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GOURAVA AND HYPER-GOURAVA INDICES OF SOME CACTUS CHAINS

B. BASAVANAGOUD[1] AND SHRUTI POLICEPATIL[2]

[1,2]**Department of Mathematics, Karnatak University**
Dharwad - 580 003 Karnataka, India
[1]**b.basavanagoud@gmail.com**
[2]**shrutipatil300@gmail.com**

Abstract. The physico-chemical characteristics of molecules are theoretically explored using the theory of graphs and mathematical chemistry. A graph's topological index is a numerical value derived from the graph mathematically. The Gourava and hyper-Gourava indices of various cactus chains are determined in this study.

Key words and Phrases: Gourava indices, hyper-Gourava indices, cactus chains.

1. INTRODUCTION

A molecular graph, also known as a chemical graph, is a graph in which the atoms are represented by the vertices, while the bonds are represented by the edges. Topological indices are numeric quantities obtained from a molecular graph that correlate the molecular graph's physico-chemical characteristics and have been shown to be beneficial in isomer discrimination, QSAR and QSPR analysis.

Only simple, finite, connected graphs with $V(G)$ as vertex set and $E(G)$ as edge set are considered throughout this study. The degree $d_G(a)$ of a vertex a is the number of vertices adjacent to a.

A cactus graph is a connected graph in which no edge lies in more than one cycle. Every cactus graph cycle is chordless, and every cactus graph block is either an edge or a cycle. A cactus graph is said to be triangular if all of its blocks are triangular. A triangular cactus graph is described as a chain triangular cactus if all of its triangles have at most two cut-vertices and each cut-vertice is shared by precisely two triangles. A square cactus graph is a type of cactus graph and all of its blocks are square. A square cactus graph is said to be a chain square cactus if all of its squares have at most two cut-vertices and each cut-vertice is shared by precisely two squares. It's worth noting that the internal squares' connections

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to their neighbours may vary. A chain square cactus is called ortho-chain square cactus if the cut-vertices are nearby. A para-chain square cactus is one in which the cut-vertices are not contiguous in a chain square cactus. The Gourava and hyper-Gourava indices of various generic ortho and para cactus chains are studied in this paper, and particular situations such as the triangular chain cactus T_n, ortho-chain square cactus O_n, and para-chain square cactus Q_n are considered. Latest investigations on several cactus chains can be found in [1, 3, 13, 14] and references cited therein. For undefined terms and notations refer to [5].

The first and second Gourava indices of a molecular graph were introduced by Kulli [6] and are defined as:

$$GO_1(G) = \sum_{ab\in E(G)} \big[(d_G(a)+d_G(b)) + d_G(a)d_G(b)\big],$$

$$GO_2(G) = \sum_{ab\in E(G)} \big[\big(d_G(a)+d_G(b)\big)\big(d_G(a)d_G(b)\big)\big].$$

Kulli proposed the first and second hyper-Gourava indices of a molecular graph G in [7], and they are defined as

$$HGO_1(G) = \sum_{ab\in E(G)} \big[d_G(a)+d_G(b)+d_G(a)d_G(b)\big]^2,$$

$$HGO_2(G) = \sum_{ab\in E(G)} \big[\big(d_G(a)+d_G(b)\big)\big(d_G(a)d_G(b)\big)\big]^2.$$

Several topological indices were investigated. For further information, see [2, 4, 8, 9, 10, 11, 12].

2. MAIN RESULTS

We look at two types of cactus chains in this section: the para cacti chain and the ortho cacti chain of cycles. We start with a para cacti chain of length n cycles C_m, where each block is a cycle C_m. Let C_m^n be the symbol for it. We compute an exact expression of GO_1, GO_2, HGO_1 and HGO_2 of C_m^n in the following theorem.

TABLE 1. Partitioning at the edge of C_m^n.

$d_{C_m^n}(a), d_{C_m^n}(b) : ab \in E(C_m^n)$	$(2,2)$	$(2,4)$
Edge count	$mn-4n+4$	$4(n-1)$

Theorem 2.1. *For a para cacti chain of cycles C_m^n ($m \geq 4$, $n \geq 2$),*

1. $GO_1(C_m^n) = 8[mn + 3(n-1)]$.

2. $GO_2(C_m^n) = 16[mn + 8(n-1)]$.
3. $HGO_1(C_m^n) = 16[4mn + 33(n-1)]$.
4. $HGO_2(C_m^n) = 256[mn + 32(n-1)]$.

Proof. 1. By utilizing the definition of GO_1 and entries in Table 1, we have

$$\begin{aligned} GO_1(C_m^n) &= \sum_{ab\in E(C_m^n)} \left[\left(d_{C_m^n}(a) + d_{C_m^n}(b)\right) + \left(d_{C_m^n}(a)d_{C_m^n}(b)\right)\right] \\ &= (mn-4n+4)(4+4) + 4(n-1)(2+4+8) \\ &= 8[mn+3(n-1)]. \end{aligned}$$

2. By making use the definition of GO_2 and values in Table 1, we have

$$\begin{aligned} GO_2(C_m^n) &= \sum_{ab\in E(C_m^n)} \left[\left(d_{C_m^n}(a) + d_{C_m^n}(b)\right)\left(d_{C_m^n}(a)d_{C_m^n}(b)\right)\right] \\ &= (mn-4n+4)(4\times 4) + 4(n-1)(6\times 8) \\ &= 16[mn+8(n-1)]. \end{aligned}$$

3. By the usage of the definition of HGO_1 and facts in table 1, we have

$$\begin{aligned} HGO_1(C_m^n) &= \sum_{ab\in E(C_m^n)} \left[\left(d_{C_m^n}(a) + d_{C_m^n}(b)\right) + \left(d_{C_m^n}(a)d_{C_m^n}(b)\right)\right]^2 \\ &= (mn-4n+4)(4+4)^2 + 4(n-1)(6+8)^2 \\ &= 16[4mn+33(n-1)]. \end{aligned}$$

4. By using the concept of HGO_2 as well as the data in Table 1, we have

$$\begin{aligned} HGO_2(C_m^n) &= \sum_{ab\in E(C_m^n)} \left[\left(d_{C_m^n}(a) + d_{C_m^n}(b)\right)\left(d_{C_m^n}(a)d_{C_m^n}(b)\right)\right]^2 \\ &= (mn-4n+4)(4\times 4)^2 + 4(n-1)(6\times 8)^2 \\ &= 256[mn+32(n-1)]. \end{aligned}$$

□

The graph Q_n is pictured in Figure 1.

Corollary 2.2. *For a para-chain square cactus graph $Q_n (n \geq 2)$,*

1. $GO_1(Q_n) = 8(7n-3)$.

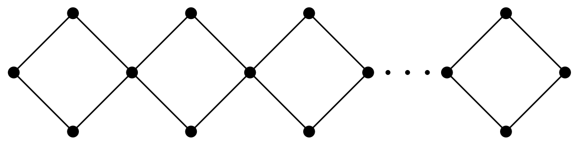

FIGURE 1. The graph Q_n.

2. $GO_2(Q_n) = 3n^3 + 9n^2 + 60n$.
3. $HGO_1(Q_n) = 16(49n - 33)$.
4. $HGO_2(Q_n) = 1024(9n - 8)$.

PROOF. Replace $m = 4$ in Theorem 2.1 to complete the proof. □

The graph L_n is indicated in Figure 2.

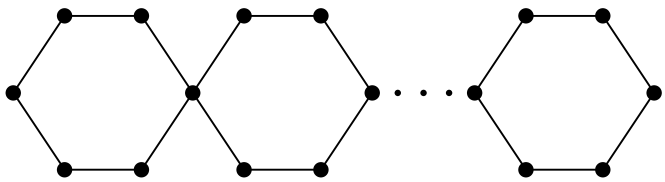

FIGURE 2. The graph L_n.

Corollary 2.3. *For a para-chain hexagonal cactus graph $L_n (n \geq 3)$,*

1. $GO_1(L_n) = 24(3n - 1)$.
2. $GO_2(L_n) = 32(7n - 4)$.
3. $HGO_1(L_n) = 16(57n - 33)$.
4. $HGO_2(L_n) = 512(19n - 16)$.

PROOF. We get the required outcome if we set $m = 6$ in the Theorem 2.1. □

The ortho-chain cacti of cycles with neighbouring cut-vertices is now considered. Let CO_m^n be an ortho-chain cactus graph, where m is the cycle length and n is the chain length. $|V(CO_m^n)| = mn - n + 1$ and $|E(CO_m^n)| = mn$ are self-evident. GO_1, GO_2, HGO_1 and HGO_2 of CO_m^n are obtained by utilizing the following theorem.

TABLE 2. Partitioning at the edge of CO_m^n.

$d_{CO_m^n}(a), d_{CO_m^n}(b) : ab \in E(CO_m^n)$	$(2,2)$	$(2,4)$	$(4,4)$
Edge count	$mn - 3m + 2$	$2n$	$n - 1$

Theorem 2.4. *For a ortho cacti chain of cycles $CO_m^n (m \geq 3,\ n \geq 2)$,*

1. $GO_1(CO_m^n) = 8mn - 24m + 52n - 8$.

2. $GO_2(CO_m^n) = 16mn - 48m + 224n - 96$.
3. $HGO_1(CO_m^n) = 64mn - 192m + 968n - 448$.
4. $HGO_2(CO_m^n) = 256mn - 768m + 20992n - 15872$.

PROOF. 1. By using the concept of GO_1 as well as the data in Table 2, we have

$$\begin{aligned} GO_1(CO_m^n) &= \sum_{ab \in E(CO_m^n)} \left[\left(d_{CO_m^n}(a) + d_{CO_m^n}(b)\right) + \left(d_{CO_m^n}(a) d_{CO_m^n}(b)\right) \right] \\ &= (mn - 3m + 2)(4 + 4) + 2n(6 + 8) + (n - 1)(8 + 16) \\ &= 8mn - 24m + 52n - 8. \end{aligned}$$

2. By making use the definition of GO_2 and values in Table 2, we have

$$\begin{aligned} GO_2(CO_m^n) &= \sum_{ab \in E(CO_m^n)} \left[\left(d_{CO_m^n}(a) + d_{CO_m^n}(b)\right) + \left(d_{CO_m^n}(a) d_{CO_m^n}(b)\right) \right] \\ &= (mn - 3m + 2)(4 \times 4) + 2n(6 \times 8) + (n - 1)(8 \times 16) \\ &= 16mn - 48m + 224n - 96. \end{aligned}$$

3. By utilizing the description of HGO_1 and entries in Table 2, we have

$$\begin{aligned} HGO_1(CO_m^n) &= \sum_{ab \in E(CO_m^n)} \left[\left(d_{CO_m^n}(a) + d_{CO_m^n}(b)\right) + \left(d_{CO_m^n}(a) d_{CO_m^n}(b)\right) \right]^2 \\ &= (mn - 3m + 2)(4 + 4)^2 + 2n(6 + 8)^2 + (n - 1)(8 + 16)^2 \\ &= 64mn - 192m + 968n - 448. \end{aligned}$$

4. By the usage of the definition of HGO_2 and facts in table 2, we have

$$\begin{aligned} HGO_2(CO_m^n) &= \sum_{ab \in E(CO_m^n)} \left[\left(d_{CO_m^n}(a) + d_{CO_m^n}(b)\right) + \left(d_{CO_m^n}(a) d_{CO_m^n}(b)\right) \right]^2 \\ &= (mn - 3m + 2)(4 \times 4)^2 + 2n(6 \times 8)^2 + (n - 1)(8 \times 16)^2 \\ &= 256mn - 768m + 20992n - 15872. \end{aligned}$$

□

Then, as illustrated in Figure 3, we consider a chain triangular cactus, designated by T_n, where n is the length of the T_n. For $m = 3$, T_n is a special case of CO_m^n.

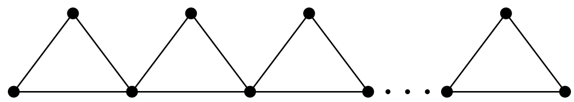

FIGURE 3. The graph T_n.

Corollary 2.5. *For a chain triangular cactus $T_n (n \geq 2)$,*

1. $GO_1(T_n) = 76n - 80$.
2. $GO_2(T_n) = 272n - 240$.
3. $HGO_1(T_n) = 1160n - 1024$.
4. $HGO_2(T_n) = 21760n - 18176$.

PROOF. Replace $m = 3$ in Theorem 2.4 to complete the proof. $\square$

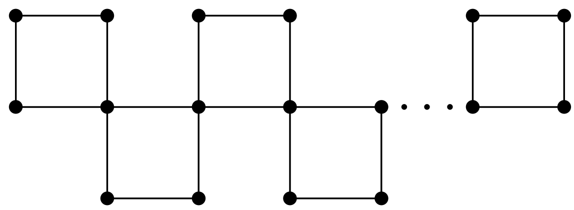

FIGURE 4. The graph O_n.

Corollary 2.6. *For the ortho-chain square cactus $O_n (n \geq 2)$,*

1. $GO_1(O_n) = 84n - 104$.
2. $GO_2(O_n) = 288(n - 1)$.
3. $HGO_1(O_n) = 1224n - 1216$.
4. $HGO_2(O_n) = 22016n - 18944$.

PROOF. We get the required outcome if we set $m = 4$ in the Theorem 2.4. $\square$

By identifying every node of K_m with a node of one K_y, the graph $Q(m, y)$ is formed from K_m and m copies of K_y. GO_1, GO_2, HGO_1 and HGO_2 of $Q(m, y)$ are computed in the following theorem. Figure 5 depicts the graph $Q(m, y)$.

TABLE 3. Partitioning at the edge of $Q(m, y)$.

$d_{Q(m,y)}(a), d_{Q(m,y)}(b) : ab \in E(Q(m, y))$	Edge count
$(y - 1, y - 1)$	$\frac{m(y-1)(y-2)}{2}$
$(y - 1, m + y - 2)$	$m(y - 1)$
$(m + y - 2, m + y - 2)$	$\frac{m(y-1)}{2}$

Theorem 2.7. *For a ortho-chain $Q(m, y) (m, y \geq 2)$,*

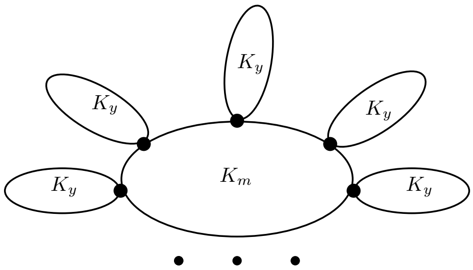

FIGURE 5. The graph $Q(m, y)$.

1. $GO_1(Q(m,y)) = \frac{m(y-1)(y-2)(y^2-1)}{2} + m(y-1)(y^2+ym-y-1) + \frac{m(y-1)(m+y-2)(m+y)}{2}$.
2. $GO_2(Q(m,n)) = m(y-1)^4(y-2) + m(y-1)[(2y^2-9y+13) + m(5-m) + my(3y+m-8) - 6] + m(y-1)[(m+y-2)^3]$.
3. $HGO_1(Q(m,y)) = \frac{m(y-1)(y-2)(y^2-1)^2}{2} + m(y-1)(y^2+ym-y-1)^2 + \frac{m(y-1)(m+y-2)(m+y)^2}{2}$.
4. $HGO_2(Q(m,y)) = 2m(y-1)[(y-1)^6(y-2) + (m+y-2)^6] + m(n-1)[(m+2y-3)(y-1)(m+y-2)]^2$.

PROOF. 1. By using the concept of GO_1 as well as the data in Table 3, we have

$$\begin{aligned} GO_1(Q(m,y)) &= \sum_{ab\in E(Q(m,y))} \left[\left(d_{Q(m,y)}(a) + d_{Q(m,y)}(b)\right) + \left(d_{Q(m,y)}(a)d_{Q(m,y)}(b)\right)\right] \\ &= \frac{m(y-1)(y-2)(y^2-1)}{2} + m(y-1)(y^2+ym-y-1) \\ &\quad + \frac{m(y-1)(m+y-2)(m+y)}{2}. \end{aligned}$$

2. By utilizing the description of GO_2 and entries in Table 3, we have

$$\begin{aligned} GO_2(Q(m,n)) &= \sum_{ab\in E(Q(m,n))} \left[\left(d_{Q(m,y)}(a) + d_{Q(m,y)}(b)\right)\left(d_{Q(m,y)}(a)d_{Q(m,y)}(b)\right)\right] \\ &= m(y-1)^4(y-2) + m(n-1)[(2y^2-9y+13) + m(5-m) \\ &\quad + my(3y+m-8) - 6] + m(y-1)[(m+y-2)^3]. \end{aligned}$$

3. By the usage of the definition of HGO_1 and facts in Table 3, we have

$$\begin{aligned} HGO_1(Q(m,y)) &= \sum_{ab\in E(Q(m,y))} \left[\left(d_{Q(m,y)}(a)+d_{Q(m,y)}(b)\right)+\left(d_{Q(m,y)}(a)d_{Q(m,y)}(b)\right)\right]^2 \\ &= \frac{m(y-1)(y-2)(y^2-1)^2}{2}+m(y-1)(y^2+ym-n-1)^2 \\ &\quad +\frac{m(y-1)(m+y-2)(m+y)^2}{2}. \end{aligned}$$

4. By making use the definition of HGO_2 and values in Table 3, we have

$$\begin{aligned} HGO_2(Q(m,y)) &= \sum_{ab\in E(Q(m,y))} \left[\left(d_{Q(m,y)}(a)+d_{Q(m,y)}(b)\right)\left(d_{Q(m,y)}(a)d_{Q(m,y)}(b)\right)\right]^2 \\ &= 2m(y-1)^7(y-2)+m(y-1)[(m+2y-3)(y-1)(m+y-2)]^2 \\ &\quad +2m(y-1)(m+y-2)^6. \end{aligned}$$

The join of each cycle of length $m \geq 3$ and a new vertex in C_m^n. That is $(C_m + K_1)$. We term it a wheel chain. W_m^n is the symbol for it. GO_1, GO_2, HGO_1 and HGO_2 of W_m^n are derived in the following theorem.

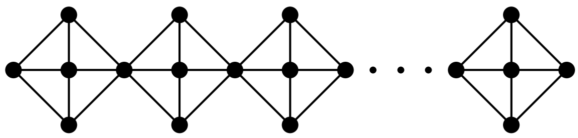

FIGURE 6. The graph W_4^n.

TABLE 4. Partitioning at the edge of W_m^n.

$d_{W_m^n}(a), d_{W_m^n}(b) : ab \in E(W_m^n)$	Edge count
$(3,3)$	$mn-4n+4$
$(3,6)$	$4(n-1)$
$(3,m)$	$mn-2n+2$
$(6,m)$	$2(n-1)$

Theorem 2.8. *For wheel chain W_m^n ($m \geq 3$, $n \geq 2$),*

1. $GO_1(W_m^n) = 4m^2n + 24mn + 54n - 6m - 54$.
2. $GO_2(W_m^n) = 3m^3n + 15m^2n - 6m^2 + 108mn + 432n - 54m - 432$.
3. $HGO_1(W_m^n) = 16m^3n + 354nm + 2070n + 90m^2n - 66m^2 - 120m - 2070$.
4. $HGO_2(W_m^n) = 9nm^5 + 108nm^4 + 837nm^3 + 2430nm^2 - 72m^4 - 864m^3$
$- 2592m^2 + 2916nm + 93312n - 93312$.

PROOF. 1. By making use the definition of GO_1 and values in Table 4, we have

$$\begin{aligned}
GO_1(W_m^n) &= \sum_{ab\in E(W_m^n)} \left[\left(d_{W_m^n}(a)+d_{W_m^n}(b)\right)+\left(d_{W_m^n}(a)d_{W_m^n}(b)\right)\right] \\
&= (mn-4n+4)[6+9]+4(n-1)[9+18] \\
&\quad +(mn-2n+2)[3+m+3m]+2(n-1)[6+m+6m] \\
&= 4m^2n+24mn+54n-6m-54.
\end{aligned}$$

2. By the usage of the definition of GO_2 and facts in Table 4, we have

$$\begin{aligned}
GO_2(W_m^n) &= \sum_{ab\in E(W_m^n)} \left[\left(d_{W_m^n}(a)+d_{W_m^n}(b)\right)\left(d_{W_m^n}(a)d_{W_m^n}(b)\right)\right] \\
&= (mn-4n+4)[6\times 9]+4(n-1)[9\times 18] \\
&\quad +(mn-2n+2)[(3+m)3m]+2(n-1)[(6+m)6m] \\
&= 3m^3n+15m^2n-6m^2+108mn+432n-54m-432.
\end{aligned}$$

3. By using the expression for HGO_1 and data in Table 4, we have

$$\begin{aligned}
HGO_1(W_m^n) &= \sum_{ab\in E(W_m^n)} \left[\left(d_{W_m^n}(a)+d_{W_m^n}(b)\right)+\left(d_{W_m^n}(a)d_{W_m^n}(b)\right)\right]^2 \\
&= (mn-4n+4)[6+9]^2+4(n-1)[9+18]^2 \\
&\quad +(mn-2n+2)[3+m+3m]^2+2(n-1)[6+m+6m]^2 \\
&= 16m^3n+354nm+2070n+90m^2n-66m^2-120m-2070.
\end{aligned}$$

4. By utilizing the description of HGO_2 and entries in Table 4, we have

$$\begin{aligned}
HGO_2(W_m^n) &= \sum_{ab\in E(W_m^n)} \left[\left(d_{W_m^n}(a)+d_{W_m^n}(b)\right)\left(d_{W_m^n}(a)d_{W_m^n}(b)\right)\right] \\
&= (mn-4n+4)[6\times 9]^2+4(n-1)[9\times 18]^2 \\
&\quad +(mn-2n+2)[(3+m)3m]^2+2(n-1)[(6+m)6m]^2 \\
&= 9nm^5+108nm^4+837nm^3+2430nm^2-72m^4-864m^3-2592m^2 \\
&\quad +2916nm+93312n-93312.
\end{aligned}$$

□

3. COMPARATIVE ANALYSIS

The plotting of GO_1, GO_2, HGO_1 and HGO_2 for the cactus graphs are shown in Figures 7 and 8. We have built the figures using Origin software taking m=4. $GO_1(C_m^n)$, $GO_1(C_m^n)$, $GO_1(CO_m^n)$, $GO_1(W_m^n)$, $GO_2(C_m^n)$, $GO_2(CO_m^n)$, $GO_2(W_m^n)$, $HGO_1(C_m^n)$, $HGO_1(CO_m^n)$, $HGO_1(W_m^n)$, $HGO_2(C_m^n)$, $HGO_2(CO_m^n)$

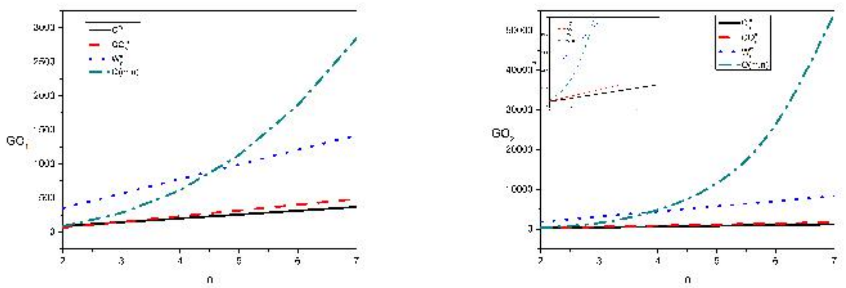

Figure 7. Plot of GO_1(left) and GO_2(right) for cactus chains.

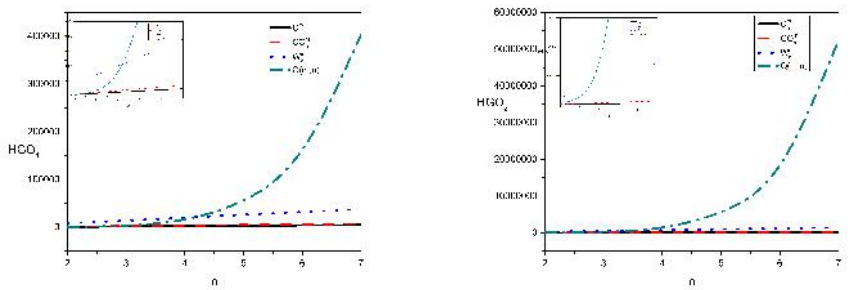

Figure 8. Plot of HGO_1(left) and HGO_2(right) for cactus chains.

and $HGO_2(W_m^n)$ are linearly increasing and $GO_1(Q(m,y))$, $GO_2(Q(m,y))$, HGO_1 $(Q(m,y))$ and $HGO_2(Q(m,y))$ are exponentially increasing.

4. CONCLUDING REMARKS

In this paper, para cactus chain, ortho cactus chain and wheel cactus chain are discussed and explicit expressions of GO_1, GO_2, HGO_1 and HGO_2 are derived for them.

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