

## Some recent results in the theory of the Wiener number

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Received 24 March 1993

The Wiener number ( $W$ ) is equal to the sum of distances between all pairs of vertices of the molecular graph. This important topological index was invented in the 1940s, but vigorous research on both its theory and its applications is still going on. The aim of this article is to outline the state of the art of the theory of the Wiener number, with emphasis on the progress achieved in the last few years. In particular, we present (a) the recent results on the relation between  $W$  and intermolecular forces (which, for the first time, provide a sound physico-chemical basis for various applications of  $W$ ), (b) several novel techniques for the calculation of  $W$ , (c) methods for the calculation of  $W$  of composite and highly branched molecular graphs, (d) the problem of isomer degeneracy of  $W$ , and (e) some novel mathematical results relevant to the theory of  $W$ .

### The Wiener number: Discovery & history

The topological index which is nowadays commonly known as the *Wiener number* or *Wiener index* ( $W$ ) was put forward in 1947 by the American physical chemist Harold Wiener<sup>1</sup>. This work was followed by a whole series of Wiener's publications<sup>2-5</sup> in which he reported the existence of correlations between the new index and a large number of physico-chemical properties of alkanes. Stiel and Thodos<sup>6</sup> seem to be the first scientists who followed up Wiener's work; they related the Wiener number to the critical constants of alkanes.

Wiener defined  $W$  only for alkanes (as the sum of the number of carbon-carbon bonds between all pairs of carbon atoms). Hosoya<sup>7</sup>, in 1971, was the first to conceive the relation between  $W$  and the distances in the molecular graph. He, in particular, pointed out that  $W$  is equal to the half of the sum of all elements of the distance matrix of the respective molecular graph. By this, the concept of Wiener number could be extended to cyclic molecules also.

In 1975, Rouvray<sup>8,9</sup> examined the sum of the elements of the distance matrix, considering it as a new topological index. The fact that Rouvray's index is equal to  $2W$  was, of course, soon recognized.

In the 1970s and 1980s, numerous studies of the Wiener number were undertaken. Eventually,  $W$  became one of the most frequently and most successfully employed descriptors of molecular

shape, that can be deduced from the molecular graph. A remarkable variety of chemical applications of  $W$  were proposed.

These researches, as well as the underlying mathematical formalism, are outlined in detail in several monographs<sup>10-13</sup> and numerous reviews<sup>14-21</sup>. In view of this, we will focus our attention on some of the most recent developments in this area.

### Molecular graphs and the Wiener number

A graph is a mathematical arrangement consisting of two types of elements: vertices and edges. Every edge is defined over a pair of vertices—the two vertices are said to be adjacent. A graph is usually represented by means of a diagram. In such a diagram the vertices are drawn either as small circles or as big dots. The edges are then indicated by means of lines which connect the respective two adjacent vertices.

In Fig. 1 two graphs are displayed, each having 10 vertices.

The applications of graphs in chemistry are based on the fact that a close analogy exists be-

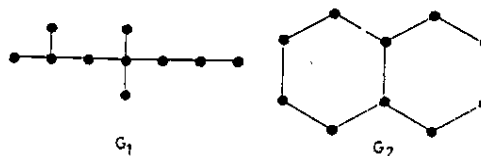


Fig. 1—Molecular graphs of 2,4,4-trimethylheptane ( $G_1$ ) and naphthalene ( $G_2$ )

tween a structural formula and a graph. The graphs  $G_1$  and  $G_2$  in Fig. 1 can be understood as representing the carbon-atom skeletons of 2,4,4-trimethylheptane and naphthalene, respectively; we say that  $G_1$  is the molecular graph of 2,4,4-trimethylheptane whereas  $G_2$  is the molecular graph of naphthalene. (Observe that the hydrogen atoms and the double bonds are disregarded in  $G_1$  and  $G_2$ . This is not necessary, but has proved to be convenient in practice).

Further details on graph theory and its chemical applications can be found elsewhere<sup>11-13</sup>.

In order to define the Wiener number, we have to first explain the notion of the distance in a graph<sup>22</sup>.

Let  $G$  be a graph and let its vertices be labelled by  $1, 2, \dots, n$ . Let  $v_0, v_1, v_2, \dots, v_k$  be  $k+1$  distinct vertices of the graph  $G$ , such that for  $j=1, 2, \dots, k$ ,  $v_{j-1}$  and  $v_j$  are adjacent. Then these vertices form a path in the graph  $G$ , whose length is  $k$ . The length of the shortest path that connects the vertices  $x$  and  $y$  is called the distance between these vertices and is denoted by  $d(x, y)$ .

Consider as an example the graph  $G_3$  in Fig. 2, which is the molecular graph of 1,1,3-trimethylcyclobutane. Its vertices are labelled by  $1, 2, \dots, 7$ . The sequence  $4, 3, 6, 5, 7$  is a path of  $G_3$ , connecting the vertices 4 and 7, and having length 4. This, however, is not the shortest path between 4 and 7. There is another path, namely  $4, 5, 7$ , that has length of only 2. Because  $4, 5, 7$  is the shortest path between the vertices 4 and 7, we have  $d(4, 7) = 2$ .

In this manner one verifies that for the graph  $G_3$ ,

$$\begin{aligned} d(1, 2) = 2, d(1, 3) = 1, d(1, 4) = 2, d(1, 5) = 3, d(1, 6) = 2, d(1, 7) = 4 \\ d(2, 3) = 1, d(2, 4) = 2, d(2, 5) = 3, d(2, 6) = 2, d(2, 7) = 4 \\ d(3, 4) = 1, d(3, 5) = 2, d(3, 6) = 1, d(3, 7) = 3 \\ d(4, 5) = 1, d(4, 6) = 2, d(4, 7) = 2 \\ d(5, 6) = 1, d(5, 7) = 1 \\ d(6, 7) = 2 \end{aligned}$$

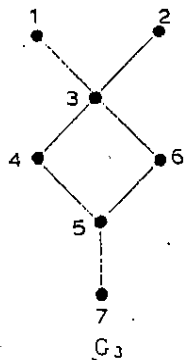


Fig. 2—The molecular graph of 1,1,3-trimethylcyclobutane: its Wiener number is 42

Now, the Wiener number is equal to the sum of distances between all pairs of vertices of the respective graph:

$$W = W(G) = \sum_{x < y} d(x, y)$$

Bearing in mind the above calculated distances in the graph  $G_3$ , we have,

$$\begin{aligned} W(G_3) &= (2+1+2+3+2+4) + (1+2+3+2+4) \\ &\quad + (1+2+1+3) + (1+2+2) + (1+1) + (2) \\ &= 42 \end{aligned}$$

Such a direct computation of the Wiener number may look very easy, but it is so only when the number of vertices of the graph considered is small.

### Physico-chemical applications of the Wiener number

The first application<sup>1</sup> of the Wiener number was for predicting the boiling points (b.p.) of alkanes based on the formula:

$$\text{b.p.} = \alpha W + \beta w(3) + \gamma$$

where  $\alpha$ ,  $\beta$  and  $\gamma$  are empirical constants and  $w(3)$  is the so-called "path number", namely, the number of pairs of vertices whose distance is equal to 3. In a series of papers<sup>2-5</sup> published in 1947 and 1948, Wiener pointed out the versatility of his index in structure-property investigations. He used  $W$  to estimate boiling points, molar volumes, refractive indices, heats of isomerization and heats of vaporization of alkanes.

It is nowadays well understood that the Wiener number measures the extent of branching of the carbon-atom skeleton, and, consequently, the compactness of a given molecule<sup>18,23</sup>. Therefore,  $W$  reflects the molecular surface-to-volume ratio. In connection with this,  $W$  was claimed to be related to the intermolecular forces<sup>18,24-26</sup>, especially in the case of non-polar molecules like hydrocarbons. However, this plausible hypothesis was directly tested only quite recently<sup>27</sup> (see the subsequent section).

Those physical and chemical properties of substances which are expected to depend on the volume-to-surface ratio of their molecules and/or on the extent of branching of the molecular carbon-atom skeleton, are usually well correlated with  $W$ . Among them are the heats of formation, atomization, isomerization and vaporization, density, boiling point, critical pressure, refractive index, surface tension and viscosity of various hydrocarbon species, both acyclic and cyclic, and both aliphatic and aromatic. For an extensive study of this

aspect see ref. 28. By means of the Wiener number, it was possible to determine the mean conformation of long-chain alkanes near their boiling points<sup>29</sup>. Correlations between  $W$  and melting points were also reported<sup>30,31</sup>, but the results in this case were not completely satisfactory. Of particular practical importance is the prediction of the behaviour of organic substances in gas chromatography. For instance, the chromatographic retention times (CRT) of monoalkyl- and  $\alpha$ -dialkylbenzenes were shown<sup>31</sup> to obey the following functional dependence on  $W$ :

$$\text{CRT} = \alpha W^\beta + \gamma$$

where  $\alpha$ ,  $\beta$  and  $\gamma$  are empirically determined parameters (different, of course, from those in Wiener's formula for b.p.). Numerous results of this kind were obtained<sup>33-36</sup>.

A somewhat less standard result along the same line is the connection between  $W$  and the velocity of ultra-sound in alkanes and alcohols<sup>37</sup>.

Bearing in mind that the pharmacological activity of a substance is often related to some of its physico-chemical properties, it is not surprising that attempts have been made to use  $W$  in designing new drugs<sup>38,41</sup>. Lukovits established correlations between  $W$  and cytostatic and antihistaminic activities of certain pharmacologically interesting compounds, as well as between  $W$  and their estrogen-binding affinities<sup>39</sup>. In a recent study, he employed  $W$  for estimating the partition coefficient of octan-1-ol and water<sup>41</sup>, a parameter of profound importance for forecasting pharmacological activities of many compounds.

The Wiener number found several noteworthy applications in polymer chemistry. The melting points and other physical properties of polymers (e.g. of polyethylene) were predicted on the basis of their  $W$ -values<sup>42,43</sup>. The average  $\pi$ -electron energies and the energy gaps in conjugated polymers (as calculated by means of the HMO and PPP methods) were also shown to depend on  $W$ <sup>44,45</sup>.

In studies of crystals, Bonchev, Mekenyan and Fritsche put forward a hypothesis that the stability of a crystal lattice depends on its  $W$ -value. (The configuration whose Wiener number is minimal, would be the most stable one). Based on this conjecture, they characterized crystal defects and predicted vacancy-favoured positions in a crystal lattice<sup>46-48</sup>. Some implications with regard to crystal growth were also considered<sup>49</sup>.

Of the newest applications of the Wiener number, we may mention its use in the rationalization of the mechanism of electroreduction of chlorobenzene derivatives<sup>50</sup> and for distinguishing be-

tween fullerene isomers<sup>51</sup>, as well as its role in the recent approaches towards the quantification of molecular similarity<sup>52</sup>.

### The Wiener number and intermolecular forces

The fact that  $W$  is correlated with so many physico-chemical properties of non-polar organic substances leads to the conclusion that it must be a rough measure of the intermolecular forces. Curiously, however, in spite of the extensive research on the Wiener number in the last fifteen years, this fundamental feature was directly tested only quite recently<sup>27</sup>.

In the kinetic theory of gases and liquids, one distinguishes between so-called simple fluids and so-called normal fluids<sup>53,54</sup>. A fluid is said to be simple if its molecules can be viewed as small spheres and if the energy of the interaction between two molecules obeys a law in which the only variable is the intermolecular distance ( $r$ ). Typical substances of this kind are those composed of monoatomic molecules (e.g. Ar, Kr, Xe) or of highly symmetric polyatomic molecules (e.g. CH<sub>4</sub>). A typical and most frequently employed interaction-energy-function<sup>55</sup> is the Lennard-Jones 12-6 potential,  $\psi(r)$ :

$$\psi(r) = 4 \epsilon \left[ \left( \frac{r}{r_0} \right)^{-12} - \left( \frac{r}{r_0} \right)^{-6} \right] \quad \dots (1)$$

Simple fluids obey a universal equation of state<sup>53,55</sup>.

$$F(P_r, V_r, T_r) = 0 \quad \dots (2)$$

where  $P_r = P/P_c$ ,  $V_r = V/V_c$  and  $T_r = T/T_c$  are the reduced pressure, reduced volume and reduced temperature, respectively. [ $P$ ,  $V$  and  $T$  are the ordinary pressure, volume and temperature, whereas  $P_c$ ,  $V_c$  and  $T_c$  are the corresponding values at the critical point].

In normal fluids, the molecules can no longer be regarded as spheres, but the energy of the intermolecular interaction still conforms to a law of type (1). However, the variable  $r$  is now not the intermolecular distance, but the distance between two particular atoms of the molecules and the total interaction-energy-function is obtained by summing terms of type (1) over all pairs of atoms. As a consequence of this, Eq. (2) is no longer satisfied.

In 1955, Pitzer<sup>54</sup> showed that the behaviour of normal fluids can be described by introducing only one additional structural parameter, the so-called acentric factor<sup>54,56,57</sup>:

$$\omega = -\log P_r - 1.00 \quad \text{at } T_r = 0.7.$$

The choice  $T_r = 0.7$  is conventional, making  $\omega$  easily accessible to direct experimental determina-

tion. In the case of simple fluids,  $\omega = 0$ , whereas in the case of normal fluids  $\omega$  measures the deviation of the intermolecular potential from that of simple fluids.

The acentric factor is used for the estimation of properties of gases and liquids<sup>53</sup>. By means of  $\omega$  one can compute the second virial coefficient, the pressure dependence of the heat capacity<sup>56,57</sup>, density of liquids<sup>57</sup>, vapour pressure<sup>57</sup>, etc.

In Fig. 3, the acentric factor of alkanes is plotted against  $W$ <sup>27</sup>. Within groups of isomers, a remarkably good linear correlation is observed. In Table 1 are given the respective correlation coefficients.

Another way to measure the intermolecular forces is to use an appropriate real-gas equation of state. In the well known van der Waals' equation,

$$(P + aV^{-2})(V - b) = RT$$

the parameter  $a$  is interpreted in terms of the mutual attraction of the molecules in the gas. This parameter is readily obtained from the critical constants<sup>53,55</sup>:

$$a = \frac{27}{64} (RT_c)^2 / P_c$$

For sets of isomeric alkanes, a linear correlation between  $a$  and  $W$  is found<sup>27</sup>, similar to that in the case of the acentric factor. The respective results are given in Table 1.

The data collected in Table 1 show that the  $a$ - $W$  correlation is somewhat worse than the  $\omega$ - $W$  correlation. This is in harmony with the fact that  $\omega$  is a direct, whereas  $a$  is an indirect measure of

the intermolecular forces. Anyway, both the  $\omega$ - $W$  and the  $a$ - $W$  results corroborate (in a quantitative manner) the previously anticipated (qualitative) assertion that the Wiener number measures the intermolecular forces in normal fluids.

#### Methods for computing the Wiener number

The finding of the shortest path (i.e. distance) between the vertices of a graph or of a network is a topic that has been extensively studied by mathematicians. In a review by Deo and Pang<sup>58</sup>, as many as 222 references are collected, all dealing with the minimum-distance problem. Several algorithms for the calculation of the Wiener number have been proposed in the chemical literature<sup>1,59-64</sup> also. Thus, the computation of the numerical value of  $W$  of a molecular graph (by means of a computer) is a completely resolved task, even if the respective graphs have weighted edges and/or vertices. Some of the algorithms offered<sup>62,63</sup> were demonstrated to be linear in the number of vertices.

On the other hand, chemists are often interested in paper-and-pencil methods for the evaluation of  $W$  as well as in methods by means of which general expressions for  $W$  for classes of molecular graphs can be deduced. Several procedures of this kind have been specifically designed<sup>1,60,64</sup> for acyclic molecules. An algorithm, originally put forward by Wiener<sup>1</sup>, is especially convenient for the calculation of  $W$  of moderately large molecular graphs. Because many researchers in this field seem to be unaware of Wiener's algorithm, we briefly outline it in this section. Another, a much more recent method by Gutman<sup>64</sup> readily yields analytical expressions for  $W$  of homologous series of acyclic molecules.

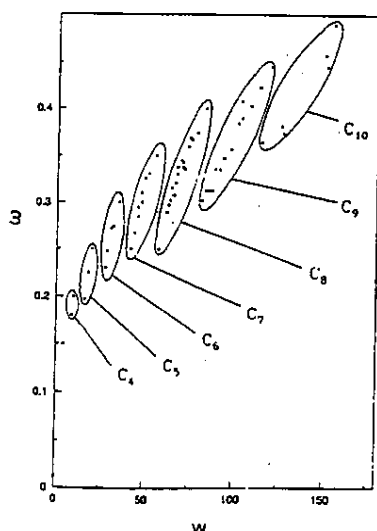


Fig. 3—Correlation between the acentric factors of alkanes and their Wiener numbers<sup>27</sup>; for details see Table 1

Table 1—Correlation between the Wiener number ( $W$ ) of isomeric alkanes and Pitzer's acentric factor ( $\omega$ ), and between  $W$  and the van der Waals' constant  $a$ ; experimental data for  $\omega$

and  $a = \frac{27}{64} (RT_c)^2 / P_c$  are taken from ref. 53.

isomer set	correlation $\omega - W$		correlation $a - W$	
	Correlation coeff.	No. of points	Correlation coeff.	No. of points
C <sub>5</sub> -alkanes	0.998	3	0.997	3
C <sub>6</sub> -alkanes	0.982	5	0.988	5
C <sub>7</sub> -alkanes	0.973	9	0.973	9
C <sub>8</sub> -alkanes	0.968	18	0.963	18
C <sub>9</sub> -alkanes	0.986	14	0.952	11
C <sub>10</sub> -alkanes	0.986	6	0.966	4

In order to describe these algorithms, we first have to specify a few graph-theoretic notions. A connected acyclic graph is called a tree. Hence, the molecular graphs of alkanes are trees. Let  $G$  be a graph and  $e$  its edge. Let  $G-e$  be the graph obtained by deleting from  $G$  the edge  $e$  (but retaining the vertices which are the endpoints of  $e$ ). Note that if  $G$  is a tree, then for any of its edges,  $G-e$  is disconnected, possessing exactly two components.

**Theorem 1<sup>1</sup>.** Let  $G$  be a tree on  $n$  vertices and  $e$  its edge. Let  $n_1(e)$  and  $n_2(e) = n - n_1(e)$  be the numbers of vertices of the two components of  $G-e$ . Then,

$$W(G) = \sum_e n_1(e)n_2(e)$$

where the summation embraces all the  $n-1$  edges of  $G$ .

Consider as an example the molecular graph  $G_4$ , displayed in Fig. 4, which possesses 11 vertices and represents 2,3,4-trimethyl-3-ethylhexane.

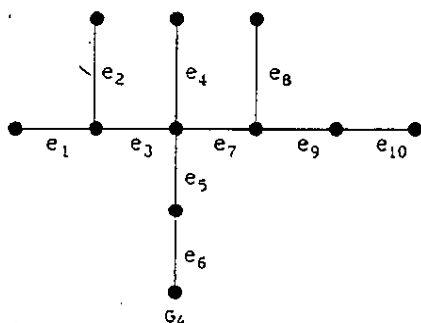


Fig. 4—The molecular graph of 2,3,4-trimethyl-3-ethylhexane; its Wiener number is 148

Its Wiener number is equal to the sum of the following ten terms:

$$\begin{aligned} n_1(e_1)n_2(e_1) &= 1 \times 10 = 10 \\ n_1(e_2)n_2(e_2) &= 1 \times 10 = 10 \\ n_1(e_3)n_2(e_3) &= 3 \times 8 = 24 \\ n_1(e_4)n_2(e_4) &= 1 \times 10 = 10 \\ n_1(e_5)n_2(e_5) &= 2 \times 9 = 18 \\ n_1(e_6)n_2(e_6) &= 1 \times 10 = 10 \\ n_1(e_7)n_2(e_7) &= 4 \times 7 = 28 \\ n_1(e_8)n_2(e_8) &= 1 \times 10 = 10 \\ n_1(e_9)n_2(e_9) &= 2 \times 9 = 18 \\ n_1(e_{10})n_2(e_{10}) &= 1 \times 10 = 10. \end{aligned}$$

$$\text{This gives } W(G_4) = 10 + 10 + 24 + 10 + 18 + 10 + 28 + 10 + 18 + 10 = 148.$$

The number of first neighbours of a vertex  $x$  is called the degree of this vertex and is denoted by  $d = d(x)$ . If  $G$  is a tree and  $d(x) \geq 3$ , then  $x$  is said to be a branching point of  $G$ .

**Theorem 2<sup>64</sup>.** Let  $G$  be a tree on  $n$  vertices and let  $x$  be its branching point. If the number of vertices in the branches attached to  $x$  are denoted by  $n_1, n_2, \dots, n_d, n_1 + n_2 + \dots + n_d + 1 = n$ . Then,

$$W(G) = \binom{n+1}{3} - \sum_x \sum_{i < j < k} n_i n_j n_k \quad \dots (3)$$

The first summation on the right-hand side of Eq. (3) goes over all branching points  $x$  of  $G$ .

An example illustrating the application of Theorem 2 is given in the subsequent section.

Denote by  $A$  the adjacency matrix<sup>11-13</sup> of the molecular graph  $G$ . The eigenvalues of  $A$  form the (ordinary) spectrum of the graph  $G$ . This spectrum has several well-known and well-elaborated chemical applications<sup>11-13</sup>.

Let the vertices of the graph  $G$  be labelled by  $1, 2, \dots, n$ . Let  $D$  be the matrix whose diagonal elements are  $d(1), d(2), \dots, d(n)$ , and whose off-diagonal elements are all equal to zero. Then  $L = D - A$  is the Laplacian matrix of the graph  $G$ . Its eigenvalues  $\lambda_1, \lambda_2, \dots, \lambda_{n-1}, \lambda_n$  form the Laplacian spectrum of  $G$ . They will be labelled in a non-increasing order, i.e.,  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_{n-1} \geq \lambda_n$ .

The Laplacian spectrum of a graph was studied in detail by mathematicians; for review and further references see refs 65-67.

The following interesting result seems to have been discovered in the late 1980s independently by Merris<sup>68,69</sup> and McKay (unpublished, referred to as private communication in refs 66, 69, 70). The chemist community was informed about the Merris-McKay theorem quite recently<sup>71</sup>.

**Theorem 3.** If  $G$  is a tree with  $n$  vertices, then

$$W(G) = n \sum_{i=1}^{n-1} \frac{1}{\lambda_i}$$

The significance of Theorem 3 lies in the fact that the Wiener number (a graph-distance based quantity) is expressed by means of the Laplacian graph eigenvalues (that have their origin in linear algebra). One can thus expect that the powerful mathematical techniques of linear algebra can be utilized in the theory of the Wiener number. Some preliminary results along these lines have already been obtained<sup>72</sup>.

#### Wiener numbers of dendrimers

The study of dendritic molecules is a relatively new and rapidly expanding field of experimental chemistry. *Dendrimers* are extremely branched molecules, mainly synthesized from identical

building blocks that contain branching sites. The synthesis proceeds in repeatable steps, each reaction cycle resulting in a new, larger generation of the respective dendrimer. The majority of the known dendrimers are organic molecules (for review see refs 73, 74); the first inorganic systems of this kind (whose branching points are ruthenium atoms) were recently reported<sup>75</sup>.

Because of their peculiar and unprecedented structural features, dendritic molecules are an evident challenge for the theoretical and mathematical chemists. The authors of a recent review<sup>74</sup> on dendrimers have expressed the opinion that "the properties of strongly branched molecules are largely unknown and await discovery".

In this section we apply Theorem 2 for the computation of the Wiener numbers of dendrimers, and establish expressions for  $W$  of some highly branched molecular graphs<sup>76</sup>. We first determine the  $W$ -value of Newkome's arborol.

Newkome and coworkers<sup>77-80</sup> synthesized a class of dendrimers which they named *arborols*. The arborol reported in ref. 77 consists of a saturated hydrocarbon skeleton, to the termini of which  $3 \times 3 \times 4 = 36$  OH groups are attached; its formula is  $C_{253}H_{472}(OH)_{36}$ . The graph  $G_5$ , displayed in Fig. 5, represents the carbon-atom skeleton of this arborol. Observe that  $G_5$  has 36 vertices of degree one, and a total of 253 vertices.

In order to compute  $W(G_5)$  by means of Theorem 2, we first have to examine the branching points of  $G_5$ . All branching points of  $G_5$  are of degree four. They are of three types:  $\alpha$ ,  $\beta$  and  $\gamma$  (see Fig. 5). There is a single branching point of type  $\alpha$ , four branching points of type  $\beta$  and  $4 \times 3 = 12$  branching points of type  $\gamma$ .

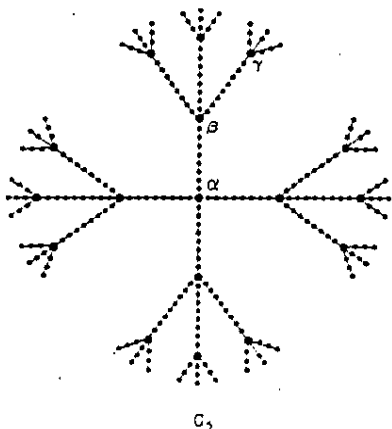


Fig. 5—The molecular graph of the highly branched carbon-atom skeleton of Newkome's arborol<sup>77</sup>  $C_{253}H_{472}(OH)_{36}$ ; this graph possesses 253 vertices; its Wiener number is 826,608

The branching point  $\alpha$  has four identical branches, each with 63 vertices. Hence, it contributes to the right-hand side of Eq. (3) by  $-\begin{bmatrix} 4 \\ 3 \end{bmatrix} 63^3 = -1,000,188$ .

A  $\beta$ -type branching point has three identical branches with 18 vertices each, and a branch with  $253 - 3 \times 18 - 1 = 198$  vertices. Its contribution is thus equal to  $-(18^3 + 3 \times 18^2 \times 198) = -198,288$ .

A  $\gamma$ -type branching point has three identical branches with 3 vertices each, and a branch with  $253 - 3 \times 3 - 1 = 243$  vertices. Its contribution is equal to  $-(3^3 + 3 \times 3^2 \times 243) = -6,588$ .

According to formula (3), the Wiener number of  $G_5$  is now equal to,

$$W(G_5) = \begin{bmatrix} 254 \\ 3 \end{bmatrix} - [1,000,188 + 4 \times 198,288 + 12 \times 6,588] = 826,608.$$

By means of Theorem 2 it was possible to deduce<sup>76</sup> a general formula (4) for the Wiener numbers of the highly branched trees  $T_{k,d}$ , called *regular dendrimer graphs* (of degree  $d$ ). Their structure should be evident from the examples shown in Fig. 6. Note that the parameter  $k$  corresponds to what in dendrimer chemistry is called "number of generations"<sup>73,74</sup>.

The respective formula reads<sup>76</sup>:

$$W(T_{k,d}) = \begin{bmatrix} kd^3 - 2(k+1)d^2 + d \\ (d-1)^{2k} + 2d^2(d-1)^k - d \end{bmatrix} (d-2)^{-1} \quad \dots (4)$$

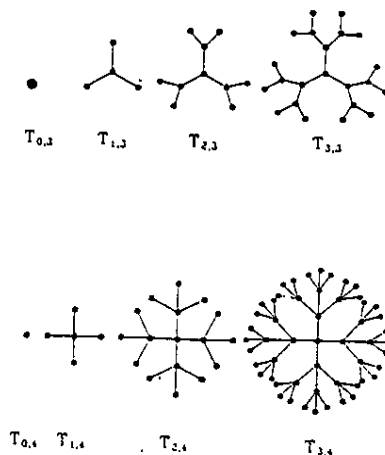


Fig. 6—The first four representatives of regular dendrimer graphs of degree three and four<sup>76</sup>

The chemically most interesting special cases of

$$\text{Eq. (14) are: } W(T_{k,3}) = (9k - 15)2^{2k} + 18 \cdot 2^k - 3$$

and

$$W(T_{k,4}) = \left( 4k - \frac{7}{2} \right) 3^{2k} + 4 \cdot 3^k - \frac{1}{2}$$

As the number of vertices of  $T_{k,d}$  is

$$n(T_{k,d}) = 1 + \frac{d-2}{d} \left[ (d-1)^k - 1 \right]$$

it follows that for large values of  $k$ ,  $W \sim n^2$ , irrespective of the value of the parameter  $d$ ,  $d \geq 3$ . This observation may be of relevance for the understanding of the fractal nature of dendritic molecules.<sup>74</sup>

#### Wiener numbers of composite graphs

There have been several attempts<sup>60,81-86</sup> to find

formulae for the calculation of the Wiener number of a composite (molecular) graph by using the  $W$ -values of certain of its fragments. This problem has not been satisfactorily solved so far. Recently, however, a systematic study of the so-called graph products has been undertaken<sup>87</sup>. In what follows, we briefly repeat the definitions of the respective graph products and state the formulae obtained for their Wiener numbers. Then we point out a number of chemically relevant applications. More details on graph products can be found in textbooks of graph theory.<sup>88</sup>

If  $G$  is a graph, then the sets of its vertices and edges are denoted by  $V(G)$  and  $E(G)$ , respectively. The number of vertices and edges of  $G$  are  $n(G)$  and  $m(G)$ , respectively. Further, if  $A$  and  $B$  are two sets, then their Cartesian product  $A \times B$  is the set containing all ordered pairs  $(a, b)$ , such that  $a \in A$  and  $b \in B$ . The following are standard graph, theoretical definitions<sup>88</sup>.

(a) *The Cartesian product*  $G_1 \times G_2$ :  
 $V(G_1 \times G_2) = V(G_1) \times V(G_2)$ ; the vertices  $u = (u_1, u_2)$  and  $v = (v_1, v_2)$  of  $G_1 \times G_2$  are adjacent if and only if  $[u_1 = v_1 \text{ and } (u_2, v_2) \in E(G_2)]$  or  $[u_2 = v_2 \text{ and } (u_1, v_1) \in E(G_1)]$ .

(b) *The join*  $G_1 + G_2$ :  
 $V(G_1 + G_2) = V(G_1) \cup V(G_2)$ ;  
 $E(G_1 + G_2) = E(G_1) \cup E(G_2) \cup \{(u_1, u_2) | u_1 \in V(G_1), u_2 \in V(G_2)\}$ .

(c) *The composition*  $G_1[G_2]$ :  
 $V(G_1[G_2]) = V(G_1) \times V(G_2)$ ; the vertices

where  $d(x|G_2)$  stands for the sum of the distances

between the vertex  $x$  and all other vertices of  $G_2$ .

In order to apply Theorem 4 to certain composite molecular graphs, we need the expressions for the Wiener numbers of two simple graphs, namely, the path  $(P_n)$  and the circuit  $(C_n)$ . The structures of  $P_n$  and  $C_n$  are displayed in Fig. 7;  $n$  stands for the number of vertices.

The following well known formulae seem to be first reported by Etringer, Jackson & Snyder<sup>90</sup>

and eventually rediscovered many times:

$$W(P_n) = \frac{1}{6} n(n^2 - 1)$$

**Theorem 4<sup>87</sup>**. (a) For  $G_1$  and  $G_2$  being connected

$$W(G_1 \times G_2) = n(G_2)^2 W(G_1) + n(G_1) W(G_2)$$

(b) For  $G_1$  and  $G_2$  being arbitrary graphs,

$$W(G_1 + G_2) = n(G_1)^2 + n(G_2)^2 - n(G_2)$$

(c) For  $G_1$  being a connected graph,

$$W(G_1[G_2]) = n(G_2)^2 W(G_1) + n(G_1) m(G_2)$$

(d) For  $G_1$  being a connected graph,

$$W(G_1 \circ G_2) = [n(G_2) + 1]^2 W(G_1) + n(G_2) [n(G_2)^2 - m(G_2)] + [n(G_1)^2 - n(G_1)] [n(G_2) + 1] \times n(G_2)$$

(e) For  $G_1$  and  $G_2$  being connected graphs and  $x$  being the root of  $G_2$ ,

$$W(G_1[G_2]) = n(G_2)^2 W(G_1) + n(G_1) W(G_2) + [n(G_1)^2 - n(G_1)] n(G_2) d(x|G_2)$$

More examples of this kind can be found in ref. 87. For the studies of clusters, the knowledge of the Wiener number of the complete graph  $K_n$  and of the complete bipartite graph  $K_{a,b}$  may be of interest:

$$W(K_n) = \frac{1}{2}n(n-1)$$

$$W(K_{a,b}) = a^2 - a + b^2 + ab$$

$$W(\text{radialene}) = \begin{cases} \frac{1}{2}a^3 + 2a^2 - a & \text{if } a \text{ is even} \\ \frac{1}{2}a^3 + 2a^2 - \frac{2}{3}a & \text{if } a \text{ is odd} \end{cases}$$

$$W(\text{square lattice}) = \frac{1}{6}ab(a+b)(ab-1).$$

**Wiener numbers of benzenoid systems**

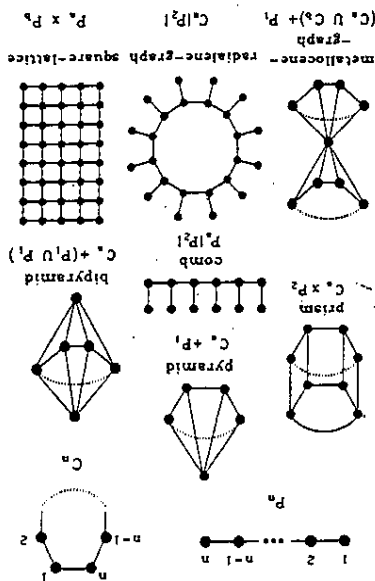
The Wiener numbers of benzenoid systems attracted a particular attention of researchers in mathematical chemistry, and a variety of results are reported in this field. Because this topic is covered by a recent review<sup>91</sup>, we skip its details here. The only noteworthy result, not included in the above mentioned review<sup>91</sup>, is the recent work by Dobrynin<sup>92</sup> in which he reports on non-isometric benzenoid molecules with equal W-values.

**The problem of isomer degeneracy of the Wiener number**

For several chemical applications of the Wiener number (e.g., in chromatography), it would be desirable that chemical compounds possess distinctive values of W. This condition, however, is far from reality. Numerous pairs, triplets, etc., of molecular structures have been found, of which W is the same<sup>19,92-95</sup>. With regard to this, the so-called *mean isomer degeneracy* of the Wiener numbers<sup>19,94</sup> was defined as  $\mu = N/t$ , where N is the number of distinct structural isomers considered, and t is the number of distinct values that the Wiener number assumes for these isomers. In the ideal case, when each isomer is associated with a distinct W, we have  $\mu = 1$ . Otherwise  $\mu$  is greater than unity and shows how many isomers (on average) share the same value of W. Evidently, the larger the  $\mu$ , the smaller is the isomer-discriminating power of W.

The concept of mean isomer degeneracy can be illustrated by considering the isomeric alkanes with seven C-atoms. There exist nine structural isomers whose formula is  $C_7H_{16}$  ( $N=9$ ), but they have only seven distinct values for the Wiener

Fig. 7—The path ( $P_n$ ), the circuit ( $C_n$ ) and some composite graphs of chemical interest that can be represented as products of paths and circuits; their Wiener numbers are obtained using Theorem 4



Combining these formulae with the results given in Theorem 4, we immediately obtain expressions for Wiener numbers of the composite graphs shown in Fig. 7. Thus, with the notation from Fig. 7, we have:

$$W(\text{prism}) = \begin{cases} \frac{1}{2}a^3 + a^2 & \text{if } a \text{ is even} \\ \frac{1}{2}a^3 + a^2 - \frac{1}{2}a & \text{if } a \text{ is odd} \end{cases}$$

For the special case of  $a=4$ , we have  $W(\text{cube})=48$ .

$W(\text{pyramid})=a^2-a$

For the special case of  $a=3$ , we have  $W(\text{tetrahedron})=6$ .

$W(\text{bipyramid})=a^2+2$ .

For the special case of  $a=4$ , we have  $W(\text{octahedron})=18$ .

$W(\text{metalocene})=(a+b)(a+b-1)$ .

For the special case of  $a=b=5$ , we have  $W(\text{ferrocene})=90$ .

$$W(\text{comb}) = \frac{2}{3}a^3 + 2a^2 - \frac{1}{3}a$$



and minimum Wiener numbers have been identified for: (a) connected graphs with  $n$  vertices<sup>90</sup>, (b) connected graphs with  $n$  vertices and  $m$  edges<sup>90</sup>, (c) trees with  $n$  vertices<sup>90</sup>, (d) trees with  $n$  vertices and a fixed maximum vertex degree<sup>102</sup>. In some cases the graphs with second, third, ... maximum and minimum  $W$ -values are also known<sup>102</sup>.

In the class of all-connected graphs,  $W$  can assume any value, except 2 and 5 (ref. 103). In the class of all-connected bipartite graphs,  $W$  can assume any value, except 2, 3, 5, 6, 7, 11, 12, 13, 15, 17, 19, 33, 37 and 39 (ref. 104).

**Concluding remarks**

The aim of this review is to present a cross-section of the contemporary investigations of the Wiener number. We hope to have demonstrated that in this field of mathematical chemistry active research is being conducted, both fundamental and applied.

In spite of numerous results obtained in the theory of the Wiener number, some basic problems still remain open. We mention here only two:

No recursive method is known for the calculation of  $W$  of a general (molecular) graph. This especially applies to polycyclic graphs. As a consequence, very little is known about the relations between the Wiener number of a graph  $G$  and the Wiener numbers of various fragments (subgraphs) of  $G$ . This, in turn, means that the dependence of  $W$  on the structure of  $G$  is far from being understood.

It is not known how  $W$  behaves when the size (= number of vertices) of the graph  $G$  increases. In particular, if  $G_1, G_2, \dots, G_k, \dots$  is a sequence of graphs, such that  $G_{k+1}$  is obtained by attaching a new vertex to  $G_k$ , then the limit value  $L = \lim_{k \rightarrow \infty} [W(G_k)/\ln n(G_k)]$  may, but need not exist. If  $L$  does exist, then  $2 \leq L \leq 3$ . The existence and value

$$\lim_{n \rightarrow \infty} N(n,m)/t(n,m) = \infty$$

of  $m - n + 1$ ,  
 a more precise formulation<sup>97</sup>, for any fixed value

The above result implies that isomeric molecules with sufficiently high number of atoms ( $n$ ) cannot be distinguished by means of their Wiener numbers. What "sufficiently high" is in reality, has been recently determined<sup>95</sup>. It was found that already for  $n \approx 10$  the isomer degeneracy of  $W$  is significantly large and rapidly increases with  $n$ . This calls for caution in various practical applications of the Wiener numbers, even in the case of medium-sized molecules.

The isomer degeneracies of connected six- and seven-vertex graphs<sup>95</sup> are collected in Table 2.

**Some mathematical connections**

Quantities identical with, or closely related to the Wiener number were extensively studied by mathematicians<sup>22</sup>. Instead of "Wiener number" they used names such as "gross status"<sup>98</sup>, "total status"<sup>22</sup>, "graph distance"<sup>99</sup> and "transmission"<sup>96,99</sup>. Instead of  $W(G)$ , some authors examined the closely related "mean distance"  $\bar{W} = [n(n-1)/2]^{-1}W$ .

For chemical applications, it may be especially interesting to note that the graphs with maximum

Table 2—Mean isomer degeneracies ( $\mu$ ) of connected graphs with  $n$  vertices and  $m$  edges<sup>95</sup>;  $\mu$  is given only if the respective graphs have at least two different  $W$ -values

n = 6		n = 7	
m	$\mu$	m	$\mu$
5	1.00	6	2.17
6	2.17	7	3.17
7	3.17	8	5.50
8	5.50	9	6.67
9	6.67	10	7.00
10	7.00	11	—
11	—	12	—
12	—	13	—
13	—	14	—
14	—	15	—
15	—	16	—
16	—	17	—
17	—	18	—
18	—	19	—
19	—	20	—
20	—	21	—
21	—	22	—
22	—	23	—
23	—	24	—
24	—	25	—
25	—	26	—
26	—	27	—
27	—	28	—
28	—	29	—
29	—	30	—
30	—	31	—
31	—	32	—
32	—	33	—
33	—	34	—
34	—	35	—
35	—	36	—
36	—	37	—
37	—	38	—
38	—	39	—
39	—	40	—
40	—	41	—
41	—	42	—
42	—	43	—
43	—	44	—
44	—	45	—
45	—	46	—
46	—	47	—
47	—	48	—
48	—	49	—
49	—	50	—
50	—	51	—
51	—	52	—
52	—	53	—
53	—	54	—
54	—	55	—
55	—	56	—
56	—	57	—
57	—	58	—
58	—	59	—
59	—	60	—
60	—	61	—
61	—	62	—
62	—	63	—
63	—	64	—
64	—	65	—
65	—	66	—
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68	—	69	—
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98	—	99	—
99	—	100	—
100	—	101	—
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102	—	103	—
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164	—	165	—
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187	—	188	—
188	—	189	—
189	—	190	—
190	—	191	—
191	—	192	—
192	—	193	—
193	—	194	—
194	—	195	—
195	—	196	—
196	—	197	—
197	—	198	—
198	—	199	—
199	—	200	—

- of L depend on the structure of the graphs  $G_n$ , but the mode of dependence is not known. With-out having an (at least partial) answer to this question, it is not possible to design reliable approximate expressions for W. On the other hand, the recent synthesis of macromolecules with highly branched skeletons (e.g., dendrimers), increases the need for estimating W via pertinent approximate formulae.
- In view of this, it seems certain that the theory of the Wiener number will continue to thrive.
- Acknowledgement**
- The authors are indebted to the National Science Council of the Republic of China for financial support under the grants NSC-82-0208-M001-042 and VRP-92029. I. Gutman thanks the staff of the Institute of Chemistry, Academia Sinica for kind hospitality.
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