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Calculating Wiener Numbers of Molecular Graphs with Symmetry*

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Abstract

This paper uses the symmetry of graphs to calculate their Wiener numbers. The methods apply to a great mumber of symmetric molecular graphs. Some illustrative examples are presented.

1 Introduction

One of the most important 'topological' (i.e. graph-theoretical) indices associated with molecular graphs is the number W, which is used to quantify the structure of organic molecules and was introduced in 1947 by Harold Wiener in the seminal article[1] (and quoted in several other articles), as the 'sum of the topological distances', that is,

Definition If $G=(V,E)$ is a connected graph, and $d: V\times V \to N=\{0, 1, 2, \cdots\}$ is the distance function on the graph, then we define the **Wiener number** to be

$$W = W(G) \equiv \sum_{\{u,v\}\subset V} d(u,v),$$

and for any given vertex u in $V = V(G)$, we define

$$W(u \mid G) \equiv \sum_{v\in V} d(u,v),$$

where $d(u,v)$ is the distance between u and v, to be the **partial Wiener number** of u (with respest to G).

In short, the Wiener number of a graph is the sum of all topological (graph-theoretical) distances between pairs of its vertices. Obviously we have

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$$W = \frac{1}{2}\sum_{u \in V} W(u \mid G).$$

Physical chemists have found that there are strong correlations between the Wiener number W and a large number of physico-chemical properties such as the boiling points, the heats of formation, atomization, isomerization and vaporization, density, critical pressure, etc. A lot of chemical applications of W have been proposed, [5][10][11] since the shortest path algorithm can be used to find the Wiener number of molecular graphs. Thus the computation of W by means of a computer is a solved task. However Chemists are often interested in paper-and-pencil methods for the evaluation of W. Several powerful methods have been developed by Wiener, Gutman, Yeh and others, [1][6][8][9] for some classes of molecular graphs.

These results can be found in the recent review of I. Gutman *et al*.[7]

In this paper, we will give a new method to evaluate the Wiener number for molecular graphs with symmetry. Our main idea is to use the orbits of the automorphism groups to simplify the calculation so that we may give an effective algorithm.

2 Symmetry and Point Groups

In order to discuss molecular symmetry, we first introduce *symmetry operations*. A symmetry operation is defined as an operation that moves a given molecule (or generally, a three-dimentional object) from an initial state to another, where the two states cannot be differentiated from each other. Clearly all the symmetry operations of a molecule (or a 3-D object) form a group (the multiplication of two operations in the group is the natural composition of the operations). This group is called the *point group* of the molecule. For more detailed discussion about the axioms and theories of group theory the reader can refer to any group theory textbook.

Next we recall the concept of *orbits* of a point group P as follows. Regard the molecule as a graph with its elements as the vertices and the bonds between elements as the edges of the graph. When an element p of P (that is, a symmetry operation on the graph) operates on the graph, it gives the vertices of the graph a permutation, that is, a one-to-one mapping. Let $p(x)$ denote the image of x under the mapping (operation). When there exists a $p \in P$ that satisfies $y = p(x)$ for two elements x and y, we define a binary relation as being $x \sim y$. This relation can be easily proved to be an equivalence relation. According to this equivalence relation, the vertices are partitioned into an appropriate number of equivalence classes: $\triangle_1, \cdots, \triangle_r$. Each $\triangle_i$ is called an *orbit* of P. The number of members of each orbit ($|\triangle_i|$) is called the *length* of the orbit($\triangle_i$). Group theory tells us that if $x \in \triangle_i$ then the length of $\triangle_i$ is $\frac{|P|}{|P_x|}$, where $P_x = \{p \mid p \in P, p(x) = x\}$. If the group has only one orbit, it is called *transitive*. Otherwise it is called *intransitive*. If H is a subgroup of G, we can define the orbits of H similarly which could also be either transitive or intransitive.

3 Calculation of Wiener Number

In section 1, we have that the Wiener number of a graph is

$$W = \frac{1}{2}\sum_{u \in V} W(u \mid G). \qquad (*)$$

We first give the following theorem for general-case calculation when the point group is not necessarily transitive.

Theorem 1 Let $H \trianglelefteq P_G$, that is, H is a subgroup of P_G, and $\triangle_1, \triangle_2, \cdots \triangle_r$ are the orbits of H. For each orbit, put $y_i \in \triangle_i$, and $\alpha_i = |\triangle_i|$, $i = 1, 2, \ldots, r$. We have

$$W = \sum_{i=1}^{r}\sum_{j=i+1}^{r} \alpha_i \sum_{y \in \triangle_j} d(y, y_i) + \frac{1}{2}\sum_{i=1}^{r} \alpha_i \sum_{x \in \triangle_i} d(x, y_i).$$

Proof Since $W(u \mid G)$ are equel for all vertices in the same orbit,

$$\begin{aligned}\sum_{u \in V} W(u \mid G) &= \sum_{i=1}^{r}\sum_{u \in \triangle_i} W(u \mid G) = \sum_{i=1}^{r} \alpha_i W(y_i \mid G)\\ &= \sum_{i=1}^{r} \alpha_i \sum_{j=1}^{r}\sum_{v \in \triangle_j} d(y_i, v) = \sum_{i=1}^{r}\sum_{j=1}^{r} \alpha_i \sum_{v \in \triangle_j} d(y_i, v)\\ &= 2\sum_{i=1}^{r}\sum_{j=i+1}^{r} \alpha_i \sum_{v \in \triangle_j} d(v, y_i) + \sum_{i=1}^{r} \alpha_i \sum_{z \in \triangle_i} d(z, y_i)\end{aligned}$$

Thus by ($*$),

$$W = \frac{1}{2}\sum_{u\in V} W(u \mid G) = \sum_{i=1}^{r}\sum_{j=i+1}^{r}\alpha_i \sum_{y\in\triangle_j} d(y, y_i) + \frac{1}{2}\sum_{i=1}^{r}\alpha_i \sum_{x\in\triangle_i} d(x, y_i). \quad \square$$

Before we proceed to give some examples it is worthwhile to develop a method of calculation when the point group of the molecule is transitive, in which case, all the partial Wiener numbers $W(u \mid G)$ will be the same. Thus we get the following

Lemma 2 If the point group P_G of the molecule is transitive, then for any element $u \in V$, the Wiener number W is

$$W = \frac{n}{2} W(u \mid G),$$

where $n = |V|$. □

By this lemma, to find the Wiener number of the molecule with transitive point group, it suffices to choose any element in V and count the distances between it and the rest elements in V. In addition, if we choose the element properly, the counting steps can also be greatly reduced. For this purpose, consider a subgroup H of P_G (for differentiation we use P_G in place of P). H is not necessarily transitive even if P_G is transitive. In this case, V is partitioned into a number of orbits of H: $\triangle_1, \triangle_2, \cdots, \triangle_r$. Assume that $|\triangle_1| \le |\triangle_2| \le \cdots \le |\triangle_r|$. Let $|\triangle_i| = \alpha_i$, for $i = 1, 2, \cdots, r$.

Theorem 3 Let $x_i \in \triangle_i$, $i = 1, 2, \cdots, r$. Then the partial Wiener number of x_1 is

$$W(x_1 \mid G) = \frac{1}{\alpha_1}\sum_{y\in\triangle_1}\sum_{i=1}^{r}\alpha_i d(y, x_i).$$

Proof Because P_G is transitive, we have that

$$W(x_1 \mid G) = \frac{1}{\alpha_1}\sum_{y\in\triangle_1}\sum_{z\in V} d(y, z)$$

$$= \frac{1}{\alpha_1} \sum_{y \in \triangle_1} \sum_{i=1}^{r} \sum_{z \in \triangle_i} d(y, z)$$

$$= \frac{1}{\alpha_1} \sum_{i=1}^{r} \sum_{z \in \triangle_i} \sum_{y \in \triangle_1} d(y, z).$$

But for any i, and any $z \in \triangle_i$, there is an $h_i \in H$ such that $h_i(z) = x_i$. Hence

$$\begin{aligned} & \sum_{z \in \triangle_i} \sum_{y \in \triangle_1} d(y, z) \\ = & \sum_{z \in \triangle_i} \sum_{y \in \triangle_1} d(h_i(y), h_i(z)) \\ = & \sum_{z \in \triangle_i} \sum_{h_i(y) \in \triangle_1} d(h_i(y), x_i) \\ = & \alpha_i \sum_{h_i(y) \in \triangle_1} d(h_i(y), x_i) \\ = & \alpha_i \sum_{v \in \triangle_1} d(v, x_i). \end{aligned}$$

Consequently we get

$$\begin{aligned} W(x_1 \mid G) & = \frac{1}{\alpha_1} \sum_{i=1}^{r} \sum_{y \in \triangle_1} \sum_{z \in \triangle_i} d(y, z) \\ & = \frac{1}{\alpha_1} \sum_{i=1}^{r} \alpha_i \sum_{v \in \triangle_1} d(v, x_i) \\ & = \frac{1}{\alpha_1} \sum_{v \in \triangle_1} \sum_{i=1}^{r} \alpha_i d(v, x_i). \end{aligned}$$ □

From this theorem, we know that for an element $x_1 \in \triangle_1$, we need not count all the distances between it and the rest in G. For the elements in $\triangle_i$, choosing one of them is enough ($i = 2, 3, \cdots, r$). In practice, it is natural to choose the subgroup H such that α_1 is as small as possible to simplify our calculation. In particular, when $\alpha_1 = 1$, that is, H fixes x_1, we count only r-1 times. Thus we get the following

Corollary 4 Let $x_i \in \triangle_i$, $i = 1, 2, \cdots, r$. Suppose that $|\triangle_1| = 1$.

Then the partial Wiener number of x_1 is

$$W(x_1 \mid G) = \sum_{i=2}^{r} \alpha_i d(x_1, x_i). \qquad \square$$

To further reduce the counting steps of the Wiener numbers, we note that many of the molecular graghs have a 'layered' structure in the sense that the different orbits have consecutive distances from a fixed point. In this case, we add 1 to the distance of an orbit to get that of the next, instead of counting them separately. This method is based on the following theorem.

Theorem 5 Suppose that P_G is transitive and $H \trianglelefteq P_G$ is a subgroup with orbits $\triangle_1, \triangle_2, \cdots, \triangle_r$. Let $\alpha_i = \mid \triangle_i \mid$ and $x_i \in \triangle_i, i = 1, 2, \cdots, r$. Suppose that $\alpha_i = 1$. If there is an x_k such that $d(x_1, x_k) \geq r - 1$, then x_1, $x_2, \cdots, x_r$ can be permuted into $x_{k_1}, x_{k_2}, \cdots, x_{k_r}$ with $k_1 = 1$ and $k_r = k$ such that $d(x_1, x_{k_j}) = j - 1, j = 1, 2, \cdots, r$. Then the Wiener number is

$$W = \frac{n}{2} \sum_{j=2}^{r} (j - 1) \alpha_{k_j}.$$

Proof Because molecular graghs are connected and elements in the same orbit have equal distances from x_1, the orbits must saturate the vacancy between $\triangle_1$ and $\triangle_k$ in terms of their distances from x_1. While $d(x_1, x_k) \geq r - 1$ and there are only $r - 1$ orbits different from $\triangle_1$, the orbits are forced to run consecutively between $\triangle_1$ and $\triangle_k$, which implies that the vertices $x_1, x_2, \cdots, x_r$. can be permuted into $x_{k_1}, x_{k_2}, \cdots, x_{k_r}$ with $k_1 = 1$ and $k_r = k$ such that $d(x_1, x_{k_j}) = j - 1, j = 1, 2, \cdots, r$. Hence

$$\begin{aligned} W = \frac{n}{2} W(x_1 \mid G) &= \frac{n}{2} \sum_{i=2}^{r} \alpha_i d(x_1, x_i) \\ &= \frac{n}{2} \sum_{j=2}^{r} \alpha_{k_j} d(x_1, x_{k_j}) \\ &= \frac{n}{2} \sum_{j=2}^{r} (j - 1) \alpha_{k_j}. \qquad \square \end{aligned}$$

We would like to metion that all the regular polyhedrons satisfy the conditions of Theorem 5.

4 Examples

Now we give some illustrative examples which show that our approach can be carried out by pen and paper not only for small graphs.

Example 1 Tetrahedron (see Fig. 1(a)). In Fig. 1, the subscripts of the x's indicate the orbits they are in. Suppose the point group is P_G. We first decide the subgroup $R \trianglelefteq P_G$ of all the rotations in P_G. The elements of R consist of rotations through angles of $\frac{2\pi}{3}$ and $\frac{4\pi}{3}$ about each of four axes joining vertices with centers of opposite faces, rotations through the angle π about each of three axes joining the midpoints of opposite edges, and the identity. Thus

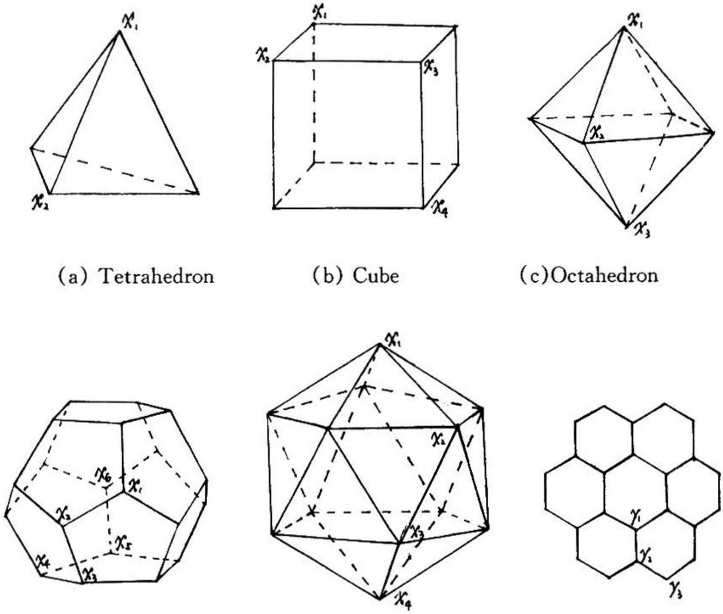
$$|R| = 4 \times 2 + 3 \times 1 + 1 = 12.$$

Obviously R is transitive and so is P_G. Choose H to be the set of all rotations around the axis joining x_1 with the center of the opposite face through angles of $\frac{2\pi}{3}, \frac{4\pi}{3}$ anticlockwise, plus the identity. We get two orbits with representatives x_1, x_2 as shown in the figure. Using $\alpha_i = \frac{|P|}{|P_x|}$, we get $\alpha_1 = 1$, $\alpha_2 = 3$. Applying Theorem 5,

$$W = \frac{n}{2}\sum_{j=2}^{r}(j-1)\alpha_{k_j} = \frac{4}{2} \times 3 = 6 \qquad \square$$

Example 2 Cube (see Fig. 1(b)). In this case the subgroup $R \trianglelefteq P_G$ of all the the rotations consists of rotations through angles of $\frac{\pi}{2}$, π, and $\frac{3\pi}{2}$ about each of three axes joining the centers of opposite faces, rotations through angles of $\frac{2\pi}{3}$ and $\frac{4\pi}{3}$ about each of four axes joining extreme opposite vertices, and rotations through the angle π about each of six axes joining midpoints of diagonally opposite edges. Thus

$$|R| = 3 \times 3 + 4 \times 2 + 6 \times 1 + 1 = 24$$



(a) Tetrahedron (b) Cube (c)Octahedron

(d) Dodecahedron (e)Icosahedron (f)coronene

Fig. 1 Regular polyhedrons and coronene

That R is transitive implies so is P_G. Now choose H as in Example 1 except that the rotations are around the axis joining the two opposite vertices x_1 and x_3. Here we have four orbits with representatives x_1, x_2, x_3 and x_4 as shown in the figure and using $\alpha_i = \frac{|P_G|}{|P_x|}$, $\alpha_1 = 1$, $\alpha_2 = 3$, $\alpha_3 = 3$, $\alpha_4 = 1$. By Theorem 5

$$W = \frac{n}{2} \sum_{j=2}^{r} (j-1) \alpha_{k_j}$$

$$= \frac{8}{2}(1 \times 3 + 2 \times 3 + 3 \times 1) = 48 \qquad \square$$

Example 3 Octahedron (see Fig. 1(c)). We first note that the point group is the same as that of the cube, for if we join the midpoints of adjacent faces of the cube with edges, we get the octahedron. Thus P_G is transitive. We choose all the rotations around the axis joining x_1 and x_3 which keep the octahedron invariant. We get three orbits with representatives x_i, $i = 1, 2, 3$, as shown in the figure and $\alpha_1 = 1$, $\alpha_2 = 4$, $\alpha_3 = 1$. By the same theorem

$$W = \frac{6}{2}(1 \times 4 + 2 \times 1) = 18 \qquad \square$$

Example 4 Icosahedron (see Fig. 1(e)). The rotation subgroup R of the point group consists of rotations through angles of $\frac{2\pi}{5}$, $\frac{4\pi}{5}$, $\frac{6\pi}{5}$ and $\frac{8\pi}{5}$ about each of 6 axes joining extreme opposite vertices, rotations through angles of $\frac{2\pi}{3}$ and $\frac{4\pi}{3}$ about each of ten axes joinjng centers of opposite faces, rotations through angle π about each of fifteen axes joining midpoints of opposite edges, and the identity. Thus

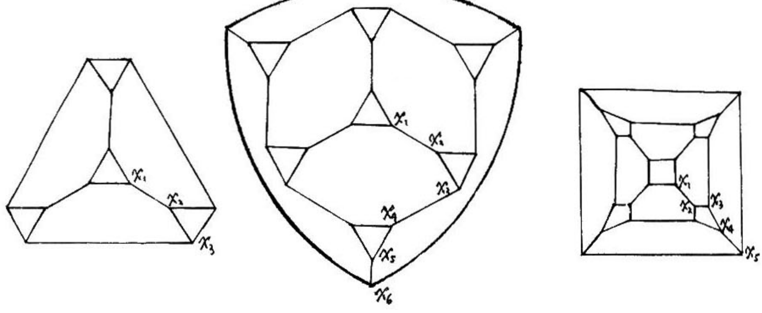
$$|R| = 6 \times 4 + 10 \times 2 + 15 \times 1 + 1 = 60$$

R is transitive and so is P_G. We choose the H to be the group generated by the $\frac{2\pi}{5}$-rotation around the axis joining x_1 and x_4. We get four orbits with representatives as shown in the figure and $\alpha_1 = 1$, $\alpha_2 = \alpha_3 = 5$, $\alpha_4 = 1$. Hence by Theorem 5 we have

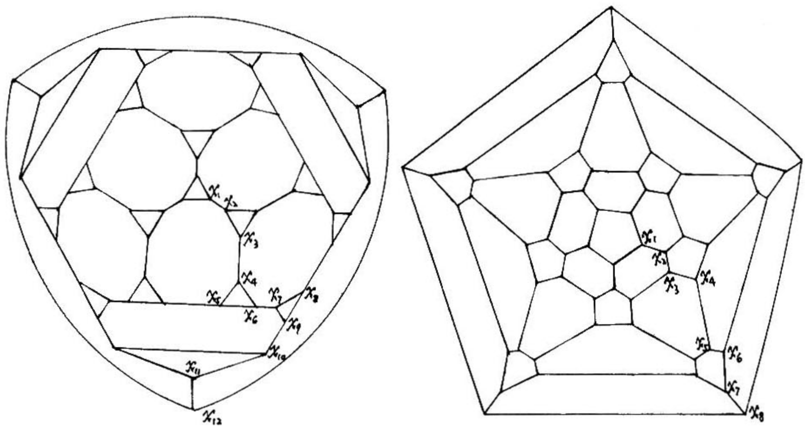
$$W = \frac{n}{2}\sum_{j=2}^{r}(j-1)\alpha_{k_j}$$

$$= \frac{12}{2} \times (1 \times 5 + 2 \times 5 + 3 \times 1) = 108 \qquad \square$$

Example 5 Dodecahedron (see Fig. 1(d)). Similar remarks in Example 3 imply that dodecahedron and icosahedron have the same point group. Choose H to be the group generated by the $\frac{2\pi}{3}$-rotation around the axis joining x_1 and x_6 and the reflection with respect to the plane containing x_1, x_2 and x_6.



(a) Truncated tetrahedron (b) Truncated cube (c) Truncated octahedron



(d) Truncated dodecahedron (e) Truncated icosahedron

Fig. 2 Truncated regular polyhedrons

Here we have 6 orbits with representatives x_i, $i = 1, 2, \cdots, 6$, as shown in the figure. $\alpha_1 = 1$, $\alpha_2 = 3$, $\alpha_3 = 6$, $\alpha_4 = 6$, $\alpha_5 = 3$, $\alpha_6 = 1$. Thus by Theorem 5 we have

$$
\begin{aligned}
W &= \frac{n}{2}\sum_{j=2}^{r}(j-1)\alpha_{k_j} \\
&= \frac{20}{2} \times (1 \times 3 + 2 \times 6 + 3 \times 6 + 4 \times 3 + 5 \times 1) = 500 \qquad \square
\end{aligned}
$$

Now we truncate the above polyhedrons and count their Wiener numbers using the above methods. Before proceeding we note that the truncated graphs have the same point groups as their corresponding ones and have the same transitivity.

Example 6 Truncated tetrahedron (see Fig. 2(a)). For convenience we have unravelled the polyhedrons on a plane. Choose H to be the group generated by the $\frac{2\pi}{3}$-rotation about the center of the graph and the reflection with respect to the line joining the center and x_1. We have three orbits with representatives x_i, $i = 1, 2, 3$, as shown in the figure. $\alpha_1 = 3$, $\alpha_2 = 3$, $\alpha_3 = 6$. Though it does not satisfy the conditions of Theorem 5, we can still count its Wiener number by Theorem 3. We have

$$\sum_{z \in \Delta_1} d(z, x_1) = 2,\ \sum_{z \in \Delta_1} d(z, x_2) = 5,\ \sum_{z \in \Delta_1} d(z, x_3) = 8.$$

Hence by Theorem 1 we have

$$
\begin{aligned}
W &= \frac{n}{2}\frac{1}{\alpha_1}\sum_{i=1}^{3}\alpha_i \sum_{z \in \Delta_1} d(z, x_i) \\
&= 6 \times \frac{1}{3}(3 \times 2 + 3 \times 5 + 6 \times 8) = 138 \qquad \square
\end{aligned}
$$

Example 7 Truncated cube (see Fig. 2(b)). We choose H to be the group generated by the $\frac{2\pi}{3}$-rotation about the center of the graph and the tacit reflection. We have 6 orbits here with representatives x_i, $i = 1, 2, \ldots, 6$, as shown in the figure. $\alpha_1 = 3$, $\alpha_2 = 3$, $\alpha_3 = 6$, $\alpha_4 = 6$, $\alpha_5 = 3$, $\alpha_6 = 3$.

$$\sum_{z \in \Delta_1} d(z, x_1) = 2, \quad \sum_{z \in \Delta_1} d(z, x_2) = 5, \quad \sum_{z \in \Delta_1} d(z, x_3) = 8,$$

$$\sum_{z \in \Delta_1} d(z, x_4) = 11, \quad \sum_{z \in \Delta_1} d(z, x_5) = 13, \quad \sum_{z \in \Delta_1} d(z, x_6) = 16$$

Thus by Theorem 3 we have

$$W = \frac{n}{2}\frac{1}{\alpha_1}\sum_{i=1}^{6}\alpha_i\sum_{z\in\Delta_1}d(z,x_i)$$
$$= 12 \times \frac{1}{3}(3\times 2 + 3\times 5 + 6\times 8 + 6\times 11 + 3\times 13 + 3\times 16)$$
$$= 888 \qquad \square$$

Example 8 Truncated octahedron (Fig. 2(c)). Choose similarly H to be generated by the rotation through $\frac{\pi}{2}$ angle about the center of the graph and a reflection . We have 5 orbits with representatives x_i, $i = 1, 2, \ldots, 5$, as shown in the figure. $\alpha_1 = 4$, $\alpha_2 = 4$, $\alpha_3 = 8$, $\alpha_4 = 4$, $\alpha_5 = 4$, $\alpha_6 = 1$.

$$\sum_{z\in\Delta_1}d(z,x_1) = 4, \quad \sum_{z\in\Delta_1}d(z,x_2) = 8, \quad \sum_{z\in\Delta_1}d(z,x_3) = 12,$$
$$\sum_{z\in\Delta_1}d(z,x_4) = 16, \quad \sum_{z\in\Delta_1}d(z,x_5) = 20,$$

and by Theorem 3 we have

$$W = \frac{n}{2}\frac{1}{\alpha_1}\sum_{i=1}^{5}\alpha_i\sum_{z\in\Delta_1}d(z,x_i)$$
$$= 12 \times \frac{1}{4}\times(4\times 4 + 4\times 8 + 8\times 12 + 4\times 16 + 4\times 20) = 864 \qquad \square$$

Example 9 Truncated dodecahedron (see Fig. 2(d)). Choose the same H as in Example 5. There are 12 orbits with representatives x_i, $i = 1, 2, \ldots, 12$, as shown in the figure. $\alpha_1 = 3$, $\alpha_2 = 3$, $\alpha_i = 6$, $i = 3, \ldots, 10$, $\alpha_{11} = 3$, $\alpha_{12} = 3$.

$$\sum_{z\in\triangle_1} d(z,x_1) = 2, \quad \sum_{z\in\triangle_1} d(z,x_2) = 5, \quad \sum_{z\in\triangle_1} d(z,x_3) = 8,$$
$$\sum_{z\in\triangle_1} d(z,x_4) = 11, \quad \sum_{z\in\triangle_1} d(z,x_5) = 14, \quad \sum_{z\in\triangle_1} d(z,x_6) = 14,$$
$$\sum_{z\in\triangle_1} d(z,x_7) = 17, \quad \sum_{z\in\triangle_1} d(z,x_8) = 20, \quad \sum_{z\in\triangle_1} d(z,x_9) = 20,$$
$$\sum_{z\in\triangle_1} d(z,x_{10}) = 23, \quad \sum_{z\in\triangle_1} d(z,x_{11}) = 25, \quad \sum_{z\in\triangle_1} d(z,x_{12}) = 28$$

Hence by Theorem 3 we have

$$\begin{aligned} W &= 10 \times (3 \times 2 + 3 \times 5 + 6 \times 8 + 6 \times 11 + 6 \times 14 + 6 \times 14 + \\ &\quad 6 \times 17 + 6 \times 20 + 6 \times 20 + 6 \times 23 + 3 \times 25 + 3 \times 28) \\ &= 9420 \end{aligned}$$

□

Example 10 Truncated icosahedron (Fig. 2(e)). Actually it is the graph of the fullerence (C_{60}). Choose H to be generated by the rotation through $\frac{2\pi}{5}$ angle about the center of the graph and a reflection. We get 8 orbits with representatives x_i, $i = 1, 2, \ldots, 8$, as shown in the figure. $\alpha_1 = 5$, $\alpha_2 = 5$, $\alpha_3 = 10$, $\alpha_4 = 10$, $\alpha_5 = 10$, $\alpha_6 = 10$, $\alpha_7 = 5$, $\alpha_8 = 5$.

$$\sum_{z\in\triangle_1} d(z,x_1) = 6, \quad \sum_{z\in\triangle_1} d(z,x_2) = 11, \quad \sum_{z\in\triangle_1} d(z,x_3) = 16,$$
$$\sum_{z\in\triangle_1} d(z,x_4) = 21, \quad \sum_{z\in\triangle_1} d(z,x_5) = 26, \quad \sum_{z\in\triangle_1} d(z,x_6) = 31,$$
$$\sum_{z\in\triangle_1} d(z,x_7) = 34, \quad \sum_{z\in\triangle_1} d(z,x_8) = 39$$

Hence by Theorem 3

$$\begin{aligned} W &= 6 \times (5 \times 6 + 5 \times 11 + 10 \times 6 + 10 \times 21 + 10 \times 26 + \\ &\quad 10 \times 31 + 5 \times 34 + 5 \times 39) \\ &= 8340 \end{aligned}$$

□

Example 11 We use Theorem 1 to calculate the Wiener number of the graph of coronene shown in Fig. 1(f). Choose K to be the subgroup generated by the $\frac{\pi}{3}$-rotation around the center of the graph and a reflection. We have three orbits: $\triangle_1$, $\triangle_2$, $\triangle_3$ from the innermost to the outermost with representatives y_1, y_2, y_3 as shown in the figure. By Theorem 1. we have

$$W = \sum_{i=1}^{r}\sum_{j=i+1}^{r}\alpha_j \sum_{y\in\triangle_i} d(y, y_j) + \frac{1}{2}\sum_{i=1}^{r}\alpha_i \sum_{x\in\triangle_i} d(x, y_i)$$

$$= 6\times 15 + 12\times 21 + 12\times 23 + \frac{1}{2}(6\times 9 + 6\times 19 + 12\times 50)$$

$$= 1002 \qquad \square$$

Finally we would like it to be known that in the collection of papers from the '96 Nankai International Symposium on Combinatorics, some Taiwanese have solved the Wiener number problem in general case.

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