

MOLECULAR DESCRIPTION OF COPPER (I) OXIDE AND COPPER (II) OXIDE

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The topological index of a molecular structure correlate certain physicochemical properties such as boiling point and stability of that molecular structure. Recently several topological indices have been introduced and studies have shown their association with certain physical and chemical properties of other molecules. Specifically, Zagreb, Atom-bound connectivity (ABC) and Sanskruti indices have been correlated with extent of branching, enthalpy and entropy of some organic molecules. In this study we have calculated Zagreb, Atom-bound connectivity (ABC) and Sanskruti indices (S) for Copper (I) oxide and Copper (II) oxide CuO. Additionally, from the experimentally available data, we calculated entropy and enthalpy per unit cell for both the oxides and compared with Atom-bound connectivity and Sanskruti indices. It appears that these indices have very poor relation with these physical properties in both oxides of copper and they may need some modifications to show considerable compliance as reported in other organic molecules.”

Keywords: molecular graphs; zagreb indices; atom-bound connectivity index; sanskruti index; copper oxide.

INTRODUCTION

“A graph that shows constituents of a molecule and their connectivity is known as molecular graph and such representation is usually referred as topological representation of molecule.¹ Molecular graphs

“are usually characterized by different topological indices for correlation of chemical structure of a molecule with biological, chemical or physical properties. Studies have reported several applications of different topological indices in quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR), virtual screening and computational drug designing.²⁻⁷

“So far, many different topological indices have been developed, and most of them are only graph descriptors.⁸⁻¹⁸ Only a few indices have shown their correlation with biological, chemical or physical chemical properties of certain molecules.¹⁹⁻²¹ For example, Zagreb indices (M_1 & M_2) were first reported by Gutman and Trinajestic for the correlation of chemical structure with π electrons.²² However, later M_1 and M_2 were associated with extent of branching in a molecule. They are described by equation (1) & (2) for a graph $G=(V,E)$, where V to be the vertex set and E to be the edge set of G. The degree d_p of the vertex p is the quantity of edges of G incident with p. The length of a most limited path in a graph G is a distance $d(p,q)$ amongst p and q.”

$$M_1(G) = \sum_{pq \in E(G)} (d_p + d_q) \quad (1)$$

$$M_2(G) = \sum_{pq \in E(G)} (d_p \cdot d_q) \quad (2)$$

“Another topological index is atom-bound connectivity (ABC) that was introduced by Estrada *et al.*^{23,24} Later, studies have reported its exceptional correlation with thermodynamic

properties of organic molecules, specifically with heat of formation of alkanes. This index is characterized by Equation (3) considering the graph similar to Zagreb indices”

$$ABC(G) = \sum_{pq \in E(G)} \sqrt{\frac{d_p + d_q - 2}{d_p \cdot d_q}} \quad (3)$$

“Another molecular descriptor that was correlated with thermodynamic properties is Sanskruti index. This index was introduced in 2016 by S. M. Hosamani and it shows considerable correlation with entropy of some organic molecules.²⁵ It is characterized as equation (4) considering the above mentioned graph conditions”

$$S(G) = \sum_{pq \in E(G)} \left(\frac{s_p \times s_q}{s_p + s_q - 2} \right)^3 \quad (4)$$

“This study is designed to calculate Zagreb, ABC and Sanskruti indices for two oxides of Cu (CuO & Cu_2O). It will allow us to compare these indices with the experimentally determined entropy, enthalpy and other physical properties of CuO and Cu_2O .”

THEORY AND METHODS

Structure of copper (I) oxide (Cu_2O)

Cu_2O is a naturally occurring reddish ore that is mainly used in chemical sensors, solar oriented cells, photo-catalysis and batteries.²⁶⁻²⁸ Crystal structure of Cu_2O is composed on small cubic unit cells based on Cu and O atoms (Figure. 1a). Analysis of the crystal lattice showed that each Cu atom is linked with two O atoms; in turn every O atom is connected with four Cu atoms (Figure 1b)”

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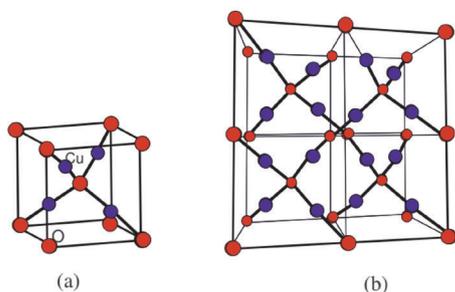


Figure 1. Copper(I) oxide . A) Unit cell of. B) Three dimensional crystal lattice of Cu and O are shown in blue and red spheres, respectively

Here, we have considered monolayer of Cu_2O for convenience. To determine the indices for Cu_2O we choose the settings of this graph as; $G \cong Cu_2O[m,n]$ be the chemical graph of Cu_2O with $(m \times n)$ unit cells in the plane. More precisely, m represents the number of unit cells in row and n represents the number of unit cells in column. Also for our convenience we represents $Cu_2O[m,n]$ as a graph G . The Figure 1(b) is representing $Cu_2O[2,2]$. Also Figure 2 represent one sheet view of Copper(I) oxide $Cu_2O[4,4]$. Computational analysis showed that the quantity 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 (Table 1)."

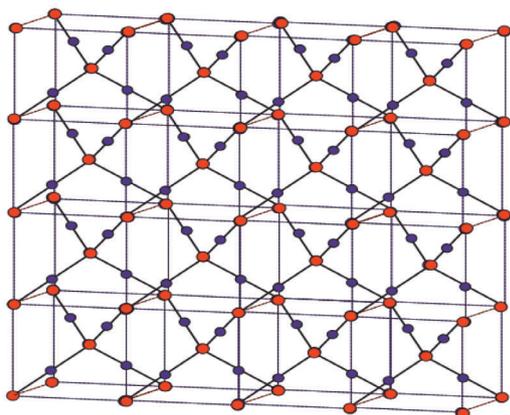


Figure 2. One sheet view of copper(I) oxide [4, 4]

Table 1. Degree based partition of edges of $Cu_2O[m, n]$ for end vertices of each edge (Degree based partition edges of Cu_2O)

(dp, dq)	Frequency
(1, 2)	$4n + 4m - 4$
(2, 2)	$4mn - 4n - 4m + 4$
(2, 4)	$4mn$

In the next Theorem, we have computed the exact result of first and second Zagreb index for the chemical graph $Cu_2O[m, n]$."

Theorem 1. "Consider the graph of $G \cong Cu_2O[m,n]$ with $m, n \geq 1$, then its first and second Zagreb index is equal to,"

$$M_1(G) = 40mn - 4m - 4n + 4$$

$$M_2(G) = 48mn - 8m - 8n + 8$$

Proof. "Let G be the crystallographic structure of $[m, n]$.The first Zagreb index is computed as below:"

$$M_1(G) = \sum_{pq \in E(G)} (d_p + d_q)$$

" $M_1(G) = (4n+4m-4)(1+2) + (4mn-4n-4m-4)(2+2) + (4mn)(2+4)$
 $M_1(G) = 40mn - 4m - 4n + 4.$ "

"By using Table 1 and Equation 1 the second Zagreb index are computed as below:"

$$M_2(G) = \sum_{pq \in E(G)} (d_p \cdot d_q)$$

" $M_2(G) = (4m+4n-4)(1 \times 2) + (4mn-4m-4n+4)(2 \times 2) + (4mn)(2 \times 4)$
 $M_2(G) = 48mn - 8m - 8n + 8.$ "

"In the next Theorem, we have computed the exact result of ABC index for the chemical graph $Cu_2O[m, n]$."

Theorem 2. "Consider the graph of $G \cong Cu_2O[m,n]$ with $m, n \geq 1$, then its ABC index is equal to,"

$$ABC(G) = 4\sqrt{2} (mn - 1)$$

Proof. "Let G be the chemical graph of $Cu_2O[m,n]$. Then by using Table 1 and equation (3) the ABC index is computed as below:"

$$ABC(G) = \sum_{pq \in E(G)} \sqrt{\frac{d_p + d_q - 2}{d_p \cdot d_q}}$$

$$ABC(G) = (4n + 4m - 4) \sqrt{\frac{1+2-2}{1 \times 2}} + (4mn - 4n - 4m - 4) \sqrt{\frac{2+2-2}{2 \times 2}}$$

$$+ 4mn \sqrt{\frac{4+2-2}{4 \times 2}}$$

$$ABC(G) = 4\sqrt{2} (mn - 1)$$

"The Table 2 shows partition of edges of the chemical graph $Cu_2O[m,n]$ depending on the sum of degrees of the neighbouring vertices of end vertices of each edge."

"The next Theorem shows the exact value of Sanskruti index of $Cu_2O[m,n]$."

Table 2. Edge partition of the graph of $Cu_2O[m, n]$ with $m, n \geq 2$, based on the degree sum of vertices lying at unit distance from end vertices of each edge

(Sp, Sq)	Frequency
(2, 4)	$4m + 4n - 4$
(4, 6)	$4mn - 4m - 4n + 4$
(5, 8)	$4n + 4m - 4$
(6, 8)	$4mn - 4m - 4n + 4$

Theorem 3. "Consider the graph $G \cong Cu_2O[m,n]$ with $m, n \geq 2$, then its Sanskruti index $S(G)$ is equal"

$$S(G) = 64mn - \frac{185892m}{1331} - \frac{185892n}{1331} + \frac{185892}{1331}$$

Proof. "Let G be the crystallographic structure of $Cu_2O[m,n]$. Then by using Table 2 and equation (4) the Sanskruti index $S(G)$ is computed as follows."

$$S(G) = \sum_{pq \in E(G)} \left(\frac{s_p \times s_q}{s_p + s_q - 2} \right)^3$$

$$S(G) = (4m+4n-4) \left(\frac{2 \times 4}{2+4-2} \right)^3 + (4mn-4m-4n-4) \left(\frac{6 \times 4}{6+4-2} \right)^3$$

$$+ (4m+4n-4) \left(\frac{5 \times 8}{5+8-2} \right)^3 + (4mn-4m-4n-4) \left(\frac{6 \times 8}{6+8-2} \right)^3$$

$$S(G) = 64mn - \frac{185892m}{1331} - \frac{185892n}{1331} + \frac{185892}{1331}$$

Structure of copper(II) oxide (CuO)

The crystal structure of Copper(II) oxide (**CuO**) is composed on monoclinic unit cells (Figure 3a). Here we have considered monolayer of **CuO** for convenience. To find the indices we choose the settings of this graph as; let $G \cong \text{CuO}[m, n]$ be the chemical graph of **CuO** with $(m \times n)$ unit cells in the plane. The Figure 3b is representing the lattice of **CuO**[4,4]. 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 $2mn-2m$."

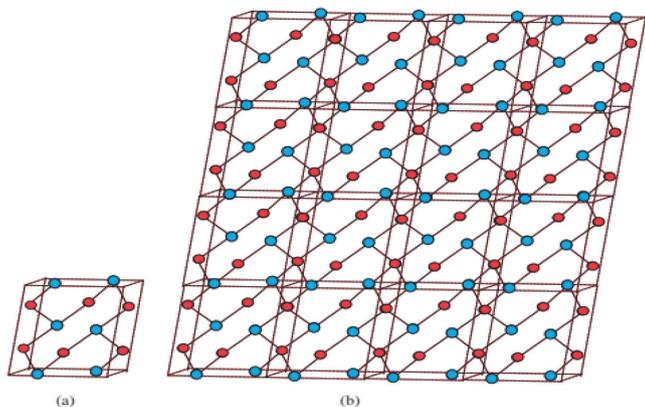


Figure 3. Copper (II) oxide CuO: (a) is the unit cell with blue and red circles represents copper and oxygen atom, respectively (b) shows the lattice CuO[4, 4]

In the next Theorem, we have computed the exact value of first and second Zagreb index for the chemical graph **CuO**[m, n]."

Table 3. Degree based partition of edges of **CuO**[m, n], of end vertices of each edge

(d_p, d_q)	Frequency
(1, 2)	2
(1, 4)	$2n - 2$
(2, 2)	$2n + 2$
(2, 3)	$4mn + 8m - 6$
(3, 4)	$8mn - 8m - 4n + 4$

Theorem 4. "Consider the graph of $G \cong \text{CuO}[m, n]$ with $m, n \geq 1$, then its first and second Zagreb index is equal to,"

$$M_1(G) = 76mn - 16m - 10n + 2$$

$$M_2(G) = 120mn - 48m - 32n + 16$$

Proof. "Let G be the crystallographic structure of **CuO**[m, n]. The first Zagreb index is computed as:

$$M_1(G) = \sum_{pq \in E(G)} (d_p + d_q)$$

$$"M_1(G) = (2)(1 + 2) + (2n - 2)(1 + 4) + (2n + 2)(2 + 2)$$

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

$$M_1(G) = 76mn - 16m - 10n + 2"$$

$$M_2(G) = \sum_{pq \in E(G)} (d_p \cdot d_q)$$

$$"M_2(G) = (2)(1 \times 2) + (2n - 2)(1 \times 4) + (2n + 2)(2 \times 2) +$$

$$(4mn + 8m - 6)(2 \times 3) + (8mn - 8m - 4n + 4)(3 \times 4)$$

$$M_2(G) = 120mn - 48m - 32n + 16"$$

"In the next Theorem, we have computed the exact result of ABC index for the chemical graph **CuO**[m, n]."

Theorem 5. "Consider the graph of $G \cong \text{CuO}[m, n]$ with $m, n \geq 1$, then its ABC index is equal to"

$$ABC(G) = \sqrt{2} + \frac{(2n-2)\sqrt{3}}{2} + \frac{(2n+2)\sqrt{2}}{2} + \frac{(4mn+8m-6)\sqrt{2}}{2}$$

$$+ \frac{(8mn-8m-4n+6)\sqrt{15}}{6}$$

Proof. Let G be the chemical graph of **CuO**[m, n]. Then by using Table 3 and equation (3) the ABC index is computed as below:

$$ABC(G) = \sum_{pq \in E(G)} \sqrt{\frac{d_p + d_q - 2}{d_p \cdot d_q}}$$

$$ABC(G) = (2)\sqrt{\frac{1+2-2}{1 \times 2}} + (2n-2)\sqrt{\frac{1+4-2}{1 \times 4}} + (2n+2)\sqrt{\frac{2+2-2}{2 \times 2}}$$

$$+ (4mn+8m-6)\sqrt{\frac{3+2-2}{3 \times 2}} + (8mn-8m-4n+4)\sqrt{\frac{3+4-2}{3 \times 4}}$$

$$ABC(G) = \sqrt{2} + \frac{(2n-2)\sqrt{3}}{2} + \frac{(2n+2)\sqrt{2}}{2} + \frac{(4mn+8m-6)\sqrt{2}}{2}$$

$$+ \frac{(8mn-8m-4n+6)\sqrt{15}}{6}$$

"The Table 4 shows partition of edges of the chemical graph **CuO**[m, n], which depends on the sum of degrees of the neighboring vertices."

Table 4. Edge partition of the graph of **CuO**[m, n] with $m, n \geq 2$

(S_p, S_q)	Frequency
(2, 4)	2
(4, 5)	4
(4, 6)	2
(4, 9)	$2n - 2$
(5, 6)	$2n + 2$
(6, 6)	$12m - 12$
(6, 9)	$2n - 2$
(5, 10)	$2n - 2$
(6, 10)	$4mn - 4m - 4n + 4$
(9, 10)	$4n - 4$
(10, 12)	$8mn - 8m - 8n + 8$

The next Theorem shows the exact value of Sanskruti index of **CuO**[m, n].

Theorem 6. “Consider the graph $G \sim \text{CuO}[m, n]$ with $m, n \geq 2$, then its Sanskruti index $S(G)$ is equal to:”

$$S(G) = \frac{101843355285146}{137310366375} - \frac{7613496016592n}{7689380517} - \frac{63583488m}{42875} + \frac{700704mn}{343}$$

Proof. Let G be the crystallographic structure of $\text{CuO}[m, n]$. Then by using Table 4 and equation (4) the Sanskruti index $S(G)$ is computed as follows:

$$S(G) = \sum_{pq \in E(G)} \left(\frac{S_p \times S_q}{S_p + S_q - 2} \right)^3$$

$$S(G) = (2) \left(\frac{2 \times 4}{2+4-2} \right)^3 + (4) \left(\frac{4 \times 5}{4+5-2} \right)^3 + (2) \left(\frac{4 \times 6}{4+6-2} \right)^3 + (2n-2) \left(\frac{4 \times 9}{4+9-2} \right)^3$$

$$+ (2n+2) \left(\frac{5 \times 6}{5+6-2} \right)^3 + (12m-12) \left(\frac{6 \times 6}{6+6-2} \right)^3 + (2n-2) \left(\frac{6 \times 9}{6+9-2} \right)^3$$

$$+ (2n-2) \left(\frac{5 \times 10}{5+10-2} \right)^3 + (4n-4) \left(\frac{9 \times 10}{9+10-2} \right)^3 + (4mn-4m-4n+4) \left(\frac{6 \times 10}{6+10-2} \right)^3$$

$$+ (8mn-8m-8n+8) \left(\frac{10 \times 12}{10+12-2} \right)^3$$

$$S(G) = \frac{101843355285146}{137310366375} - \frac{7613496016592n}{7689380517} - \frac{63583488m}{42875} + \frac{700704mn}{343}$$

RESULTS AND DISCUSSIONS

“In this section we have compared the first ($M1$) and second Zgrab ($M2$) indices of Copper(I) oxide Cu_2O and Copper(II) oxide CuO which is shown in Table 5. Analysis of the data showed that both the indices are higher in CuO compared to those of Cu_2O . For instance, $M1(\text{CuO})/M1(\text{Cu}_2\text{O})$ for [1,1] cell is 1.44 and the ratio increases to 1.943 for [7,7] and then it decrease to 1.87 for [10,10] cell. On the other hand, $M2(\text{CuO})/M2(\text{Cu}_2\text{O})$ for [1,1] is 1.40 and the ratio gradually increases to 2.413 for [10,10] cell.”

“Comparison of ABC indices for both the oxides of Copper showed higher values for CuO compared to those of Cu_2O (Table 6). For example, ratio of $ABC(\text{CuO})/ABC(\text{Cu}_2\text{O})$ for [2,2] cell is 1.95 and it decreases to 1.44 for [10,10]. This shows its decreasing trend with the increase of cells.”

“In the Table 7, we gave a comparison of the Sanskruti indices of Copper(I) oxide Cu_2O and Copper(II) oxide CuO . Analysis of the data showed that host higher Sanskruti index

Table 5. Comparison of the first and second Zgrab indices of Copper(I) oxide Cu_2O and Copper(II) oxide CuO

$[n, m]$	$M_1(\text{Cu}_2\text{O})$	$M_1(\text{CuO})$	$M_2(\text{Cu}_2\text{O})$	$M_2(\text{CuO})$
[1,1]	36	52	40	56
[2,2]	148	254	168	336
[3,3]	340	608	392	856
[4,4]	612	1114	712	1616
[5,5]	964	1772	1128	2616
[6,6]	1396	2582	1640	3856
[7,7]	1908	3544	2248	5336
[8,8]	2500	4858	2952	7056
[9,9]	3172	5924	3752	9016
[10,10]	3924	7342	4648	11216

Table 6. Comparison of the ABC index of Copper(I) oxide Cu_2O and Copper(II) oxide CuO

$[n, m]$	Formula Units		ABC		(Heat of formation) $\times (10)^{-23}$ kJ	
	Cu_2O	CuO	Cu_2O	CuO	Cu_2O	CuO
[1,1]	4	6	0	8.4852	112.88	155.4
[2,2]	16	20	16.970	33.519	451.52	518
[3,3]	36	42	45.254	74.538	1592	1087.8
[4,4]	66	65	64.254	102.42	1947	1836.5
[5,5]	100	110	135.76	204.53	2822	2849
[6,6]	144	156	197.99	293.50	4063.68	4040.4
[7,7]	196	210	271.53	398.46	5531.12	5439
[8,8]	256	272	356.38	519.41	7224.32	7044.8
[9,9]	324	342	452.54	656.34	9143.28	8857.8
[10,10]	400	420	560.02	809.25	11288	10878

Table 7. Comparison of the Sanskruti indices of Copper(I) oxide Cu_2O and Copper(II) oxide CuO

$[n, m]$	Formula Units		$S(\text{Cu}_2\text{O})$	$S(\text{CuO})$	(Entropy) $\times(10^{-23})$ kJ	
	Cu_2O	CuO			Cu_2O	CuO
[2,2]	16	20	1037.0	3966.9	247.04	142.8
[3,3]	36	42	2577.682945	11708.13692	555.84	299.88
[4,4]	64	72	4846.356123	23535.09049	988.16	514.08
[5,5]	100	110	7843.029301	39447.78166	1544	785.4
[6,6]	144	156	11567.70248	59446.21045	2223.36	1113.84
[7,7]	196	210	16020.37566	83530.37685	3026.24	1499.4
[8,8]	256	272	21201.04884	111700.2809	3952.64	1942.08
[9,9]	324	342	27109.72201	143955.9225	5002.56	2441.88
[10,10]	400	420	33746.39519	180297.3017	6176	2998.8

compared to CuO . The $S(\text{CuO})/S(\text{Cu}_2\text{O})$ for [2,2] is 3.825 and it increases to 5.34 for [10,10]. This shows its increasing trend with the increase of cells.”

A topological index is a numerical value that is calculate form molecular graph for explaining the relationship of chemical structure with physiochemical properties. So far, several applications of different indices have been reported for organic molecules, such as entropy and enthalpy determination, chirality identification,⁹ ZE-isomerism¹⁰ and heterosystem studies.¹⁸ The topological indices can be very helpful for crystalline compounds to correlate their structure with physiochemical properties. Therefore, we have determined Zagreb, ABC and Sunskurti indices for Cu_2O and CuO . Additionally, we compared these indices with the physical properties these oxides as described in Pubchem (<https://pubchem.ncbi.nlm.nih.gov/>).

“Zagreb indices ($M1$ & $M2$) were initially considered for total energy of π -electrons in organic molecules.¹² However, later they were associated with extent of branching in a molecular graph [10,11]. Analyses revealed higher $M1$ and $M2$ for CuO compared to those of Cu_2O at any cubic level i.e. at any equal value of $(m \times n)$ (Table 5). It suggests more branching in CuO compared to Cu_2O . It may cause more compact CuO (Density: 6.315 g/cm³) structure compared to Cu_2O (6.0 g/cm³).

Moreover, higher melting point of CuO (1599 K) compared to that of Cu_2O (1505 K) may also be associated to the higher branching.”

“ABC indices of Cu_2O and CuO were calculated at different unit cells as shown in Table 6. Analysis of the data showed higher ABC indices for CuO compared to those of Cu_2O (Table 6). Figure 4 shows that ABC indices increase exponentially with number of cells ($m \times n$) for both the oxides of copper. On the other hand, a linear relation of ABC index was observed with formula units (Figure 5). Since, ABC index has previously been linked with the thermodynamic properties” of different alkanes,^{7,11} “therefore, we determined the heat of formation per different units cells of both the oxides from the reported real molar enthalpy of formations (Table 6). For example, experimental molar enthalpy for CuO is -156 kJ mol^{-1} so for one formula unit it will be $-156/6.022 \times 10^{-23} \text{ kJ}$. The obtained value then multiplied with the number of formula units present in each cell to get the enthalpy for the cell. Similarly, enthalpy for Cu_2O calculated considering standard molar enthalpy -170 kJ mol^{-1} (Table 6). Analysis of the data showed that ABC index is not strongly associated with enthalpy of formation for the oxides of copper as reported in case of alkanes.^{6,13}” Therefore we determined a mathematical relationship, by using equation generator (<http://www.1728.org/threeps.htm>), between the ABC indices and the heat of formation of both the oxides of copper as below:

$$\text{Heat of formation for } \text{Cu}_2\text{O} = [\{ 3.045 \times 10^{-6} (\text{ABC})^2 \} + \{ 19.95 (\text{ABC}) \} + 112] \times 10^{-23}$$

$$\text{Heat of formation for } \text{CuO} = [\{ 3.75 \times 10^{-4} (\text{ABC})^2 \} + \{ 13.67 (\text{ABC}) \} + 60.17] \times 10^{-23}$$

These equations can be used for the transformation of ABC indices into the approximate heat of formation of the oxides of Cu at any cubic level.

Figure 6 shows a linear relation of Sanskriti indices with number of formula units and analysis showed higher indices for Cu_2O compared to CuO . Previous studies have shown an association of Sanskriti indices with entropy of octane.¹⁵ Here we calculated the entropy of both the oxides at different cells from the standard molar entropy. For instance, standard molar entropy for CuO is $93 \text{ J mol}^{-1} \text{ K}^{-1}$ so for one formula unit it will be $93/6.022 \times 10^{-23} \text{ J K}^{-1}$, and for each cell we just multiplied the obtained value with the no. of formula units present in the cell. Similarly entropy for Cu_2O calculated considering standard molar entropy $43 \text{ J mol}^{-1} \text{ K}^{-1}$ (Table 7). Analysis of the data showed a considerable difference between the Sanskriti indices and entropies for the oxides of Cu (Table 7). Therefore, we determined a mathematical relation for the transformation of Sanskriti indices into approximate entropies of both the oxides of copper as below:

$$\text{Entropy of } \text{Cu}_2\text{O} = [\{ -2.89 \times 10^{-7} (S)^2 \} + \{ 0.1913 (S) \} + 48.89] \times 10^{-23}$$

$$\text{Entropy of } \text{CuO} = [\{ -1.081 \times 10^{-8} (S)^2 \} + \{ 0.1819 (S) \} + 70.82] \times 10^{-23}$$

CONCLUSIONS

In conclusion, ABC and Sanskriti indices of Cu_2O and CuO showed considerable difference with the experimentally reported entropy and enthalpy of these oxides. On the other hand, Zagreb index and all these indices showed exponential

increase with the number of unit cells. On the other hand, these indices showed a linear behavior with number of formula units, suggesting that we may need a slight transformation of these indices for better explanation of physical properties of crystalline compounds.”

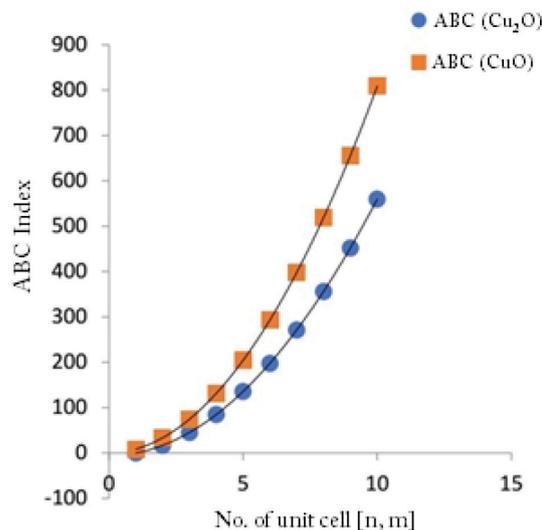


Figure 4. ABC indices of Cu_2O and CuO showing exponential increase with number of units cells (at x-axis)

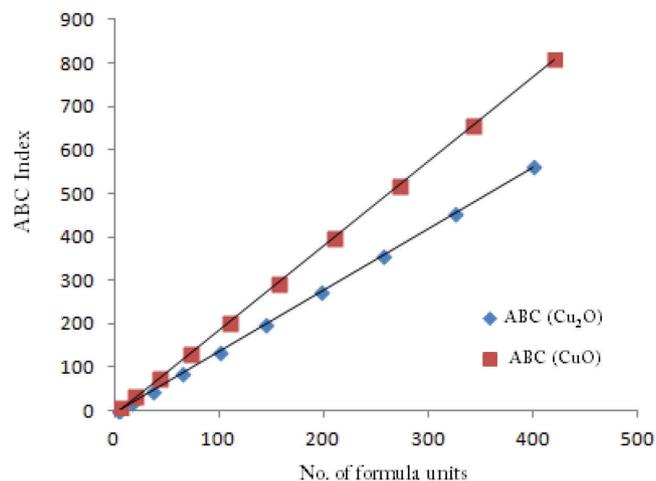


Figure 5. ABC indices of Cu_2O and CuO showing linear increase with number of formula units (at x-axis)

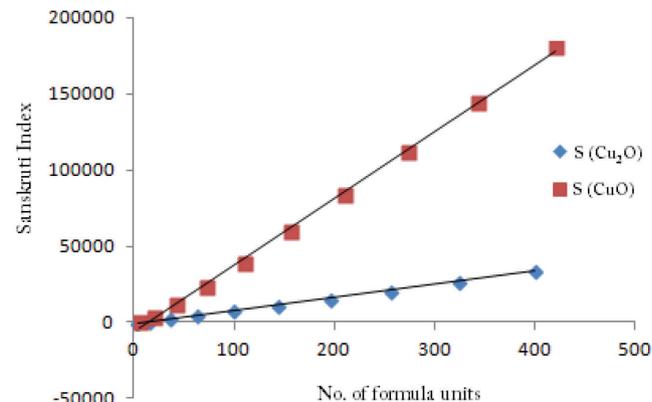


Figure 6. Sanskriti indices of Cu_2O and CuO showing linear increase with number of formula units (at x-axis)

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