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Reciprocal Degree Distance of Circumcoronene

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Abstract: Chemical compounds and drugs are often modeled as graphs where each vertex represents an atom of molecule and covalent bounds between atoms are represented by edges between the corresponding vertices. This graph derived from a chemical compounds is called its molecular graph. The reciprocal degree distance defined over this molecular graph has been shown to be strongly correlated to properties of the compounds. In this article, by virtue of molecular structural analysis, the reciprocal degree distance of H_3 is reported. The theoretical results achieved in this article illustrate the promising prospects of the application for the chemical and pharmacy engineering.

Keywords: Theoretical chemistry, reciprocal degree distance, circumcoronene

I. INTRODUCTION

Investigations of degree or distance based topological indices have been conducted over 35 years. Topological indices are numerical parameters of molecular graph, and play significant roles in physics, chemistry and pharmacology science. For example, the reciprocal degree distance reflect the oxidizing property of chemical compounds.

Specifically, let G be a molecular graph, then a topological index can be regarded as a score function f: $G \to \square^+$, with this property that f(G1) = f(G2) if G1 and G2 are isomorphic. As numerical descriptors of the molecular structure obtained from the corresponding molecular graph, topological indices have found several applications in theoretical chemistry, especially in QSPR/QSAR study. For instance, Wiener index, Zagreb index, harmonic index and sum connectivity index are introduced to reflect certain structural features of organic molecules. Several papers contributed to determine these distance-based indices of special molecular graph (See Yan et al., [1, 2], Gao et al., [3, 4], Gao and Shi [5], Gao and Wang [6], Xi and Gao [7, 8], Xi et al., [9], Gao et al., [10] for more detail). The notation and terminology used but undefined in this paper can be found in [11].

The graphs considered in this paper are simple and connected. The vertex and edge sets of G are denoted by V(G) and E(G), respectively. The reciprocal degree distance (also called additively weighted Harary index) of molecular graph G is defined as:

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

This index has been shown to be strongly correlated to oxidizing properties of the compounds.

As the generalizations of benzene molecule C_6, circumcoronene homologous series of benzenoid is a class of molecular structures. In this paper, we discuss the base member of this family which is planar of benzene. The first three molecular structures (H_1, H_2, and H_3) of this series of Benzenoid are presented in Figure 1.

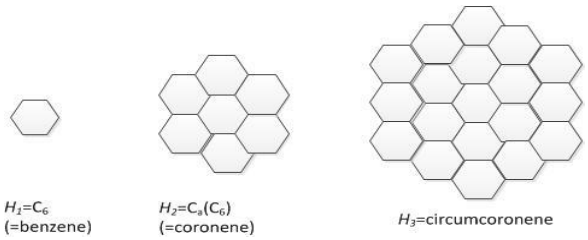

Figure 1. The first, second and third molecular graphs H_1, H_2 and H_3 from the circumcoronene series of benzenoid.

As presented in Figures 1 and 2, the first terms of this series are H_1 =benzene, H_2 =coronene, H_3 =circumcoronene, H_4 =circumcircumcoronene, and the circumcoronene homologous series of benzenoid is just family of molecular graph consist several copy of benzene C_6 on circumference.

For a planar molecular graph, a mapping is just a new drawing on the plane. The Capra operation is

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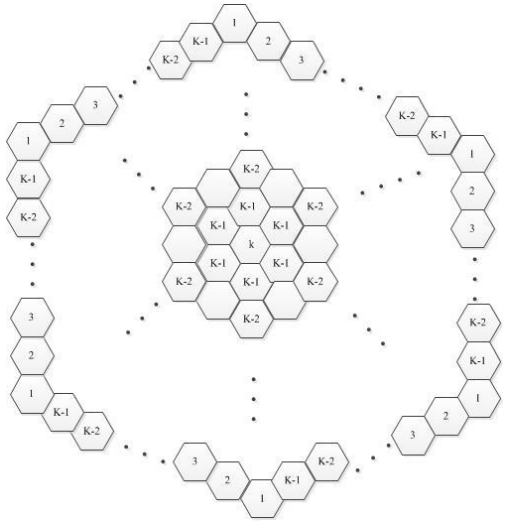

Figure 2. The circumcoronene series of benzenoid H_k for $k \geq 1$.

used to construct a new structure of a planar molecular graph. For a cyclic planar molecular graph *G*, the Capra map operation is obtained as follows:

(i) insert two vertices on each edge of *G*;

(ii) add pendant vertices to the above inserted ones and

(iii) connect the pendant vertices in order (-1,+3) around the boundary of a face of *G*. In terms of running these steps for each cycle of *G*, the Capra-transform of *G*, $Ca(G)$ is achieved.

Hence, the benzenoid series (see Figures 3 and 4) can be designed in view of iterating the Capra-operation on the hexagon (i.e. benzene molecular graph C_6) and its Ca-transforms. In what follows, the Capra operation is denoted by Ca. Thus, Capra operation of arbitrary molecular graph *G* is $Ca(G)$, and we use $CaCa(G)$ (or $Ca_2(G)$) to express the iteration of Capra operation.

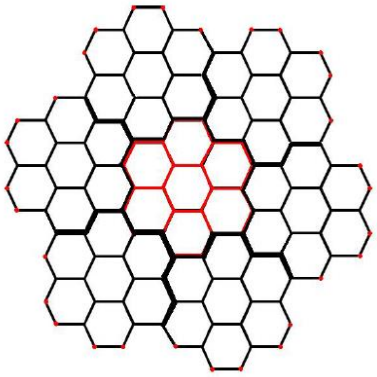

Figure 3. The structure of $Ca_2(C_6)$.

Although there have been several advances in Wiener index, Zagreb index, PI index, hyper-Wiener index and sum connectivity index of molecular

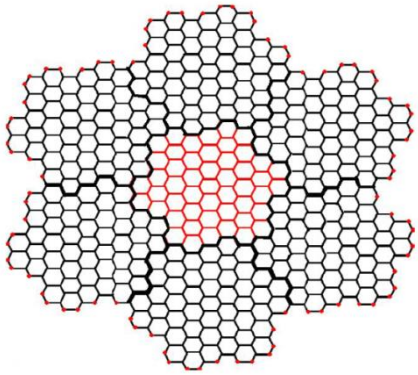

Figure 4. The structure of $Ca_3(C_6)$.

graphs, and sum connectivity index of molecular graphs, the study of reciprocal degree distance for special chemical structures has been largely limited. In addition, as widespread and critical chemical structures, Capra-designed planar benzenoids are widely used in medical science and pharmaceutical field. As an example, circumcoronene is one of the basic chemical structures and exists widely in benzene and alkali molecular structures. For these reasons, we have attracted tremendous academic and industrial interests to research the reciprocal degree distance of this molecular structure from a mathematical point of view.

The contribution of this paper is to determine the reciprocal degree distance of H_3.

II. Main Results and Proof

In this section, we consider the reciprocal degree distance of circumcoronene $= H_3$. We present the main results below.

A. *Theorem 1.*

Let $G = H_3$ be the circumcoronene. Then the reciprocal degree distance of *G* is equal to:

$$RDD(G) = 1962\frac{12539}{13860}.$$

Before proving Theorem 1, we first introduce some notations, related to Figure 5.

Suppose $\mathbb{Z}_6 = \{0,1,2,3,4,5\}$ is the cycle finite group of order 6 (it can be regarded as the integer number of module 6). Let $V(G)$ be the vertex set of $G = H_3$ with $|V(H_3)| = 54$ and $E(G)$ the edge set with $|E(H_3)| = 72$. We show each vertex of H_3 by automorphism *f* (*f* is bijection), such that:

$$f: V(G) \to \{u_i, v_i, x_i, y_i, z_i, t_i, a_i, b_i, c_i \mid i \in \mathbb{Z}_6\},$$

and

$$f: E(G) \to \begin{matrix}\{v_iv_{i+1}, v_iu_i, u_ix_i, u_iy_i, x_iy_{i+1}, x_iz_i, y_it_i,\\ z_ia_i, z_ic_i, t_ib_i, t_ic_i, a_ib_{i+1} \mid i \in \mathbb{Z}_6\}\end{matrix}$$

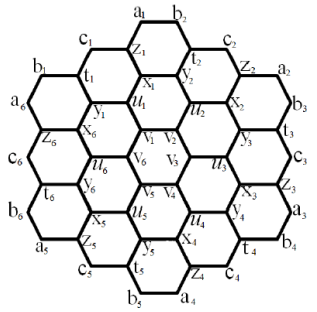

Figure 5. H_3 and the notations used in the article.

In terms of the Figure 5, we verify the degree of vertices $u_i, v_i, x_i, y_i, z_i, t_i$ is 3 and the degree of vertices a_i, b_i, c_i is 2, for all $i \in \mathbb{Z}_6$. Let $d(u,v)=i$ is distance between vertices *u* and *v* of *G*. Then,

$$D_i(d_1,d_2) = \begin{matrix}\{(u,v) \mid u,v \in V(G), d(u,v) \\ = i, d_1 = d(u) \text{ and } d_2 = d(v)\}\end{matrix}$$

is the set of dual (u,v) of vertex set *V*(*G*).

Clearly, if $G= H_3$, let

$$D_i = \{(u,v) \mid u,v \in V(H_3), d(u,v) = i\}$$

$$= D_i(3,3) \cup D_i(3,2) \cup D_i(2,2).$$

B. *Proof of Theorem 1.*

Let $G= H_3$ be the second member of circumcoronene series of benzenoid. It exists 54 different vertices and 1431 different shortest paths between vertices *u* and *v* of H_3. Furthermore, there are distances from 1 to 11, for each pair of vertices $u,v \in V(G)$. That is to say,

$$\forall \ \ u,v \in V(G), \ \ \exists d(u,v) \in \{1,2,\cdots,11\}.$$

Thus, we split following seven situations for our proving.

Case 1.

If $d(u,v)$=1, then $D_1 = |E(G)|$. Hence, we have three subcase of this situation.

Subcase1.1

$$D_1(3,3) = \begin{matrix}\{(v_i,v_{i+1}),(v_i,u_i),(u_i,x_i),(u_i,y_i), \\ (x_i,y_{i+1}),(x_i,z_i),(y_i,t_i) \mid i \in \mathbb{Z}_6\}\end{matrix}.$$

Hence, $|D_1(3,3)|$=42. Therefore, this part contribute total 252 of the reciprocal degree distance.

Subcase1.2

$$D_1(3,2) = \{(z_i,a_i),(z_i,c_i),(t_i,b_i),(t_i,c_i) \mid i \in \mathbb{Z}_6\}.$$

Hence, $|D_1(3,2)|$=24. Therefore, this part contribute total 120 of the reciprocal degree distance.

Subcase 1.3

$$D_1(2,2) = \{(a_i,b_{i+1}) \mid i \in \mathbb{Z}_6\}.$$

Therefore, this part contribute total 24 of the reciprocal degree distance.

In general, case 1 contribute total 396 for the reciprocal degree distance.

Now, we list all existent sets $D_d(d_1,d_2)$, $\forall i \in \mathbb{Z}_6$, *d*=2,⋯,11 and d_1, d_2 =2 or 3, as follows:

Case2.

$$D_2(3,3) = \begin{matrix}\{(v_i,v_{i+2}),(v_i,u_{i+1}),(v_i,u_{i-1}),(v_i,x_i),(v_i,y_i), \\ (u_i,x_{i-1}),(u_i,y_{i+1}),(u_i,z_i),(u_i,t_i),(x_i,y_i), \\ (x_i,t_{i+1}),(y_i,z_{i-1}),(z_i,t_i) \mid i \in \mathbb{Z}_6\}.\end{matrix}$$

$$D_2(3,2) = \begin{matrix}\{(x_i,a_i),(x_i,c_i),(y_i,b_i),(y_i,c_i), \\ (z_i,b_{i+1}),(t_i,a_{i-1}) \mid i \in \mathbb{Z}_6\}\end{matrix}$$

$$D_2(2,2) = \{(a_i,c_i),(b_i,c_i) \mid i \in \mathbb{Z}_6\}.$$

Case3.

$$D_3(3,3) = \begin{matrix}\{(v_i,v_{i+3}),(v_i,u_{i+2}),(v_i,u_{i-2}),(v_i,x_{i-1}),(v_i,y_{i-1}), \\ (v_i,x_{i+1}),(v_i,y_{i+1}),(v_i,z_i),(v_i,t_i),(u_i,u_{i+1}), \\ (u_i,t_{i+1}),(u_i,z_{i-1}),(y_i,z_i),(y_i,y_{i+1}),(x_i,x_{i+1}),(x_i,t_i),(z_i,t_{i+1}) \mid i \in \mathbb{Z}_6\}.\end{matrix}$$

$$D_3(3,2) = \begin{matrix}\{(u_i,a_i),(u_i,b_i),(u_i,c_i),(x_i,b_{i+1}),(x_i,c_{i+1}), \\ (y_i,a_{i-1}),(y_i,c_{i-1}),(z_i,b_i),(t_i,a_i) \mid i \in \mathbb{Z}_6\}\end{matrix}.$$

$$D_3(2,2) = \{(a_i,c_{i+1}),(b_i,c_{i-1}) \mid i \in \mathbb{Z}_6\}.$$

Case4.

$$D_4(3,3) = \begin{matrix}\{(v_i,u_{i+3}),(v_i,x_{i+2}),(v_i,x_{i-2}),(v_i,y_{i+2}),(v_i,y_{i-2}), \\ (v_i,t_{i+1}),(v_i,z_{i+1}),(v_i,t_{i-1}),(v_i,z_{i-1}),(u_i,u_{i+2}), \\ (u_i,x_{i+1}),(u_i,y_{i-1}),(x_i,y_{i+2}),(x_i,z_{i-1}),(x_i,z_{i+1}),(y_i,t_{i-1}),(y_i,t_{i+1}) \mid i \in \mathbb{Z}_6\}.\end{matrix}$$

$$D_4(3,2) = \begin{matrix}\{(v_i,a_i),(v_i,b_i),(v_i,c_i),(u_i,b_{i+1}),(u_i,c_{i+1}),(u_i,a_{i-1}), \\ (u_i,c_{i-1}),(x_i,b_i),(y_i,a_i),(t_i,b_{i+1}),(t_i,c_{i-1}), \\ (z_i,a_{i-1}),(z_i,c_{i+1}) \mid i \in \mathbb{Z}_6\}.\end{matrix}$$

$$D_4(2,2) = \{(a_i,b_i) \mid i \in \mathbb{Z}_6\}.$$

Case5.

$$D_5(3,3) = \begin{matrix}\{(v_i,y_{i+3}),(v_i,x_{i+3}),(v_i,t_{i+2}),(v_i,t_{i-2}),(v_i,z_{i+2}), \\ (v_i,z_{i-2}),(u_i,u_{i+3}),(u_i,x_{i+2}),(u_i,x_{i-2}),(u_i,y_{i+2}), \\ (u_i,y_{i-2}),(u_i,z_{i+1}),(u_i,t_{i-1}),(x_i,y_{i-1}),(x_i,t_{i+2}), \\ (t_i,t_{i+1}),(z_i,z_{i+1}),(y_i,z_{i-2}) \mid i \in \mathbb{Z}_6\}\end{matrix}$$

$$D_5(3,2) = \begin{matrix}\{(v_i,a_{i+1}),(v_i,b_{i+1}),(v_i,c_{i+1}),(v_i,a_{i-1}),(v_i,b_{i-1}), \\ (v_i,c_{i-1}),(x_i,a_{i+1}),(x_i,a_{i-1}),(x_i,c_{i-1}),(y_i,b_{i+1}), \\ (y_i,b_{i-1}),(y_i,c_{i+1}) \mid i \in \mathbb{Z}_6\}.\end{matrix}$$

$$D_5(2,2) = \{(a_i,a_{i+1}),(b_i,b_{i+1}),(c_i,c_{i+1}) \mid i \in \mathbb{Z}_6\}.$$

Case6.

$$D_6(3,3)=\begin{matrix}\{(v_i,t_{i+3}),(v_i,z_{i+3}),(v_i,y_{i+3}),(u_i,x_{i+3}),(u_i,t_{i+2}),\\(u_i,t_{i-2}),(u_i,z_{i+2}),(u_i,z_{i-2}),(x_i,x_{i+2}),(x_i,y_{i-2}),\end{matrix}$$

$$(x_i,t_{i-1}),(y_i,y_{i+2}),(y_i,z_{i+1}),(z_i,t_{i+2})\mid i\in\square_6\}.$$

$$D_6(3,2)=\begin{matrix}\{(v_i,a_{i+2}),(v_i,b_{i+2}),(v_i,c_{i+2}),(v_i,a_{i-2}),(v_i,b_{i-2}),\\(v_i,c_{i-2}),(u_i,a_{i-1}),(u_i,b_{i+1}),(x_i,b_{i+2}),(x_i,c_{i+2}),\end{matrix}$$

$$(y_i,a_{i-2}),(y_i,c_{i-2}),(z_i,c_{i-1}),(z_i,a_{i+1}),(t_i,b_{i-1}),(t_i,c_{i+1})\mid i\in\square_6\}$$

$$D_6(2,2)=\{(a_i,b_{i+2})\mid i\in\square_6\}.$$

Case7.

$$D_7(3,3)=\begin{matrix}\{(u_i,t_{i+3}),(u_i,z_{i+3}),(x_i,x_{i+3}),(x_i,y_{i+3}),(x_i,z_{i+2}),\\(x_i,z_{i-2}),(x_i,t_{i-2}),(y_i,y_{i+3}),(y_i,t_{i+2}),(y_i,t_{i-2}),\end{matrix}$$

$$(y_i,z_{i+2}),(z_i,t_{i-1})\mid i\in\square_6\}.$$

$$D_7(3,2)=\begin{matrix}\{(v_i,a_{i+3}),(v_i,b_{i+3}),(v_i,c_{i+3}),(u_i,a_{i+2}),(u_i,b_{i+2}),\\(u_i,c_{i+2}),(u_i,a_{i-2}),(u_i,b_{i-2}),(u_i,c_{i-2}),(x_i,b_{i-1}),\end{matrix}$$

$$(y_i,a_{i+1}),(y_i,b_{i-2}),(z_i,c_{i+1}),(z_i,a_{i-2}),(t_i,c_{i-2})\mid i\in\square_6\}$$

$$D_7(2,2)=\{(a_i,c_{i-1}),(b_i,c_{i+1})\mid i\in\square_6\}.$$

Case8.

$$D_8(3,3)=\begin{matrix}\{(x_i,t_{i+3}),(x_i,z_{i+3}),(y_i,t_{i+3}),(y_i,z_{i+3}),\\(z_i,z_{i+2}),(z_i,t_{i-2}),(t_i,t_{i+2})\mid i\in\square_6\}\end{matrix}$$

$$D_8(3,2)=\begin{matrix}\{(u_i,a_{i+3}),(u_i,b_{i+3}),(u_i,c_{i+3}),(x_i,a_{i+2}),(x_i,a_{i-1}),\\(x_i,b_{i-1}),(x_i,c_{i-1}),(y_i,a_{i+2}),(y_i,b_{i+2}),(y_i,b_{i-1}),\end{matrix}$$

$$(y_i,c_{i+2}),(z_i,b_{i-1}),(t_i,a_{i+1})\mid i\in\square_6\}.$$

$$D_8(2,2)=\{(a_i,c_{i+2}),(b_i,c_{i-2}),(c_i,c_{i+2})\mid i\in\square_6\}.$$

Case 9.

$$D_9(3,3)=\{(z_i,z_{i+3}),(z_i,t_{i+3}),(t_i,t_{i+3})\mid i\in\square_6\}.$$

$$D_9(3,2)=\begin{matrix}\{(x_i,a_{i+3}),(x_i,b_{i+3}),(x_i,c_{i+3}),(y_i,a_{i+3}),(y_i,b_{i+3}),\\(y_i,c_{i+3}),(z_i,a_{i+2}),(z_i,a_{i-2}),(z_i,b_{i-2}),(z_i,c_{i-2}),\end{matrix}$$

$$(t_i,a_{i+2}),(t_i,b_{i+2}),(t_i,b_{i-2}),(t_i,c_{i+2})\mid i\in\square_6\}.$$

$$D_9(2,2)=\{(a_i,b_{i-1})\mid i\in\square_6\}.$$

Case10.

$$D_{10}(3,2)=\begin{matrix}\{(z_i,a_{i+3}),(z_i,b_{i+3}),(z_i,c_{i+3}),(t_i,a_{i+3}),\\(t_i,b_{i+3}),(t_i,c_{i+3})\mid i\in\square_6\}\end{matrix}$$

$$D_{10}(2,2)=\{(a_i,a_{i+2}),(a_i,b_{i-2}),(a_i,c_{i-2}),(b_i,b_{i+2}),$$

$$(b_i,c_{i+2})\mid i\in\square_6\}$$

Case11.

$$D_{11}=\begin{matrix}\{(a_i,a_{i+3}),(a_i,b_{i+3}),(a_i,c_{i+3}),(b_i,b_{i+3}),\\(b_i,c_{i+3}),(c_i,c_{i+3})\mid i\in\square_6\}\end{matrix}$$

By our analysis in Case 1-11, we infer

$$RDD(G)=396+\frac{696}{2}+\frac{912}{3}+\frac{1026}{4}+\frac{1062}{5}+\frac{1008}{6}+\frac{894}{7}$$
$$+\frac{714}{8}+\frac{515}{9}+\frac{300}{10}+\frac{108}{11}=1962\frac{12539}{13860}$$

III. CONCLUSIONS

In our article, by virtue of the molecular graph structural analysis and mathematical derivation, we mainly report reciprocal degree distance of H_3. As the reciprocal degree distance is widely used in the analysis of oxidation procedure for chemical compounds, the theoretical conclusion obtained in this article illustrates the promising prospects of the application for the chemical and pharmacy engineering.

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