Molecular Descriptors and Topological Analysis of Cyclooctane Derivatives

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Abstract. Cyclooctane is mainly used in the synthesis of cyclooctanone, cyclooctanol, caprolactam and octanoic acid. At the same time, it can also be used as an intermediate in organic synthesis and a chemical reagent. By discussing the resistance distance between any two points of cyclooctane derivative $T_n(C_8)$, some invariants about resistance distance are obtained, such as Kirchhoff index, multiplicative degree-Kirchhoff index, and additive degree-Kirchhoff index. Topological index can help scholars better understand some physical and chemical properties of compounds, and we obtain the closed expressions of valency-based topological indices for $T_n(C_8)$, such as ABC index, GA index, etc.

Keywords: Valency-based topological index, Resistance distance, Kirchhoff index, (multiplicative /additive)Degree-Kirchhoff index.

1. Introduction

Topological descriptor is a numerical constant related to the composition of chemical structure, physical properties, chemical reactions and other biological activities. $QSAR$ model is a regression or classification model, which is often used in chemistry and control system engineering. Historically, $QSAR$ model was first used to predict the boiling point of compounds. In organic chemistry, we view atoms as vertices and covalent bonds between atoms as edges. Chemical graph theory is a topological branch of mathematical chemistry. Graph theory is usually applied to the mathematical modeling of chemical phenomena. Suppose the graph G is a simple connected graph. Vertex set and edge set are $V(G)$ and $E(G)$, respectively. If there is an edge between two vertices $i,\ j$, we say it is adjacent, and this edge is represented as ij. Take $|V(G)| = n,\ |E(G)| = m$, and let d_i be recorded as the degree of vertex i. For terms in the text, please refer to [1]. The shortest length of path between vertices $i\ and\ j$ is recorded as $d(i, j)$ [2] in the graph G. If each side of the graph G is replaced by unit resistor, then simple graph G can be transformed into a circuit diagram in physics. Using Ohm's law, and the Kirchhoff's law, the resistance distance between any two vertices can be obtained. The resistance distance between any two vertices i and j is defined as r_{ij}, also called effective resistance [3]. It is a tool to measure distance driven by point network and chemical Applications. It has been proved to be of significant help in the study of graph structure and chemistry. It has been proved to be of significant help in the study of graph structure and chemistry.

The specific expression of Kirchhoff index $Kf(G)$ [3]is

$$Kf(G) = \frac{1}{2} \sum_{i,j \in V(G)} r_{ij}.$$

The Kirchhoff index is a relatively successful topological descriptor. For its specific applications, you can refer to [4–7].

Chen and Zhang [8] proposed multiplicative degree-Kirchhoff index,

$$Kf^*(G) = \sum_{i,j \in V(G)} d_i \cdot d_j r_{ij}.$$

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The additive degree-Kirchhoff index [9] is proposed by *Gutman* and recorded as

$$Kf^{+}(G) = \sum_{i,j \in V(G)} (d_i + d_j) r_{ij}.$$

From the definitions of Kirchhoff index, multiplicative degree-Kirchhoff index, and additive degree-Kirchhoff index, it can be seen that these three invariants are all functions of resistance distance r_{ij}. For their applications in other aspects, please refer to [10–15].

In addition to the Kirchhoff index, there are other successful indices. These indices are about valency-based topological indices. The geometric-arithmetic index $GA(G)$ [16] is defined as

$$GA(G) = \sum_{ij \in E(G)} \frac{2\sqrt{d_i \cdot d_j}}{d_i + d_j}.$$

Gutman puts forward the second multiplication Zagreb index [17], and the expression is

$$\pi_2(G) = \prod_{ij \in E(G)} d_i \cdot d_j.$$

The atom-bond connectivity index was proposed by Estrada [18] and defined as

$$ABC(G) = \sum_{ij \in E(G)} \sqrt{\frac{d_i + d_j - 2}{d_i \cdot d_j}}.$$

For more extensive applications of $M_2(G)$, you can refer to [20, 21].

The most successful index is the *Randić* index [22], which is defined as

$$R(G) = \sum_{ij \in E(G)} \frac{1}{\sqrt{d_i \cdot d_j}}.$$

The general *Randić* [23] is regarded as

$$R_\alpha(G) = \sum_{ij \in E(G)} [d_i \cdot d_j]^\alpha; \alpha = 1, -1, -\frac{1}{2}, \frac{1}{2}.$$

In addition, when $\alpha = \frac{1}{2}$, and$\alpha = 1$ is used in this paper, it is called reciprocal *Randić* index [24] and the second Zagreb index [19], abbreviated as $RR(G)$ and $M_2(G)$.

It is widely used in physical chemistry and mathematics [25, 26]. The topological indices used in other papers as shown in Table 1. As everyone knows, New Corona virus has swept the world in recent years. It poses a great threat to the safety of people's lives and property all over the world. The topological index provides the possibility of selecting drugs for the treatment of New Corona virus. By calculating the topological index of drugs, it can better understand the physical, chemical and biological activities of drugs [27–29].

Inspired by reference [30], this paper naturally came up with the idea of calculating the resistance distance of any two points in a new cyclic compounds $T_n(C_8)$, as shown in Fig. 1, so as to obtain the invariant of $T_n(C_8)$ about the resistance distance and some related indices based on the degree of this compound.

For the rest of the paper, the second section mainly makes some preparations and introduces some Lemmas and theorems. The third section is main results. The last section is a general conclusion.

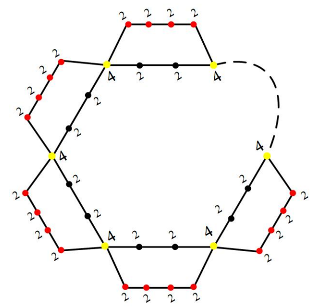

Figure 1: The cyclooctane derivatives $T_n(C_8)$.

Table 1: The rest of valency-based topological indices in this paper.

Topological indices	Mathematical expressions
hyper Zagreb	$HM(G)=\sum_{ij\in E(G)}(d_i+d_j)^2$
harmonic	$H(G)=\sum_{ij\in E(G)}\frac{2}{d_i+d_j}$
reduced reciprocal Randić	$RRR(G)=\sum_{ij\in E(G)}\sqrt{(d_i-1)\cdot(d_j-1)}$
modified first-multiplicative Zagreb	$\pi_1^*(G)=\prod_{ij\in E(G)}(d_i+d_j)$
general sum-connectivity	$\chi_\alpha(G)=\prod_{ij\in E(G)}(d_i+d_j)^\alpha$
reduced second Zagreb	$RM_2(G)=\prod_{ij\in E(G)}((d_i-1)+(d_j-1))$
augmented Zagreb	$AZ(G)=\prod_{ij\in E(G)}(\frac{d_i\cdot d_j}{d_i+d_j-2})^3$
sum-connectivity	$SC(G)=\prod_{ij\in E(G)}\frac{1}{\sqrt{d_i+d_j}}$

2. Preliminaries

The resistance distance we derive mainly depends on the definition. The graph is divided into subgraphs with n vertices. On the hand, the resistance distance of the subgraphs is calculated, and on the other hand the resistance distance of the whole graph is calculated.

2.1. N-division of Graphs

Definition 2.1. [31]The graph T is divided into two subgraphs T_1 and T_2 by n-separation, then

(a.)$V(T)=V(T_1)\bigcup V(T_2)$.

(b.)$|V(T_1)\bigcap V(T_2)|=n$.

(c.)$E(T)=E(T_1)\bigcup E(T_2)$.

(d.)$E(T_1)\bigcap E(T_2)=\emptyset$.

The set $V(T_1)\bigcap V(T_2)=\{t_1,t_2...t_n\}$ is known as n-separation of T.

Lemma 2.1. [31] Suppose G is a 1-separation graph with vertex $j\in V(T)$, and G is divided into T_1 and T_2 subgraphs through vertex j. If $a\in V(T_1)$, and $b\in V(T_2)$,

$$r_T(a,b)=r_{T_1}(a,j)+r_{T_2}(j,b).$$

Lemma 2.2. [31] Suppose T is a 2-separation graph with two vertices $u,v\in V(T)$, and T is divided into T_1 and T_2 subgraphs through vertices $u,\ v$. If $a,b\in V(T_1)$,

$$r_T(a,b)=r_{T_1}(a,b)-\frac{[r_{T_1}(a,u)+r_{T_1}(b,u)-r_{T_1}(a,v)-r_{T_1}(b,u)]^2}{4[r_{T_1}(u,v)+r_{T_2}(u,v)]}.$$

2.2. Cyclooctane Derivatives

In this paper, the cyclic compound we consider is composed of a cyclic graph with a base graph of 8 vertices C_8.

Definition 2.2. [32] A class of cyclooctane derivatives, defined as $T_n(C_8)$, is to copy n subgraphs and paste a_{d-1} vertex from each subgraph. Subgraphs G_d and G_{d-1} share a_{i-1} vertex, while G_d and G_{d+1} are connected by a vertices. The set I is the common vertices of each base graph, $I = \{a_1, a_2, ...a_n\}$.

Definition 2.3. Let $T = C_8$, take any two vertices $i,\ j$ from this circle and construct it in the way shown in the figure below. The shorter path between vertices i, j is D_1 and the longer path is D_2. The set of O represents other vertices excluding vertices i and j in the base graph(C_8). Take $p = d(i, j)$.

Theorem 2.1 Let $T_n(G) = T_n(C_8)$ be cyclooctane derivatives with $i,\ j$ in different (C_8), and $i \in V(T_1)$. Take f be the number of base graphs between vertices i and j inclusive, and $j \in V(T_f)$. Let vertices $a,\ b$ be the connecting vertices of graphs $T_{t-1}T_t$ and T_tT_{t+1}, respectively. Then

$$\begin{aligned} r_{T_n(G)}(i,j) &= r_T(i,b) + r_T(j,a) + (f-2)r_T(a,b) \\ &\quad - \frac{[r_T(i,a) + r_T(j,b) - r_T(i,y) - r_T(j,a) - 2(f-1)r_T(a,b)]^2}{4nr_T(a,b)}. \end{aligned}$$

If i, j in the same base graphs,

$$r_{T_n(G)}(i,j) = r_T(i,j) - \frac{[r_T(i,a) + r_T(j,b) - r_T(i,b) - r_T(j,a)]^2}{4nr_T(a,b)}.$$

Proof. We derive $i,\ j$ in different base graphs T, i.e set $i\ \in V(T_1),\ j \in V(T_f)$. Let $T_n(C_8)$ be the cyclooctane derivatives with the 2-separation $u,\ v$, and $i, j \in T_n(C_8)$. Take $i = u,\ j = v$. Let T_1 be the graph where vertices i and j are located, and the remaining graph is T_2. (As shown in Figure 1.) Using Lemma 2.1, where we have

$$r_{T_1}(i,j) = r_T(i,v) + (f-2)r_T(u,v) + r_T(u,j),$$
$$r_{T_1}(i,u) = r_T(i,a), r_{T_1}(j,v) = r_T(j,b).$$

Similarly,

$$\begin{aligned} r_{T_1}(i,v) &= r_T(i,b) + (f-1)r_T(a,b), \\ r_{T_1}(j,u) &= r_T(j,a) + (f-1)r_T(a,b), \\ r_{T_1}(u,v) = fr_T(a,b),\ and\ r_{T_2}(u,v) &= (n-f)r_T(a,b). \end{aligned}$$

Substitute the results of the above formulas into Lemma 2.2,

$$\begin{aligned} r_{T_n(G)}(i,j) &= r_T(i,b) + r_T(j,a) + (f-2)r_T(a,b) \\ &\quad - \frac{[r_T(i,a) + r_T(j,b) - r_T(i,b) - (f-1)r_T(a,b) - r_T(j,a) - (f-1)r_T(a,b)]^2}{4[fr_T(a,b) + (n-f)r_T(a,b)]} \\ &= r_G(i,b) + r_G(j,a) + (f-2)r_G(a,b) \\ &\quad - \frac{[r_T(i,a) + r_T(j,b) - r_T(i,b) - r_T(j,a) - 2(f-1)r_T(a,b)]^2}{4nr_T(a,b)}. \end{aligned}$$

In another case, when $i, j \in T$, one has

$$r_{T_1}(u,v) + r_{T_2}(u,v) = nr_T(a,b),$$

as desired.

3. Main results

In this section, we mainly derive the degree Kirchhoff index and its topological indices of cyclooctane derivatives $T_n(C_8)$, as shown in Table 1.

3.1. Resistance Distance

Theorem 3.1. Let C_8 be represented as a cyclic graph with 8 vertices. In this circle, the formulas of the $r_{C_8}(i,j)$ between any $i,\ j$ are

$$r_{C_8}(i,j)=\frac{(8-d(i,j))d(i,j)}{8},$$

where $d(i,j)$ is the distance between vertices $i,\ j$. The results can be easily verified by reference [4].
Theorem 3.2. Let G be cyclooctane derivatives $T_n(C_8)$. If $i\in C_{m_p},\ j\in C_{m_q},\ p\neq q$, then

$$\begin{aligned} r_G(i,j) \quad = \quad & \frac{(p_i+a)(8-p_i-a)+b(8-b)+p_i(8-p_i)(d-2)}{8} \\ & -\frac{[p_j(8-p_j-2b)+p_i(8-p_i-2a)-2dp_i(8-p_i)]^2}{32np_i(8-p_i)}. \end{aligned}$$

If $i,j\in C_{m_p}$, one has

$$r_G(i,j)=\begin{cases} \frac{(b-a)(8-b+a)}{8}-\frac{p_i(b-a)^2}{8n(8-p_i)};\ i,j\in D_p \\ \frac{(b+a)(8-b-a)}{8}-\frac{[p_i^2+p_i(2a-8)+p_j(8-2b-p_j)]^2}{32np_i(8-p_i)};\ i\in D_p,\ j\in D_q\ and\ p\neq q \end{cases},$$

where, d represents the number of base graph between vertices i and j, inclusive, p_i is the path length between u_t and v_t without vertex i, p_j is the path length between u_i and v_i without vertex j, a is the distance from vertex u to vertex i containing i, b is the distance from vertex u to vertex j containing j. If $i,j\in I$, replace the distance between vertices $x,\ y$ in the base graph with p_i. If $p_i=p_j$, at this point, note that $b\geq a$.
Proof. In the first case, if $i\in C_{8p},\ j\in C_{8q}$, set $p=1,\ q=d$. According to Theorem 3.1 has

$$r_{C_8}(i,y)=\frac{p_i+a}{8-p_i-a}, r_{C_8}(j,x)=\frac{a(8-a)}{8},$$

$$r_{C_8}(j,y)=\frac{p_j+b}{8-p_j-b}, r_{C_8}(i,x)=\frac{b(8-b)}{8}, r_{C_8}(x,y)=\frac{p_i(8-p_i)}{8},$$

by substituting these equations into Theorem 2.1, specific results can be obtained.

Next, we consider that i and j are in the same C_8. In the first case, if $i,\ j\ \in\ C_8$, and $b\geq a$, the path length between vertices $i,\ j$ is $b-a$, substitute it into Theorem 2.1 and simplify it $r_{C_8}(i,j)=\frac{(b-a)}{8-b+a}$. This contains $p_i=p_j$. One can get the desired results.

Another case, if $i\ \in\ D_p,\ j\ \in\ D_q$, and $d(i,j)=a+b$, similarly, $r_{C_8}(i,j)=\frac{(a+b)(8-b-a)}{8}$. Using Theorem 2.1, we can get the desired results.

3.2. The Kirchhoff Index

Theorem 3.3. The Kirchhoff index of cyclooctane derivatives $T_n(C_8)$ is

$$Kf(T_n(C_8))=\frac{1}{48}(915n^3+2304n^2-1343n+496).$$

Proof. Our purpose is to derive the resistance distance between any two points $i,\ j$ in the $T_n(C_8)$. Therefore, it is discussed in detail in the following six cases.
Case 1. $i,\ j$ in the different base graphs, and $i, j \in D_1$,

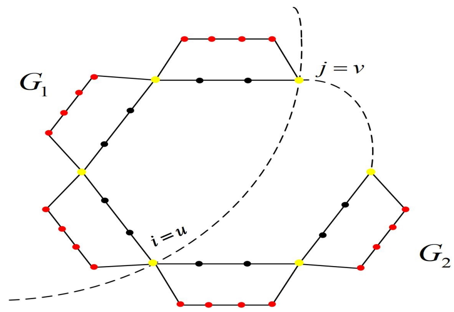

Figure 2: The $T_n(C_8)$ is divided into two subgraphs G_1 and G_2, in the **Case 1.**

$$Kf_1(T_n(C_8)) \quad = \quad n\sum_{d=2}^{n}\sum_{a=0}^{2}\sum_{b=0}^{2}\Big(\frac{k(8-b)+(3-a)(5+a)+15(d-2)}{8} - \frac{5(b-a+3(d-1))^2}{24n}\Big).$$

Case 2. $i,\ j$ in the different base graphs, and $i, j \in D_2$,

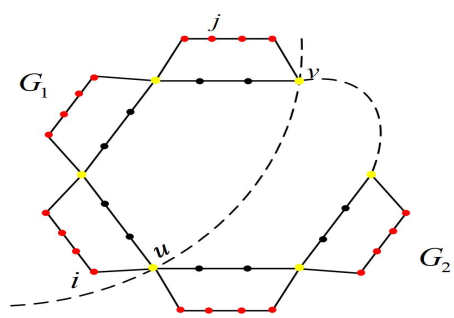

Figure 3: The $T_n(C_8)$ is divided into two subgraphs G_1 and G_2, in the **Case 2.**

$$Kf_2(T_n(C_8)) \quad = \quad n\sum_{d=2}^{n}\sum_{a=1}^{4}\sum_{b=1}^{4}\Big(\frac{(3+a)(5-a)+b(8-b)+15(d-2)}{8} - \frac{3(a-b+8+3(d-1)-8d)^2}{24n}\Big).$$

Case 3. $i,\ j$ in the different base graph, and $i \in D_2,\ j \in D_1$,

$$Kf_3(T_n(C_8)) \quad = \quad n\sum_{d=2}^{n}\sum_{a=1}^{4}\sum_{b=1}^{3}\Big(\frac{(3+a)(5-a)+b(8-b)+15(d-2)}{8} - \frac{(9(d-1)+3(a+b+8-8d)-8b)^2}{120n}\Big).$$

Case 4. $i,\ j$ in the same base graph, and $i, j \in D_1$,

$$Kf_4(T_n(C_8)) \quad = \quad n\sum_{a=2}^{n}\sum_{b=a+1}^{2}\Big(\frac{(b-a)(8-b+a)}{8} - \frac{5(b-a)^2}{120n}\Big).$$

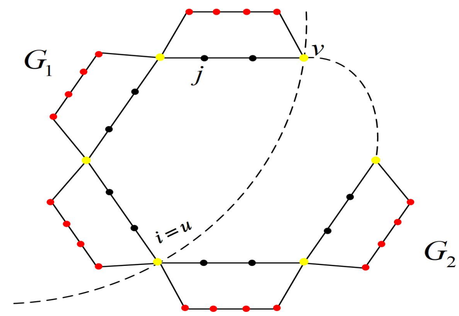

Figure 4: The $T_n(C_8)$ is divided into two subgraphs G_1 and G_2, in the **Case 3.**

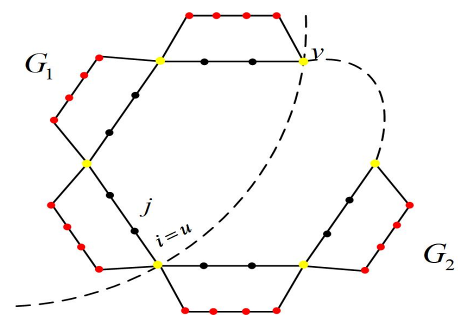

Figure 5: The $T_n(C_8)$ is divided into two subgraphs G_1 and G_2, in the **Case 4.**

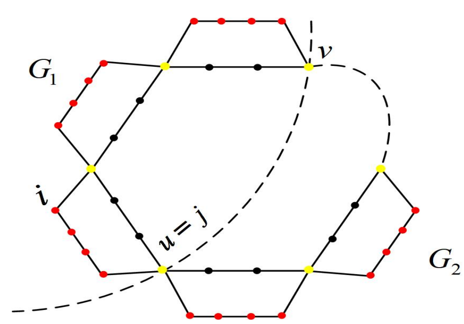

Figure 6: The $T_n(C_8)$ is divided into two subgraphs G_1 and G_2, in the **Case 5.**

Case 5. $i,\ j$ in the same base graph, and $i \in D_2,\ j \in D_1$,

$$Kf_5(T_n(C_8)) \quad = \quad n\sum_{a=1}^{4}\sum_{b=l}^{3}\Big(\frac{(b+a)(8-b-a)}{8} - \frac{(3(b+a)-8b)^2}{120n}\Big).$$

Case 6. $i,\ j$ in the same base graph, and $i, j \in D_2$

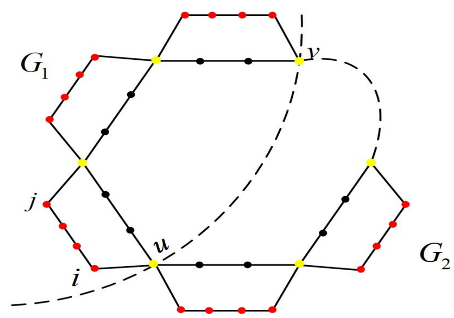

Figure 7: The $T_n(C_8)$ is divided into two subgraphs G_1 and G_2, in the **Case 6.**

$$Kf_6(T_n(C_8)) \quad = \quad n\sum_{a=1}^{4}\sum_{b=a+1}^{4}\Big(\frac{(b-a)(8-b+a)}{8} - \frac{3(b-a)^2}{40n}\Big).$$

Thus,

$$\begin{aligned} Kf(T_n(C_8)) &= \frac{1}{2}(Kf_1(F_n(C_8)) + Kf_2(F_n(C_8)) + 2Kf_3(F_n(C_8)) \\ &\quad +2Kf_4(F_n(C_8)) + 2Kf_5(F_n(C_8)) + 2Kf_6(F_n(C_8))) \\ &= \frac{1}{48}(915n^3 + 2304n^2 - 1343n + 496). \end{aligned}$$

3.3. The degree-Kirchhoff index

Theorem 3.4. The expressions of multiplicative degree-Kirchhoff index and additive degree-Kirchhoff index of a class of cyclooctane derivatives $T_n(C_8)$ are expressed as

$$Kf^+(T_n(C_8)) = \quad = \quad 2n(-13 + 90n + 35n^2),$$

$$Kf^*(T_n(C_8)) = \quad = \quad \frac{16n}{3}(-5 + 36n + 15n^2).$$

Proof. Let G be the cyclooctane derivatives $T_n(C_8)$. The degree-Kirchhoff index is calculated by using a similar method to calculate Kirchhoff index. If $i \in F,\ d_i = 4$. Otherwise, $d_i = 2$.
Case 1. $i,\ j$ in the different base graphs, $i, j \in D_1$, and this case just includes that i or j belongs to set I,

$$Kf_1^+(G) \quad = \quad (4+2)\cdot 2n \cdot \sum_{d=2}^{n}\sum_{b=a}^{2}\Big(\frac{b(8-b)+15(d-1)}{8} - \frac{5[b+3(d-1)]^2}{24n}\Big).$$

Similarly,

$$Kf_1^*(G) \quad = \quad 4*2\cdot 2n\cdot\sum_{d=2}^{n}\sum_{b=a}^{2}\Big(\frac{b(8-b)+15(d-1)}{8}-\frac{5[b+3(d-1)]^2}{24n}\Big).$$

Case 2. $i,\ j$ in the different base graphs, and $i,j\in I$,

$$Kf_2^+(G) \quad = \quad (4+4)\cdot n\cdot\sum_{d=2}^{n}\sum_{b=1}^{2}\Big(\frac{15(n-d+a)(d-1)}{8}\Big).$$

Similarly,

$$Kf_2^*(G) \quad = \quad 4*4\cdot n\cdot\sum_{d=2}^{n}\sum_{b=1}^{2}\Big(\frac{15(n-d+1)(d-1)}{8}\Big).$$

Case 3. $i,\ j$ in the different base graphs, $i,j\in O$, and $i,j\in D_1$,

$$Kf_3^+(G) \quad = \quad (2+2)\cdot n\cdot\sum_{d=2}^{n}\sum_{a=1}^{2}\sum_{b=a}^{2}\Big(\frac{b(8-b)+(3-a)(5+a)+15(d-2)}{8}-\frac{5[b-a+3(d-1)]^2}{24n}\Big).$$

Similarly,

$$Kf_3^*(G) \quad = \quad 2*2\cdot n\cdot\sum_{d=2}^{n}\sum_{a=1}^{2}\sum_{b=1}^{2}\Big(\frac{b(8-b)+(3-a)(5+a)+15(d-2)}{8}-\frac{5[b-a+3(d-1)]^2}{24n}\Big).$$

Case 4. $i,\ j$ in the different base graphs, $i,j\in O$, and $i,j\in D_2$,

$$Kf_4^+(G) \quad = \quad (2+2)\cdot n\cdot\sum_{d=2}^{n}\sum_{a=1}^{4}\sum_{b=1}^{4}\Big(\frac{b(8-b)+(3+a)(5-a)+15(d-2)}{8}-\frac{3[a-b+8+3(d-1)-8d]^2}{40n}\Big).$$

Similarly,

$$Kf_4^*(G) \quad = \quad 2*2\cdot n\cdot\sum_{d=2}^{n}\sum_{a=1}^{4}\sum_{b=1}^{4}\Big(\frac{b(8-b)+(3+a)(5-a)+15(d-2)}{8}-\frac{3[a-b+8+3(d-1)-8d]^2}{40n}\Big).$$

Case 5. $i,\ j$ in the different base graphs, $j\in I$, and $i\in D_1$,

$$Kf_5^+(G) \quad = \quad (4+2)\cdot 2n\cdot\sum_{d=2}^{n}\sum_{a=1}^{4}\Big(\frac{(3+a)(5-a)+15(d-1)}{8}-\frac{3[a+5d]^2}{40n}\Big).$$

Similarly,

$$Kf_5^*(G) \quad = \quad 4*2\cdot 2n\cdot\sum_{d=2}^{n}\sum_{a=1}^{4}\Big(\frac{(3+a)(5-a)+15(d-1)}{8}-\frac{3[a+5d]^2}{40n}\Big).$$

Case 6. $i,\ j$ in the different base graphs, $j \in D_1$, and $i \in D_2$,

$$\begin{aligned} Kf_6^{+}(G) &= (2+2)\cdot 2n\cdot \sum_{d=2}^{n}\sum_{a=1}^{4}\sum_{b=1}^{2}\Big(\frac{(3+a)(5-a)+b(8-b)+15(d-2)}{8} \\ &\qquad - \frac{[9(d-1)+3(b+a-8-8d)-8k]^2}{120n}\Big). \end{aligned}$$

Similarly,

$$\begin{aligned} Kf_6^{*}(G) &= 2*2\cdot 2n\cdot \sum_{d=2}^{n}\sum_{a=1}^{4}\sum_{b=1}^{2}\Big(\frac{(3+a)(5-a)+b(8-b)+15(d-2)}{8} \\ &\qquad - \frac{[9(d-1)+3(b+a-8-8d)-8k]^2}{120n}\Big). \end{aligned}$$

Case 7. $i,\ j$ in the same base graphs, $i,j \in D_1$, and $i \in I$,

$$Kf_7^{+}(G) = (2+4)\cdot 2n\cdot \sum_{b=1}^{2}\Big(\frac{b(8-b)}{8} - \frac{5b^2}{24n}\Big).$$

Similarly,

$$Kf_7^{*}(G) = 2*4\cdot 2n\cdot \sum_{b=1}^{2}\Big(\frac{b(8-b)}{8} - \frac{5b^2}{24n}\Big).$$

Case 8. $i,\ j$ in the same base graphs, $i,j \in D_1$, and $i,j \in O$,

$$Kf_8^{+}(G) = (2+2)\cdot 2n\cdot \sum_{a=1}^{2}\sum_{b=a+1}^{2}\Big(\frac{(b-a)(8-b+a)}{8} - \frac{5(b-a)^2}{24n}\Big).$$

Similarly,

$$Kf_8^{*}(G) = 2*2\cdot 2n\cdot \sum_{a=1}^{2}\sum_{b=a+1}^{2}\Big(\frac{(b-l)(8-b+a)}{8} - \frac{5(b-a)^2}{24n}\Big).$$

Case 9. $i,\ j$ in the same base graphs, $i \in D_2$, and $j \in I$,

$$Kf_9^{+}(G) = (2+4)\cdot 2n\cdot \sum_{a=1}^{4}\Big(\frac{(3+a)(5-a)}{8} - \frac{3(5-a)^2}{40n}\Big).$$

Similarly,

$$Kf_9^{*}(G) = 2*4\cdot 2n\cdot \sum_{a=1}^{4}\Big(\frac{(3+a)(5-a)}{8} - \frac{3(5-a)^2}{40n}\Big).$$

Case 10. i, j in the same base graphs, $i \in D_2,\ j \in D_1$, and $i, j \in O$,

$$Kf_{10}^{+}(G) \quad = \quad (2+2) \cdot 2n \cdot \sum_{a=1}^{4} \sum_{b=1}^{2} \Big(\frac{(b+a)(8-b-a)}{8} - \frac{[3(b+a)-8b]^2}{120n} \Big).$$

Similarly,

$$Kf_{10}^{*}(G) \quad = \quad 2 * 2 \cdot 2n \cdot \sum_{a=1}^{4} \sum_{b=1}^{2} \Big(\frac{(b+a)(8-b-a)}{8} - \frac{[3(b+l)-8b]^2}{120n} \Big).$$

Case 11. i, j in the same base graphs, $i, j \in D_2$, and $i, j \in O$,

$$Kf_{11}^{+}(G) \quad = \quad (2+2) \cdot 2n \cdot \sum_{a=1}^{4} \sum_{b=1}^{4} \Big(\frac{(b-a)(8-b+a)}{8} - \frac{3(b-a)^2}{40n} \Big).$$

Similarly,

$$Kf_{11}^{*}(G) \quad = \quad 2 * 2 \cdot 2n \cdot \sum_{a=1}^{4} \sum_{b=1}^{4} \Big(\frac{(b-a)(8-b+a)}{8} - \frac{3(b-l)^2}{40n} \Big).$$

Thus,

$$\begin{aligned} Kf^{+}(G) &= Kf_1^{+}(G) + Kf_2^{+}(G) + Kf_3^{+}(G) ... + Kf_{11}^{+}(G) \\ &= 2n(-13 + 90n + 35n^2), \end{aligned}$$

as desired.

Similarly,

$$\begin{aligned} Kf^{*}(G) &= Kf_1^{*}(G) + Kf_2^{*}(G) + Kf_3^{*}(G) + ... + Kf_{11}^{*}(G) \\ &= \frac{16n}{3}(-5 + 36n + 15n^2). \end{aligned}$$

The proof is completed.

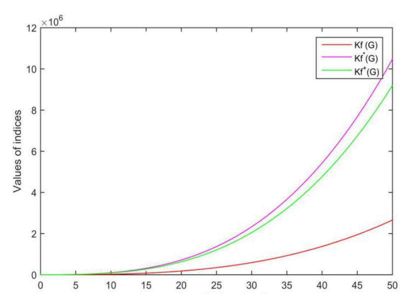

Figure 8: The function images of the (degree) Kirchhoff index in $T_n(C_8)$.

Table 2: Vertex partition of $T_n(C_8)$ degree-based on vertices.

(d_u, d_v)	(4,2)	(2,2)
number of edges	4n	4n

3.4. Others topological indices

Theorem 3.5. Suppose G is a cyclooctane derivatives, then its related topological indices are

$$\begin{aligned}
(1)GA(G) &= (\frac{8\sqrt{2}}{3}+4)n. \\
(2)ABC(G) &= 4\sqrt{2}n. \\
(3)HM(G) &= 208n \\
(4)H(G) &= \frac{10}{3}n. \\
(5)R(G) &= (2+\sqrt{2})n. \\
(6)R_\alpha(G) &= 4n(4^\alpha+8^\alpha). \\
(7)RR(G) &= (\sqrt{2}+1)8n. \\
(8)RRR(G) &= (\sqrt{3}+1)4n. \\
(9)M_2(G) &= 48n. \\
(10)\pi_2(G) &= (32)^{4n}. \\
(11)\pi_1^*(G) &= (24)^{4n}. \\
(12)\chi_\alpha(G) &= (24)^{4n\alpha} \\
(13)RM_2(G) &= (2)^{8n}. \\
(14)AZ(G) &= (8)^{8n}. \\
(15)SC(G) &= (\frac{\sqrt{6}}{12})^{4n}.
\end{aligned}$$

Proof. Let G be a kind of Cyclooctane derivatives. It's easy to know that $V(G) = 7n$, and $E(G) = 8n$. If vertex $i \in I,\ d_i = 4$, else $\ d_i = 2$. According to the degree of vertices, we can get the results shown in Table 2. Combined with the topological descriptor formula, we have

$$\begin{aligned}
GA(G) &= \sum_{ij\in E(G)} \frac{2\sqrt{d_i \cdot d_j}}{d_i+d_j} \\
&= 4n * \frac{2*\sqrt{4*2}}{4+2} + 4n * \frac{2*\sqrt{2*2}}{2+2} \\
&= (\frac{8\sqrt{2}}{3}+4)n.
\end{aligned}$$

$$
\begin{aligned}
ABC(G) &= \sum_{ij\in E(G)} \sqrt{\frac{d_i+d_j-2}{d_i\cdot d_j}} \\
&= 4n*\sqrt{\frac{4+2-2}{4*2}}+4n*\sqrt{\frac{2+2-2}{2*2}} \\
&= 4\sqrt{2}n.
\end{aligned}
$$

$$
\begin{aligned}
HM(G) &= \sum_{ij\in E(G)} (d_i+d_j)^2 \\
&= 4n*(4+2)^2+4n*(2+2)^2 \\
&= 208n.
\end{aligned}
$$

$$
\begin{aligned}
H(G) &= \sum_{ij\in E(G)} \frac{2}{d_i+d_j} \\
&= 4n*\frac{2}{4+2}+4n*\frac{2}{2+2} \\
&= \frac{10}{3}n.
\end{aligned}
$$

$$
\begin{aligned}
R(G) &= \sum_{ij\in E(G)} \frac{1}{\sqrt{d_i\cdot d_j}} \\
&= 4n*\frac{1}{\sqrt{4+2}}+4n*\frac{1}{\sqrt{2+2}} \\
&= (2+\sqrt{2})n.
\end{aligned}
$$

$$
\begin{aligned}
R_\alpha(G) &= \sum_{ij\in E(G)} [d_i\cdot d_j]^\alpha \\
&= 4n*8^\alpha+4n*4^\alpha \\
&= 4n(4^\alpha+8^\alpha).
\end{aligned}
$$

$$
\begin{aligned}
RR(G) &= \sum_{ij\in E(G)} \sqrt{d_i\cdot d_j} \\
&= 4n*\sqrt{4*2}+4n*\sqrt{2*2} \\
&= (\sqrt{2}+1)8n.
\end{aligned}
$$

$$
\begin{aligned}
RRR(G) &= \sum_{ij\in E(G)} \sqrt{(d_i-1)\cdot(d_j-1)} \\
&= 4n*\sqrt{(4-1)\cdot(2-1)}+4n*\sqrt{(2-1)\cdot(2-1)} \\
&= (\sqrt{3}+1)4n.
\end{aligned}
$$

$$
\begin{aligned}
M_2(G) &= \sum_{ij\in E(G)} d_i \cdot d_j \\
&= 4n*4*2+4n*2*2 \\
&= 48n.
\end{aligned}
$$

$$
\begin{aligned}
\pi_2(G) &= \prod_{ij\in E(G)} d_i \cdot d_j \\
&= (4*2)^{4n}\cdot(2\cdot 2)^{4n} \\
&= (32)^{4n}.
\end{aligned}
$$

$$
\begin{aligned}
\pi_1^*(G) &= \prod_{ij\in E(G)} (d_i + d_j) \\
&= (4+2)^{4n}\cdot(2+2)^{4n} \\
&= (24)^{4n}.
\end{aligned}
$$

$$
\begin{aligned}
\chi_\alpha(G) &= \prod_{ij\in E(G)} (d_i + d_j)^\alpha \\
&= (4+2)^{\alpha 4n}\cdot(2+2)^{\alpha 4n} \\
&= (24)^{4n\alpha}.
\end{aligned}
$$

$$
\begin{aligned}
RM_2(G) &= \prod_{ij\in E(G)} ((d_i-1)+(d_j-1)) \\
&= [(4-1)+(2-1)]^{4n}\cdot[(2-1)+(2-1)]^{4n} \\
&= (2)^{8n}.
\end{aligned}
$$

$$
\begin{aligned}
AZ(G) &= \prod_{ij\in E(G)} (\frac{d_i\cdot d_j}{d_i+d_j-2})^3 \\
&= [(\frac{4*2}{4+2-2})^3]^{4n}\cdot[(\frac{2*2}{2+2-2})^3]^{4n} \\
&= (8)^{8n}.
\end{aligned}
$$

$$
\begin{aligned}
SC(G) &= \prod_{ij\in E(G)} \frac{1}{\sqrt{d_i+d_j}} \\
&= [\frac{1}{\sqrt{4+2}}]^{4n} \cdot [\frac{1}{\sqrt{2+2}}]^{4n} \\
&= (\frac{\sqrt{6}}{12})^{4n}.
\end{aligned}
$$

Finally, in order to intuitively see the change trend of several indexes,we draw the curves of several indices in the same coordinate. From the Figure 9, we can clearly see that the change of $M_2(G)$ is significantly higher than that of other indices.

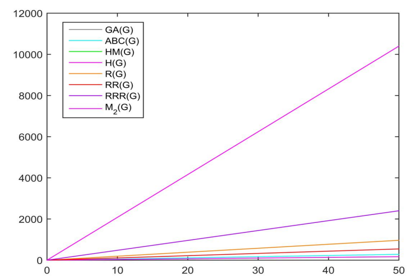

Figure 9: Variation trend of several indices of $T_n(C_8)$.

4. Conclusion

In this paper, we mainly define a cyclic compound $T_n(C_8)$, which can also be called cyclic network. We mainly derive the resistance distance between any two vertices of $T_n(C_8)$, and obtain its Kirchhoff expression. Using its vertex degree distribution, its (degree) Kirchhoff index and other related topological indexes are calculated. Using these invariants, we can predict some physical or properties of this compound, and provide some references for others to study this compound.

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