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DISTANCE-BASED INDICES COMPUTATION OF SYMMETRY MOLECULAR STRUCTURES

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ABSTRACT. Most of molecular structures have symmetrical characteristics. It inspires us to calculate the topological indices by means of group theory. In this paper, we present the formulations for computing the several distance-based topological indices using group theory. We solve some examples as applications of our results.

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1. Introduction

In early years, many chemical experiments showed the evidence that the biochemical properties of chemical compounds, materials and drugs are closely related to their molecular structures. As a result, topological indices are introduced as numerical parameters of molecular graph, which play a vital role in understanding the properties of chemical compounds and are applied in disciplines such as chemistry, physics and medicine science.

In chemical graph theory, a molecular structure is expressed as a molecular graph G in which atoms are taken as vertices and chemical bonds are taken as edges. A topological index can be considered as a function $f : G \to \mathcal{R}^+$. In the past 40 years, scholars introduced many topological indices, such as Wiener index, Zagreb index, harmonic index, sum connectivity index, etc which reflect certain structural characteristics of organic molecules. There were many works contributing to report these distance-based or degree-based indices of special

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molecular structures (See Farahani *et al.* [1], Jamil *et al.* [2], Gao and Farahani [3], Gao *et al.* [4, 5, 6] and Gao and Wang [7, 8, 9] for details). The notation and terminology that were used but were undefined in this paper can be found in [10].

One of oldest indices, the Wiener index was defined as the sum of distance for all pair of vertices,

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v).$$

The modified Wiener index was introduced by Nikolić *et al.* [11] as the extension of the Wiener index which was defined as

$$W_\lambda(G) = \sum_{\{u,v\} \subseteq V(G)} d^\lambda(u,v).$$

Several conclusions on modified Wiener index can be referred to Vukićević and Źerovnik [12], Vukićević and Gutman [13], Lim [14], Gorse and Źerovnik [15], Vukićević and Graovac [16], and Gutman *et al.* [17].

Moreover, the hyper-Wiener index and λ-modified hyper-Wiener index are defined as

$$WW(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{2}(d(u,v) + d^2(u,v))$$

and

$$WW_\lambda(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{2}(d^\lambda(u,v) + d^{2\lambda}(u,v)),$$

respectively. Some important contributions on hyper-Wiener index can be found in Gutman [18], Gutman and Furtula [19], Eliasi and Taeri [20, 21], Iranmanesh *et al.* [22], Yazdani and Bahrami [23], Behtoei *et al.* [24], Mansour and Schork [25], Heydari [26], Ashrafi *et al.* [27], and Heydari [28].

The Harary index was introduced independently by Plavšić *et al.* [29] and Ivanciuc *et al.* [30] in 1993, as

$$H(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d(u,v)}.$$

Its corresponding Harary polynomial can be defined as

$$H(G,x) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d(u,v)} x^{d(u,v)}.$$

The second and third Harary indices are defined as

$$H_1(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d(u,v)+1},$$

$$H_2(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d(u,v)+2}.$$

More generally, the generalized Harary index was introduced by Das *et al.* [31] which is defined as

$$H_t(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{1}{d(u,v)+t},$$

where $t \in \mathcal{N}$ is a non-negative integer. Hence, Harary index is a special case of generalized Harary index when $t = 0$.
One topological index related to Wiener index is the reciprocal complementary Wiener (RCW) index which is defined by Zhou *et al.* [32] and can be defined as

$$RCW(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{1}{D(G)+1-d(u,v)},$$

where $D(G)$ is the diameter of molecular graph G. In what follows, we always denote $D(G)$ as the diameter of molecular graph G.
Furthermore, the multiplicative version of the Wiener index was defined by Gutman *et al.* [33, 34] as

$$\pi(G) = \prod_{\{u,v\}\subseteq V(G)} d(u,v).$$

The logarithm of multiplicative Wiener index was defined as

$$\Pi(G) = \ln \sqrt{2 \prod_{\{u,v\}\subseteq V(G)} d(u,v)}.$$

So far, many mathematical approaches are given to calculate different topological indices and received good results. Since most of the chemical compounds have symmetric structures. It inspires us to consider the computation of topological indices by using group theory. We use the automorphism groups and its orbits to simplify the computation of molecular graphs for some distance-based indices.

2. Main results and proofs

To discuss the symmetry molecular structures, we should first introduce symmetry operations which are defined as operations that move a fixed molecule structure from a previous condition to another, and any two states can't be differentiated from each other. Obviously, all the symmetry operations on a molecular structure constitute a group which is called the point group of the molecular structure.
When an element p of point group P (i.e., a symmetry operation on the molecular structure) operates on the molecular graph, it provides the vertices of the molecular graph a permutation. We denote $p(v)$ as the image of vertex v under the operation p. If there exists a $p \in P$ that satisfies $p(v) = u$ for two vertices v and u, then we define an equivalence binary relation denoted by $v \sim u$. By means of this equivalent relation, the vertex set is divided into several equivalence classes: $\Theta_1, \cdots, \Theta_r$. Each Θ_i can be called an orbit of point group P, and the number of vertices of each orbit $|\Theta_i|$ is called the length of the orbit Θ_i. By

the knowledge of group theory, we know that if $v \in \Theta_i$ then $|\Theta_i| = \frac{|P|}{|P_v|}$, where $P_v = \{p|p \in P, p(v) = v\}$. The group called transitive if it has only one orbit, and it is called intransitive otherwise. Moreover, we can define the orbits of subgroup H in similar way which could also be either transitive or intransitive. Set

- $W_\lambda(v,G) = \sum_{u\in V(G)} d^\lambda(u,v)$,
- $WW(v,G) = \frac{1}{2}\sum_{u\in V(G)}(d(u,v) + d^2(u,v))$,
- $WW_\lambda(v,G) = \frac{1}{2}\sum_{u\in V(G)}(d^\lambda(u,v) + d^{2\lambda}(u,v))$,
- $H(v,G) = \sum_{u\in V(G)} \frac{1}{d(u,v)}$,
- $H(v,G,x) = \sum_{u\in V(G)} \frac{1}{d(u,v)} x^{d(u,v)}$,
- $H_1(v,G) = \sum_{u\in V(G)} \frac{1}{d(u,v)+1}$,
- $H_2(v,G) = \sum_{u\in V(G)} \frac{1}{d(u,v)+2}$,
- $H_t(v,G) = \sum_{u\in V(G)} \frac{1}{d(u,v)+t}$,
- $RCW(v,G) = \sum_{u\in V(G)} \frac{1}{D(G)+1-d(u,v)}$,
- $\pi(v,G) = \prod_{u\in V(G)} d(u,v)$.

Hence, we have

- $W_\lambda(G) = \frac{1}{2}\sum_{v\in V(G)} W_\lambda(v,G)$, (1)
- $WW(G) = \frac{1}{2}\sum_{v\in V(G)} WW(v,G)$,
- $WW_\lambda(G) = \frac{1}{2}\sum_{v\in V(G)} WW_\lambda(v,G)$,
- $H(G) = \frac{1}{2}\sum_{v\in V(G)} H(v,G)$,
- $H(G,x) = \frac{1}{2}\sum_{v\in V(G)} H(v,G,x)$,
- $H_1(G) = \frac{1}{2}\sum_{v\in V(G)} H_1(v,G)$,
- $H_2(G) = \frac{1}{2}\sum_{v\in V(G)} H_2(v,G)$,
- $H_t(G) = \frac{1}{2}\sum_{v\in V(G)} H_t(v,G)$,
- $RCW(G) = \frac{1}{2}\sum_{v\in V(G)} RCW(v,G)$,
- $\pi(G) = \sqrt{\prod_{v\in V(G)} \pi(v,G)}$,
- $\Pi(G) = \ln\sqrt{2\sqrt{\prod_{v\in V(G)} \pi(v,G)}}$.

Following theorem is about the calculation of different topological indices when the point group is not necessarily transitive.

Theorem 2.1. *Let $H \trianglelefteq P_G$ be a subgroup of P_G, and $\Theta_1, \Theta_2, \cdots, \Theta_r$ are the orbits of H and $u_i \in \Theta_i$, $i = 1, 2, \cdots, r$. Then, we have*

(1) $W_\lambda(G) = \sum_{i=1}^r \sum_{j=i+1}^r |\Theta_i| \sum_{u\in\Theta_j} d^\lambda(u,u_i) + \frac{1}{2}\sum_{i=1}^r |\Theta_i| \sum_{v\in\Theta_i} d^\lambda(v, u_i)$,

(2) $WW(G) = \frac{1}{2}\sum_{i=1}^r \sum_{j=i+1}^r |\Theta_i| \sum_{u\in\Theta_j}(d(u,u_i)+d^2(u,u_i))+\frac{1}{2}\sum_{i=1}^r |\Theta_i| \sum_{v\in\Theta_i}(d(v,u_i) + d^2(v,u_i))$,

(3) $WW_\lambda(G) = \frac{1}{2}\sum_{i=1}^{r}\sum_{j=i+1}^{r}|\Theta_i|\sum_{u\in\Theta_j}(d^\lambda(u,u_i)+d^{2\lambda}(u,u_i))+\frac{1}{2}\sum_{i=1}^{r}|\Theta_i|\sum_{v\in\Theta_i}(d^\lambda(v,u_i)+d^{2\lambda}(v,u_i))$,

(4) $H(G) = \sum_{i=1}^{r}\sum_{j=i+1}^{r}|\Theta_i|\sum_{u\in\Theta_j}\frac{1}{d(u,u_i)}+\frac{1}{2}\sum_{i=1}^{r}|\Theta_i|\sum_{v\in\Theta_i}\frac{1}{d(v,u_i)}$,

(5) $H(G,x) = \sum_{i=1}^{r}\sum_{j=i+1}^{r}|\Theta_i|\sum_{u\in\Theta_j}\frac{1}{d(u,u_i)}x^{d(u,u_i)}+\frac{1}{2}\sum_{i=1}^{r}|\Theta_i|\sum_{v\in\Theta_i}\frac{1}{d(v,u_i)}x^{d(v,u_i)}$,

(6) $H_t(G) = \sum_{i=1}^{r}\sum_{j=i+1}^{r}|\Theta_i|\sum_{u\in\Theta_j}\frac{1}{d(u,u_i)+t}+\frac{1}{2}\sum_{i=1}^{r}|\Theta_i|\sum_{v\in\Theta_i}\frac{1}{d(v,u_i)+t}$,

(7) $RCW(G) = \sum_{i=1}^{r}\sum_{j=i+1}^{r}|\Theta_i|\sum_{u\in\Theta_j}\frac{1}{D(G)+1-d(u,u_i)}+\frac{1}{2}\sum_{i=1}^{r}|\Theta_i|\sum_{v\in\Theta_i}\frac{1}{D(G)+1-d(v,u_i)}$,

(8) $\pi(G) = \prod_{i=1}^{r}\prod_{j=i+1}^{r}\prod_{u\in\Theta_j}d^{|\Theta_i|}(u,u_i)\times\sqrt{\prod_{i=1}^{r}\prod_{v\in\Theta_i}d^{|\Theta_i|}(v,u_i)}$,

(9) $\Pi(G) = \ln\sqrt{2\prod_{i=1}^{r}\prod_{j=i+1}^{r}\prod_{u\in\Theta_j}d^{|\Theta_i|}(u,u_i)\times\sqrt{\prod_{i=1}^{r}\prod_{v\in\Theta_i}d^{|\Theta_i|}(v,u_i)}}$.

Proof. We only prove for $W_\lambda(G)$. The remaining cases can be proved in similar fashion.
Since $W_\lambda(u,G)$ is equal to the sum of all vertices in the same orbit, we infer

$$\begin{aligned}
\sum_{w\in V(G)}W_\lambda(w,G) &= \sum_{i=1}^{r}\sum_{w\in\Theta_i}W_\lambda(w,G)\\
&= \sum_{i=1}^{r}|\Theta_i|W_\lambda(u_i,G)\\
&= \sum_{i=1}^{r}|\Theta_i|\sum_{j=1}^{r}\sum_{y\in\Theta_i}d^\lambda(u_i,y)\\
&= \sum_{i=1}^{r}\sum_{j=1}^{r}|\Theta_i|\sum_{y\in\Theta_i}d^\lambda(u_i,y)\\
&= 2\sum_{i=1}^{r}\sum_{j=i+1}^{r}|\Theta_i|\sum_{y\in\Theta_i}d^\lambda(y,u_i)+\sum_{i=1}^{r}|\Theta_i|\sum_{z\in\Theta_i}d^\lambda(z,u_i).
\end{aligned}$$

Hence, in terms of (1),

$$\begin{aligned}
W_\lambda(G) &= \frac{1}{2}\sum_{w\in V(G)}W_\lambda(w,G)\\
&= \sum_{i=1}^{r}\sum_{j=i+1}^{r}|\Theta_i|\sum_{u\in\Theta_j}d^\lambda(u,u_i)+\frac{1}{2}\sum_{i=1}^{r}|\Theta_i|\sum_{v\in\Theta_i}d^\lambda(v,u_i).
\end{aligned}$$

Hence, the desired result is obtained. □

The next result is about the computation of topological indices when the point group of the molecular graph is transitive.

Lemma 2.2. *If the point group P_G of the molecular graph is transitive. Then for any $v \in V(G)$, we have*

(1) $W_\lambda(G) = \frac{|V(G)|}{2} W_\lambda(v, G)$,
(2) $WW(G) = \frac{|V(G)|}{4} WW(v, G)$,
(3) $WW_\lambda(G) = \frac{|V(G)|}{4} WW_\lambda(v, G)$,
(4) $H(G) = \frac{|V(G)|}{2} H(v, G)$,
(5) $H(G, x) = \frac{|V(G)|}{2} H(v, G, x)$,
(6) $H_t(G) = \frac{|V(G)|}{2} H_t(v, G)$,
(7) $RCW(G) = \frac{|V(G)|}{2} RCW(v, G)$,
(8) $\pi(G) = \sqrt{\pi^{|V(G)|}(v, G)}$,
(9) $\Pi(G) = \ln \sqrt{2\sqrt{\pi^{|V(G)|}(v, G)}}$.

In terms of Lemma 2.2, to calculate the distance-based topological indices of the molecular graph with transitive point group, we only need to choose any vertex $v \in V(G)$ and calculate the distances between v and $u \in V(G) - \{v\}$. Take a subgroup H of P_G, which is not necessarily transitive even if P_G is transitive. Now, the vertex set $V(G)$ can be divided into orbits of H such that $\Theta_1, \Theta_2, \cdots, \Theta_r$ with $|\Theta_1| \le |\Theta_2| \le \cdots |\Theta_r|$.

Theorem 2.3. *Let $v_i \in \Theta_i$, $i = 1, 2, \cdots, r$. Then,*

(1) $W_\lambda(v_1, G) = \frac{1}{|\Theta_1|} \sum_{u \in \Theta_1} \sum_{i=1}^{r} |\Theta_i| d^\lambda(u, v_i)$,
(2) $WW(v_1, G) = \frac{1}{|\Theta_1|} \sum_{u \in \Theta_1} \sum_{i=1}^{r} \frac{|\Theta_i|}{2} (d(u, v_i) + d^2(u, v_i))$,
(3) $WW_\lambda(v_1, G) = \frac{1}{|\Theta_1|} \sum_{u \in \Theta_1} \sum_{i=1}^{r} \frac{|\Theta_i|}{2} (d^\lambda(u, v_i) + d^{2\lambda}(u, v_i))$,
(4) $H(v_1, G) = \frac{1}{|\Theta_1|} \sum_{u \in \Theta_1} \sum_{i=1}^{r} \frac{|\Theta_i|}{d(u, v_i)}$,
(5) $H(v_1, G, x) = \frac{1}{|\Theta_1|} \sum_{u \in \Theta_1} \sum_{i=1}^{r} \frac{|\Theta_i|}{d(u, v_i)} x^{d(u, v_i)}$,
(6) $H_t(v_1, G) = \frac{1}{|\Theta_1|} \sum_{u \in \Theta_1} \sum_{i=1}^{r} \frac{|\Theta_i|}{d(u, v_i) + t}$,
(7) $RCW(v_1, G) = \frac{1}{|\Theta_1|} \sum_{u \in \Theta_1} \sum_{i=1}^{r} \frac{|\Theta_i|}{D(G) + 1 - d(u, v_i)}$.

Proof. Since P_G is transitive, we get

$$\begin{aligned} W_\lambda(v_1, G) &= \frac{1}{|\Theta_1|} \sum_{u \in \Theta_1} \sum_{z \in V(G)} d^\lambda(u, z) \\ &= \frac{1}{|\Theta_1|} \sum_{u \in \Theta_1} \sum_{i=1}^{r} \sum_{z \in \Theta_i} d^\lambda(u, z) \\ &= \frac{1}{|\Theta_1|} \sum_{i=1}^{r} \sum_{z \in \Theta_i} \sum_{u \in \Theta_1} d^\lambda(u, z). \end{aligned}$$

For any i and any $z \in \Theta_i$, there exist $h_i \in H$ satisfying $h_i(z) = v_i$. Therefore,

$$\sum_{z \in \Theta_i} \sum_{u \in \Theta_1} d^\lambda(u, z) = \sum_{z \in \Theta_i} \sum_{u \in \Theta_1} d^\lambda(h_i(u), h_i(z))$$

$$= \sum_{z\in\Theta_i}\sum_{h_i(u)\in\Theta_1} d^{\lambda}(h_i(u),v_i)$$
$$= |\Theta_i|\sum_{h_i(u)\in\Theta_1} d^{\lambda}(h_i(u),v_i)$$
$$= |\Theta_i|\sum_{v\in\Theta_1} d^{\lambda}(v,v_i).$$

Consequently, we yield

$$\begin{aligned} W_\lambda(v_1,G) &= \frac{1}{|\Theta_1|}\sum_{i=1}^{r}\sum_{u\in\Theta_1}\sum_{z\in\Theta_i} d^{\lambda}(u,z) \\ &= \frac{1}{|\Theta_1|}\sum_{i=1}^{r}|\Theta_i|\sum_{v\in\Theta_1} d^{\lambda}(v,v_i) \\ &= \frac{1}{|\Theta_1|}\sum_{v\in\Theta_1}\sum_{i=1}^{r}|\Theta_i| d^{\lambda}(v,v_i). \end{aligned}$$

The remaining parts follows similarly, hence, we complete the proof. □

In theorem 2.3, we can see that for a vertex $v_1 \in \Theta_1$, we do not need to compute all distances between v_1 and $V(G)-\{v_1\}$. It is enough to select one vertex from Θ_i. In real practice, we select a subgroup H so that Θ_1 is as small as possible in order to simplify the calculation. Specially, if $|\Theta_1| = 1$ (H fixes v_1), we only count $r-1$ times. Hence, we can give the following corollary.

Corollary 2.4. *Let $v_i \in \Theta_i$, $i = 1,2,\cdots,r$. Assume that $|\Theta_1| = 1$. We get*

(1) $W_\lambda(v_1,G) = \sum_{i=2}^{r}|\Theta_i| d^{\lambda}(v_1,v_i)$,
(2) $WW(v_1,G) = \sum_{i=2}^{r}|\Theta_i|\frac{d(v_1,v_i)+d^2(v_1,v_i)}{2}$,
(3) $WW_\lambda(v_1,G) = \sum_{i=2}^{r}|\Theta_i|\frac{d^{\lambda}(v_1,v_i)+d^{2\lambda}(v_1,v_i)}{2}$,
(4) $H(v_1,G) = \sum_{i=2}^{r}|\Theta_i|\frac{1}{d(v_1,v_i)}$,
(5) $H(v_1,G,x) = \sum_{i=2}^{r}|\Theta_i|\frac{1}{d(v_1,v_i)}x^{d(v_1,v_i)}$,
(6) $H_t(v_1,G) = \sum_{i=2}^{r}|\Theta_i|\frac{1}{d(v_1,v_i)+t}$,
(7) $RCW(v_1,G) = \sum_{i=2}^{r}|\Theta_i|\frac{1}{D(G)+1-d(v_1,v_i)}$,
(8) $\pi(v_1,G) = \prod_{i=2}^{r} d^{|\Theta_i|}(v_1,v_i)$,
(9) $\Pi(v_1,G) = \ln\sqrt{2\prod_{i=2}^{r} d^{|\Theta_i|}(v_1,v_i)}$.

In order to reduce the computation steps of the distance-based topological indices, note that a large number of the molecular structures have the layered structure such that the different orbits have consecutive distances from a fixed vertex. In such a situation, we have following theorem.

Theorem 2.5. *Assume that P_G is transitive and $H \trianglelefteq P_G$ is a subgroup with orbits $\Theta_1,\Theta_2,\cdots,\Theta_r$ such that $|\Theta_i| = 1$. Let $v_i \in \Theta_i$ for $i = 1,2,\cdots,r$. Then we have*

(1) $W_\lambda(G)=\frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|(j-1)^\lambda$,
(2) $WW(G)=\frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|\frac{j^2-j}{2}$,
(3) $WW_\lambda(G)=\frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|\frac{(j-1)^\lambda+(j-1)^{2\lambda}}{2}$,
(4) $H(G)=\frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|\frac{1}{j-1}$,
(5) $H(G,x)=\frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|\frac{1}{j-1}x^{j-1}$,
(6) $H_t(G)=\frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|\frac{1}{j+t-1}$,
(7) $RCW(G)=\frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|\frac{1}{D(G)+2-j}$,
(8) $\pi(G)=(\prod_{j=2}^{r}(j-1)^{|\Theta_{k_j}|})^{\frac{n}{2}}$,
(9) $\Pi(G)=\ln\sqrt{(\prod_{j=2}^{r}(j-1)^{|\Theta_{k_j}|})^{\frac{n}{2}}}$.

Proof. Science the molecular graphs are connected and all the elements in the same orbit have equal distances from v_1, the orbits saturate the vacancy between Θ_1 and Θ_k by means of their distances from v_1. Since only $r-1$ orbits different from Θ_1 and $d(v_1,v_k)\geq r-1$, we infer that the orbits run consecutively between Θ_1 and Θ_k, which reveals that the vertices $v_1,v_2,\cdots,v_r$ can be permuted into $v_{k_1},v_{k_2},\cdots,v_{k_r}$ with $k_1=1$ and $k_r=k$ satisfies $d(v_1,v_{k_j})=j-1$, $j=1,2,\cdots,r$. Therefore,

$$\begin{aligned}W_\lambda(G) &= \frac{n}{2}W_\lambda(v_1,G)\\ &= \frac{n}{2}\sum_{i=2}^{r}|\Theta_i|d^\lambda(v_1,v_i)\\ &= \frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|d^\lambda(v_1,v_{k_j})\\ &= \frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|(j-1)^\lambda.\end{aligned}$$

The remaining cases can be easily proved in similar fashion. □

3. Computation Examples

In this section, we give five illustrative examples to explain our method. In the following contexts, we always assume that n is the number of vertex in molecular graph G and the regular polyhedrons meet the conditions of the theorem 2.5.

Example 3.1 (Computation on tetrahedron)**.** The structure of tetrahedron (denoted by G_1) can refer to Figure 1. Let P_{G_1} be its point group. We need first determine the subgroup $R\trianglelefteq P_{G_1}$ of all the rotation in P_{G_1}. The elements consisting of R are as follows: (1) the identity; (2) rotations through the angle π about each of three axes joining the midpoints of opposite edges; (3) rotations through angles of $\frac{2\pi}{3}$ and $\frac{4\pi}{3}$ on the each of four axes joining vertices with centers of opposite faces. So, we have $|R|=12$. Clearly, R and P_{G_1} are transitive. Select

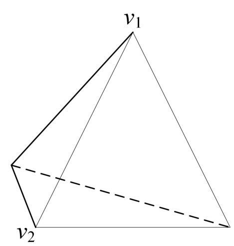

FIGURE 1. The structure of tetrahedron G_1

H as the identity plus the set of all rotations around the axis joining v_1 with the center of the opposite face through angles of $\frac{2\pi}{3}$ and $\frac{4\pi}{3}$ anticlockwise. We yield two orbits with representatives v_1, v_2 as presented in the Figure 1. Applying $|\Theta_i| = \frac{|P|}{|P_v|}$, we infer $|\Theta_1| = 1$, $|\Theta_2| = 3$. According to theorem 2.5, we get

(1) $W_\lambda(G_1) = \frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|(j-1)^\lambda = \frac{4}{2}\cdot 3 = 6$,
(2) $WW(G_1) = \frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|\frac{j^2-j}{2} = \frac{4}{2}\cdot 3\cdot\frac{1}{2}(1+1^2) = 6$,
(3) $WW_\lambda(G_1) = \frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|\frac{(j-1)^\lambda+(j-1)^{2\lambda}}{2} = \frac{4}{2}\cdot 3\cdot\frac{1}{2}(1^\lambda+1^{2\lambda}) = 6$,
(4) $H(G_1) = \frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|\frac{1}{j-1} = \frac{4}{2}\cdot 3 = 6$,
(5) $H(G_1,x) = \frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|\frac{1}{j-1}x^{j-1} = \frac{4}{2}\cdot 3\cdot x = 6x$,
(6) $H_t(G_1) = \frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|\frac{1}{j+t-1} = \frac{4}{2}\cdot 3\cdot\frac{1}{1+t} = \frac{6}{1+t}$,
(7) $RCW(G_1) = \frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|\frac{1}{D(G)+2-j} = \frac{4}{2}\cdot 3\cdot\frac{1}{1+1-1} = 6$,
(8) $\pi(G_1) = (\prod_{j=2}^{r}(j-1)^{|\Theta_{k_j}|})^{\frac{n}{2}} = 1$,
(9) $\Pi(G_1) = \ln\sqrt{(\prod_{j=2}^{r}(j-1)^{|\Theta_{k_j}|})^{\frac{n}{2}}} = \ln\sqrt{2}$.

Example 3.2 (Computation on cube)**.** The structure of cube (denoted as G_2) can refer to Figure 2. In this case, the subgroup $R \trianglelefteq P_{G_2}$ of all the rotations consists of the follows: (1) rotations through the angle π on each of six axes joining midpoints of diagonally opposite edges; (2) rotations through angles of $\frac{\pi}{2}$ and $\frac{3\pi}{2}$ about each of four axes joining extreme opposite vertices; (3) rotations through angles of $\frac{\pi}{2}, \pi$, and $\frac{3\pi}{2}$ about each of three axes joining the centers of opposite faces. Thus, by simple computation, we get $|R| = 24$. Clearly, R and P_{G_2} are both transitive. H is selected as in the first instance but the rotations are around the axis joining the two opposite vertices v_1 and v_3. We get four orbits with representatives v_1, v_2, v_3 and v_4 as presented in the Figure 2. In view of $|\Theta_i| = \frac{|P|}{|P_v|}$, we yield $|\Theta_1| = |\Theta_4| = 1$, $|\Theta_2| = |\Theta_3| = 3$. Applying theorem 2.5, we get

(1) $W_\lambda(G_2) = \frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|(j-1)^\lambda = \frac{8}{2}(3+3\cdot 2^\lambda+3^\lambda) = 12+12\cdot 2^\lambda+4\cdot 3^\lambda$,
(2) $WW(G_2) = \frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|\frac{j^2-j}{2} = \frac{8}{2}(\frac{3}{2}(1+1)+\frac{3}{2}(2+4)+\frac{3+9}{2}) = 72$,

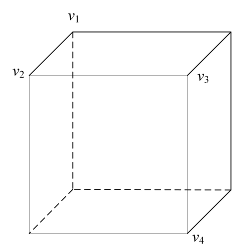

FIGURE 2. The structure of cube G_2

(3) $WW_\lambda(G_2) = \frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|\frac{(j-1)^\lambda+(j-1)^{2\lambda}}{2} = \frac{8}{2}(\frac{3}{2}(1+1)+\frac{3}{2}(2^\lambda+4^\lambda)+\frac{3^\lambda+9^\lambda}{2}) = 12+6(2^\lambda+4^\lambda)+2(3^\lambda+9^\lambda)$,
(4) $H(G_2) = \frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|\frac{1}{j-1} = \frac{8}{2}(3+\frac{3}{2}+\frac{1}{3}) = \frac{58}{3}$,
(5) $H(G_2,x) = \frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|\frac{1}{j-1}x^{j-1} = \frac{8}{2}(3x+\frac{3}{2}x^2+\frac{1}{3}x^3) = 12x+6x^2+\frac{4}{3}x^3$,
(6) $H_t(G_2) = \frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|\frac{1}{j+t-1} = 4(\frac{3}{1+t}+\frac{3}{2+t}+\frac{1}{3+t})$,
(7) $RCW(G_2) = \frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|\frac{1}{D(G)+2-j} = \frac{8}{2}(\frac{3}{3}+\frac{3}{2}+\frac{1}{1}) = 14$,
(8) $\pi(G_2) = (\prod_{j=2}^{r}(j-1)^{|\Theta_{k_j}|})^{\frac{n}{2}} = (1^3\cdot 2^3\cdot 3)^{\frac{8}{2}} = 331776$,
(9) $\Pi(G_2) = \ln\sqrt{(\prod_{j=2}^{r}(j-1)^{|\Theta_{k_j}|})^{\frac{n}{2}}} = \ln 576\sqrt{2}$.

Example 3.3 (Computation on octahedron)**.** The structure of octahedron (denoted by G_3) can refer to Figure 3. Obviously, we can get the octahedron by adding the midpoints of adjacent faces of the cube with edges. Form this point of view, its point group is the same as that of the cube. Furthermore, P_{G_3} is

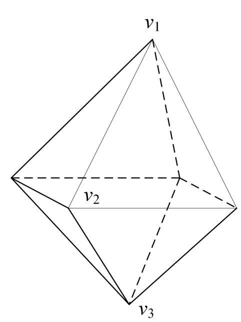

FIGURE 3. The structure of octahedron G_3

transitive, and all the rotations can be selected around the axis joining v_1 and

v_3 which keep the octahedron invariant. Three orbits are obtained with representatives v_i, $i = 1, 2, 3$ as depicted in the Figure 3 and $|\Theta_1| = |\Theta_3| = 1$ and $|\Theta_2| = 4$. By theorem 2.5, we get

(1) $W_\lambda(G_3) = 12 + 3 \cdot 2^\lambda$,
(2) $WW(G_3) = 21$,
(3) $WW_\lambda(G_3) = 12 + \frac{3}{2}(2^\lambda + 4^\lambda)$,
(4) $H(G_3) = \frac{27}{2}$,
(5) $H(G_3, x) = 12x + 3x^2$,
(6) $H_t(G_3) = \frac{12}{1+t} + \frac{3}{2+t}$,
(7) $RCW(G_3) = 9$,
(8) $\pi(G_3) = 8$,
(9) $\Pi(G_3) = \ln 4$.

Example 3.4 (Computation on icosahedron)**.** The structure of icosahedron (denoted by G_4) can refer to Figure 4. The rotation subgroup R of the point group consists: (1)the identity; (2) rotations through the angle π about each of fifteen axes joining midpoints of opposite edges; (3) rotations through angles of $\frac{2\pi}{3}$ and $\frac{4\pi}{3}$ about each of ten axes joining centers of opposite faces; (4) rotations through angles of $\frac{2\pi}{5}, \frac{4\pi}{5}, \frac{6\pi}{5}$, and $\frac{8\pi}{5}$ about each of six axes joining extreme opposite vertices. Therefore, we have $|R| = 60$. Furthermore, R and P_{G_4} are

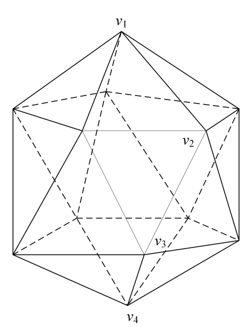

FIGURE 4. The structure of icosahedron G_4

transitive. H can be selected as the group generated by the $\frac{2\pi}{5}$-rotation around the axis joining v_1 and v_4. There are four orbits with representatives as shown in the Figure 4 and by $|\Theta_i| = \frac{|P|}{|P_v|}$ we get $|\Theta_1| = |\Theta_4| = 1$, $|\Theta_2| = |\Theta_3| = 5$. Applying theorem 2.5, we get

(1) $W_\lambda(G_4) = \frac{n}{2}\sum_{j=2}^{r} |\Theta_{k_j}|(j-1)^\lambda = \frac{12}{2}(5+5\cdot 2^\lambda+3^\lambda) = 30+30\cdot 2^\lambda+6\cdot 3^\lambda$,
(2) $WW(G_4) = \frac{n}{2}\sum_{j=2}^{r} |\Theta_{k_j}|\frac{j^2-j}{2} = \frac{12}{2}(\frac{5}{2}(1+1) + \frac{5}{2}(2+4) + \frac{3+9}{2}) = 156$,
(3) $WW_\lambda(G_4) = \frac{n}{2}\sum_{j=2}^{r} |\Theta_{k_j}|\frac{(j-1)^\lambda+(j-1)^{2\lambda}}{2} = \frac{12}{2}(\frac{5}{2}(1+1) + \frac{5}{2}(2^\lambda + 4^\lambda) + \frac{3^\lambda+9^\lambda}{2}) = 30 + 15(2^\lambda + 4^\lambda) + 3(3^\lambda + 9^\lambda)$,

(4) $H(G_4) = \frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|\frac{1}{j-1} = \frac{12}{2}(5+\frac{5}{2}+\frac{1}{3}) = 47$,
(5) $H(G_4,x) = \frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|\frac{1}{j-1}x^{j-1} = \frac{12}{2}(5x+\frac{5}{2}x^2+\frac{1}{3}x^3) = 30x+15x^2+2x^3$,
(6) $H_t(G_4) = \frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|\frac{1}{j+t-1} = 6(\frac{5}{1+t}+\frac{5}{2+t}+\frac{1}{3+t})$,
(7) $RCW(G_4) = \frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|\frac{1}{D(G)+2-j} = \frac{12}{2}(\frac{5}{3}+\frac{5}{2}+\frac{1}{1}) = 31$,
(8) $\pi(G_4) = (\prod_{j=2}^{r}(j-1)^{|\Theta_{k_j}|})^{\frac{n}{2}} = (1^5\cdot 2^5\cdot 3)^{\frac{12}{2}} = 96^6$,
(9) $\Pi(G_4) = \ln\sqrt{(\prod_{j=2}^{r}(j-1)^{|\Theta_{k_j}|})^{\frac{n}{2}}} = \ln 96^3\sqrt{2}$.

Example 3.5 (Computation on dodecahedron)**.** The structure of dodecahedron (denoted by G_5) can refer to Figure 5. Similar as we discussed in the above examples, one can see that the dodecahedron and icosahedron have the same point group. Hence, H can be selected to be the group generated by the $\frac{2\pi}{3}$-rotation around the axis joining v_1 and v_6, and the reflection with respect to the plane containing v_1, v_2 and v_6. There are six orbits with representatives

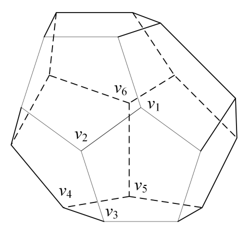

FIGURE 5. The structure of dodecahedron G_5

v_i, $i = 1, 2, \cdots, 6$ as shown in the Figure 5. By simple computation, we get $|\Theta_1| = |\Theta_6| = 1$, $|\Theta_2| = |\Theta_5| = 3$ and $|\Theta_3| = |\Theta_4| = 6$. Thus, in terms of Theorem 2.5, we get

(1) $W_\lambda(G_5) = \frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|(j-1)^\lambda = \frac{20}{2}(3+6\cdot 2^\lambda+6\cdot 3^\lambda+3\cdot 4^\lambda+5^\lambda) = 30+60\cdot 2^\lambda+60\cdot 3^\lambda+30\cdot 4^\lambda+10\cdot 5^\lambda$,
(2) $WW(G_5) = \frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|\frac{j^2-j}{2} = \frac{20}{2}(\frac{3}{2}(1+1)+3(2+4)+3(3+9)+\frac{3}{2}(4+16)+\frac{1}{2}(5+25)) = 1020$,
(3) $WW_\lambda(G_5) = \frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|\frac{(j-1)^\lambda+(j-1)^{2\lambda}}{2} = \frac{20}{2}(\frac{3}{2}(1+1)+3(2^\lambda+4^\lambda)+3(3^\lambda+9^\lambda)+\frac{3}{2}(4^\lambda+16^\lambda)+\frac{1}{2}(5^\lambda+25^\lambda)) = 30+30(2^\lambda+4^\lambda)+30(3^\lambda+9^\lambda)+15(4^\lambda+16^\lambda)+5(5^\lambda+25^\lambda)$,
(4) $H(G_5) = \frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|\frac{1}{j-1} = \frac{20}{2}(3+\frac{6}{2}+\frac{6}{3}+\frac{3}{4}+\frac{1}{5}) = \frac{179}{2}$,
(5) $H(G_5,x) = \frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|\frac{1}{j-1}x^{j-1} = \frac{20}{2}(3x+\frac{6}{2}x^2+\frac{6}{3}x^3+\frac{3}{4}x^4+\frac{1}{5}x^5) = 30x+30x^2+20x^3+\frac{15}{2}x^4+2x^5$,
(6) $H_t(G_5) = \frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|\frac{1}{j+t-1} = \frac{20}{2}(\frac{3}{1+t}+\frac{6}{2+t}+\frac{6}{3+t}+\frac{3}{4+t}+\frac{1}{5+t}) = \frac{30}{1+t}+\frac{60}{2+t}+\frac{60}{3+t}+\frac{30}{4+t}+\frac{10}{5+t}$,
(7) $RCW(G_5) = \frac{n}{2}\sum_{j=2}^{r}|\Theta_{k_j}|\frac{1}{D(G)+2-j} = \frac{20}{2}(\frac{3}{5}+\frac{6}{4}+\frac{6}{3}+\frac{3}{2}+\frac{1}{1}) = 66$,

(8) $\pi(G_5) = (\prod_{j=2}^{r}(j-1)^{|\Theta_{k_j}|})^{\frac{n}{2}} = (2^6 3^6 4^3 5)^{10}$,

(9) $\Pi(G_5) = \ln\sqrt{(\prod_{j=2}^{r}(j-1)^{|\Theta_{k_j}|})^{\frac{n}{2}}} = \ln\sqrt{2^{61}3^{60}4^{30}5^{10}}$.

4. Conclusion

In this paper, we mainly report the approach on how to use group theory to determine the distance-based topological indices for certain important symmetry chemical structures. Since these Wiener related and other distance-based topological indices are widely applied in the analysis of both the boiling point and melting point of chemical compounds and QSPR/QSAR study, the promising prospects of their application for the chemical, medical and pharmacy engineering will be illustrated in the theoretical conclusion that is obtained in this article.

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Competing Interests

The author(s) do not have any competing interests in the manuscript.

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