On analysis of thermodynamic properties of cuboctahedral bi-metallic structure

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 metalorganic 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 metalorganic 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, Cu$_2$(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 PdIIIMII (M = Ni,
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 $\Delta(a)$ 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:

$$R_1 = R_1(G) = \sum_{a \in V} \frac{1}{\sqrt{\Delta(a) \times \Delta(b)}}$$

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

$$R_\alpha = R_\alpha(G) = \sum_{a \in V} (\Delta(a) \times \Delta(b))^\alpha$$

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

$$ABC = ABC(G) = \sum_{a \in V} \sqrt{\Delta(a) + \Delta(b) - 2}$$

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

$$GA(G) = \sum_{a \in V} \sqrt{\frac{\Delta(a) \times \Delta(b)}{\Delta(a) + \Delta(b)}}$$
The first and second Zagreb index is formulated by Gutman and Trinajsti (1972) and Gutman and Das (2004) as:

\[ M_1 = M_1(G) = \sum_{ab \in E(G)} (\bar{\Delta}(a) + \bar{\Delta}(b)) \]
\[ M_2 = M_2(G) = \sum_{ab \in E(G)} (\bar{\Delta}(a) \times \bar{\Delta}(b)) \]

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

\[ M_1^1 = M_1^1(G) = \sum_{ab \in E(G)} (\bar{\Delta}(a) + \bar{\Delta}(b)) \]
\[ M_2^1 = M_2^1(G) = \sum_{ab \in E(G)} (\bar{\Delta}(a) \times \bar{\Delta}(b)) \]

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

**Theorem 1:**
Let \( G \) be a graph with \( |V(G)| \) vertices and \( |E(G)| \) edges. Then:

\[ M_1^1(G) = 2|E(G)|(|V(G)| - 1) - M_1(G) \]

**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:

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

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

\[ PM_1 = PM_1(G) = \prod_{ab \in E(G)} (\bar{\Delta}(a) + \bar{\Delta}(b)) \]
\[ PM_2 = PM_2(G) = \prod_{ab \in E(G)} (\bar{\Delta}(a) \times \bar{\Delta}(b)) \]

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

\[ F = F(G) = \sum_{ab \in E(G)} (\bar{\Delta}(a))^2 + (\bar{\Delta}(b))^2 \]

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

\[ AZI = AZI(G) = \sum_{ab \in E(G)} \left( \frac{\bar{\Delta}(a) \times \bar{\Delta}(b)}{\bar{\Delta}(a) + \bar{\Delta}(b) - 2} \right)^3 \]

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

\[ J = J(G) = \frac{q}{q - p + 2} \sum_{ab \in E(G)} \frac{1}{\sqrt{\bar{\Delta}(a) \times \bar{\Delta}(b)}} \]

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:

\[ ReZG_1 = ReZG_1(G) = \sum_{ab \in E(G)} \frac{\bar{\Delta}(a) + \bar{\Delta}(b)}{\bar{\Delta}(a) \times \bar{\Delta}(b)} \]
\[ ReZG_2 = ReZG_2(G) = \sum_{ab \in E(G)} \frac{\bar{\Delta}(a) \times \bar{\Delta}(b)}{\bar{\Delta}(a) + \bar{\Delta}(b)} \]
\[ ReZG_3 = ReZG_3(G) = \sum_{ab \in E(G)} (\bar{\Delta}(a) + \bar{\Delta}(b))(\bar{\Delta}(a) \times \bar{\Delta}(b)) \]

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 196\( n \) and 240\( n \), 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.
3.1 The general Randic index

3.1.1 For $\alpha = 1$

\[ R_1(G) = \sum_{ab \in E(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{\alpha} \]
\[ = \sum_{ab \in E_1(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b)) + \sum_{ab \in E_2(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \]
\[ + \sum_{ab \in E_3(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \]
\[ + \sum_{ab \in E_4(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b)) \]
\[ = 36n(1 \times 4) + 16n(2 \times 2) + 120n(2 \times 3) \]
\[ + 42n(2 \times 4) + 24n(3 \times 3) + 12n(3 \times 4) \]
\[ = 1624n. \]

3.1.2 For $\alpha = -1$

\[ R_{-1}(G) = \sum_{ab \in E(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{-1} \]
\[ = \sum_{ab \in E_1(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{-1} + \sum_{ab \in E_2(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{-1} \]
\[ + \sum_{ab \in E_3(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{-1} \]

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

| $\Delta(a)$ | 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)

| $\Delta(a)$ | 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)       | $16n$     | $E_6$           |

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

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

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

\[ R_{-\frac{1}{2}}(G) = \sum_{ab \in E(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{-\frac{1}{2}} \]
\[ = \sum_{ab \in E_1(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{-\frac{1}{2}} + \sum_{ab \in E_2(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{-\frac{1}{2}} \]
\[ + \sum_{ab \in E_3(G)} (\tilde{\Delta}(a) \times \tilde{\Delta}(b))^{-\frac{1}{2}} \]
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

\[
ABC(G) = \sum_{a \in E(G)} \sqrt{\frac{\Delta(a) + \Delta(b) - 2}{\Delta(a) \times \Delta(b)}}
\]

\[
= 36n \left( 1 + 4 \right)^{-1/2} + 16n \left( 2 \times 2 \right)^{-1/2}
\]

\[
+ 120n \left( 2 \times 3 \right)^{-1/2} + 42n \left( 2 \times 4 \right)^{-1/2}
\]

\[
+ 24n \left( 3 \times 3 \right)^{-1/2} + 12n \left( 3 \times 4 \right)^{-1/2}
\]

\[
+ 36n + 10n \sqrt{2} + 27n \sqrt{3}
\]
3.3 The geometric arithmetic index

\[ GA(G) = \sum_{ab \in E(G)} \frac{2\sqrt{\Delta(a) \times \Delta(b)}}{\Delta(a) + \Delta(b)} \]

\[ = \sum_{ab \in E_1(G)} \frac{2\sqrt{\Delta(a) \times \Delta(b)}}{\Delta(a) + \Delta(b)} + \sum_{ab \in E_2(G)} \frac{2\sqrt{\Delta(a) \times \Delta(b)}}{\Delta(a) + \Delta(b)} \]

\[ + \sum_{ab \in E_3(G)} \frac{2\sqrt{\Delta(a) \times \Delta(b)}}{\Delta(a) + \Delta(b)} \]

\[ + \sum_{ab \in E_4(G)} \frac{2\sqrt{\Delta(a) \times \Delta(b)}}{\Delta(a) + \Delta(b)} \]

\[ + \sum_{ab \in E_5(G)} \frac{2\sqrt{\Delta(a) \times \Delta(b)}}{\Delta(a) + \Delta(b)} \]

\[ = 36n \left( \frac{2\sqrt{1 \times 4}}{1 + 4} \right) + 16n \left( \frac{2\sqrt{2 \times 2}}{2 + 2} \right) \]

\[ + 12n \left( \frac{2\sqrt{2 \times 3}}{2 + 3} \right) \]

\[ + 42n \left( \frac{2\sqrt{2 \times 4}}{2 + 4} \right) + 24n \left( \frac{2\sqrt{3 \times 3}}{3 + 3} \right) \]

\[ + 12n \left( \frac{2\sqrt{3 \times 4}}{3 + 4} \right) \]

\[ = \frac{344}{5}n + 48n \sqrt{6} + 28n \sqrt{2} + \frac{48}{7}n \sqrt{3}. \]

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

3.4 The first Zagreb index

\[ M_1(G) = \sum_{ab \in E(G)} (\Delta(a) + \Delta(b)) \]

\[ = \sum_{ab \in E_1(G)} (\Delta(a) + \Delta(b)) + \sum_{ab \in E_2(G)} (\Delta(a) + \Delta(b)) \]

\[ + \sum_{ab \in E_3(G)} (\Delta(a) + \Delta(b)) \]

\[ + \sum_{ab \in E_4(G)} (\Delta(a) + \Delta(b)) \]

\[ + \sum_{ab \in E_5(G)} (\Delta(a) + \Delta(b)) \]

\[ = 18n \sqrt{3} + 89n \sqrt{2} + 16n + 2n \sqrt{5} \sqrt{3}. \]

3.5 The second Zagreb index

\[ M_2(G) = \sum_{ab \in E(G)} (\Delta(a) \times \Delta(b)) \]

\[ = \sum_{ab \in E_1(G)} (\Delta(a) \times \Delta(b)) + \sum_{ab \in E_2(G)} (\Delta(a) \times \Delta(b)) \]

\[ + \sum_{ab \in E_3(G)} (\Delta(a) \times \Delta(b)) \]

\[ + \sum_{ab \in E_4(G)} (\Delta(a) \times \Delta(b)) \]

\[ + \sum_{ab \in E_5(G)} (\Delta(a) \times \Delta(b)) \]

\[ = 36n(1 + 4) + 16n(2 + 2) \]

\[ + 120n(2 + 3) + 42n(2 + 4) \]

\[ + 24n(3 + 3) + 12n(3 + 4) \]

\[ = 1324n. \]
3.6 The first Zagreb coindex

\[\overline{M}_1(G) = \sum_{ab \in E(G)} (\tilde{d}(a) + \tilde{d}(b))\]

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

\[= 2(240n)(196n - 1) - 1324n\]

\[= 94080n^2 - 1804n.\]

3.7 The second Zagreb coindex

\[\overline{M}_2(G) = \sum_{ab \in E(G)} (\tilde{d}(a)\tilde{d}(b))\]

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

\[= 2(240n)^2 - \frac{1}{2}1324n - 1624n\]

\[= 68160n^2 - 722n.\]

3.8 The hyper Zagreb index

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

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

\[= \sum_{ab \in E_1(G)} (\tilde{d}(a) \times \tilde{d}(b))^2 + \sum_{ab \in E_2(G)} (\tilde{d}(a) \times \tilde{d}(b))^2\]

\[+ \sum_{ab \in E_3(G)} (\tilde{d}(a) \times \tilde{d}(b))^2\]

\[= 36n(1 \times 4) + 16n(2 \times 2)\]

\[+ 120n(2 \times 3) + 42n(2 \times 4)\]

\[+ 24n(3 \times 3) + 12n(3 \times 4)\]

\[= 1624n.\]

3.9 The first and second multiplicative Zagreb index

The first multiplicative Zagreb index is computed as:

\[PM_1(G) = \prod_{ab \in E(G)} (\tilde{d}(a) + \tilde{d}(b))\]

\[= \prod_{ab \in E_1(G)} (\tilde{d}(a) + \tilde{d}(b)) \times \prod_{ab \in E_2(G)} (\tilde{d}(a) + \tilde{d}(b))\]
The second multiplicative Zagreb index is computed as:

\[ \prod_{ab \in E_3(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b)) \]
\[ \prod_{ab \in E_4(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b)) \times \prod_{ab \in E_5(G)} (\tilde{\Delta}(a) + \tilde{\Delta}(b)) \]
\[ = 36n(1+4) \times 16n(2+2) \times 120n(2+3) \times 42n(2+4) \times 24n(3+3) \times 12n(3+4) \]
\[ = 21069103104000 n^6. \]

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

Table 6: Comparison of HM(G), PM₁(G), and PM₂(G)

| n | HM(G) | PM₁(G) | PM₂(G) |
|---|-------|--------|--------|
| 1 | 7120  | 21069103104000 | 69347447930880 |
| 2 | 14240 | 1348422598656000 | 4438236667576320 |
| 3 | 21360 | 15359376162816000 | 50554289541611520 |
| 4 | 28480 | 86299046313984000 | 28404714672488480 |
| 5 | 35600 | 329204736000000000 | 108355387392000000 |
| 6 | 42720 | 9830000074420224000 | 323547450663137280 |
| 7 | 49840 | 2478758911082496000 | 8158657901620101120 |

Figure 7: Comparison of $\tilde{M}_1(G)$ and $\tilde{M}_3(G)$.

Figure 8: Comparison of HM(G), PM₁(G), and PM₂(G).

3.10 The forgotten index

The forgotten index is computed as:

\[ F(G) = \sum_{ab \in E(G)} (\tilde{\Delta}(a))^2 + (\tilde{\Delta}(b))^2 \]
\[ = \sum_{ab \in E_1(G)} (\tilde{\Delta}(a))^2 + (\tilde{\Delta}(b))^2 + \sum_{ab \in E_2(G)} (\tilde{\Delta}(a))^2 + (\tilde{\Delta}(b))^2 \]
\[ + \sum_{ab \in E_3(G)} (\tilde{\Delta}(a))^2 + (\tilde{\Delta}(b))^2 \]
\[ + \sum_{ab \in E_4(G)} (\tilde{\Delta}(a))^2 + (\tilde{\Delta}(b))^2 \]
\[ + \sum_{ab \in E_5(G)} (\tilde{\Delta}(a))^2 + (\tilde{\Delta}(b))^2 \]
\[ = 36n(1^2 + 4^2) + 16n(1^2 + 2^2) + 24n(1^2 + 4^2) + 12n(1^2 + 4^2) \]
\[ = 3872n. \]
3.11 The augmented Zagreb index

The augmented Zagreb index is computed as below:

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

\[
= \sum_{ab \in E_1(G)} \left( \frac{\Delta(a) \times \Delta(b)}{\Delta(a) + \Delta(b) - 2} \right)^3
+ \sum_{ab \in E_2(G)} \left( \frac{\Delta(a) \times \Delta(b)}{\Delta(a) + \Delta(b) - 2} \right)^3
+ \sum_{ab \in E_3(G)} \left( \frac{\Delta(a) \times \Delta(b)}{\Delta(a) + \Delta(b) - 2} \right)^3
+ \sum_{ab \in E_4(G)} \left( \frac{\Delta(a) \times \Delta(b)}{\Delta(a) + \Delta(b) - 2} \right)^3
+ \sum_{ab \in E_5(G)} \left( \frac{\Delta(a) \times \Delta(b)}{\Delta(a) + \Delta(b) - 2} \right)^3
+ \sum_{ab \in E_6(G)} \left( \frac{\Delta(a) \times \Delta(b)}{\Delta(a) + \Delta(b) - 2} \right)^3
\]

\[
= 36n \left( \frac{1 \times 4}{1 + 4 - 2} \right)^3 + 16n \left( \frac{2 \times 2}{2 + 2 - 2} \right)^3
+ 120n \left( \frac{2 \times 3}{2 + 3 - 2} \right)^3
+ 42n \left( \frac{3 \times 4}{3 + 4 - 2} \right)^3
+ 3 \times 4 \left( \frac{3 \times 4}{3 + 4 - 2} \right)^3
\]

\[
= \frac{5845789}{3000} n .
\]

3.12 The Balaban index

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

\[
= \frac{q}{q - p + 2} \left[ \sum_{ab \in E_1(G)} \frac{1}{\sqrt{\Delta(a) \times \Delta(b)}}
+ \sum_{ab \in E_2(G)} \frac{1}{\sqrt{\Delta(a) \times \Delta(b)}}
+ \sum_{ab \in E_3(G)} \frac{1}{\sqrt{\Delta(a) \times \Delta(b)}}
+ \sum_{ab \in E_4(G)} \frac{1}{\sqrt{\Delta(a) \times \Delta(b)}} \right]
\]

\[
= \frac{240n}{240n - 196n + 2} \left[ \frac{36n(1 \times 4)}{2} \right]^{1/2}
+ 16n(2 \times 2)^{-1/2} + 120n(2 \times 3)^{-1/2}
+ 42n(2 \times 4)^{-1/2} + 24n(3 \times 3)^{-1/2} + 12n(3 \times 4)^{-1/2}
\]

\[
= \frac{240n[34n + 2n\sqrt{n} + n^{1/2} + 2n^{1/2}]}{44n + 2} .
\]

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:

\[
ReZG_1(G) = \sum_{ab \in E(G)} \frac{\Delta(a) + \Delta(b)}{\Delta(a) \times \Delta(b)}
\]

\[
= \sum_{ab \in E_1(G)} \frac{\Delta(a) + \Delta(b)}{\Delta(a) \times \Delta(b)}
+ \sum_{ab \in E_2(G)} \frac{\Delta(a) + \Delta(b)}{\Delta(a) \times \Delta(b)}
+ \sum_{ab \in E_3(G)} \frac{\Delta(a) + \Delta(b)}{\Delta(a) \times \Delta(b)}
+ \sum_{ab \in E_4(G)} \frac{\Delta(a) + \Delta(b)}{\Delta(a) \times \Delta(b)}
+ \sum_{ab \in E_5(G)} \frac{\Delta(a) + \Delta(b)}{\Delta(a) \times \Delta(b)}
+ \sum_{ab \in E_6(G)} \frac{\Delta(a) + \Delta(b)}{\Delta(a) \times \Delta(b)}
\]
The numerical and graphical representation of above computed results are presented in Table 8 and in Figure 10.

\[ ReZ_{\overline{G}}(G) = \sum_{ab \in E_{3}(G)} \frac{\Delta(a) \times \Delta(b)}{\Delta(a) + \Delta(b)} \]
\[ = \sum_{ab \in E_{3}(G)} \frac{\Delta(a) \times \Delta(b)}{\Delta(a) + \Delta(b)} \]
\[ + \sum_{abc \in E_{3}(G)} \frac{\Delta(a) \times \Delta(b)}{\Delta(a) + \Delta(b)} \]
\[ + \sum_{abc \in E_{3}(G)} \frac{\Delta(a) \times \Delta(b)}{\Delta(a) + \Delta(b)} \]
\[ + \sum_{abc \in E_{3}(G)} \frac{\Delta(a) \times \Delta(b)}{\Delta(a) + \Delta(b)} \]
\[ + \sum_{abc \in E_{3}(G)} \frac{\Delta(a) \times \Delta(b)}{\Delta(a) + \Delta(b)} \]
\[ + \sum_{abc \in E_{3}(G)} \frac{\Delta(a) \times \Delta(b)}{\Delta(a) + \Delta(b)} \]

\[ = 36n \left( \frac{1}{1 \times 4} + 16n \left( 2 + 2 \right) \right) \]
\[ + 12n \left( \frac{2}{2 \times 3} + 42n \left( 2 \times 4 \right) \right) \]
\[ + 24n \left( \frac{3}{3 \times 3} + 12n \left( 3 \times 4 \right) \right) \]
\[ = \frac{431}{2} n. \]

\[ ReZ_{\overline{G}}(G) = \sum_{ab \in E_{3}(G)} \left( \frac{\Delta(a) \times \Delta(b)}{\Delta(a) + \Delta(b)} \right) \]
\[ = \sum_{ab \in E_{3}(G)} \left( \frac{\Delta(a) \times \Delta(b)}{\Delta(a) + \Delta(b)} \right) \]
\[ + \sum_{abc \in E_{3}(G)} \left( \frac{\Delta(a) \times \Delta(b)}{\Delta(a) + \Delta(b)} \right) \]
\[ + \sum_{abc \in E_{3}(G)} \left( \frac{\Delta(a) \times \Delta(b)}{\Delta(a) + \Delta(b)} \right) \]
\[ + \sum_{abc \in E_{3}(G)} \left( \frac{\Delta(a) \times \Delta(b)}{\Delta(a) + \Delta(b)} \right) \]
\[ + \sum_{abc \in E_{3}(G)} \left( \frac{\Delta(a) \times \Delta(b)}{\Delta(a) + \Delta(b)} \right) \]
\[ + \sum_{abc \in E_{3}(G)} \left( \frac{\Delta(a) \times \Delta(b)}{\Delta(a) + \Delta(b)} \right) \]

\[ = 36n \left( 1 \times 4 \right) \left( \frac{2 + 2}{2 \times 2} \right) \]
\[ + 12n \left( 2 \times 3 \right) \left( \frac{2 + 4}{2 \times 4} \right) \]
\[ + 24n \left( 3 \times 3 \right) \left( \frac{3 + 4}{3 \times 4} \right) \]
\[ = \frac{10548}{35} n. \]

4 Conclusion

In this paper, we discuss the structure of Hetero-bimetallic metalorganic polyhedra (cuboctahedral bi-metalic). Also, we computed the topological indices based on the degree of atoms in this cuboctahedral bi-metallic structure. More precisely 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

| N   | ReZ_{\overline{G}}(G) | ReZ_{\overline{G}}(G) | ReZ_{\overline{G}}(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                |
hetero-bimetallic metalorganic polyhedra (cuboctahedral bi-metallic structure).

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**References**

Amic D., Belo D., Luci B., Nikol S., Trinajstic N., The vertex-connectivity index revisited. J Chem Inf Comp Sci, 1998, 38(5), 819-822.

Akhter S., Imran M., Raza Z., On the general sum-connectivity index and general Randic index of cacti. J. Inequal. Appl., 2019, 30, 1-18.

Ali A., Raza Z., Bhatti A.A., Some vertex-degree-based topological indices of cacti. Ars Combinatoria, 2019, 144, 195-206.

Ali A., Bhatti A.A., Raza Z., Vertex-degree based topological indices of a smart polymer and some dendrimer nanostars. Optoelectron. Adv. Mat., 2015, 9, 256-259.

Balaban A.T., Highly discriminating distance-based topological index. Chem. Phys. Lett., 1982, 89(5), 399-404.

Balaban A.T., Quintas L.V., The smallest graphs, trees, and 4-trees with degenerate topological index. J. Math. Chem, 1983, 14, 213-233.

Bollobás B., Erds P., Graphs of extremal weights. Ars Combinatoria, 1998, 50, 225-233.

Day V.W., Klemperer W.G., Yaghi O.M., Synthesis and characterization of a soluble oxide inclusion complex, [CH3CN. cntnd. (V 120324-)]. J. Am. Chem. Soc., 1989, 111(15), 5959-5961.

Došlić T., Vertex-weighted Wiener polynomials for composite graphs. Ars Math. Contemp., 2008, 1(1), 66-80.
Raza Z., The expected values of some indices in random phenylene chains. Eur. Phys. J. Plus, 2021, 136, 91-99.
Raza Z., The expected values of arithmetic bond connectivity and geometric indices in random phenylene chains. Helion, 2020, 6 (7), 44-49.
Shirdel G.H., Rezapour H., Sayadi A.M., The hyper-Zagreb index of graph operations. Iran. J. Math. Chem., 2013, 4(2), 213-220.
Shao Z., Siddiqui M.K., Muhammad M.H., Computing Zagreb indices and Zagreb polynomials for symmetrical nanotubes. Symmetry, 2016, 10(7), 244-260.
Teo J. M., Coghlan C.J., Evans J.D., Tsivion E., Head-Gordon M., Sumby C.J., et al., Hetero-bimetallic metalorganic polyhedra. Chem. Commun., 2016, 52(2), 276-279.
Vukicevic D., Furtula B., Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges. J. Math. Chem., 2009, 46(4), 1369-1376.
Yang H., Imran M., Akhter S., Iqbal Z., Siddiqui M.K., On Distance-Based Topological Descriptors of Subdivision Vertex-Edge Join of Three Graphs. IEEE Access, 2019, 7(1), 143381-143391.