + 2 + 2 + \\ & 2 + 2 + 2 + 2 + 2 + 2 + 2 + 2 + 2 + 2 + \\ & 2 + 2 + 2 + 2 + 2 + 2 + 2 + 2 + 2 + 2 + \\ & 2 + 2 + 2 + 2 + 2 + 2 + 2 + 2 + 2 + 2 + \\ & 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + \\ & 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + \\ & 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + \\ & 1 = 71 = P_{1,2} \end{aligned} \quad (20)$$

where the first entry in row 1 denotes the contribution of paths  $\pi_{1,2}$ , the second entry  $\pi_{1,3}$ , etc., and the first entry of the second row  $\pi_{2,3}$ , the second entry of the second row  $\pi_{2,4}$ , etc. A similar calculation yields for the other bonds  $P_{2,3} = 68$ ,  $P_{3,4} = 67$ , and  $P_{1,6} = 61$ . Therefore by using the symmetry of naphthalene we obtain

$$P(\text{naphthalene}) = 4P_{1,2} + 4P_{2,3} + 2P_{3,4} + P_{1,6} = (4 \times 71) + (4 \times 68) + (2 \times 67) + 61 = 751 \quad (21)$$

the value obtained by using eq 7 or by adding the entries in the upper triangle of matrix  $\Omega$  (eq 5).

## DISCUSSION AND CONCLUSIONS

The proposed all-path number is a graph invariant, that is, at least for cycle-containing structures, more discriminatory than previously proposed Wiener-type indices. However, this does not mean that no pairs of distinct structures, with identical values of  $P(G)$ , may exist.

Because  $P(G)$  is an exponential function in terms of  $N$ ,  $P(G)$  is clearly not appropriate for use in quantitative structure–activity/property studies such as the Wiener index itself, which has to be divided by  $N^2$  in series of molecules of various sizes.<sup>1</sup> It is easy to transform  $P(G)$  to obtain a

**Table 2.** Wiener-Type Indices of Simple Cycles

$N$	$W(C_N)$	$w(C_N)$	$Sz(C_N)$	$P(C_N)$	$V(C_N)$
3	3	6	3	9	4.5
4	8	16	16	24	12.0
5	15	35	20	50	25.0
6	27	63	54	90	45.0
7	42	105	63	147	73.5
8	64	160	128	224	112.0
9	90	234	144	324	162.0
10	125	325	250	450	225.0

new invariant  $V(G)$ , which is larger than  $W(G)$  but is less than  $w(G)$ :

$$V(G) = P(G)/k \quad (22)$$

where  $k$  is the total number of paths in  $G$  divided by  $N(N-1)/2$ . For simple cycles,  $k = 2$ , and Table 2 shows the Wiener-type indices of cycles. The usefulness of  $V(G)$  in quantitative structure–activity/property studies (QSAR/QSPR) still has to be investigated.

Previous investigations<sup>27</sup> showed that in a series (consisting of acyclic as well as cyclic structures) of octane isomers  $W(G)$  completely failed to explain the variation of boiling points, whereas in the same series, moderate correlation could be detected between boiling points and  $w(G)$ . In the original study by Wiener,<sup>1</sup> it was found that  $W(G)$  together with the number of distances equal to 3,  $p(G)$ , accounts for the variation of different physical properties of acyclic alkanes. The importance of  $p(G)$  and the number of paths of length two in QSAR/QSPR studies was also confirmed by other investigations.<sup>33–35</sup> If  $p(G)$  or other path numbers are combined with  $V(G)$ , the problem of extending the definition of the path numbers for cycle-containing systems has to be solved. Instead of path numbers, other supplementary descriptors<sup>36</sup> combined with  $V(G)$  could also be considered.

It should be emphasized that most graph invariants that were applied successfully in QSAR/QSPR studies are " $N$ -dependent", that is, they increase more or less proportionally with  $N$ . Therefore, Balaban's suggestion<sup>37</sup> to use a graph invariant together with  $N$  should be taken seriously in series of structures of different sizes because it may happen that the " $N$ -dependence" deceives the investigator: it is the  $N$ -dependence rather than the discriminatory ability of the index that accounts for the bulk of variation in the experimental results. Another possibility is to investigate structures containing an identical number of carbons. It is important that the series contain both acyclic and cyclic structures.

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CI9700541