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On analysis of thermodynamic properties of cuboctahedral bi-metallic structure

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Abstract: Porous materials, for example, metal-natural structures (MOFs) and their discrete partners metal-natural polyhedra (MOPs), that are built from coordinatively unsaturated inorganic hubs show incredible potential for application in gas adsorption/partition cycles, catalysis, and arising openings in hardware, optics, detecting, and biotechnology. A well-known hetero-bimetallic metal-organic polyhedra of this discrete partners metal-natural polyhedra (MOPs) class is cuboctahedral bi-metallic structure. In this paper, we discuss the structure of Hetero-bimetallic metal-organic polyhedra (cuboctahedral bi-metallic). Also, we computed the topological indices based on the degree of atoms in this cuboctahedral bi-metallic structure.

Keywords: topological indices, general Randic index, atom bond connectivity index, geometric arithmetic index, Zagreb type indices, cuboctahedral bi-metallic

1 Introduction

Development of large molecules that are amiable to plan also, functionalization is of essential current interest as it speaks to a significant advance in the accomplishment of atomic complexity. We accept that enormous permeable atoms fill in as charming beginning protests toward this path since the openings to their voids might be helpful in

directing the specific delivery and official of more modest molecules (Eddaoudi et al., 2001; Müller et al., 1998).

At present there are in any event two difficulties that must be tended to for bigger and more intricate frameworks to be figured it out. To begin with, single precious stones of huge particles are hard to get, accordingly blocking their full primary portrayal; second, plan of unbending substances that keep up their structure without visitors to take into consideration reversible admittance to the voids also as compound functionalization of their voids and outside surface remains generally unexplored (Fujita et al., 1999).

Given these difficulties and considering our ongoing work on metal-natural structures (MOFs), where we have illustrated the utilization of optional structure units (SBUs) as intends to the development of unbending organizations with perpetual porosity, we looked for to utilize the oar wheel group embraced by copper (II) acetic acid derivation, $\text{Cu}_2(\text{CO}_2)_4$, as an unbending SBU for tending to these difficulties. Fundamentally, the gathering of such SBUs with polytopic carboxylate linkers produced unbending permeable systems with open metal destinations where it is conceivable to functionalize the pores with various ligands (Day et al., 1989; Hong et al., 2000).

The clusters investigated of unit cell of cuboctahedral bi-metallic by DFT methods is dedicated in Figure 1. In which Hydrogen bound structures were advanced and checked to be at least on the potential energy surface with zero negative eigenvalue of the Hessian. Critically, the Pd site indicated no considerable cooperation with H_2 by and large no minima were found. The bimetallic groups were contrasted with the scandalous CuCu bunch, which was demonstrated in the trio state. All hydrogen communication energies were adjusted for premise set superposition error and zero-point energy commitments (Teo et al., 2016).

Here we depict the amalgamation and characterization of an arrangement of permeable metal-natural polyhedra developed from bimetallic paddle wheels that are, up to this point, uncommon building blocks for structure materials. The bimetallic metal units depend on a PdIIMII ($M = \text{Ni}$,

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Figure 1: Clusters investigated of unit cell of cuboctahedral bi-metallic by DFT methods: (a) formate, (b) benzoate, and (c) water solvated.

Figure 2: Schematic representations of the synthesis of the cuboctahedral bi-metallic (MOPs).

Cu, or Zn) theme (Figure 2), where the Pd(II) particles transcendently dwell on the inside of the cuboctahedral confines. As an outcome, the outside of the MOPs can be specifically enhanced with a progression of first column change metals that can be responded to give open coordination locales. We misuse this element and decide the gas adsorption properties of these extraordinary materials tentatively, utilizing a hypothetical examination to additionally clarify the adsorption. Eminently, they show incredibly high take-up of hydrogen for discrete permeable particles (Teo *et al.*, 2016).

2 Degree-based topological indices

Let $G = (V; E)$ be a graph where V be the vertex set and E be the edge set of G . The degree $\tilde{\Delta}(a)$ of a vertex a is the number of edges of G incident with a . Mathematical chemistry connects graph theory to science and focuses its consideration on the ideas of chemical graphs known as a molecular graph where atoms in the molecules are represented by vertices and bonds by edges. In fact, topological theories have often been used in the field of chemistry, the topology of an atom determines the form

of prominent Huckel sub-atomic orbitals. Normally the vertex degree is referred to its valency in a chemical graph.

The first degree-based index is introduced by Randic (1975) as:

$$R_{\frac{1}{2}} = R_{\frac{1}{2}}(G) = \sum_{ab \in E(G)} \frac{1}{\sqrt{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}} \quad (1)$$

Amic *et al.* (1998) and Bollobás and Erds (1988) proposed the general Randic index as:

$$R_{\alpha} = R_{\alpha}(G) = \sum_{ab \in E(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{\alpha} \quad (2)$$

The atom bond connectivity index is introduced by Estrada *et al.* (1998) as:

$$ABC = ABC(G) = \sum_{ab \in E(G)} \sqrt{\frac{\tilde{\Delta}(a) + \tilde{\Delta}(b) - 2}{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}} \quad (3)$$

The geometric arithmetic index is introduced by Vukicevic and Furtula (2009) as:

$$GA(G) = \sum_{ab \in E(G)} \frac{2\sqrt{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}}{\tilde{\Delta}(a) + \tilde{\Delta}(b)} \quad (4)$$

The first and second Zagreb index is formulated by Gutman and Trinajsti (1972) and Gutman and Das (2004) as:

$$M_1 = M_1(G) = \sum_{ab \in E(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b)) \quad (5)$$

$$M_2 = M_2(G) = \sum_{ab \in E(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \quad (6)$$

In 2008, Došlić put forward the first Zagreb coindex and second Zagreb coindex (Došlić, 2008), defined as:

$$\overline{M}_1 = \overline{M}_1(G) = \sum_{ab \notin E(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b)) \quad (7)$$

$$\overline{M}_2 = \overline{M}_2(G) = \sum_{ab \notin E(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \quad (8)$$

Gutman et al. (2016) proved the following Theorems:

Theorem 1:

Let G be a graph with $|V(G)|$ vertices and $|E(G)|$ edges. Then:

$$\overline{M}_1(G) = 2|E(G)|(|V(G)| - 1) - M_1(G)$$

Theorem 2:

Let G be a graph with $|V(G)|$ vertices and $|E(G)|$ edges. Then:

$$\overline{M}_2(G) = 2|E(G)|^2 - \frac{1}{2}M_1(G) - M_2(G)$$

For more details about these indices see Gao et al. (2016, 2017, 2018), Imran et al. (2018, 2019), Kang et al. (2018), Nadeem et al. (2019), and Yang et al. (2019).

In 2013, Shirdel et al. introduced a hyper-Zagreb index (Shirdel et al., 2013) as:

$$HM = HM(G) = \sum_{ab \in E(G)} [\tilde{\Delta}(a) \times \tilde{\Delta}(b)]^2 \quad (9)$$

In 2012, Ghorbani and Azimi defined two new versions of Zagreb indices of a graph G (Ghorbani and Azimi, 2012) as:

$$PM_1 = PM_1(G) = \prod_{ab \in E(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b)) \quad (10)$$

$$PM_2 = PM_2(G) = \prod_{ab \in E(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \quad (11)$$

Gutman and Trinajsti (1972) and Furtula and Gutman (2015) presented forgotten topological indices which was characterized as:

$$F = F(G) = \sum_{ab \in E(G)} (\tilde{\Delta}(a)^2 + \tilde{\Delta}(b)^2) \quad (12)$$

Furtula et al. (2010) defined augmented Zagreb index as:

$$AZI = AZI(G) = \sum_{ab \in E(G)} \left(\frac{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}{\tilde{\Delta}(a) + \tilde{\Delta}(b) - 2} \right)^3 \quad (13)$$

The Balaban index (Balaban, 1982; Balaban and Quintas, 1983) is defined as for a graph G of order n , size is defined as:

$$J = J(G) = \frac{q}{q - p + 2} \sum_{ab \in E(G)} \frac{1}{\sqrt{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}} \quad (14)$$

The redefined version of the Zagreb indices was defined by Ranjini et al. (2013), namely, the redefined first, second and third Zagreb indices for a graph G as:

$$ReZG_1 = ReZG_1(G) = \sum_{ab \in E(G)} \frac{\tilde{\Delta}(a) + \tilde{\Delta}(b)}{\tilde{\Delta}(a) \times \tilde{\Delta}(b)} \quad (15)$$

$$ReZG_2 = ReZG_2(G) = \sum_{ab \in E(G)} \frac{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}{\tilde{\Delta}(a) + \tilde{\Delta}(b)} \quad (16)$$

$$ReZG_3 = ReZG_3(G) = \sum_{ab \in E(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b))(\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \quad (17)$$

For more details about these indices see Akhter et al. (2019), Ali et al. (2015, 2019), Liu et al. (2020), Raza (2020, 2021), Raza and Sukaiti (2020), Shao et al. (2016).

3 Results for cuboctahedral bi-metallic (MOPs)

The number of vertices and edges of cuboctahedral bi-metallic (MOPs) are $196n$ and $240n$, respectively. Since there are four type of vertices in cuboctahedral bi-metallic (MOPs) namely the vertices of degree 1, 2, 3, 4, respectively. The vertex partition of the vertex set cuboctahedral bi-metallic (MOPs) is presented in Table 1. Also, the edge partition of cuboctahedral bi-metallic (MOPs) based on degrees of end vertices of each edge are depicted in Table 2.

Table 1: Vertex partition of cuboctahedral bi-metallic (MOPs) based on degree of vertex

$\tilde{\Delta}(a)$	Frequency	Set of vertices
1	$36n$	V_1
2	$84n$	V_2
3	$60n$	V_3
4	$16n$	V_4

Table 2: Edge partition of cuboctahedral bi-metallic (MOPs)

$\tilde{\Delta}(a)$	Frequency	Set of vertices
(1,4)	$36n$	E_1
(2,2)	$16n$	E_2
(2,3)	$120n$	E_3
(2,4)	$42n$	E_4
(3,3)	$24n$	E_5
(3,4)	$16n$	E_6

3.1 The general Randic index

3.1.1 For $\alpha = 1$

$$\begin{aligned}
 R_1(G) &= \sum_{ab \in E(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^1 \\
 &= \sum_{ab \in E_1(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b)) + \sum_{ab \in E_2(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \\
 &\quad + \sum_{ab \in E_3(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \\
 &\quad + \sum_{ab \in E_4(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b)) + \sum_{ab \in E_5(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \\
 &\quad + \sum_{ab \in E_6(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \\
 &= 36n(1 \times 4) + 16n(2 \times 2) + 120n(2 \times 3) \\
 &\quad + 42n(2 \times 4) + 24n(3 \times 3) + 12n(3 \times 4) \\
 &= 1624n.
 \end{aligned}$$

3.1.2 For $\alpha = -1$

$$\begin{aligned}
 R_{-1}(G) &= \sum_{ab \in E(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{-1} \\
 &= \sum_{ab \in E_1(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{-1} + \sum_{ab \in E_2(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{-1} \\
 &\quad + \sum_{ab \in E_3(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{-1}
 \end{aligned}$$

$$\begin{aligned}
 &+ \sum_{ab \in E_4(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{-1} + \sum_{ab \in E_5(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{-1} \\
 &+ \sum_{ab \in E_6(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{-1} \\
 &= 36n \left(\frac{1}{1 \times 4} \right) + 16n \left(\frac{1}{2 \times 2} \right) \\
 &\quad + 120n \left(\frac{1}{2 \times 3} \right) + 42n \left(\frac{1}{2 \times 4} \right) \\
 &\quad + 24n \left(\frac{1}{3 \times 3} \right) + 12n \left(\frac{1}{3 \times 4} \right) \\
 &= \frac{503}{12}n.
 \end{aligned}$$

3.1.3 For $\alpha = \frac{1}{2}$

$$\begin{aligned}
 R_{\frac{1}{2}}(G) &= \sum_{ab \in E(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{\frac{1}{2}} \\
 &= \sum_{ab \in E_1(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{\frac{1}{2}} + \sum_{ab \in E_2(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{\frac{1}{2}} \\
 &\quad + \sum_{ab \in E_3(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{\frac{1}{2}} \\
 &\quad + \sum_{ab \in E_4(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{\frac{1}{2}} + \sum_{ab \in E_5(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{\frac{1}{2}} \\
 &\quad + \sum_{ab \in E_6(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{\frac{1}{2}} \\
 &= 36n(1 \times 4)^{\frac{1}{2}} + 16n(2 \times 2)^{\frac{1}{2}} \\
 &\quad + 120n(2 \times 3)^{\frac{1}{2}} + 42n(2 \times 4)^{\frac{1}{2}} \\
 &\quad + 24n(3 \times 3)^{\frac{1}{2}} + 12n(3 \times 4)^{\frac{1}{2}} \\
 &= 176n + 120n\sqrt{6} + 48n\sqrt{2} + 24n\sqrt{3}.
 \end{aligned}$$

3.1.4 For $\alpha = -\frac{1}{2}$

$$\begin{aligned}
 R_{-\frac{1}{2}}(G) &= \sum_{ab \in E(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{-\frac{1}{2}} \\
 &= \sum_{ab \in E_1(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{-\frac{1}{2}} \\
 &\quad + \sum_{ab \in E_2(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{-\frac{1}{2}}
 \end{aligned}$$

$$\begin{aligned}
& + \sum_{ab \in E_3(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{-\frac{1}{2}} \\
& + \sum_{ab \in E_4(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{-\frac{1}{2}} \\
& + \sum_{ab \in E_5(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{-\frac{1}{2}} \\
& + \sum_{ab \in E_6(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{-\frac{1}{2}} \\
& = 36n(1 \times 4)^{-\frac{1}{2}} + 16n(2 \times 2)^{-\frac{1}{2}} \\
& \quad + 120n(2 \times 3)^{-\frac{1}{2}} + 42n(2 \times 4)^{-\frac{1}{2}} \\
& \quad + 24n(3 \times 3)^{-\frac{1}{2}} + 12n(3 \times 4)^{-\frac{1}{2}} \\
& = 34n + 20n\sqrt{6} + \frac{21}{2}n\sqrt{2} + 2n\sqrt{3}.
\end{aligned}$$

The numerical and graphical representation of above computed results are presented in Table 3 and Figures 3 and 4, respectively.

3.2 The atom bond connectivity index

$$\begin{aligned}
ABC(G) &= \sum_{ab \in E(G)} \sqrt{\frac{\tilde{\Delta}(a) + \tilde{\Delta}(b) - 2}{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}} \\
&= \sum_{ab \in E_1(G)} \sqrt{\frac{\tilde{\Delta}(a) + \tilde{\Delta}(b) - 2}{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}} \\
& \quad + \sum_{ab \in E_2(G)} \sqrt{\frac{\tilde{\Delta}(a) + \tilde{\Delta}(b) - 2}{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}} \\
& \quad + \sum_{ab \in E_3(G)} \sqrt{\frac{\tilde{\Delta}(a) + \tilde{\Delta}(b) - 2}{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}} \\
& \quad + \sum_{ab \in E_4(G)} \sqrt{\frac{\tilde{\Delta}(a) + \tilde{\Delta}(b) - 2}{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}} \\
& \quad + \sum_{ab \in E_5(G)} \sqrt{\frac{\tilde{\Delta}(a) + \tilde{\Delta}(b) - 2}{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}} \\
& \quad + \sum_{ab \in E_6(G)} \sqrt{\frac{\tilde{\Delta}(a) + \tilde{\Delta}(b) - 2}{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}}
\end{aligned}$$

Table 3: Comparison of Randic index for $\alpha = 1, -1, \frac{1}{2}, -\frac{1}{2}$

n	$R_1(G)$	$R_{-1}(G)$	$R_{\frac{1}{2}}(G)$	$R_{-\frac{1}{2}}(G)$
1	1624	41.9167	630.302	101.303
2	3248	83.833	1260.604	202.606
3	4872	125.75	1890.906	303.909
4	6496	167.67	2521.207	405.213
5	8120	209.583	3151.509	506.516
6	9744	251.5	3781.8116	607.818
7	11368	293.4167	4412.1135	709.122

Figure 3: Comparison of $\alpha = 1, -1$.

Figure 4: Comparison of $\alpha = \frac{1}{2}, -\frac{1}{2}$.

$$\begin{aligned}
& = 36n \left(\sqrt{\frac{1+4-2}{1 \times 4}} \right) + 16n \left(\sqrt{\frac{2+2-2}{2 \times 2}} \right) \\
& \quad + 120n \left(\sqrt{\frac{2+3-2}{2 \times 3}} \right)
\end{aligned}$$

$$\begin{aligned}
& + 42n \left(\sqrt{\frac{2+4-2}{2 \times 4}} \right) + 24n \left(\sqrt{\frac{3+3-2}{3 \times 3}} \right) \\
& + 12n \left(\sqrt{\frac{3+4-2}{3 \times 4}} \right) \\
& = 18n\sqrt{3} + 89n\sqrt{2} + 16n + 2n\sqrt{5}\sqrt{3}.
\end{aligned}$$

3.3 The geometric arithmetic index

$$\begin{aligned}
GA(G) &= \sum_{ab \in E(G)} \frac{2\sqrt{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}}{\tilde{\Delta}(a) + \tilde{\Delta}(b)} \\
&= \sum_{ab \in E_1(G)} \frac{2\sqrt{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}}{\tilde{\Delta}(a) + \tilde{\Delta}(b)} + \sum_{ab \in E_2(G)} \frac{2\sqrt{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}}{\tilde{\Delta}(a) + \tilde{\Delta}(b)} \\
&\quad + \sum_{ab \in E_3(G)} \frac{2\sqrt{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}}{\tilde{\Delta}(a) + \tilde{\Delta}(b)} \\
&\quad + \sum_{ab \in E_4(G)} \frac{2\sqrt{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}}{\tilde{\Delta}(a) + \tilde{\Delta}(b)} \\
&\quad + \sum_{ab \in E_5(G)} \frac{2\sqrt{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}}{\tilde{\Delta}(a) + \tilde{\Delta}(b)} \\
&\quad + \sum_{ab \in E_6(G)} \frac{2\sqrt{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}}{\tilde{\Delta}(a) + \tilde{\Delta}(b)} \\
&= 36n \left(\frac{2\sqrt{1 \times 4}}{1+4} \right) + 16n \left(\frac{2\sqrt{2 \times 2}}{2+2} \right) \\
&\quad + 120n \left(\frac{2\sqrt{2 \times 3}}{2+3} \right) \\
&\quad + 42n \left(\frac{2\sqrt{2 \times 4}}{2+4} \right) + 24n \left(\frac{2\sqrt{3 \times 3}}{3+3} \right) \\
&\quad + 12n \left(\frac{2\sqrt{3 \times 4}}{3+4} \right) \\
&= \frac{344}{5}n + 48n\sqrt{6} + 28n\sqrt{2} + \frac{48}{7}n\sqrt{3}.
\end{aligned}$$

The numerical and graphical representation of above computed results are presented in Table 4 and in Figure 5.

3.4 The first Zagreb index

$$\begin{aligned}
M_1(G) &= \sum_{ab \in E(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b)) \\
&= \sum_{ab \in E_1(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b)) + \sum_{ab \in E_2(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b))
\end{aligned}$$

Table 4: Comparison of $ABC(G)$ and $GA(G)$ indices for TbO_2

n	$ABC(G)$	$GA(G)$
1	180.78	237.85
2	361.58	475.7
3	542.36	713.55
4	723.15	951.4
5	903.94	1189.25
6	1084.73	1427.1
7	1265.52	1664.95

Figure 5: Comparison of $ABC(G)$ and $GA(G)$.

$$\begin{aligned}
& + \sum_{ab \in E_3(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b)) \\
& + \sum_{ab \in E_4(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b)) + \sum_{ab \in E_5(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b)) \\
& + \sum_{ab \in E_6(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b)) \\
& = 36n(1+4) + 16n(2+2) \\
& \quad + 120n(2+3) + 42n(2+4) \\
& \quad + 24n(3+3) + 12n(3+4) \\
& = 1324n.
\end{aligned}$$

3.5 The second Zagreb index

$$\begin{aligned}
M_2(G) &= \sum_{ab \in E(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \\
&= \sum_{ab \in E_1(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b)) + \sum_{ab \in E_2(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \\
&\quad + \sum_{ab \in E_3(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))
\end{aligned}$$

$$\begin{aligned}
& + \sum_{ab \in E_4(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b)) + \sum_{ab \in E_5(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \\
& + \sum_{ab \in E_6(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \\
& = 36n(1 \times 4) + 16n(2 \times 2) \\
& \quad + 120n(2 \times 3) + 42n(2 \times 4) \\
& \quad + 24n(3 \times 3) + 12n(3 \times 4) \\
& = 1624n.
\end{aligned}$$

3.6 The first Zagreb coindex

$$\begin{aligned}
\overline{M}_1(G) &= \sum_{ab \notin E(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b)) \\
\overline{M}_1(G) &= 2|E(G)|(|V(G)| - 1) - M_1(G) \\
&= 2(240n)(196n - 1) - 1324n \\
&= 94080n^2 - 1804n.
\end{aligned}$$

3.7 The second Zagreb coindex

$$\begin{aligned}
\overline{M}_2(G) &= \sum_{ab \notin E(G)} (\tilde{\Delta}(a)\tilde{\Delta}(b)) \\
\overline{M}_2(G) &= 2|E(G)|^2 - \frac{1}{2}M_1(G) - M_2(G) \\
&= 2(240n)^2 - \frac{1}{2}1324n - 1624n \\
&= 68160n^2 - 722n.
\end{aligned}$$

3.8 The hyper Zagreb index

The hyper Zagreb index is computed by using Table 2 as follows:

$$\begin{aligned}
HM(G) &= \sum_{ab \in E(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^2 \\
&= \sum_{ab \in E_1(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^2 \\
&\quad + \sum_{ab \in E_2(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^2 \\
&\quad + \sum_{ab \in E_3(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^2
\end{aligned}$$

Table 5: Comparison of $M_1(G)$, $M_2(G)$, $\overline{M}_1(G)$, and $\overline{M}_2(G)$

n	$M_1(G)$	$M_2(G)$	$\overline{M}_1(G)$	$\overline{M}_2(G)$
1	1324	1624	92276	67438
2	2648	3248	372712	271196
3	3972	4872	841308	611274
4	5296	6496	1498064	1087672
5	6620	8120	2342980	1700390
6	7944	9744	3376056	2449428
7	9268	11368	4597292	3334786

Figure 6: Comparison of $M_1(G)$ and $M_2(G)$.

$$\begin{aligned}
& + \sum_{ab \in E_4(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^2 + \sum_{ab \in E_5(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^2 \\
& + \sum_{ab \in E_6(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^2 \\
& = 36n(1 \times 4)^2 + 16n(2 \times 2)^2 \\
& \quad + 120n(2 \times 3)^2 + 42n(2 \times 4)^2 \\
& \quad + 24n(3 \times 3)^2 + 12n(3 \times 4)^2 \\
& = 7120n.
\end{aligned}$$

3.9 The first and second multiplicative Zagreb index

The first multiplicative Zagreb index is computed as:

$$\begin{aligned}
PM_1(G) &= \prod_{ab \in E(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b)) \\
&= \prod_{ab \in E_1(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b)) \times \prod_{ab \in E_2(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b))
\end{aligned}$$

Figure 7: Comparison of $\overline{M}_1(G)$ and $\overline{M}_2(G)$.

$$\begin{aligned}
 & \times \prod_{ab \in E_3(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b)) \\
 & \times \prod_{ab \in E_4(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b)) \times \prod_{ab \in E_5(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b)) \\
 & \times \prod_{ab \in E_6(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b)) \\
 & = 36n(1+4) \times 16n(2+2) \times 120n(2+3) \\
 & \quad \times 42n(2+4) \times 24n(3+3) \times 12n(3+4) \\
 & = 21069103104000 n^6.
 \end{aligned}$$

The second multiplicative Zagreb index is computed as:

$$\begin{aligned}
 PM_2(G) &= \prod_{ab \in E(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \\
 &= \prod_{ab \in E_1(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \times \prod_{ab \in E_2(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \\
 & \quad \times \prod_{ab \in E_3(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \\
 & \quad \times \prod_{ab \in E_4(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \times \prod_{ab \in E_5(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \\
 & \quad \times \prod_{ab \in E_6(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \\
 &= 36n(1 \times 4) \times 16n(2 \times 2) \times 120n(2 \times 3) \\
 & \quad \times 42n(2 \times 4) \times 24n(3 \times 3) \times 12n(3 \times 4) \\
 &= 69347447930880 n^6.
 \end{aligned}$$

The numerical and graphical representation of above computed results are presented in Table 6 and in Figure 8.

Table 6: Comparison of $HM(G)$, $PM_1(G)$, and $PM_2(G)$

n	$HM(G)$	$PM_1(G)$	$PM_2(G)$
1	7120	21069103104000	69347447930880
2	14240	1348422598656000	4438236667576320
3	21360	15359376162816000	50554289541611520
4	28480	86299046313984000	284047146724884480
5	35600	3292047360000000000	1083553873920000000
6	42720	983000074420224000	3235474530663137280
7	49840	2478758911082496000	8158657901620101120

Figure 8: Comparison of $HM(G)$, $PM_1(G)$, and $PM_2(G)$.

3.10 The forgotten index

The forgotten index is computed as:

$$\begin{aligned}
 F(G) &= \sum_{ab \in E(G)} (\tilde{\Delta}(a)^2 + \tilde{\Delta}(b)^2) \\
 &= \sum_{ab \in E_1(G)} (\tilde{\Delta}(a)^2 + \tilde{\Delta}(b)^2) + \sum_{ab \in E_2(G)} (\tilde{\Delta}(a)^2 + \tilde{\Delta}(b)^2) \\
 & \quad + \sum_{ab \in E_3(G)} (\tilde{\Delta}(a)^2 + \tilde{\Delta}(b)^2) \\
 & \quad + \sum_{ab \in E_4(G)} (\tilde{\Delta}(a)^2 + \tilde{\Delta}(b)^2) \\
 & \quad + \sum_{ab \in E_5(G)} (\tilde{\Delta}(a)^2 + \tilde{\Delta}(b)^2) \\
 & \quad + \sum_{ab \in E_6(G)} (\tilde{\Delta}(a)^2 + \tilde{\Delta}(b)^2) \\
 &= 36n(1^2 + 4^2) + 16n(1^2 + 4^2) \\
 & \quad + 120n(1^2 + 4^2) + 42n(1^2 + 4^2) \\
 & \quad + 24n(1^2 + 4^2) + 12n(1^2 + 4^2) \\
 &= 3872n.
 \end{aligned}$$

3.11 The augmented Zagreb index

The augmented Zagreb index is computed as below:

$$\begin{aligned}
 AZI(G) &= \sum_{ab \in E(G)} \left(\frac{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}{\tilde{\Delta}(a) + \tilde{\Delta}(b) - 2} \right)^3 \\
 &= \sum_{ab \in E_1(G)} \left(\frac{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}{\tilde{\Delta}(a) + \tilde{\Delta}(b) - 2} \right)^3 \\
 &\quad + \sum_{ab \in E_2(G)} \left(\frac{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}{\tilde{\Delta}(a) + \tilde{\Delta}(b) - 2} \right)^3 \\
 &\quad + \sum_{ab \in E_3(G)} \left(\frac{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}{\tilde{\Delta}(a) + \tilde{\Delta}(b) - 2} \right)^3 \\
 &\quad + \sum_{ab \in E_4(G)} \left(\frac{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}{\tilde{\Delta}(a) + \tilde{\Delta}(b) - 2} \right)^3 \\
 &\quad + \sum_{ab \in E_5(G)} \left(\frac{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}{\tilde{\Delta}(a) + \tilde{\Delta}(b) - 2} \right)^3 \\
 &\quad + \sum_{ab \in E_6(G)} \left(\frac{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}{\tilde{\Delta}(a) + \tilde{\Delta}(b) - 2} \right)^3 \\
 &= 36n \left(\frac{1 \times 4}{1 + 4 - 2} \right)^3 + 16n \left(\frac{2 \times 2}{2 + 2 - 2} \right)^3 \\
 &\quad + 120n \left(\frac{2 \times 3}{2 + 3 - 2} \right)^3 \\
 &\quad + 42n \left(\frac{2 \times 4}{2 + 4 - 2} \right)^3 + 24n \left(\frac{3 \times 3}{3 + 3 - 2} \right)^3 \\
 &\quad + 12n \left(\frac{3 \times 4}{3 + 4 - 2} \right)^3 \\
 &= \frac{5845789}{3000} n.
 \end{aligned}$$

3.12 The Balaban index

$$\begin{aligned}
 J(G) &= \frac{q}{q-p+2} \sum_{ab \in E(G)} \frac{1}{\sqrt{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}} \\
 &= \frac{q}{q-p+2} \left[\sum_{ab \in E_1(G)} \frac{1}{\sqrt{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}} \right. \\
 &\quad + \sum_{ab \in E_2(G)} \frac{1}{\sqrt{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}} \\
 &\quad + \sum_{ab \in E_3(G)} \frac{1}{\sqrt{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}} + \sum_{ab \in E_4(G)} \frac{1}{\sqrt{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}} \\
 &\quad + \sum_{ab \in E_5(G)} \frac{1}{\sqrt{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}} + \sum_{ab \in E_6(G)} \frac{1}{\sqrt{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}} \left. \right] \\
 &= \frac{240n}{240n - 196n + 2} \left[36n(1 \times 4)^{-\frac{1}{2}} \right. \\
 &\quad + 16n(2 \times 2)^{-\frac{1}{2}} + 120n(2 \times 3)^{-\frac{1}{2}} \\
 &\quad + 42n(2 \times 4)^{-\frac{1}{2}} + 24n(3 \times 3)^{-\frac{1}{2}} + 12n(3 \times 4)^{-\frac{1}{2}} \left. \right] \\
 &= \frac{240n \left(34n + 20n\sqrt{6} + \frac{21}{2}n\sqrt{6} + 2n\sqrt{3} \right)}{44n + 2}.
 \end{aligned}$$

Table 7: Comparison of $F(G)$, $AZI(G)$, and $J(G)$

n	$F(G)$	$AZI(G)$	$J(G)$
1	3872	1948.596333	528.5381158
2	7744	3897.192667	1080.566814
3	11616	5845.789000	1632.946119
4	15488	7794.385333	2185.416030
5	19360	9742.981667	2737.922673
6	23232	11691.57800	3290.447819
7	27104	13640.17433	3842.983591

Figure 9: Comparison of $F(G)$, $AZI(G)$, and $J(G)$.

$$\begin{aligned}
 &+ \sum_{ab \in E_5(G)} \frac{1}{\sqrt{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}} + \sum_{ab \in E_6(G)} \frac{1}{\sqrt{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}} \left. \right] \\
 &= \frac{240n}{240n - 196n + 2} \left[36n(1 \times 4)^{-\frac{1}{2}} \right. \\
 &\quad + 16n(2 \times 2)^{-\frac{1}{2}} + 120n(2 \times 3)^{-\frac{1}{2}} \\
 &\quad + 42n(2 \times 4)^{-\frac{1}{2}} + 24n(3 \times 3)^{-\frac{1}{2}} + 12n(3 \times 4)^{-\frac{1}{2}} \left. \right] \\
 &= \frac{240n \left(34n + 20n\sqrt{6} + \frac{21}{2}n\sqrt{6} + 2n\sqrt{3} \right)}{44n + 2}.
 \end{aligned}$$

The numerical and graphical representation of above computed results are presented in Table 7 and in Figure 9.

3.13 The redefine Zagreb indices

The redefine Zagreb indices are computed as:

$$\begin{aligned}
 ReZG_1(G) &= \sum_{ab \in E(G)} \frac{\tilde{\Delta}(a) + \tilde{\Delta}(b)}{\tilde{\Delta}(a) \times \tilde{\Delta}(b)} \\
 &= \sum_{ab \in E_1(G)} \frac{\tilde{\Delta}(a) + \tilde{\Delta}(b)}{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}
 \end{aligned}$$

$$\begin{aligned}
& + \sum_{ab \in E_2(G)} \frac{\tilde{\Delta}(a) + \tilde{\Delta}(b)}{\tilde{\Delta}(a) \times \tilde{\Delta}(b)} \\
& + \sum_{ab \in E_3(G)} \frac{\tilde{\Delta}(a) + \tilde{\Delta}(b)}{\tilde{\Delta}(a) \times \tilde{\Delta}(b)} \\
& + \sum_{ab \in E_4(G)} \frac{\tilde{\Delta}(a) + \tilde{\Delta}(b)}{\tilde{\Delta}(a) \times \tilde{\Delta}(b)} \\
& + \sum_{ab \in E_5(G)} \frac{\tilde{\Delta}(a) + \tilde{\Delta}(b)}{\tilde{\Delta}(a) \times \tilde{\Delta}(b)} \\
& + \sum_{ab \in E_6(G)} \frac{\tilde{\Delta}(a) + \tilde{\Delta}(b)}{\tilde{\Delta}(a) \times \tilde{\Delta}(b)} \\
& = 36n \left(\frac{1+4}{1 \times 4} \right) + 16n \left(\frac{2+2}{2 \times 2} \right) \\
& + 120n \left(\frac{2+3}{2 \times 3} \right) + 42n \left(\frac{2+4}{2 \times 4} \right) \\
& + 24n \left(\frac{3+3}{3 \times 3} \right) + 12n \left(\frac{3+4}{3 \times 4} \right) \\
& = \frac{431}{2} n.
\end{aligned}$$

$$\begin{aligned}
ReZG_2(G) &= \sum_{ab \in E(G)} \frac{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}{\tilde{\Delta}(a) + \tilde{\Delta}(b)} \\
&= \sum_{ab \in E_1(G)} \frac{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}{\tilde{\Delta}(a) + \tilde{\Delta}(b)} \\
&+ \sum_{ab \in E_2(G)} \frac{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}{\tilde{\Delta}(a) + \tilde{\Delta}(b)} \\
&+ \sum_{ab \in E_3(G)} \frac{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}{\tilde{\Delta}(a) + \tilde{\Delta}(b)} \\
&+ \sum_{ab \in E_4(G)} \frac{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}{\tilde{\Delta}(a) + \tilde{\Delta}(b)} \\
&+ \sum_{ab \in E_5(G)} \frac{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}{\tilde{\Delta}(a) + \tilde{\Delta}(b)} \\
&+ \sum_{ab \in E_6(G)} \frac{\tilde{\Delta}(a) \times \tilde{\Delta}(b)}{\tilde{\Delta}(a) + \tilde{\Delta}(b)} \\
&= 36n \left(\frac{1 \times 4}{1+4} \right) + 16n \left(\frac{2 \times 2}{2+2} \right) \\
&+ 120n \left(\frac{2 \times 3}{2+3} \right) + 42n \left(\frac{2 \times 4}{2+4} \right) \\
&+ 24n \left(\frac{3 \times 3}{3+3} \right) + 12n \left(\frac{3 \times 4}{3+4} \right) \\
&= \frac{10548}{35} n.
\end{aligned}$$

$$\begin{aligned}
ReZG_3(G) &= \sum_{ab \in E(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b))(\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \\
&= \sum_{ab \in E_1(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b))(\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \\
&+ \sum_{ab \in E_2(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b))(\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \\
&+ \sum_{ab \in E_3(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b))(\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \\
&+ \sum_{ab \in E_4(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b))(\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \\
&+ \sum_{ab \in E_5(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b))(\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \\
&+ \sum_{ab \in E_6(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b))(\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \\
&= 36n(1+4)(1 \times 4) + 16n(2+2)(2 \times 2) \\
&+ 120n(2+3)(2 \times 3) + 42n(2+4)(2 \times 4) \\
&+ 24n(3+3)(3 \times 3) + 12n(3+4)(3 \times 4) \\
&= 8896n.
\end{aligned}$$

The numerical and graphical representation of above computed results are presented in Table 8 and in Figure 10.

4 Conclusion

In this paper, we discuss the structure of Hetero-bimetallic metalorganic polyhedra (cuboctahedral bi-metallic). Also, we computed the topological indices based on the degree of atoms in this cuboctahedral bi-metallic structure. More preciously we have computed, Randic indices, Zagreb type indices, forgotten index, geometric arithmetic index, and Balaban indices. Also, we provide the numerical and graphical representation of computed results, which leads us to describe the thermodynamics properties of

Table 8: Comparison of $ReZG_1(G)$, $ReZG_2(G)$, and $ReZG_3(G)$

N	$ReZG_1(G)$	$ReZG_2(G)$	$ReZG_3(G)$
1	215.5	301.3714286	8896
2	431	602.7428571	17792
3	646.5	904.1142857	26688
4	862	1205.485714	35584
5	1077.5	1506.857143	44480
6	1293	1808.228571	53376
7	1508.5	2109.6	62272

Figure 10: Comparison of $ReG_1(G)$, $ReG_2(G)$, and $ReG_3(G)$.

hetero-bimetallic metalorganic polyhedra (cuboctahedral bi-metallic structure).

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