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FULL PAPER

On ve-degree atom-bond connectivity, sum-connectivity, geometric-arithmetic and harmonic indices of copper oxide

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Topological indices are important tools to modeling chemical properties of molecules. ve-degree based atom-bond connectivity, sum-connectivity, geometric-arithmetic, and harmonic indices are defined as their corresponding classical degree based counterparts recently in chemical graph theory. In this study we investigate ve-degree atom-bond connectivity, sum-connectivity, geometric-arithmetic, and harmonic topological properties of copper oxide. We calculate exact values of these novel topological indices for copper oxide and give closed formulas.

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Ve-degree atom-bond connectivity index; ve-degree sum-connectivity index; ve-degree geometric arithmetic index; ve-degree harmonic index.

Introduction

Graph theory has many applications in chemical and physical sciences. Graphs enable to model molecules and compounds as chemical graphs [1-3]. A topological index is a closed formula derived from chemical graphs. Topological index of chemical graphs sometimes provides great correlations with some physical and chemical properties of these chemical substances. The first distance based topological index was proposed by Wiener in 1947 for modeling physical properties of alcanes, and the first degree based topological index was proposed by Platt in 1947 for modeling physical properties of alcanes [4, 5]. For detailed discussions about the Platt index and Zagreb indices we refer the interested reader to [6]. More than forty years ago Gutman and Trinajstic defined Zagreb indices which are degree based topological indices [7]. These topological indices were proposed to be measures of branching of the carbon-atom skeleton [8]. Very recently Chellali et al have published very seminal study about the novel two degree concepts: ve-degrees and ev-degrees in graph theory [6]. The authors defined these novel degree concepts in relation to the vertex-edge domination and the edge-vertex domination parameters [10-12]. The ev-degree and ve-degree topological indices have been defined and their basic mathematical properties have been investigated [13-15]. It was showed that, ve-degree sum-connectivity index of octane isomers provides the highest value of correlation coefficient of the property of acentric factor than other well-known topological indices such as Zagreb, Randic, atom-bond connectivity, sum-connectivity indices [13].

The copper oxide/cupric oxide is an inorganic chemical compound CuO. It is an essential mineral found in plants and animals.

Copper has enormous applications in medical instruments, drugs, as a heat conductor and many others. In Figure 1, the copper hydroxide is depicted and when hydrogen atoms are deleted from $Cu(OH)_2$ then the resultant graph is depicted in Figure 2.

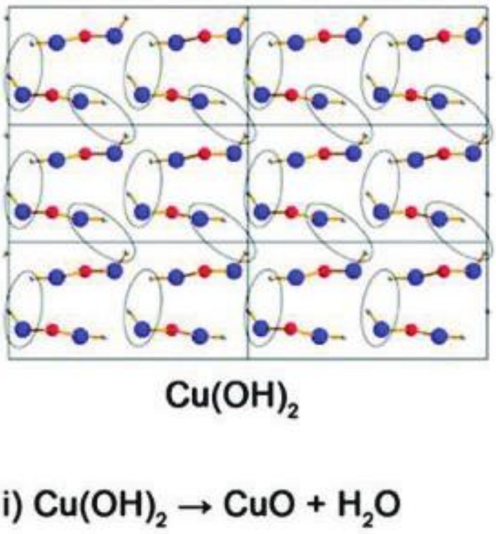

FIGURE 1 2D representation of $Cu(OH)_2$

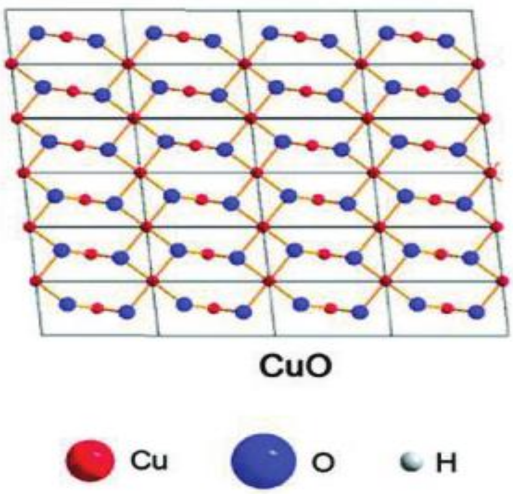

FIGURE 2 2D representation of CuO

The 3D graph of copper oxide CuO is depicted in Figure 3.

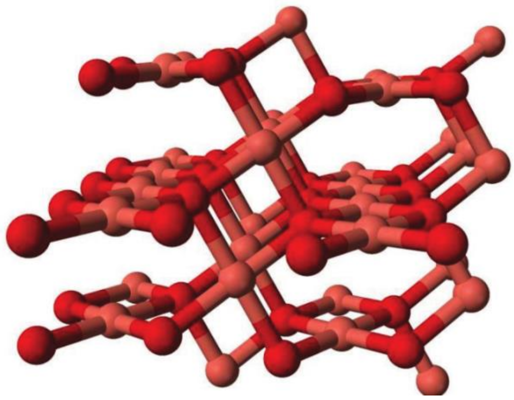

FIGURE 3 3D representation of CuO

The ABC, GA, ABC 4 , GA 5 , general Randic index and Zagreb index for copper oxide CuO were calculated [16,17].

Preliminaries

We consider only connected and simple graphs throughout this work. Let *G* be a graph with the vertex set *V (G)*, the edge set *E(G)* and $v \in V(G)$. The degree of a vertex $v \in V(G)$, deg(v), equals the number of edges incident to v that is the cardinality of the set $N(v) = \{u \mid uv \in E(G)\}$.

Definition 1. Let *G* be a connected graph and $v \in V(G)$. The ve-degree $deg_{ve}(v)$, equals the number of different edges that incident to any vertex from the closed (or open) neighborhood of v. vertex from the closed (or open) neighborhood of v.

In order to calculate the ve-degrees of the vertices of CuO we give the edge partition of its vertices with respect to classical degrees in Table 1.

TABLE 1 The degrees of the end vertices of edges for CuO

(deg(u),deg(v))	Number of Edges
(2,2)	4(n + 1)
(2,3)	2mn + 2(2m − n) − 4
(2,4)	4(n − 1)
(3,4)	4(mn − (m + n) + 1)

From Definition 1 and Table 1, the ve-degree partition of copper oxide is given the Table 2.

TABLE 2 The ve-degrees of the end vertices of edges for CuO

$(deg_{ve}(u), deg_{ve}(v))$	Number of Edges
(4,4)	4
(4,5)	4
(4,6)	4(n – 1)
(5,6)	4
(6,6)	6m – 10
(6,10)	2(mn – (m – n) – 1)
(10,10)	4(n – 1)
(10,12)	4(mn – (m + 2n) + 2)

Definition 2 (**ve-degree atom-bond connectivity (ve-ABC) index**) Let G be a connected graph and $e=uv$E(G). The ve-degree atom-bond connectivity index of the graph G defined as;

$$ABC^{ve}(G) = \sum_{uv\in E(G)} \sqrt{\frac{deg_{ve}u+deg_{ve}v-2}{deg_{ve}u\,deg_{ve}v}} \quad (1)$$

Definition 3 (**ve-degree geometric-arithmetic (ve-GA) index**) Let G be a connected graph and vV(G). Ve-degree geometric-arithmetic index of the graph G defined as;

$$GA^{ve}(G) = \sum_{uv\in E(G)} \frac{2\sqrt{deg_{ve}u\,deg_{ve}v}}{deg_{ve}u+deg_{ve}v} \quad (2)$$

Definition 4 (**ve-degree harmonic (ve-H) index**) Let G be a connected graph and uvE(G). Ve-degree harmonic index of the graph G defined as;

$$H^{ve}(G) = \sum_{uv\in E(G)} \frac{2}{deg_{ve}u+deg_{ve}v} \quad (3)$$

Definition 5 (**ve-degree sum-connectivity (ve-χ) index**) Let G be a connected graph and uvE(G). Ve-degree sum-connectivity index of the graph G defined as;

$$\chi^{ve}(G) = \sum_{uv\in E(G)} (deg_{ve}u+deg_{ve}v)^{-1/2} \quad (4)$$

Results

In this section we compute the ve-degree topological indices for copper oxide.

Theorem 1. Let G be a connected graph of copper oxide and uv ∈ E(G). The ve-degree harmonic index of the graph G is;

$$H^{ve}(G) = \frac{17}{9} + \frac{6n-6}{5} + \frac{3m-5}{3} + \frac{mn-m+n-1}{4} + \frac{4mn-4m-8n+16}{11}$$

Proof. From the Table 2 and Equation 3,

$$H^{ve}(G) = \sum_{uv\in E(G)} \frac{2}{deg_{ve}u + deg_{ve}v}$$

$$= \frac{8}{4+4} + \frac{8}{4+5} + \frac{8(n-1)}{4+6} + \frac{8}{5+6} + \frac{12m-20}{6+6} + \frac{4mn-4m+4n-4}{6+10} + \frac{8(n-1)}{10+10} + \frac{8mn-8m-16n+16}{10+12}$$

$$= \frac{17}{9} + \frac{4n-4}{5} + \frac{8}{11} + \frac{3m-5}{3} + \frac{mn-m+n-1}{4} + \frac{2n-2}{5} + \frac{4mn-4m-8n+16}{11}$$

$$= \frac{17}{9} + \frac{6n-6}{5} + \frac{3m-5}{3} + \frac{mn-m+n-1}{4} + \frac{4mn-4m-8n+16}{11}$$

Theorem 2. Let G be a connected graph of copper oxide and uv ∈ E(G). The ve-degree sum-connectivity index of the graph G is;

$$\chi^{ve}(G) = \frac{2}{\sqrt{2}} + \frac{4}{3} + \frac{4n-4}{\sqrt{10}} + \frac{4}{\sqrt{11}} + \frac{3m-5}{\sqrt{3}} + \frac{mn-m+n-1}{2} + \frac{2n-2}{\sqrt{5}} + \frac{4mn-4m-8n+8}{\sqrt{22}}$$

Proof. From the Table 2 and Equation 4;

$$\chi^{ve}(G) = \sum_{uv\in E(G)} (deg_{ve}u+deg_{ve}v)^{-1/2}$$

$$= \frac{4}{\sqrt{4+4}} + \frac{4}{\sqrt{4+5}} + \frac{4(n-1)}{\sqrt{4+6}} + \frac{4}{\sqrt{5+6}} + \frac{6m-10}{\sqrt{6+6}} + \frac{2mn-2m+2n-2}{\sqrt{6+10}} + \frac{4(n-1)}{\sqrt{10+10}} + \frac{4mn-4m-8n+8}{\sqrt{10+12}}$$

$$= \frac{2}{\sqrt{2}} + \frac{4}{3} + \frac{4n-4}{\sqrt{10}} + \frac{4}{\sqrt{11}} + \frac{3m-5}{\sqrt{3}} + \frac{mn-m+n-1}{2} + \frac{2n-2}{\sqrt{5}} + \frac{4mn-4m-8n+8}{\sqrt{22}}$$

Theorem 3. Let G be a connected graph of copper oxide and uv ∈ E(G). The ve-degree geometric-arithmetic index of the graph G is;

$$GA^{ve}(G) = 4 + \frac{16\sqrt{5}}{9} + \frac{8(n-1)\sqrt{6}}{5} + \frac{8\sqrt{30}}{11} + \frac{6m-10}{3} + \frac{(mn-m+n-1)\sqrt{15}}{2} + \frac{4(n-1)}{5} + \frac{(8mn-8m-16n+16)\sqrt{30}}{11}$$

Proof. From the Table 2 and Equation 2;

$$GA^{ve}(G) = \sum_{uv\in E(G)} \frac{2\sqrt{deg_{ve}u\, deg_{ve}v}}{deg_{ve}u + deg_{ve}v}$$

$$= \frac{8\sqrt{4x4}}{4+4} + \frac{8\sqrt{4x5}}{4+5} + \frac{8(n-1)\sqrt{4x6}}{4+6} + \frac{8\sqrt{5x6}}{5+6} + \frac{(12m-20)\sqrt{6x6}}{6+6} + \frac{(4mn-4m+4n-4)\sqrt{6x10}}{6+10} + \frac{8(n-1)\sqrt{6x10}}{6+10} + \frac{(8mn-8m-16n+16)\sqrt{10x12}}{10+12}$$

$$= 4 + \frac{16\sqrt{5}}{9} + \frac{8(n-1)\sqrt{6}}{5} + \frac{8\sqrt{30}}{11} + \frac{6m-10}{3} + \frac{(mn-m+n-1)\sqrt{15}}{2} + \frac{4(n-1)}{5} + \frac{(8mn-8m-16n+16)\sqrt{30}}{11}$$

Theorem 4. Let G be a connected graph of copper oxide and uv ∈ E(G). The ve-degree atom-bond connectivity index of the graph G is

$$ABC^{ve}(G) = \frac{2\sqrt{5}}{\sqrt{2}} + \frac{2\sqrt{7}}{\sqrt{5}} + \frac{4(n-1)\sqrt{2}}{\sqrt{6}} + \frac{12}{\sqrt{30}} + \frac{(3m-5)\sqrt{10}}{3} + \frac{(mn-m+n-1)\sqrt{10}}{\sqrt{15}} + \frac{(3n-1)\sqrt{2}}{5} + \frac{(4mn-4m-8n+8)}{\sqrt{6}}$$

Proof. From the Table 2 and Equation 1,

$$ABC^{ve}(G) = \sum_{uv\in E(G)} \sqrt{\frac{deg_{ve}u + deg_{ve}v - 2}{deg_{ve}u\, deg_{ve}v}}$$

$$= \frac{4\sqrt{4+4-2}}{\sqrt{4x4}} + \frac{4\sqrt{4+5-2}}{\sqrt{4x5}} + \frac{4(n-1)\sqrt{4+6-2}}{\sqrt{4x6}} + \frac{4\sqrt{5+6-2}}{\sqrt{5x6}} + \frac{(6m-10)\sqrt{6+6-2}}{\sqrt{6x6}} + \frac{(2mn-2m+2n-2)\sqrt{6+10-2}}{\sqrt{6x10}} + \frac{4(n-1)\sqrt{10+10-2}}{\sqrt{10x10}} + \frac{(4mn-4m-8n+8)\sqrt{10+12-2}}{\sqrt{10x12}}$$

$$= \frac{2\sqrt{5}}{\sqrt{2}} + \frac{2\sqrt{7}}{\sqrt{5}} + \frac{4(n-1)\sqrt{2}}{\sqrt{6}} + \frac{12}{\sqrt{30}} + \frac{(3m-5)\sqrt{10}}{3} + \frac{(mn-m+n-1)\sqrt{10}}{\sqrt{15}} + \frac{(3n-1)\sqrt{2}}{5} + \frac{(4mn-4m-8n+8)}{\sqrt{6}}$$

Conclusion

In this research study, we computed the ve-degree atom-bond connectivity, ve-degree sum-connectivity, ve-degree geometric-arithmetic and ve-degree harmonic indices of copper oxide. The closed formulas are as follows:

$$H^{ve}(G) = \frac{17}{9} + \frac{6n-6}{5} + \frac{3m-5}{3} + \frac{mn-m+n-1}{4} + \frac{4mn-4m-8n+16}{11}$$

$$\chi^{ve}(G) = \frac{2}{\sqrt{2}} + \frac{4}{3} + \frac{4n-4}{\sqrt{10}} + \frac{4}{\sqrt{11}} + \frac{3m-5}{\sqrt{3}} + \frac{mn-m+n-1}{2} + \frac{2n-2}{\sqrt{5}} + \frac{4mn-4m-8n+8}{\sqrt{22}}$$

$$GA^{ve}(G) = 4 + \frac{16\sqrt{5}}{9} + \frac{8(n-1)\sqrt{6}}{5} + \frac{8\sqrt{30}}{11} + \frac{6m-10}{3} + \frac{(mn-m+n-1)\sqrt{15}}{2} + \frac{4(n-1)}{5} + \frac{(8mn-8m-16n+16)\sqrt{30}}{11}$$

$$ABC^{ve}(G) = \frac{2\sqrt{5}}{\sqrt{2}} + \frac{2\sqrt{7}}{\sqrt{5}} + \frac{4(n-1)\sqrt{2}}{\sqrt{6}} + \frac{12}{\sqrt{30}} + \frac{(3m-5)\sqrt{10}}{3} + \frac{(mn-m+n-1)\sqrt{10}}{\sqrt{15}} + \frac{(3n-1)\sqrt{2}}{5} + \frac{(4mn-4m-8n+8)}{\sqrt{6}}$$

Computation of the ve-degree topological indices of other molecules and the mathematical properties of these novel indices and ve-degree and ev-degree based topological indices of other chemical compounds are interested problems for further studies.

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