

**ECCENTRICITY BASED ZAGREB INDICES
OF COPPER OXIDE CuO**

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Abstract: Graph theory has much advancement in the field of mathematical chemistry. Recently, chemical graph theory has become very popular among researchers because of its wide applications in mathematical chemistry. The molecular topological descriptors are the numerical invariants of a molecular graph and are very useful for predicting their bioactivity. A great variety of such indices are studied and used in theoretical chemistry, pharmaceutical researchers, in drugs and in different other fields. Among topological descriptor, connectivity indices are very important and they have a prominent role in chemistry. In this article, we study the chemical graph of copper oxide and compute the eccentricity based Zagreb indices for Copper oxide. Furthermore, we give analytically closed formulas of these indices which are helpful in studying the underlying topologies.

AMS Subject Classification: 05C12, 05C90

Key Words: molecular graph; eccentricity based Zagreb indices; first Zagreb index; second Zagreb index; third Zagreb index; Copper oxide

1. Introduction

There are a lot of chemical compounds, either organic or inorganic, which pos-

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sess a level of commercial, industrial, pharmaceutical chemistry and laboratory importance. A relationship exists between chemical compounds and their molecular structures. Graph theory is a very powerful area of mathematics that has wide range of applications in many areas of science such as chemistry, biology, computer science, electrical, electronics and other fields. Chemical graph theory is a branch of mathematical chemistry in which we apply tools of graph theory to model the chemical phenomenon mathematically. This theory contributes a prominent role in the field of chemical sciences. Some references are given, which hopefully demonstrate the importance of this field [6, 8, 9, 10, 12, 13, 14].

Let $G = (V, E)$ be a graph, where V is a non-empty set of vertices and E is a set of edges. The chemical graph theory applies graph theory to mathematical modeling of molecular phenomena, which is helpful for the study of molecular structure. This theory contributes a prominent role in the field of chemical sciences. Chemical compounds have a variety of applications in chemical graph theory, drug design, etc. A great variety of topological indices are studied and used in theoretical chemistry, pharmaceutical researchers. In chemical graph theory, there are many topological indices for a connected graph, which are helpful in study of chemical molecules. Development of chemical science had an important effect by this theory.

If $p, q \in V(G)$, then the distance $d(p, q)$ between p and q is defined as the length of any shortest path in G connecting p and q . Eccentricity is the distance of vertex u from the farthest vertex in G . In mathematical form,

$$\varepsilon(u) = \max\{d(u, v) | \forall u \in V(G)\}. \quad (1)$$

Recently in 2010, D. Vukičević et al., and in 2012, Ghorbani et al., proposed some new modified versions of Zagreb indices of a molecular graph G [7, 16].

These indices are eccentricity based indices, which are defined as

$$M_1^*(G) = \sum_{uv \in E(G)} [\varepsilon(u) + \varepsilon(v)],$$

$$M_1^{**}(G) = \sum_{v \in V(G)} [\varepsilon(v)]^2,$$

$$M_2^*(G) = \sum_{uv \in E(G)} \varepsilon(u)\varepsilon(v).$$

Some applications of eccentricity based Zagreb indices are given in [3, 4, 5, 17].

The Copper oxide/cupric oxide form an inorganic chemical compound CuO . This is an essential mineral found in plants and animals. Copper has enormous

applications in medical instruments, drugs, and as a heat conductor, among others. Some applications of Copper and Cupric oxide are given in [1, 11, 15].

In Fig. 1(a), the copper hydroxide is depicted and when hydrogen atoms are depleted from $Cu(OH)_2$ then the resultant graph is depicted in Fig. 1(b). The 3D graph of copper oxide CuO is depicted in Fig. 2. Copper oxide is used as the source of copper in mineral and vitamin supplements and is considered safe. Its use in medical devices, and industrial and consumer products, is novel. The safety aspects of the use of copper oxide in products that come into contact with open and closed skin must be considered [2].

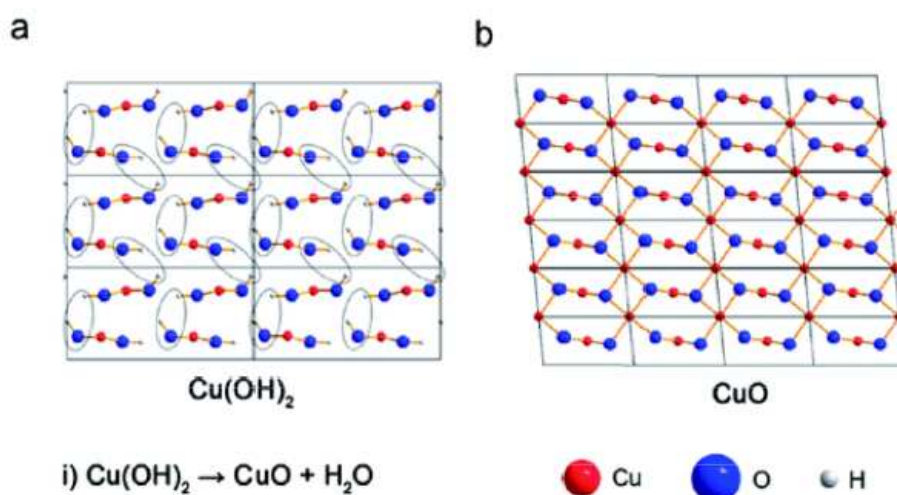


Figure 1: (a) $Cu(OH)_2$ (b) CuO

2. Main results and discussion

In this section, we discuss the first Zagreb eccentricity index $M_1^*(G)$, second Zagreb eccentricity index $M_1^{**}(G)$ and third Zagreb eccentricity index $M_2^*(G)$ of copper oxide. Here we consider the copper oxide graph $CuO = G$. In this article, we consider the copper oxide molecular graph CuO , as depicted in Fig. 1(b). The construction of the CuO graph is such that the octagons are connected to each other in columns and rows; the connection between two octagons is achieved by making one C_4 bond between two octagons. For our convenience, we take m and n as the number of octagons in rows and columns,

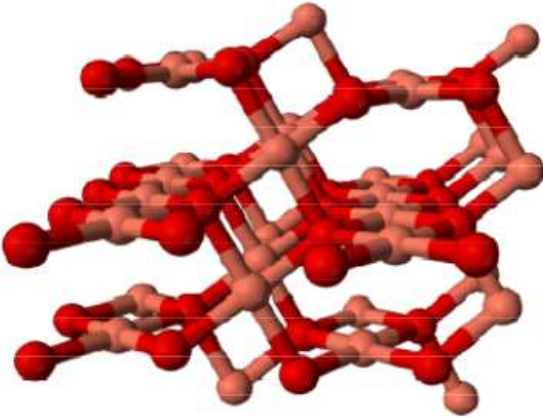


Figure 2: 3D Copper oxide CuO

respectively. The cardinality of vertices and edges in CuO are $4mn + 3n + m$ and $6mn + 2n$, respectively.

$(\varepsilon(u), \varepsilon(v))$	frequency	Range of k
$(4k + 2m, 4k + 2m + 1)$	$4m$	$\frac{n-m}{2} \leq k \leq \frac{2n-m-2}{2}$
$(4k + 2m + 1, 4k + 2m + 2)$	$2(m + 1)$	$\frac{n-m}{2} \leq k \leq \frac{2n-m-2}{2}$
$(4k + 2m + 2, 4k + 2m + 3)$	$2(m + 1)$	$\frac{n-m}{2} \leq k \leq \frac{2n-m-2}{2}$
$(4k + 2m + 3, 4k + 2m + 4)$	$4m$	$\frac{n-m}{2} \leq k \leq \frac{2n-m-2}{2}$

Table 1: Edge partition of Copper oxide for $((m, n)$ -levels) where m and n both are even and $m \geq 2$, $n \geq 2m$, based on eccentricity of end vertices of each edge with existence of their frequencies.

$(\varepsilon(u), \varepsilon(v))$	frequency	Range of k
$(4k + 2m, 4k + 2m + 1)$	$2(m + 1)$	$\frac{n-m}{2} \leq k \leq \frac{2n-m-1}{2}$
$(4k + 2m + 1, 4k + 2m + 2)$	$4m$	$\frac{n-m}{2} \leq k \leq \frac{2n-m-1}{2}$
$(4k + 2m + 2, 4k + 2m + 3)$	$4m$	$\frac{n-m}{2} \leq k \leq \frac{2n-m-3}{2}$
$(4k + 2m + 3, 4k + 2m + 4)$	$2(m + 1)$	$\frac{n-m}{2} \leq k \leq \frac{2n-m-3}{2}$

Table 2: Edge partition of Copper oxide for $((m, n)$ -levels) where m and n both are odd and $m \geq 1$, $n \geq 2m + 1$, based on eccentricity of end vertices of each edge with existence of their frequencies.

$(\varepsilon(u), \varepsilon(v))$	frequency	Range of m and n	Range of k
$(4k + 8, 4k + 9)$	$4m$	$m \geq 1, n \geq 2m$	$\frac{n-4}{2} \leq k \leq n - 3$
$(4k + 9, 4k + 10)$	$2(m + 1)$	$m \geq 1, n \geq 2m$	$\frac{n-4}{2} \leq k \leq n - 3$
$(4k + 10, 4k + 11)$	$2(m + 1)$	$m \geq 1, n \geq 2m$	$\frac{n-4}{2} \leq k \leq n - 3$
$(4k + 11, 4k + 12)$	$4m$	$m \geq 1, n \geq 2m$	$\frac{n-4}{2} \leq k \leq n - 3$

Table 3: Edge partition of Copper oxide for $((m, n)$ -levels) where m is odd and n is even, based on eccentricity of end vertices of each edge with existence of their frequencies.

$(\varepsilon(u), \varepsilon(v))$	frequency	Range of m and n	Range of k
$(4k + 6, 4k + 7)$	$2(m + 1)$	$m \geq 2, n > 2m$	$\frac{n-3}{2} \leq k \leq n - 2$
$(4k + 7, 4k + 8)$	$4m$	$m \geq 2, n > 2m$	$\frac{n-3}{2} \leq k \leq n - 2$
$(4k + 8, 4k + 9)$	$4m$	$m \geq 2, n > 2m$	$\frac{n-3}{2} \leq k \leq n - 3$
$(4k + 9, 4k + 10)$	$2(m + 1)$	$m \geq 2, n > 2m$	$\frac{n-3}{2} \leq k \leq n - 3$

Table 4: Edge partition of Copper oxide for $((m, n)$ -levels) where m is even and n is odd, based on eccentricity of end vertices of each edge with existence of their frequencies.

$\varepsilon(u)$	frequency	Range of m and n	Range of k
k	m	$m \geq 2, n \geq 2m$	$k = 2n$
$4k + 2m + 1$	$2(m + 1)$	$m \geq 2, n \geq 2m$	$\frac{n-m}{2} \leq k \leq \frac{2n-m-2}{2}$
$4k + 2m + 2$	$2(m + 1)$	$m \geq 2, n \geq 2m$	$\frac{n-m}{2} \leq k \leq \frac{2n-m-2}{2}$
$4k + 2m + 3$	$2(m + 1)$	$m \geq 2, n \geq 2m$	$\frac{n-m}{2} \leq k \leq \frac{2n-m-2}{2}$
$4k + 2m + 4$	$2m$	$m \geq 2, n \geq 2m$	$\frac{n-m}{2} \leq k \leq \frac{2n-m-2}{2}$

Table 5: Vertex partition of Copper oxide for $((m, n)$ -levels) where m and n both are even, based on eccentricity of each vertex with existence of their frequencies.

2.1. Eccentricity based first Zagreb index

In this section we find the first Zagreb eccentricity index of Copper oxide $M_1^*(G(m, n))$.

Theorem 1. *Let $G(m, n)$ for all $m, n \in N$, where m and n both are even, be the copper oxide, then the first Zagreb eccentricity index of $G(m, n)$ is*

$\varepsilon(u)$	frequency	Range of m and n	Range of k
k	$m + 1$	$m \geq 1, n \geq 2m + 1$	$k = 2n$
$4k + 2m + 1$	$2(m + 1)$	$m \geq 1, n \geq 2m + 1$	$\frac{n-m}{2} \leq k \leq \frac{2n-m-1}{2}$
$4k + 2m + 2$	$2m$	$m \geq 1, n \geq 2m + 1$	$\frac{n-m}{2} \leq k \leq \frac{2n-m-1}{2}$
$4k + 2m + 3$	$2(m + 1)$	$m \geq 1, n \geq 2m + 1$	$\frac{n-m}{2} \leq k \leq \frac{2n-m-3}{2}$
$4k + 2m + 4$	$2(m + 1)$	$m \geq 1, n \geq 2m + 1$	$\frac{n-m}{2} \leq k \leq \frac{2n-m-3}{2}$

Table 6: Vertex partition of Copper oxide for $((m, n)$ -levels) where m and n both are odd, based on eccentricity of each vertex with existence of their frequencies.

$\varepsilon(u)$	frequency	Range of m and n	Range of k
k	m	$m \geq 1, n \geq 2m$	$k = 2n$
$4k + 9$	$2(m + 1)$	$m \geq 1, n \geq 2m$	$\frac{n-4}{2} \leq k \leq n - 3$
$4k + 10$	$2(m + 1)$	$m \geq 1, n \geq 2m$	$\frac{n-4}{2} \leq k \leq n - 3$
$4k + 11$	$2(m + 1)$	$m \geq 1, n \geq 2m$	$\frac{n-4}{2} \leq k \leq n - 3$
$4k + 12$	$2m$	$m \geq 1, n \geq 2m$	$\frac{n-4}{2} \leq k \leq n - 3$

Table 7: Vertex partition of Copper oxide for $((m, n)$ -levels) where m is odd and n is even, based on eccentricity of each vertex with existence of their frequencies.

$\varepsilon(u)$	frequency	Range of m and n	Range of k
k	$m + 1$	$m \geq 2, n > 2m$	$k = 2n$
$4k + 7$	$2(m + 1)$	$m \geq 2, n > 2m$	$\frac{n-3}{2} \leq k \leq n - 2$
$4k + 8$	$2m$	$m \geq 2, n > 2m$	$\frac{n-3}{2} \leq k \leq n - 2$
$4k + 9$	$2(m + 1)$	$m \geq 2, n > 2m$	$\frac{n-3}{2} \leq k \leq n - 3$
$4k + 10$	$2(m + 1)$	$m \geq 2, n > 2m$	$\frac{n-3}{2} \leq k \leq n - 3$

Table 8: Vertex partition of Copper oxide for $((m, n)$ -levels) where m is even and n is odd, based on eccentricity of each vertex with existence of their frequencies.

$$M_1^*(G(m, n)) = 16 \sum_{m \geq 2} \{(3m + 1) \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-2}{2}} (2k + m + 1)\}.$$

Proof. Let $G(m, n)$, where m and n both are even, be the Copper oxide containing $4mn + 3n + m$ vertices and $6mn + 2n$ edges.

The formula of the first Zagreb eccentricity index is

$$M_1^*(G) = \sum_{uv \in E(G)} [\varepsilon(u) + \varepsilon(v)].$$

Using the edge partitioned from Table 1, we have the following computations:

$$\begin{aligned} M_1^*(G(m, n)) &= \sum_{m \geq 2} \left\{ 2(m+1) \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-2}{2}} ((4k+2m+1) + (4k+2m+2) + (4k+2m+2+4k+2m+3)) + 4m \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-4}{2}} ((4k+2m+3) + (4k+2m+4) + (4k+2m+4k+2m+1)) \right\} \\ &= \sum_{m \geq 2} \left\{ 2(m+1) \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-2}{2}} ((8k+4m+3) + (8k+4m+5)) + 4m \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-4}{2}} ((8k+4m+7) + (8k+4m+1)) \right\} \\ &= \sum_{m \geq 2} \left\{ 2(m+1) \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-2}{2}} (16k+8m+8) + 4m \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-4}{2}} (16k+8m+8) \right\}. \end{aligned}$$

After some simplification, we have

$$M_1^*(G(m, n)) = 16 \sum_{m \geq 2} \left\{ (3m+1) \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-2}{2}} (2k+m+1) \right\}. \quad \square$$

Theorem 2. Let $G(m, n)$, for all $m, n \in N$, where m and n both are odd, be the copper oxide, then the eccentricity based first zagreb index M_1^* of $G(m, n)$ is:

$$\begin{aligned} M_1^*(G(m, n)) &= 2 \sum_{m \geq 1} \left\{ \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-1}{2}} (12m(2k+m) + 11m + 8k + 1) \right. \\ &\quad \left. + \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-3}{2}} (12m(2k+m) + 21m + 8k + 7) \right\}. \end{aligned}$$

Proof. Let $G(m, n)$, where m and n both are odd, be the Copper oxide containing $4mn + 3n + m$ vertices and $6mn + 2n$ edges.

The formula of the first Zagreb eccentricity index is

$$M_1^*(G) = \sum_{uv \in E(G)} [\varepsilon(u) + \varepsilon(v)].$$

Using the edge partitioned from Table 2, we have the following computations:

$$M_1^*(G(m, n)) = \sum_{m \geq 1} \left\{ \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-1}{2}} (2(m+1)(4k+2m+4k+2m+1) + 4m(4k + \right.$$

$$\begin{aligned}
& 2m+1+4k+2m+2)) + \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-3}{2}} (4m(4k+2m+2+4k+2m+3) + 2(m+1)(4k+2m+3+4k+2m+4))\} \\
&= \sum_{m \geq 1} \{ \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-1}{2}} (2(m+1)(8k+4m+1) + 4m(8k+4m+3)) + \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-3}{2}} (4m(8k+4m+5) + 2(m+1)(8k+4m+7)) \} \\
&= 2 \sum_{m \geq 1} \{ \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-1}{2}} ((m+1)(8k+4m+1) + 2m(8k+4m+3)) + \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-3}{2}} (2m(8k+4m+5) + (m+1)(8k+4m+7)) \}.
\end{aligned}$$

After some simplification, we have

$$\begin{aligned}
M_1^*(G(m, n)) &= 2 \sum_{m \geq 1} \{ \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-1}{2}} (12m(2k+m) + 11m + 8k + 1) \\
&+ \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-3}{2}} (12m(2k+m) + 21m + 8k + 7) \}. \quad \square
\end{aligned}$$

Theorem 3. Let $G(m, n)$, for all $m, n \in N$, where m is odd and n is even, be the copper oxide, then the eccentricity based first zagreb index M_1^* of $G(m, n)$ is:

$$M_1^*(G(m, n)) = 16 \sum_{m \geq 1} \{ (3m+1) \sum_{k=\frac{n-4}{2}}^{n-3} (2k+5) \}.$$

Proof. Let $G(m, n)$, where m is odd and n is even, be the Copper oxide contains $4mn + 3n + m$ vertices and $6mn + 2n$ edges.

The formula of the first Zagreb eccentricity index is

$$M_1^*(G) = \sum_{uv \in E(G)} [\varepsilon(u) + \varepsilon(v)].$$

Using the edge partitioned from Table 3, we have the following computations:

$$\begin{aligned}
M_1^*(G(m, n)) &= \sum_{m \geq 1} \{ \sum_{k=\frac{n-4}{2}}^{n-3} (2(m+1)(4k+9+4k+10) + 2(m+1)(4k+10+4k+11)) + \sum_{k=\frac{n-4}{2}}^{n-3} (4m(4k+11+4k+12) + 4m(4k+8+4k+9)) \} \\
&= \sum_{m \geq 1} \{ \sum_{k=\frac{n-4}{2}}^{n-3} (2(m+1)(4k+9+4k+10+4k+10+4k+11)) + \sum_{k=\frac{n-4}{2}}^{n-3} (4m(4k+11+4k+12+4k+8+4k+9)) \} \\
&= \sum_{m \geq 1} \{ \sum_{k=\frac{n-4}{2}}^{n-3} (2(m+1)(16k+40)) + \sum_{k=\frac{n-4}{2}}^{n-3} (4m(16k+40)) \}
\end{aligned}$$

$$= \sum_{m \geq 1} \{(2(m+1) + 4m) \sum_{k=\frac{n-4}{2}}^{n-3} 8(2k+5)\}.$$

Finally, for all $m, n \in N$, where m is odd and n is even, the eccentricity based first zagreb index of copper oxide $G(m, n)$ is

$$M_1^*(G(m, n)) = 16 \sum_{m \geq 1} \{(3m+1) \sum_{k=\frac{n-4}{2}}^{n-3} (2k+5)\}. \quad \square$$

Theorem 4. Let $G(m, n)$, for all $m, n \in N$, where m is even and n is odd, be the copper oxide, then the eccentricity based first Zagreb index M_1^* of $G(m, n)$ is

$$M_1^*(G(m, n)) = 2 \sum_{m \geq 2} \left\{ \sum_{k=\frac{n-3}{2}}^{n-2} (8k(3m+1) + 43m + 13) + \sum_{k=\frac{n-3}{2}}^{n-3} (8k(3m+1) + 53m + 19) \right\}.$$

Proof. Let $G(m, n)$, where m is even and n is odd, be the copper oxide contains $4mn + 3n + m$ vertices and $6mn + 2n$ edges.

The formula of the first Zagreb eccentricity index is

$$M_1^*(G) = \sum_{uv \in E(G)} [\varepsilon(u) + \varepsilon(v)].$$

Using the edge partitioned from Table 4, we have the following computations:

$$\begin{aligned} M_1^*(G(m, n)) &= \sum_{m \geq 1} \left\{ \sum_{k=\frac{n-3}{2}}^{n-2} (2(m+1)(4k+6+4k+7) + 4m(4k+7+4k+8)) + \sum_{k=\frac{n-3}{2}}^{n-3} (4m(4k+8+4k+9) + 2(m+1)(4k+9+4k+10)) \right\} \\ &= \sum_{m \geq 1} \left\{ \sum_{k=\frac{n-3}{2}}^{n-2} (2(m+1)(8k+13) + 4m(8k+15)) + \sum_{k=\frac{n-3}{2}}^{n-3} (4m(8k+17) + 2(m+1)(8k+19)) \right\} \\ &= \sum_{m \geq 1} \left\{ 2 \sum_{k=\frac{n-3}{2}}^{n-2} (8km + 13m + 8k + 13 + 16km + 30m) + 2 \sum_{k=\frac{n-3}{2}}^{n-3} (16km + 34m + 8km + 19m + 8k + 19) \right\} \\ &= 2 \sum_{m \geq 1} \left\{ \sum_{k=\frac{n-3}{2}}^{n-2} (24km + 43m + 8k + 13) + \sum_{k=\frac{n-3}{2}}^{n-3} (24km + 53m + 8k + 19) \right\}. \end{aligned}$$

Finally, for all $m, n \in N$, where m is even and n is odd, the eccentricity based first zagreb index of copper oxide $G(m, n)$ is

$$M_1^*(G(m, n)) = 2 \sum_{m \geq 2} \left\{ \sum_{k=\frac{n-3}{2}}^{n-2} (8k(3m+1) + 43m + 13) \right. \\ \left. + \sum_{k=\frac{n-3}{2}}^{n-3} (8k(3m+1) + 53m + 19) \right\}.$$

□

2.2. Eccentricity based second Zagreb index

In this section we find the second Zagreb eccentricity index of the Copper oxide $G(m, n)$ which is denoted by $M_1^{**}(G(m, n))$.

Theorem 5. *Let $G(m, n)$, for all $m, n \in N$, where m and n both are even, be the copper oxide, then the eccentricity based second zagreb index M_1^{**} of $G(m, n)$ is*

$$M_1^{**}(G(m, n)) = \sum_{m \geq 2} \left\{ 4mn^2 + 4 \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-2}{2}} (2(2k+m)^2(4m+3) + 4(2k+m)(5m+3) + 15m + 7) \right\}.$$

Proof. Let $G(m, n)$, where m and n both are even, be the copper oxide contains $4mn + 3n + m$ vertices and $6mn + 2n$ edges.

The general formula of second Zagreb eccentricity index is

$$M_1^{**}(G) = \sum_{v \in V(G)} [\varepsilon(v)]^2.$$

Using the edge partitioned from Table 5, we have the following computations:

$$\begin{aligned} M_1^{**}(G(m, n)) &= \sum_{m \geq 2} \left\{ m \sum_{k=2n} (k)^2 + 2(m+1) \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-2}{2}} ((4k+2m+1)^2 + (4k+2m+2)^2 + (4k+2m+3)^2) \right. \\ &\quad \left. + 2m \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-2}{2}} (4k+2m+4)^2 \right\} \\ &= \sum_{m \geq 2} \left\{ m(2n)^2 + 2 \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-2}{2}} ((m+1)(48k^2 + 12m^2 + 48km + 48k + 24m + 14) + m(16k^2 + 4m^2 + 16 + 16km + 32k + 16m)) \right\} \\ &= \sum_{m \geq 2} \left\{ 4mn^2 + 2 \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-2}{2}} (m(64k^2 + 16m^2 + 64km + 80k + 40m + 30) + (48k^2 + 12m^2 + 48km + 48k + 24m + 14)) \right\} \\ &= \sum_{m \geq 2} \left\{ 4mn^2 + 2 \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-2}{2}} (m(16(2k+m)^2 + 40(2k+m) + 30) + 12(2k+m)^2 + 24(2k+m) + 14) \right\}. \end{aligned}$$

After some simplification, we have

$$M_1^{**}(G(m, n)) = \sum_{m \geq 2} \{4mn^2 + 4 \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-2}{2}} (2(2k+m)^2(4m+3) + 4(2k+m)(5m+3) + 15m + 7)\}. \quad \square$$

Theorem 6. Let $G(m, n)$, for all $m, n \in N$, where m and n both are odd, be the Copper oxide, then the eccentricity based second Zagreb index M_1^{**} of $G(m, n)$ is

$$M_1^{**}(G(m, n)) = 2 \sum_{m \geq 1} \{2n^2(m+1) + \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-1}{2}} (8(2k+m)^2 + 12(2k+m) + 5 + (4k+2m+1)^2) + (m+1) \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-3}{2}} (8(2k+m)^2 + 28(2k+m) + 25)\}.$$

Proof. Let $G(m, n)$, where m and n both are odd, be the copper oxide contains $4mn + 3n + m$ vertices and $6mn + 2n$ edges.

The general formula of second Zagreb eccentricity index is

$$M_1^{**}(G) = \sum_{v \in V(G)} [\varepsilon(v)]^2.$$

Using the edge partitioned from Table 6, we have the following computations:

$$\begin{aligned} M_1^{**}(G(m, n)) &= \sum_{m \geq 1} \{(m+1) \sum_{k=2n} (k)^2 + \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-1}{2}} (2(m+1)(4k+2m+1)^2 + 2m(4k+2m+2)^2) + 2(m+1) \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-3}{2}} ((4k+2m+3)^2 + (4k+2m+4)^2)\} \\ &= \sum_{m \geq 1} \{(m+1)(2n)^2 + \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-1}{2}} (2m(4k+2m+1)^2 + 8m(2k+m+1)^2 + 2(4k+2m+1)^2) + 2(m+1) \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-3}{2}} ((4k+2m+3)^2 + 4(2k+m+2)^2)\} \\ &= 2 \sum_{m \geq 1} \{2n^2(m+1) + \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-1}{2}} (m(32k^2 + 8m^2 + 32km + 24k + 12m + 5) + (4k+2m+1)^2) + (m+1) \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-3}{2}} (32k^2 + 8m^2 + 32km + 56k + 28m + 25)\}. \end{aligned}$$

After some simplification, we have

$$M_1^{**}(G(m, n)) = 2 \sum_{m \geq 1} \{2n^2(m+1) + \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-1}{2}} (8(2k+m)^2 + 12(2k+m) + 5 + (4k+2m+1)^2) + (m+1) \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-3}{2}} (8(2k+m)^2 + 28(2k+m) + 25)\}. \quad \square$$

Theorem 7. Let $G(m, n)$, for all $m, n \in N$, where m is odd and n is even, be the Copper oxide, then the eccentricity based second Zagreb index M_1^{**} of $G(m, n)$ is

$$M_1^{**}(G(m, n)) = 4 \sum_{m \geq 1} \{mn^2 + \sum_{k=\frac{n-4}{2}}^{n-3} (m(32k^2 + 168k + 223) + 24k^2 + 120k + 151)\}.$$

Proof. Let $G(m, n)$, where m is odd and n is even, be the Copper oxide contains $4mn + 3n + m$ vertices and $6mn + 2n$ edges.

The general formula of second Zagreb eccentricity index is

$$M_1^{**}(G) = \sum_{v \in V(G)} [\varepsilon(v)]^2.$$

Using the edge partitioned from Table 7, we have the following computations:

$$\begin{aligned} M_1^{**}(G(m, n)) &= \sum_{m \geq 1} \{m \sum_{k=2n} (k)^2 + 2(m+1) \sum_{k=\frac{n-4}{2}}^{n-3} ((4k+9)^2 + (4k+10)^2 + (4k+11)^2) + 2m \sum_{k=\frac{n-4}{2}}^{n-3} (4k+12)^2\} \\ &= \sum_{m \geq 1} \{m(2n)^2 + 2 \sum_{k=\frac{n-4}{2}}^{n-3} ((m+1)(48k^2 + 240k + 302) + m(16k^2 + 144 + 96k))\} \\ &= \sum_{m \geq 1} \{4mn^2 + 2 \sum_{k=\frac{n-4}{2}}^{n-3} (m(48k^2 + 240k + 302 + 16k^2 + 144 + 96k) + 48k^2 + 240k + 302)\} \\ &= \sum_{m \geq 1} \{4mn^2 + 2 \sum_{k=\frac{n-4}{2}}^{n-3} (m(64k^2 + 336k + 446) + 2(24k^2 + 120k + 151))\}. \end{aligned}$$

After some simplification, we have

$$M_1^{**}(G(m, n)) = 4 \sum_{m \geq 1} \{mn^2 + \sum_{k=\frac{n-4}{2}}^{n-3} (m(32k^2 + 168k + 223) + 24k^2 + 120k + 151)\}.$$

□

Theorem 8. Let $G(m, n)$, for all $m, n \in N$, where m is even and n is odd, be the Copper oxide, then the eccentricity based second Zagreb index M_1^{**} of $G(m, n)$ is

$$M_1^{**}(G(m, n)) = 2 \sum_{m \geq 2} \{2n^2(m+1) + \sum_{k=\frac{n-3}{2}}^{n-2} (m(32k^2 + 120k + 113) + (4k+7)^2) + (m+1) \sum_{k=\frac{n-3}{2}}^{n-3} (32k^2 + 152k + 181)\}.$$

Proof. Let $G(m, n)$, where m is even and n is odd, be the Copper oxide contains $4mn + 3n + m$ vertices and $6mn + 2n$ edges.

The general formula of second Zagreb eccentricity index is

$$M_1^{**}(G) = \sum_{v \in V(G)} [\varepsilon(v)]^2.$$

Using the edge partitioned from Table 8, we have the following computations:

$$\begin{aligned} M_1^{**}(G(m, n)) &= \sum_{m \geq 2} \{ (m+1) \sum_{k=2n} (k)^2 + \sum_{k=\frac{n-3}{2}}^{n-2} (2(m+1)(4k+7)^2 + 2m(4k+8)^2) + 2(m+1) \sum_{k=\frac{n-3}{2}}^{n-3} ((4k+9)^2 + (4k+10)^2) \} \\ &= \sum_{m \geq 2} \{ (m+1)(2n)^2 + 2 \sum_{k=\frac{n-3}{2}}^{n-2} (m((4k+7)^2 + (4k+8)^2) + (4k+7)^2) + 2(m+1) \sum_{k=\frac{n-3}{2}}^{n-3} (16k^2 + 72k + 81 + 16k^2 + 80k + 100) \} \\ &= \sum_{m \geq 2} \{ 4n^2(m+1) + 2 \sum_{k=\frac{n-3}{2}}^{n-2} (m((16k^2 + 49 + 56k + 16k^2 + 64 + 64k) + (4k+7)^2) + 2(m+1) \sum_{k=\frac{n-3}{2}}^{n-3} (32k^2 + 152k + 181)) \} \\ &= \sum_{m \geq 2} \{ 4n^2(m+1) + 2 \sum_{k=\frac{n-3}{2}}^{n-2} (m((32k^2 + 120k + 113) + (4k+7)^2) + 2(m+1) \sum_{k=\frac{n-3}{2}}^{n-3} (32k^2 + 152k + 181)) \}. \end{aligned}$$

After some simplification, we have

$$M_1^{**}(G(m, n)) = 2 \sum_{m \geq 2} \{ 2n^2(m+1) + \sum_{k=\frac{n-3}{2}}^{n-2} (m(32k^2 + 120k + 113) + (4k+7)^2) + (m+1) \sum_{k=\frac{n-3}{2}}^{n-3} (32k^2 + 152k + 181) \}. \quad \square$$

2.3. Eccentricity based third Zagreb index

In this section we find the third Zagreb eccentricity index of the Copper oxide $G(m, n)$ which is denoted by $M_2^*(G(m, n))$.

Theorem 9. *Let $G(m, n)$, for all $m, n \in N$, where m and n both are even, be the copper oxide, then the eccentricity based third zagreb index M_2^* of $G(m, n)$ is*

$$M_2^*(G(m, n)) = 16 \sum_{m \geq 2} \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-2}{2}} \{ m(3(2k+m)^2 + 6(2k+m) + 4) + (2k+m+1)^2 \}.$$

Proof. Let $G(m, n)$, where m and n both are even, be the Copper oxide contains $4mn + 3n + m$ vertices and $6mn + 2n$ edges.

The general formula of third Zagreb eccentricity index is

$$M_2^*(G) = \sum_{uv \in E(G)} [\varepsilon(u) \cdot \varepsilon(v)].$$

Using the edge partitioned from Table 1, we have the following computations:

$$\begin{aligned} ABC_5(G(m, n)) &= \sum_{m \geq 2} \left\{ 2(m+1) \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-2}{2}} ((4k+2m+1)(4k+2m+2) + (4k+2m+2)(4k+2m+3)) \right. \\ &\quad \left. + 4m \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-2}{2}} ((4k+2m+3)(4k+2m+4) + (4k+2m)(4k+2m+1)) \right\} \\ &= \sum_{m \geq 2} \left\{ 2(m+1) \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-2}{2}} (4k+2m+2)(4k+2m+1+4k+2m+3) + \right. \\ &\quad \left. 8m \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-2}{2}} ((4k+2m+3)(2k+m+2) + (2k+m)(4k+2m+1)) \right\} \\ &= \sum_{m \geq 2} \left\{ 16(m+1) \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-2}{2}} (2k+m+1)(2k+m+1) \right. \\ &\quad \left. + 8m \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-2}{2}} (16k^2 + 16km + 16k + 4m^2 + 8m + 6) \right\}. \end{aligned}$$

After some simplification, we have

$$M_2^*(G(m, n)) = 16 \sum_{m \geq 2} \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-2}{2}} \{m(3(2k+m)^2 + 6(2k+m) + 4) + (2k+m+1)^2\}. \quad \square$$

Theorem 10. Let $G(m, n)$, for all $m, n \in N$, where m and n both are odd, be the copper oxide, then the eccentricity based third zagreb index M_2^* of $G(m, n)$ is

$$M_2^* = 4 \sum_{m \geq 1} \left\{ \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-1}{2}} (4k+2m+1)(6km+3m^2+2k+3m) + \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-3}{2}} (4k+2m+3)(6km+3m^2+2k+5m+2) \right\}.$$

Proof. Let $G(m, n)$, where m and n both are odd, be the Copper oxide contains $4mn + 3n + m$ vertices and $6mn + 2n$ edges.

The general formula of third Zagreb eccentricity index is

$$M_2^*(G) = \sum_{uv \in E(G)} [\varepsilon(u) \cdot \varepsilon(v)].$$

Using the edge partitioned from Table 2, we have the following computations:

$$\begin{aligned}
 M_2^*(G(m, n)) &= \sum_{m \geq 1} \left\{ \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-1}{2}} (2(m+1)(4k+2m)(4k+2m+1) + 4m(4k+2m+1)(4k+2m+2)) \right. \\
 &\quad \left. + \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-3}{2}} (4m(4k+2m+2)(4k+2m+3) + 2(m+1)(4k+2m+3)(4k+2m+4)) \right\} \\
 &= \sum_{m \geq 1} \left\{ \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-1}{2}} (4(m+1)(2k+m)(4k+2m+1) + 8m(4k+2m+1)(2k+m+1)) \right. \\
 &\quad \left. + \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-3}{2}} (8m(2k+m+1)(4k+2m+3) + 4(m+1)(4k+2m+3)(2k+m+2)) \right\} \\
 &= 4 \sum_{m \geq 1} \left\{ \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-1}{2}} ((4k+2m+1)(2km+m^2+2k+m+4km+2m^2+2m)) \right. \\
 &\quad \left. + \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-3}{2}} ((4k+2m+3)(4km+2m^2+2km+2m+m^2+2m+2k+m+2)) \right\}.
 \end{aligned}$$

After some simplification, we have

$$M_2^* = 4 \sum_{m \geq 1} \left\{ \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-1}{2}} (4k+2m+1)(6km+3m^2+2k+3m) + \sum_{k=\frac{n-m}{2}}^{\frac{2n-m-3}{2}} (4k+2m+3)(6km+3m^2+2k+5m+2) \right\}. \quad \square$$

Theorem 11. Let $G(m, n)$, for all $m, n \in N$, where m is odd and n is even, be the Copper oxide, then the eccentricity based third Zagreb index M_2^* of $G(m, n)$ is

$$M_2^*(G(m, n)) = 16 \sum_{m \geq 1} \sum_{k=\frac{n-4}{2}}^{n-3} \{4m(3k^2 + 15k + 19) + (2k + 5)^2\}.$$

Proof. Let $G(m, n)$, where m is odd and n is even, be the Copper oxide contains $4mn + 3n + m$ vertices and $6mn + 2n$ edges. The general formula of third Zagreb eccentricity index is

$$M_2^*(G) = \sum_{uv \in E(G)} [\varepsilon(u) \cdot \varepsilon(v)].$$

Using the edge partitioned from Table 3, we have the following computations:

$$\begin{aligned}
 M_2^*(G(m, n)) &= \sum_{m \geq 1} \left\{ 2(m+1) \sum_{k=\frac{n-4}{2}}^{n-3} ((4k+9)(4k+10) + (4k+10)(4k+11)) \right. \\
 &\quad \left. + 4m \sum_{k=\frac{n-4}{2}}^{n-3} ((4k+11)(4k+12) + (4k+8)(4k+9)) \right\} \\
 &= \sum_{m \geq 1} \sum_{k=\frac{n-4}{2}}^{n-3} \{2(m+1)(4k+10)(8k+20) + 4m((4k+11)4(k+3) + 4(k+2)(4k+9))\}
 \end{aligned}$$

$$\begin{aligned}
&= \sum_{m \geq 1} \sum_{k=\frac{n-4}{2}}^{n-3} \{16(m+1)(4k^2 + 20k + 25) + 16m(4k^2 + 11k + 12k + 33 + 4k^2 + 8k + 9k + 18)\} \\
&= 16 \sum_{m \geq 1} \sum_{k=\frac{n-4}{2}}^{n-3} \{(m+1)(4k^2 + 20k + 25) + m(8k^2 + 40k + 51)\}.
\end{aligned}$$

After some simplification, we have

$$M_2^*(G(m, n)) = 16 \sum_{m \geq 1} \sum_{k=\frac{n-4}{2}}^{n-3} \{4m(3k^2 + 15k + 19) + (2k + 5)^2\}. \quad \square$$

Theorem 12. Let $G(m, n)$, for all $m, n \in N$, where m is even and n is odd, be the copper oxide, then the eccentricity based third zagreb index M_2^* of $G(m, n)$ is

$$\begin{aligned}
M_2^*(G(m, n)) &= 4 \sum_{m \geq 2} \left\{ \sum_{k=\frac{n-3}{2}}^{n-2} (m(24k^2 + 86k + 77) + 8k^2 + 26k + 21) + \right. \\
&\quad \left. \sum_{k=\frac{n-3}{2}}^{n-3} (m(24k^2 + 106k + 117) + 8k^2 + 38k + 45) \right\}.
\end{aligned}$$

Proof. Let $G(m, n)$, where m is even and n is odd, be the Copper oxide contains $4mn + 3n + m$ vertices and $6mn + 2n$ edges.

The general formula of third Zagreb eccentricity index is

$$M_2^*(G) = \sum_{uv \in E(G)} [\varepsilon(u) \cdot \varepsilon(v)].$$

Using the edge partitioned from Table 4, we have the following computations:

$$\begin{aligned}
M_2^*(G(m, n)) &= \sum_{m \geq 2} \left\{ \sum_{k=\frac{n-3}{2}}^{n-2} (2(m+1)(4k+6)(4k+7) + 4m(4k+7)(4k+8)) \right. \\
&\quad \left. + \sum_{k=\frac{n-3}{2}}^{n-3} (4m(4k+8)(4k+9) + 2(m+1)(4k+9)(4k+10)) \right\} \\
&= \sum_{m \geq 2} \left\{ \sum_{k=\frac{n-3}{2}}^{n-2} (4(m+1)(2k+3)(4k+7) + 16m(4k+7)(k+2)) \right. \\
&\quad \left. + \sum_{k=\frac{n-3}{2}}^{n-3} (16m(k+2)(4k+9) + 4(m+1)(4k+9)(2k+5)) \right\} \\
&= \sum_{m \geq 2} \left\{ 4 \sum_{k=\frac{n-3}{2}}^{n-2} ((4k+7)((m+1)(2k+3) + 4m(k+2))) \right. \\
&\quad \left. + 4 \sum_{k=\frac{n-3}{2}}^{n-3} ((4k+9)(4m(k+2) + (m+1)(2k+5))) \right\}.
\end{aligned}$$

After some simplification, we have

$$\begin{aligned}
M_2^*(G(m, n)) &= 4 \sum_{m \geq 2} \left\{ \sum_{k=\frac{n-3}{2}}^{n-2} (m(24k^2 + 86k + 77) + 8k^2 + 26k + 21) + \right. \\
&\quad \left. \sum_{k=\frac{n-3}{2}}^{n-3} (m(24k^2 + 106k + 117) + 8k^2 + 38k + 45) \right\}. \quad \square
\end{aligned}$$

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