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EDGE-DECOMPOSITION OF THE WIENER NUMBER

I. LUKOVITS[a] and I. GUTMAN[b]

[a] *Central Research Institute for Chemistry, Hungarian Academy of Sciences, P.O.Box 17, H-1525 Budapest, Hungary*

[b] *Institute of Physical Chemistry, Attila Jozsef University, P.O.Box 105, H-6701 Szeged, Hungary; on leave from: Faculty of Science, Kragujevac*

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Abstract

The decomposition of the Wiener number into contributions coming from the edges of the respective molecular graph is a problem that was solved already in 1947 by Wiener himself, but only for acyclic systems. We now report an edge-decomposition formula valid for arbitrary connected graphs, and examine its various special cases.

Introduction

Since 1947, when the topological index W was invented by H. Wiener [1], this quantity became one of the most frequently used descriptors of branching of the carbon-atom skeleton of organic molecules; W is nowadays commonly known under the name *Wiener number* or *Wiener index*. The Wiener number was the topic of a large number of studies, and a plethora of published papers exists on this subject (see [2-7] for review and further references). In this work we are concerned with the edge-decomposition of W, namely with the quantities W_e that satisfy the formula

$$W = \sum_e W_e \quad . \qquad (1)$$

In Eq. (1) and elsewhere $\sum_e$ denotes summation over all edges of the respective molecular graph.

The Wiener number is defined as follows [5]. Let the vertices of the molecular graph G be labeled by $1, 2, \ldots, n$. Let u and v be two vertices of G and let $d(u,v)$ be the distance [8] between them. Then the Wiener number is equal to the sum of the distances between all pairs of vertices of the respective graph, i.e.:

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

Already in the first published work [1] on the Wiener number it was observed that in the case of acyclic molecular graphs, the sum of all distances in G can be obtained by counting the paths that go through an edge e, and then summing these counts over all edges of G. This result is an immediate consequence of the following two elementary facts: (*a*) $d(u,v)$ is equal to the number of edges lying on a path of minimal length, connecting u and v; (*b*) in acyclic graphs the path connecting any two vertices u and v is unique, and is thus of minimal length. Now, in an acyclic graph G, the number of paths that include a certain edge e is equal to $n_1(e) \times n_2(e)$, where $n_1(e)$ and $n_2(e)$ denote the number of vertices of G, lying on the left and right side, respectively, of the edge e. This is because every path going through e starts on one side of e and ends on the other side of e.

The above reasoning results in *Wiener's edge-decomposition formula* [1]:

$$W = \sum_e n_1(e) \times n_2(e) \qquad \text{i.e.} \qquad W_e = n_1(e) \times n_2(e) \tag{3}$$

which holds for acyclic, but not for cyclic molecular graphs. In this paper we offer a generalization of (3), applicable to all graphs.

A general edge-decomposition formula

Consider a connected graph G, let **u** and **v** be two distinct vertices of G, and let $d(\mathbf{u},\mathbf{v})$ denote their distance in G. The total number of paths between **u** and **v**, that are of length $d(\mathbf{u},\mathbf{v})$, is denoted by π_{uv}. The number of such paths, that contain the edge **e** is denoted by $\pi_{uv}(\mathbf{e})$. Then we have the following

Theorem 1. For every connected graph G,

$$W = W(G) = \sum_{e} \sum_{u<v} \left[\pi_{uv}(e)/\pi_{uv}\right] \tag{4}$$

i.e.

$$W_e = \sum_{u<v} \left[\pi_{uv}(e)/\pi_{uv}\right] \quad . \tag{5}$$

Proof. Consider the sum $\sum_{e} \pi_{uv}(\mathbf{e})$. Because $\pi_{uv}(\mathbf{e})$ counts the shortest paths between **u** and **v**, that include **e**, in $\sum_{e} \pi_{uv}(\mathbf{e})$ every shortest path between **u** and **v** is counted as many times as there are edges in a shortest path between **u** and **v**, i.e., $d(\mathbf{u},\mathbf{v})$ times. In other words:

$$\sum_{e} \pi_{uv}(\mathbf{e}) = \pi_{uv} \times d(\mathbf{u},\mathbf{v}) \quad . \tag{6}$$

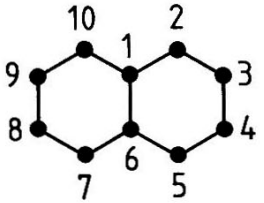
From (6) we obtain $\sum_{e} \pi_{uv}(\mathbf{e})/\pi_{uv} = d(\mathbf{u},\mathbf{v})$, which substituted back into (2) yields

$$W = \sum_{u<v} \sum_{e} \left[\pi_{uv}(e)/\pi_{uv}\right] \quad . \tag{7}$$

Exchanging the two summations in (7) we readily arrive at (4). ■

The result stated here as Theorem 1 was first reported by one of the present authors in [9], but was deduced using a completely different way of reasoning.

As an example consider the naphthalene graph and the edge **e** = **e(1,2)**, connecting its vertices **1** and **2**. According to Eq. (5), in order to find the contribution $W_{e(1,2)}$ of the edge **e** to the Wiener number, we have to compute $\pi_{uv}(e)/\pi_{uv}$ for all the vertex pairs of the naphthalene graph. There are n(n-1)/2 such pairs, with n being equal to 10.



Examine first the vertex pair **3, 8**. Its distance is **d(3,8) = 5**. There exist three distinct paths of length 5, connecting the vertices **3** and **8**. These are: **{3,2,1,10,9,8}**, **{3,2,1,6,7,8}** and **{3,4,5,6,7,8}**. The first two of them contain the edge **e = e(1,2)**, whereas the third does not. Therefore, $\pi_{38} = 3$, $\pi_{38}(e) = 2$. Consequently, the contribution of the vertex pair **3, 8** to the value of $W_{e(1,2)}$ is equal to 2/3.

For the vertex pair **7, 10** the contribution to $W_{e(1,2)}$ is zero, because neither of the two shortest paths **{7,6,1,10}** and **{7,8,9,10}** includes the edge **e(1,2)**.

Repeating such an analysis for all 45 vertex pairs of the naphthalene graph we arrive at the following results:

u	v	π_{uv}	$\pi_{uv}(e)$	u	v	π_{uv}	$\pi_{uv}(e)$	u	v	π_{uv}	$\pi_{uv}(e)$
1	**2**	1	1	**2**	**9**	1	1	**5**	**6**	1	0
1	**3**	1	1	**2**	**10**	1	1	**5**	**7**	1	0
1	**4**	2	1	**3**	**4**	1	0	**5**	**8**	1	0
1	**5**	1	0	**3**	**5**	1	0	**5**	**9**	2	0
1	**6**	1	0	**3**	**6**	2	1	**5**	**10**	1	0
1	**7**	1	0	**3**	**7**	2	1	**6**	**7**	1	0
1	**8**	2	0	**3**	**8**	3	2	**6**	**8**	1	0
1	**9**	1	0	**3**	**9**	1	1	**6**	**9**	2	0
1	**10**	1	0	**3**	**10**	1	1	**6**	**10**	1	0
2	**3**	1	0	**4**	**5**	1	0	**7**	**8**	1	0
2	**4**	1	0	**4**	**6**	1	0	**7**	**9**	1	0
2	**5**	2	1	**4**	**7**	1	0	**7**	**10**	2	0
2	**6**	1	1	**4**	**8**	1	0	**8**	**9**	1	0
2	**7**	1	1	**4**	**9**	3	1	**8**	**10**	1	0
2	**8**	2	2	**4**	**10**	2	1	**9**	**10**	1	0

By applying Eq. (5) we now readily establish that $W_{e(1,2)} = 12\frac{1}{2}$. Observe that of the 45 vertex pairs in the naphthalene graph, only 16 have non-zero contributions to $W_{e(1,2)}$.

The above example illustrates an interesting feature of the edge-decomposition of the Wiener number: whereas W is necessarily an integer, its edge-decomposition may lead to non-integer W_e-values. .

A similar calculation for the edges **e(2,3)**, **e(3,4)** and **e(1,6)** yields: $W_{e(2,3)} = 8\frac{1}{2}$, $W_{e(3,4)} = 6\frac{1}{6}$ and $W_{e(1,6)} = 12\frac{2}{3}$. This, of course, is consistent with the fact that for the naphthalene graph, W = 109. Really, $4 \times W_{e(1,2)} + 4 \times W_{e(2,3)} + 2 \times W_{e(3,4)} + W_{e(1,6)} = 109$.

We see that the edges **e(1,2)**, **e(2,3)**, **e(3,4)** and **e(1,6)** contribute to W by 11.5% , 7.8% , 5.6% and 11.6% , respectively. Observe that the more branched edges **e(1,2)** and **e(1,6)** have a significantly greater contribution to W than the less branched edges **e(2,3)** and **e(3,4)**.

The above example reveals that the edge-decomposition of the Wiener number via a direct application of Theorem 1 is a quite cumbersome and an error prone task. In what follows we demonstrate that in a number of chemically relevant cases the form of Eq. (5) can be significantly simplified.

Some corollaries of Theorem 1

The most noteworthy simplification of Theorem 1 is obtained if the edge **e** is a bridge. (Recall that an edge **e** of a connected graph G is said to be a bridge if G-**e** is disconnected.)

Let G be a connected graph on n vertices and let **e** be one of its bridges. Denote by G_1 and G_2 the two components of G-**e** and let them possess $n_1(\mathbf{e})$ and $n_2(\mathbf{e})$ vertices, respectively, $n_1(\mathbf{e}) + n_2(\mathbf{e}) = n$. Consider the quantities π_{uv} and $\pi_{uv}(\mathbf{e})$ that occur in Eq. (5).

If both vertices **u** and **v** of G belong to either G_1 or G_2, then the shortest paths between **u** and **v** lie either completely in G_1 or completely in G_2 and, consequently, do not include **e**. Therefore, for such vertex pairs, $\pi_{uv}(\mathbf{e}) = 0$ and their contribution to W_e is nil. If, on the other hand, **u** belongs to G_1 and **v** belongs to G_2, then all shortest paths between **u** and **v** must go through **e**. Therefore, for such vertex pairs, $\pi_{uv}(\mathbf{e}) = \pi_{uv}$. Each such pair contributes to W_e by $\pi_{uv}(\mathbf{e})/\pi_{uv} = 1$.

We thus have demonstrated that if **e** is a bridge, then W_e is equal to the number of vertex pairs **u**, **v**, such that **u** belongs to G_1 and **v** belongs to G_2. The number of such vertex pairs is evidently $n_1(\mathbf{e}) \times n_2(\mathbf{e})$.

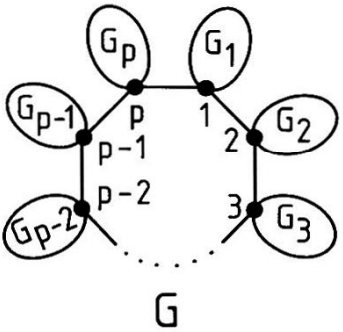
Corollary 1.1. If **e** is a bridge, then $W_e = n_1(\mathbf{e}) \times n_2(\mathbf{e})$.

Acyclic graphs have the property that all their edges are bridges.

Corollary 1.2. If G is acyclic, then relation $W_e = n_1(\mathbf{e}) \times n_2(\mathbf{e})$ is obeyed by all edges of G, i.e. Eq. (3) holds.

Thus (and of course), Wiener's edge-decomposition formula occurs to be a special case of our Theorem 1.

If the edge **e** is not a bridge, then it necessarily belongs to a circuit of the graph G. The simplest such case is when the circuit **Z** to which **e** belongs is unique. The general structure of the respective graph G is given as follows:



In the above diagram p is the size of the circuit **Z** to which the edge **e** belongs. If **Z** is an even-membered circuit, then p = 2k. If **Z** is an odd-membered circuit, then p = 2k+1. Without loss of generality we may assume that the edge **e** lies between the vertices which, in the above diagram, are labeled by **k** and **k+1** .

The structure of the subgraphs G_1 , G_2 ,..., G_p is arbitrary; they may be cyclic or acyclic, and need not be isomorphic. The number of vertices of G_i is denoted by n_i , $i = 1,2,\ldots,p$.

The following results can be deduced from Theorem 1 by elementary, but somewhat lengthy reasoning. We, therefore, state them without proof.

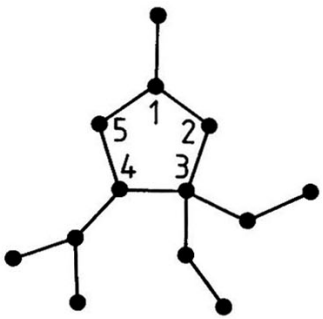
Corollary 1.3. Let G be the above described graph and **e** its above described edge. If the size p of the circuit **Z** to which **e** belongs is odd, $p = 2k + 1$, $k = 1,2,\ldots$, then

$$W_e = \sum_{i=1}^{k} \sum_{j=1}^{i} n_i \, n_{k+j} \quad . \tag{8}$$

Corollary 1.4. Let G be the above described graph and **e** its above described edge. If the size p of the circuit **Z** to which **e** belongs is even, $p = 2k$, $k = 2,3,\ldots$, then

$$W_e = \sum_{i=1}^{k} \sum_{j=1}^{i} n_i \, n_{k+j} - \frac{1}{2} \sum_{i=1}^{k} n_i \, n_{k+i} \quad . \tag{9}$$

As an illustration of the above results consider the molecular graph of 1-methyl,3,3-diethyl,4-isopropylcyclopentane. This graph has a unique 5-membered circuit (i.e. $p = 5$ and $k = 2$), and therefore Corollary 1.3 is applicable. Further, $n_1 = 2$, $n_2 = 1$, $n_3 = 5$, $n_4 = 4$, $n_5 = 1$.



Formula (8) is directly applicable to the edge **e(2,3)**:

$$W_{e(2,3)} = n_1 \times n_3 + n_2 \times n_3 + n_2 \times n_4 = 2 \times 5 + 1 \times 5 + 1 \times 4 = 19 .$$

In a fully analogous manner we can compute the contributions of the remaining four edges of the 5-membered circuit:

$$W_{e(1,2)} = n_5 \times n_2 + n_1 \times n_2 + n_1 \times n_3 = 1 \times 1 + 2 \times 1 + 2 \times 5 = 13$$

$$W_{e(3,4)} = n_2 \times n_4 + n_3 \times n_4 + n_3 \times n_5 = 1 \times 4 + 5 \times 4 + 5 \times 1 = 29$$

$$W_{e(4,5)} = n_3 \times n_5 + n_4 \times n_5 + n_4 \times n_1 = 5 \times 1 + 4 \times 1 + 4 \times 2 = 17$$

$$W_{e(5,1)} = n_4 \times n_1 + n_5 \times n_1 + n_5 \times n_2 = 4 \times 2 + 1 \times 2 + 1 \times 1 = 11 .$$

From Corollaries 1.3 and 1.4 we see that W_e depends only on the number of vertices of the subgraphs G_1 , G_2 ,..., G_p and is independent of any other structural detail of G. A noteworthy special case of Corollary 1.3 is:

Corollary 1.5. Let G and **e** be the graph and its edge, considered in Corollary 1.3. Let **Z** be a triangle, i.e. k = 1. Then $W_e = n_1 \times n_2$.

The above result should be compared with Corollary 1.1.

An interesting expression is obtained for the sum of the edge-contributions of all edges of G, belonging to the circuit **Z**.

Corollary 1.6. Let G be the graph considered in Corollaries 1.3 and 1.4. Let $\sum_e'$ symbolize summation over all edges of G that belong to the circuit **Z**. Then for both odd and even p,

$$\sum_e' W_e = \sum_{i=1}^{p-1} \sum_{j=i+1}^{p} d(i,j)\, n_i\, n_j .$$

In the special case when $n_1 = n_2 = \ldots = n_p$ (which does not require that the subgraphs G_1 , G_2 ,..., G_p be isomorphic), Eqs. (8) and (9) are much simplified:

Corollary 1.7. Let G and **e** be the graph and its edge, considered in Corollaries 1.3 and 1.4. If all the subgraphs G_1 , G_2 ,..., G_p have the same number of vertices (= n/p), then W_e does not depend on the position of the edge **e** in the circuit **Z** and

$$W_e = \begin{cases} (n^2/8)(1 - 1/p^2) & \text{if } p \text{ is odd} \\ n^2/8 & \text{if } p \text{ is even} \end{cases} . \qquad (10)$$

Corollary 1.8. Let **Z** denote the p-vertex circuit. Then under the conditions specified in Corollary 1.7, $\sum_e' W_e = (n/p)^2 W(\mathbf{Z})$.

We note in passing that if G coincides with **Z**, i.e., if in the formula (10), p = n, then the result of Corollary 1.7 reduces to the well known expression [10] for the Wiener number of the p-vertex circuit **Z** :

$$W_e = \begin{cases} (p^2 - 1)/8 \\ p^2/8 \end{cases} \quad \text{and} \quad W(\mathbf{Z}) = \begin{cases} p(p^2 - 1)/8 & \text{if } p \text{ is odd} \\ p^3/8 & \text{if } p \text{ is even} \end{cases}$$

In this case, of course, $W_e = W/p$.

Applications

The theory of the Wiener number was originally designed for, and applied to saturated hydrocarbons. For such molecules it is a plausible assumption that all carbon-carbon bonds have equal effects on various physico-chemical properties that are (expected to be) described by means of the Wiener number. In later developments, the theory of the Wiener number was extended to other types of organic systems (unsaturated and aromatic hydrocarbons, etc). For these compounds it is not clear why different types of carbon-carbon bonds should be equally treated and why the effects of such different bonds should be incorporated with equal weights in the resulting value of the Wiener index.

Theorem 1 offers a solution for this problem.

Using Theorem 1 we can identify the effect of any particular chemical bond on the Wiener index of an organic molecule. We can collect the effects

of bonds of the same kind and consider them separately. Application of this idea to the study of the water/*n*-octanol partition coefficient was already reported [9,11].

In the formulation of the Wiener index all carbon-carbon bonds are represented in the molecular graph by edges of the same type. Each edge--contribution is then simply added, so as to obtain the regular Wiener number, cf. Eq. (1). If we wish to distinguish between the effects of various bond types, then Eq. (1) provides us with the following straightforward generalization

$$WW = \sum_{e} w_e W_e$$

where w_e is a pertinently chosen weight of the edge e. (A typical weighting would be by choosing $w_e = 1$ for single carbon-carbon bonds, $w_e = w_=$ and $w_e = w_\equiv$ for the double and triple carbon-carbon bonds, respectively, and $w_e = w_{ar}$ for aromatic bonds; the parameters $w_=$, $w_\equiv$ & w_{ar} could be adjusted by optimizing the correlation between WW and some pre-selected physico--chemical property of the respective class of compounds.

The above proposed quantity WW could be named the *weighted Wiener index*. Work on the applications of the weighted Wiener index is under way.

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