Computing Revan polynomials and Revan indices of copper (I) oxide and copper (II) oxide

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ABSTRACT

The topological index shows some of the properties of the molecule. One of the practical tools for computing topological indices is to use polynomials of that index. Therefore, from a computational and mathematical point of view, determining polynomials of topological indices is very important.

In this article, first, Revan polynomials are computed for molecular graph of copper (I) oxide Cu_2O (m, n) and copper (II) oxide CuO (m, n). Then, using Revan polynomials, Revan indices are obtained. To compare the obtained values, the diagrams are drawn.

KEYWORDS: Molecular graph, Revan Polynomials, Revan indices, Copper oxide.

1 INTRODUCTION

Graph theory is used in chemistry for modelling. The chemical graph of a molecule is obtained by assuming its atoms as vertices and its chemical bonds as edges. Graph theory provides a variety of valuable tools for chemists, including topological indices.

In a molecular graph, the topological index is expressed as a real number, and this number is attributed to the graphs, uniform with that molecule.

The topological index shows some of the properties of the molecule and is one of the practical tools in studying the structure and properties of a molecule such as: boiling point, evaporation heat, surface tension, vapor pressure, etc.

Copper (I) oxide has many applications as a semiconductor. many semiconductor applications such as semiconductor diodes and phonoritons have been shown for the first time in this material [3-5]. Copper (I) oxide has many applications and is used as a pigment, fungicide and anti-fouling agent for marine paints. Copper oxide (I) is also responsible for the pink color in Benedict's positive test.

Copper (II) oxide is a solid mineral compound with the formula CuO and is the raw material of many products containing copper and chemical compounds. Copper (II) oxide as an important product is the starting point for the production of other copper salts and has many applications in the production of wood preservatives, the production of colored glazes in ceramics, feed additives in animal feed, welding with copper alloys and etc[2][7].

Topological indices can be computed using mathematical operations on polynomials. Next, Revan polynomials are obtained for copper (I) oxide and copper (II) oxide and then, with the help of mathematical relations, Revan indices are also computed.

2 PRELIMINARIES

This section provides some of the required definitions. Suppose G = (V, E) is a simple and connected graph. We represent the set of edges with E(G) and the number of edges with $|E(G)|$ and the set of vertices with V (G) and the number of vertices with $|V(G)|$. We denote the degree of vertex u by d_u and If there is an edge between two vertices u and v, denoted it by $uv \in E(G)$. In graph G, we denote the minimum vertex degree by $\delta(G)$ and the maximum vertex degree by $\Delta(G)$.

The first and second Indices of Zagreb were first introduced by Guttman et al. These Indices have been used as branching Indices. Zagreb indices have found many applications in QSPR and QSAR studies [1].

Motivated by the definitions of Zagreb indices and their wide applications, Revan indices for graph G were defined by V.R. Kulli in 2017 [6].

The degree of Revan for vertex u in graph G is expressed as follows:

$$r_G(u) = \Delta(\mathrm{G}) + \delta(\mathrm{G}) - \mathrm{d}_u .$$

Definition 2.1: The first Revan index, second Revan index and third Revan index for graph G are defined as:

$$R_1(G) = \sum_{uv \in E(G)} [r_G(u) + r_G(\mathrm{v})],$$

$$R_2(G) = \sum_{uv \in E(G)} r_G(u) r_G(\mathrm{v}),$$

$$R_3(\mathrm{G}) = \sum_{uv \in E(G)} |r_G(u) - r_G(\mathrm{v})|.$$

For each edge of $uv \in E(G)$, by defining $\psi_i = [r_G(u) + r_G(\mathrm{v})]$, $\psi_i' = r_G(u) r_G(\mathrm{v})$ and $\psi_i'' = |r_G(u) - r_G(\mathrm{v})|$ the above formulas can be defined as:

$$R_1(G) = \sum_{i=1}^{|E(G)|} \psi_i ,$$

$$R_2(G) = \sum_{i=1}^{|E(G)|} \psi_i' ,$$

$$R_3(G) = \sum_{i=1}^{|E(G)|} \psi_i'' .$$

Definition 2.2: The first, second and third Revan polynomials of a simple connected graph G are defined as [8]:

$$R_1(G, x) = \sum_{uv \in E(G)} x^{r_G(u) + r_G(\mathrm{v})},$$

$$R_2(G, x) = \sum_{uv \in E(G)} x^{r_G(u) r_G(\mathrm{v})},$$

$$R_3(\mathrm{G}, \mathrm{x}) = \sum_{uv \in E(G)} x^{|r_G(u) - r_G(\mathrm{v})|}.$$

We can obtain first Revan index $R_1(G)$, second Revan index $R_2(G)$ and third Revan index $R_3(G)$ from its polynomial, because for i= 1, 2, 3:

$$R_i(G) = \left. \frac{\partial R_i(G, x)}{\partial x} \right|_{x=1} .$$

The graph of CuO (*m*, *n*) is shown in Figure (1) and the graph of Cu_2O (*m*, *n*) is shown in Figure (2).

According to the unit cell in figure (1) and figure (2), m represents the number of times a unit cell repeats in a row and n represents the number of times a unit cell repeats in a column of copper (I) oxide and copper (II) oxide.

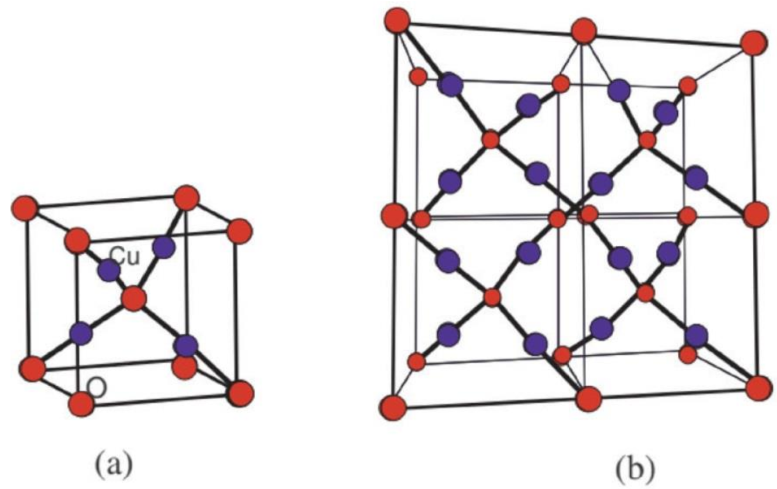

Figure 1: (a) Cu_2O (1, 1); (b) Cu_2O (2, 2).

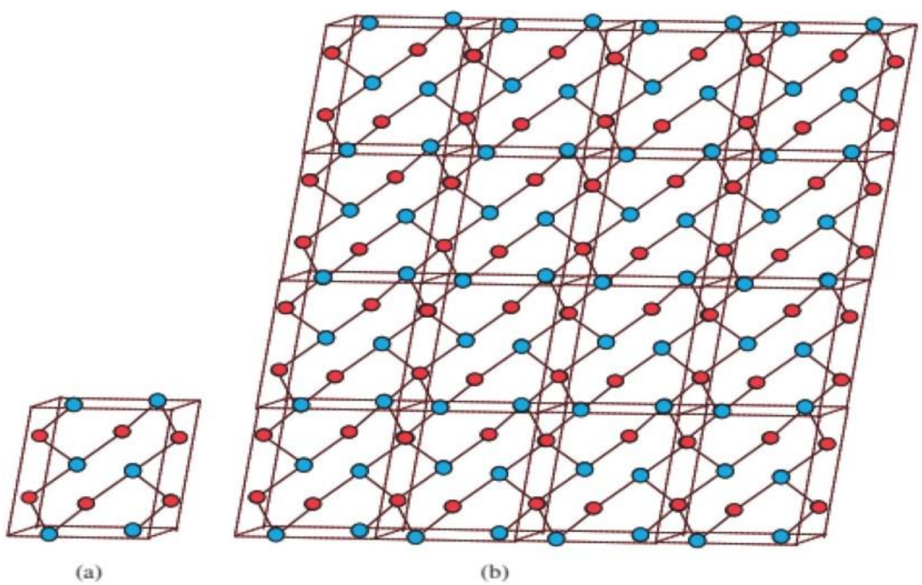

Figure 2: (a) CuO (1, 1); (b) CuO (4, 4).

Suppose H is the molecular graph of copper (I) oxide. There are three types of edges in copper (I) oxide as follows:

$$e_1 = \left\{(d_u, d_v) \middle| uv \in E(H), \mathrm{d}_u = 1, d_v = 2\right\},\ e_2 = \left\{(d_u, d_v) \middle| uv \in E(H), \mathrm{d}_u = 2, d_v = 2\right\},$$
$$e_3 = \left\{(d_u, d_v) \middle| uv \in E(H), \mathrm{d}_u = 2, d_v = 4\right\}.$$

Computational analysis showed that the number of vertices and edges of Cu_2O (m, n) are 7mn+2m+2n+2 and 8mn, respectively. In Cu_2O (m, n), the number of zero degree vertices is 4, the number of one degree vertices is 4m+4n-4, the number of two degree vertices is 6mn-2m-2n+2 and the number of four degree vertices is mn.
We have the following table for Cu_2O (m, n):

Table 1 Types and number of Cu_2O (m, n) edges.

Number of edges	$r_G(u)$	$r_G(v)$	ψ_i	ψ_i'	ψ_i''	Edge type
4n+4m - 4	1	12	7	3	4	e_1
4mn -4n- 4m + 4	0	9	6	3	3	e_2
4mn	2	3	4	1	3	e_3

Suppose G is the molecular graph of copper (II) oxide. There are five types of edges in copper (II) oxide as follows:

$$e_1 = \{(d_u, d_v) | uv \in E(\mathrm{G}), \mathrm{d}_u = 1, d_v = 2\},\ e_2 = \{(d_u, d_v) | uv \in E(\mathrm{G}), \mathrm{d}_u = 1, d_v = 4\},$$
$$e_3 = \{(d_u, d_v) | uv \in E(\mathrm{G}), \mathrm{d}_u = 2, d_v = 2\},\ e_4 = \{(d_u, d_v) | uv \in E(\mathrm{G}), \mathrm{d}_u = 2, d_v = 3\},$$
$$e_5 = \{(d_u, d_v) | uv \in E(\mathrm{G}), \mathrm{d}_u = 3, d_v = 4\}.$$

Computational analysis showed that number of vertices and edges of CuO (m, n) are 8mn+2m+2n and 12mn, respectively. In CuO (m, n) the number of one degree vertices are 2n, the number of two degree vertices are 2mn+4m+2n, the number of three degree vertices are 4mn-2n and the number of four degree vertices are 2mn-2m.
We have the following table for CuO (m, n):

Table 2 Types and number of CuO (m, n) edges.

Number of edges	$r_G(u)$	$r_G(v)$	ψ_i	ψ_i'	ψ_i''	Edge type
2	4	3	7	12	1	e_1
2n -2	4	1	5	4	3	e_2
2n +2	3	3	6	9	0	e_3
4mn + 8m – 6	3	2	5	6	1	e_4
8mn -8m- 4n + 4	2	1	3	2	1	e_5

3 MAIN RESULTS

In the following, Revan polynomials and Revan indices are computed in the general case of copper (I) oxide Cu_2O (*m*, *n*) and copper (II) oxide CuO (*m*, *n*).

Theorem 3.1: Let H be the graph of copper (I) oxide Cu_2O (m, n). Then,

$$i) R_1(H,x) = (4n+4m-4)x^7 + (4mn-4n-4m+4)x^6 + (4mn)x^4,$$
$$ii) R_2(H,x) = (4n+4m-4)x^3 + (4mn-4n-4m+4)x^3 + (4mn)x^1,$$
$$iii) R_3(H,x) = (4n+4m-4)x^4 + (4mn-4n-4m+4)x^3 + (4mn)x^3.$$

Proof:

$$i) R_1(H,x) = \sum_{uv\in E(H)} x^{r_H(u)+r_H(v)} = \sum_{uv\in e_1} x^{r_H(u)+r_G(v)} + \sum_{uv\in e_2} x^{r_H(u)+r_G(v)} + \sum_{uv\in e_3} x^{r_H(u)+r_H(v)}$$
$$= (4n+4m-4)x^7 + (4mn-4n-4m+4)x^6 + (4mn)x^4,$$
$$ii) R_2(H,x) = \sum_{uv\in E(H)} x^{r_H(u) r_H(v)} = \sum_{uv\in e_1} x^{r_H(u)+r_G(v)} + \sum_{uv\in e_2} x^{r_H(u)+r_G(v)} + \sum_{uv\in e_3} x^{r_H(u)+r_H(v)}$$
$$= (4n+4m-4)x^3 + (4mn-4n-4m+4)x^3 + (4mn)x^1,$$
$$iii) R_3(H,x) = \sum_{uv\in E(H)} x^{|r_H(u)-r_H(v)|} = \sum_{uv\in e_1} x^{r_H(u)+r_G(v)} + \sum_{uv\in e_2} x^{r_H(u)+r_G(v)} + \sum_{uv\in e_3} x^{r_H(u)+r_H(v)}$$
$$= (4n+4m-4)x^4 + (4mn-4n-4m+4)x^3 + (4mn)x^3. \square$$

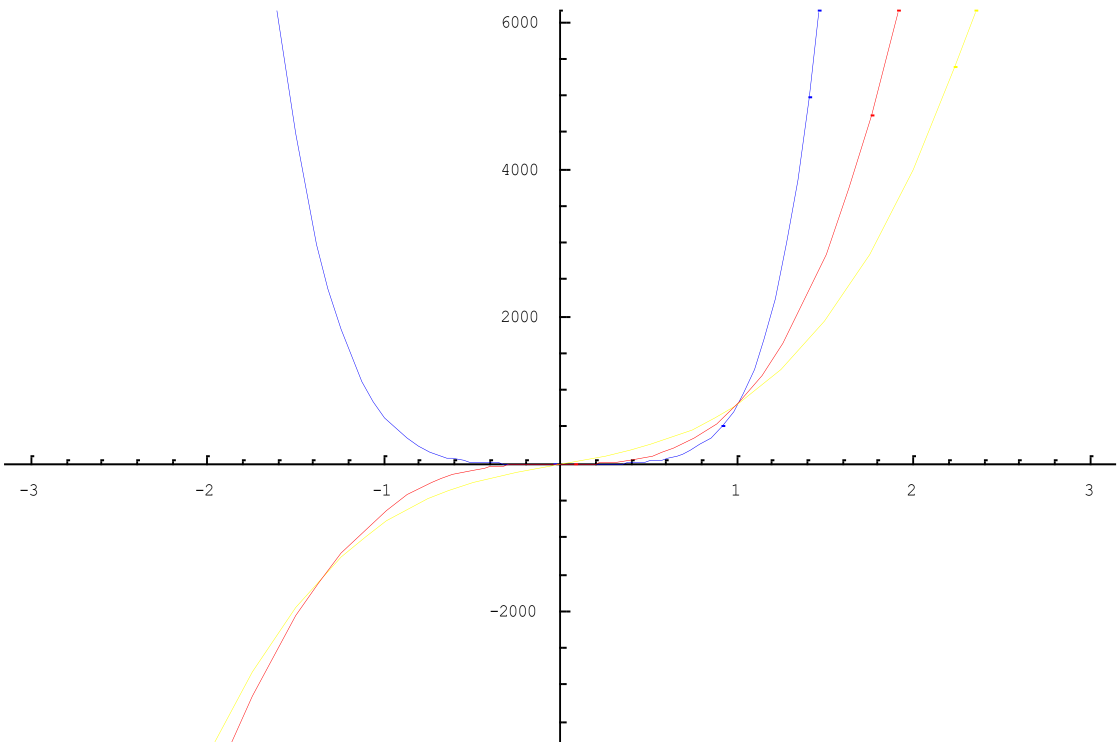

Figure 3: Shows the behavior of first, second and third Revan polynomials of copper (I) oxide, with Blue, Yellow and Red lines, respectively.

Theorem 3.2: Let G be the graph of copper (II) oxide CuO (m, n). Then,

$$i) R_1(G,x) = 2(x^7) + (2n-2)(x^5) + (2n+2)(x^6) + (4mn+8m-6)(x^5) + (8mn-8m-4n+4)(x^3),$$
$$ii) R_2(G,x) = 2(x^{12}) + (2n-2)(x^4) + (2n+2)(x^9) + (4mn+8m-6)(x^6) + (8mn-8m-4n+4)(x^2),$$
$$R_3(G,x) = 2(x^1) + (2n-2)(x^3) + (2n+2)(x^0) + (4mn+8m-6)(x^1) + (8mn-8m-4n+4)(x^1).$$

Proof:

$$i) R_1(G,x) = \sum_{uv\in E(G)} x^{r_G(u)+r_G(v)} = \sum_{uv\in e_1} x^{r_G(u)+r_G(v)} + \sum_{uv\in e_2} x^{r_G(u)+r_G(v)} + \sum_{uv\in e_3} x^{r_G(u)+r_G(v)} + \sum_{uv\in e_4} x^{r_G(u)+r_G(v)} + \sum_{uv\in e_5} x^{r_G(u)+r_G(v)}$$
$$= 2(x^7) + (2n-2)(x^5) + (2n+2)(x^6) + (4mn+8m-6)(x^5) + (8mn-8m-4n+4)(x^3),$$
$$ii) R_2(G,x) = \sum_{uv\in E(G)} x^{r_G(u)r_G(v)} = \sum_{uv\in e_1} x^{r_G(u)+r_G(v)} + \sum_{uv\in e_2} x^{r_G(u)+r_G(v)} + \sum_{uv\in e_3} x^{r_G(u)+r_G(v)} + \sum_{uv\in e_4} x^{r_G(u)r_G(v)} + \sum_{uv\in e_5} x^{r_G(u)+r_G(v)}$$
$$= 2(x^{12}) + (2n-2)(x^4) + (2n+2)(x^9) + (4mn+8m-6)(x^6) + (8mn-8m-4n+4)(x^2),$$
$$R_3(G,x) = \sum_{uv\in E(G)} x^{|r_G(u)-r_G(v)|} = \sum_{uv\in e_1} x^{r_G(u)+r_G(v)} + \sum_{uv\in e_2} x^{r_G(u)+r_G(v)} + \sum_{uv\in e_3} x^{r_G(u)+r_G(v)} + \sum_{uv\in e_4} x^{r_G(u)+r_G(v)} + \sum_{uv\in e_5} x^{r_G(u)+r_G(v)}$$
$$= 2(x^1) + (2n-2)(x^3) + (2n+2)(x^0) + (4mn+8m-6)(x^1) + (8mn-8m-4n+4)(x^1). \square$$

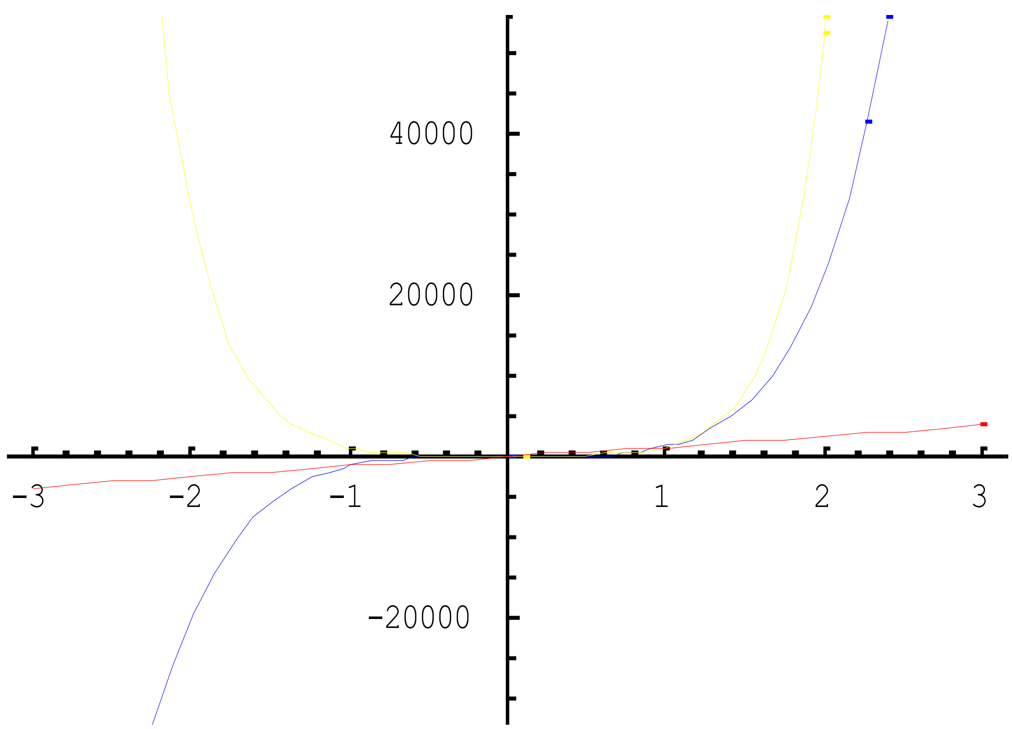

Figure 4: Shows the behavior of first, second and third Revan polynomials of copper (II) oxide, with Blue, Yellow and Red lines, respectively.

Theorem 3.3: Let H be the graph of copper (I) oxide Cu_2O (m, n). Then,

$i) R_1(H) = 4(10mn + n + m - 1),$
$ii) R_2(H) = 16mn,$
$iii) R_3(H) = 4(6mn + n + m + 2).$

Proof:

$$R_1(H) = \left.\frac{\partial R_1(H,x)}{\partial x}\right|_{x=1} = \left.\frac{\partial((4n+4m-4)x^7 + (4mn-4n-4m+4)x^6 + (4mn)x^4)}{\partial x}\right|_{x=1}$$
$$= 7(4n+4m-4) + 6(4mn-4n-4m+4) + 4(4mn)$$
$$= 40mn + 4n + 4m - 4 = 4(10mn + n + m - 1),$$

$$R_2(H) = \left.\frac{\partial R_2(H,x)}{\partial x}\right|_{x=1} = \left.\frac{\partial((4n+4m-4)x^3 + (4mn-4n-4m+4)x^3 + (4mn)x^1)}{\partial x}\right|_{x=1}$$
$$= 3(4n+4m-4) + 3(4mn-4n-4m+4) + (4mn) = 16\,\mathrm{mn},$$

$$R_3(H) = \left.\frac{\partial R_3(H,x)}{\partial x}\right|_{x=1} = \left.\frac{\partial((4n+4m-4)x^4 + (4mn-4n-4m+4)x^3 + (4mn)x^3)}{\partial x}\right|_{x=1}$$
$$= 4(4n+4m-4) + 3(4mn-4n-4m+4) + 3(4mn)$$
$$= 24mn + 4n + 4m + 8 = 4(6mn + n + m + 2).$$

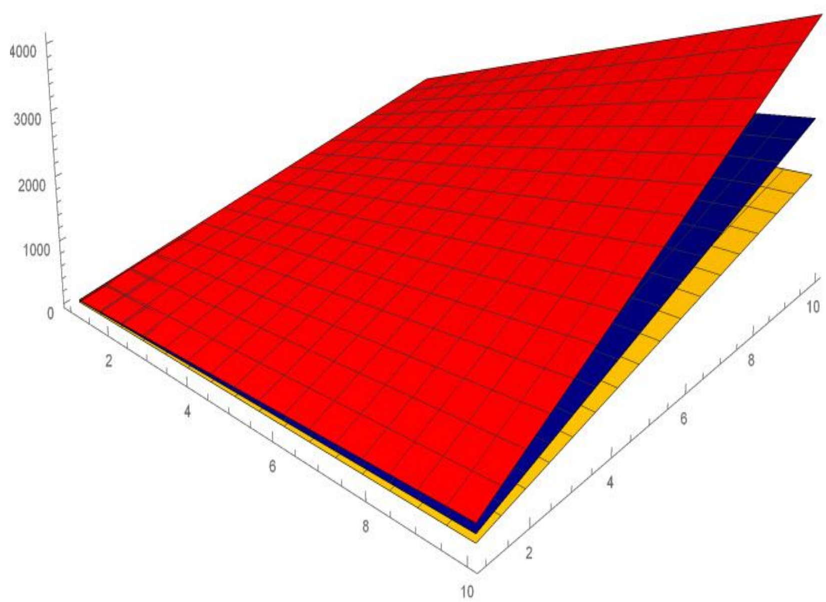

Figure 5: Shows the behavior of first, second and third Revan indices of copper (I) oxide, with Red, Yellow and Blue, respectively.

Theorem 3.4: Let G be the graph of copper (II) oxide CuO (m, n). Then,

$i) R_1(G) = 44mn + 10n + 16m - 2,$

$ii) R_2(G) = 40mn + 18n + 32m + 6,$

$R_3(\mathrm{G}) = 12\,\mathrm{mn} + 2\,\mathrm{n} - 6.$

Proof:

$$R_1(G) = \left.\frac{\partial R_1(G,x)}{\partial x}\right|_{x=1}$$

$$= \left.\frac{\partial(2(x^7) + (2n-2)(x^5) + (2n+2)(x^6) + (4mn+8m-6)(x^5) + (8mn-8m-4n+4)(x^3))}{\partial x}\right|_{x=1}$$

$$= 14 + 5(2n-2) + 6(2n+2) + 5(4mn+8m-6) + 3(8mn-8m-4n+4)$$

$$= 44mn + 10n + 16m - 2,$$

$$R_2(G) = \left.\frac{\partial R_2(G,x)}{\partial x}\right|_{x=1}$$

$$= \left.\frac{\partial(2(x^{12}) + (2n-2)(x^4) + (2n+2)(x^9) + (4mn+8m-6)(x^6) + (8mn-8m-4n+4)(x^2))}{\partial x}\right|_{x=1}$$

$$= 24 + 4(2n-2) + 9(2n+2) + 6(4mn+8m-6) + 2(8mn-8m-4n+4)$$

$$= 40mn + 18n + 32m + 6,$$

$$R_3(G) = \left.\frac{\partial R_3(G,x)}{\partial x}\right|_{x=1}$$

$$= \left.\frac{\partial(2(x^1) + (2n-2)(x^3) + (2n+2)(x^0) + (4mn+8m-6)(x^1) + (8mn-8m-4n+4)(x^1))}{\partial x}\right|_{x=1}$$

$$= 2 + 3(2n-2) + (4mn+8m-6) + (8mn-8m-4n+4) = 12\,\mathrm{mn} + 2\,\mathrm{n} - 6.$$

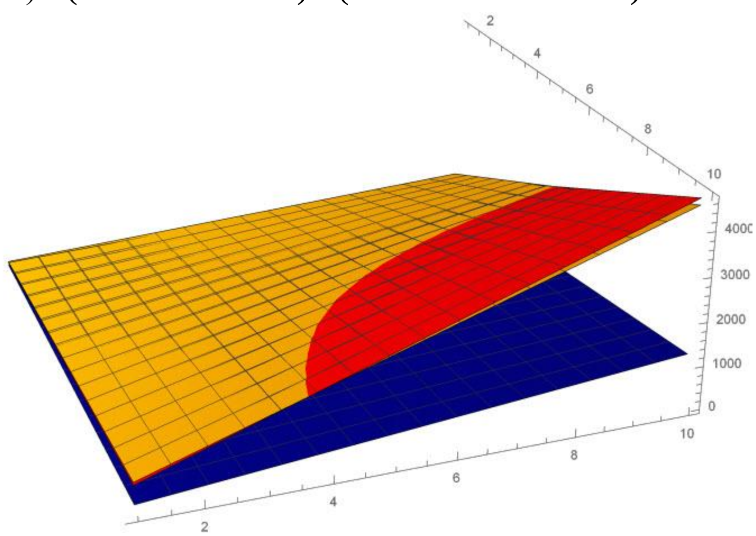

Figure 6: Shows the behavior of first, second and third Revan indices of copper (II) oxide, with Red, Yellow, and Blue, respectively.

CONCLUSION

In copper (I) oxide, the first Revan polynomial always has negative values. For x> 1, first Revan polynomial has the highest value and the second Revan polynomial has the lowest value. The first Revan index has the highest value and the third Revan index has the lowest value.

In copper (II) oxide, the second Revan polynomial always has negative values. For x> 1, the second Revan polynomial has the highest value and the third Revan polynomial has the lowest value. The third Revan index has the lowest value. For further research, other topological indices can be computing on copper oxide.

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