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Research Article

On Degree-Based Topological Indices of Thermodynamic Cuboctahedral Bi-Metallic Structure

Guozhen Ma,[1] Muhammad Ibrahim ,[2] Ghazanfar Abbas ,[2] M. K. Siddiqui,[3] and Samuel Asefa Fufa [4]

[1]*Department of Engineering Mechanics, Tsinghua University, Beijing 100084, China*
[2]*Centre for Advanced Studies in Pure and Applied Mathematics, Bahauddin Zakariya University, Multan, Pakistan*
[3]*Department of Mathematics, COMSATS University Islamabad, Lahore Campus, Lahore, Pakistan*
[4]*Department of Mathematics, Addis Ababa University, Addis Ababa, Ethiopia*

Correspondence should be addressed to Samuel Asefa Fufa; samuel.asefa@aau.edu.et

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Porous material such as metal-natural constructions and their particular partner metal-natural poly-hydra are made up of inorganic clusters with no saturation and exhibit great capability for utilization in the absorption of gas and ascending opening in optics and detecting biotechnology and hardware. Cuboctahedral bi-metallic structure is an often-quoted example of metal-natural polyhedra class. In this study, we have calculated the first and second Zagreb index, the augmented Zagreb index, and the inverse Randic, as well as general Randic index, the symmetric division, and harmonic index. We have also discussed these topological indices graphically and have found that the value of almost all indices goes higher and higher as the value of n goes higher.

1. Introduction

It has been observed that the development of large molecules that are congenial to growth and functionalization is quite necessary for its present advantage. The atoms that are permeable on large scale can act as a favorable start to fill the gap in simpler molecules [1, 2]. Two problems in the function and generation of complex on larger systems must be considered. The first problem arises when we try to acquire monolithic parts of precious stones, and their full basic portrayal is hard to find. Secondly, inflexible substances resist the change in their structure making the compound functionlization of their voids unobservable [3].

Under these problems, along with the work going on about natural metal structures, the proper application of the optional structures units, and the proper building of inflexible systems with unending porosity, basically, mustering of such (SBU), poly topic carboxylate liners for solving problems created a lot of inflexible permeable systems with open metal ends where functionalization of different ligand pores were perceived [4, 5]. $(DFT)'s$ method applied to examine the unit cell of cubactohedral bi-metallic has been illustrated where the hydrogen bond structure was advanced, and it was evaluated for potential energy surface having zero negative eigenvalues of the Hessian. Pd site displayed negligible co-operation of hydrogen.

The mixturization and characterization of orderly permeable metal-natural poly-hydra growth from bi-metallic paddle wheel forming unusual building blocks have been displayed here. If the $Pd\,(II)$ particles transcendentally depend on the interiors of cubactohedral confines, the bi-metallic metal units will rely in a $Pd\,(II) M\,(II)$ theme. The outer ($MOPs$) can be improved to a large extent with the advancement if first column changes metals. Misusing this element, we can infer that the gas absorption characteristics of the unusual materials tentatively use the supposed evaluation for further examining of absorption. For details, see [6].

Molecular structure decides the properties of a matter. The chemical graph theory depicts the structure in graph with verities showing atoms of cubactohedral and edges relating to chemical bonds. A great deal of effort was shown by chemical graph theory for displaying the chemical characteristics of bi-metallic with no use of a wet lab. A graph $G(V, E)$ with vertex set $V(G)$ and edge set $E(G)$ is associated and assuming that nearby is a way concerning any pair of vertices in G. In a substance graph diagram, the maximum degree of that chemical graph is four. The idea of degree in graph theory is thoroughly associated (but not identical) to the perception of valence in chemistry [7]. Aimed at the particular details on the ground of graph theory, any ordinary or typical manuscript can be of great assistance [8, 9]. More than a few algebraic multinomials and polynomials have valuable submissions and understanding in chemical chemistry. The Hosoya polynomial is perchance the greatest healthy-recognized specimen [10, 11], and it produces an energetic participation in influential distance-based topological descriptors. The new concept of M-polynomial was established in 2015 and revolutionized the process of defining and determining bolted and closed procedures of man lateral to ictal descriptors. These descriptors summarily capture a large range of physico-chemical properties and surface tension [12, 13].

2. Basic Definitions

The Deutsch in [14] defined the M-polynomial of graph H as follows:

$$M(H; a, b) = \sum_{s \leq t} m_{s,t}(H) s^u t^v, \tag{1}$$

where $m_{s,t}(H)$ is the counting of edges $vu \in E(H)$ such that $\{d_s, d_t\} = \{i, j\}$. The application of Wiener index has discussed in [15–17].

The Randic index was introduced by Milan Randic in 1975 and defined as follows [18]:

$$R_{-1/2}(H) = \sum_{\mathrm{st} \in E(H)} \left(\frac{1}{\sqrt{d_s d_t}} \right). \tag{2}$$

The generalized Randic index is defined as follows [19, 20]:

$$R_\alpha(H) = \sum_{st \in E(H)} \left(\frac{1}{(d_s d_t)^\alpha} \right). \tag{3}$$

For details, see [21–23].

$M_1(H)$, $M_2(H)$, and ${}^m M_2(H)$ were introduced by Gutman and Trinajstic in [24–26] as

$$\begin{aligned} M_1(H) &= \sum_{st \in E(H)} (d_s + d_t), M_2(H) \\ &= \sum_{st \in E(H)} (d_s d_t), {}^m M_2(H) = \sum_{st \in H} \left(\frac{1}{d(s) d(t)} \right). \end{aligned} \tag{4}$$

The symmetric division index is defined as [27]

$$SDD(H) = \sum_{\mathrm{st} \in E(H)} \left\{ \frac{(\min(d_s, d_t)}{\max(d_s, d_t)} + \frac{\max(d_s, d_t)}{\min(d_s, d_t)} \right\}. \tag{5}$$

The harmonic index is defined as

$$\mathbb{H}(H) = \sum_{\mathrm{st} \in E(H)} \left(\frac{2}{d_s + d_t} \right). \tag{6}$$

For details, see [28, 29].

The inverse sum index is defined as

$$I(H) = \sum_{\mathrm{st} \in E(H)} \left(\frac{d_s d_t}{d_s + d_t} \right). \tag{7}$$

For details, see [18, 30, 31].

In [32, 33], the augmented Zagreb index is defined as

$$\begin{aligned} A(H) &= \sum_{\mathrm{st} \in E(H)} \left\{ \frac{d_s d_t}{d_s + d_t - 2} \right\}^3, \\ D_s &= s \frac{\partial (f(s,t))}{\partial s}, D_t = t \frac{\partial (f(s,t))}{\partial t}, S_s = \int \frac{f(s,t)}{s} \mathrm{d}s, \\ S_t &= \int \frac{f(s,t)}{t} \mathrm{d}t, J(f(s,t)) = f(s,s), Q_\alpha(f(s,t)) \\ &= s^\alpha f(s,t). \end{aligned} \tag{8}$$

3. Computational Results of Bi-Metallic Structure

Our fundamental goals of concentrating on M-polynomial and its connected all parts are to set up a connection between different effects of M-polynomials and its connected things on bi-metallic design, see Figure 1.

3.1. Main Results. We split vertices and edges' degree of cuboctahedral bi-metallic structure in Table 1 and Table 2.

Theorem 1. *Let H be a cuboctahedral bi-metallic. Then, M-polynomial of this structure is*

$$\begin{aligned} M(H, a, b) &= 36na^1b^4 + 16na^2b^2 + 120na^2b^3 \\ &\quad + 42na^2b^4 + 24na^3b^3 + 16na^3b^4. \end{aligned} \tag{9}$$

Proof 1. The M-polynomial is constructed from Figure 1 and by the use of Table 1 and Table 2 as

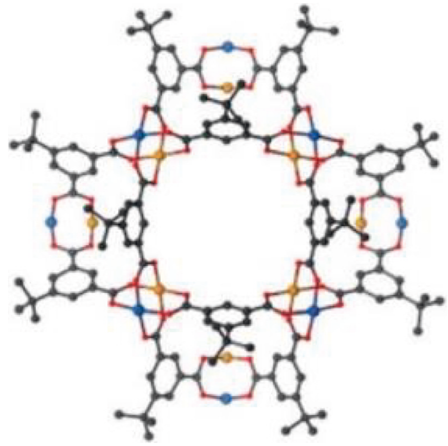

Figure 1: Cuboctahedral bi-metallic.

Table 1: Vertex partition of cuboctahedral bi-metallic structure.

Vertices	Total no. of vertices
$V(H)$	$196n$
$E(H)$	$254n$

Table 2: Edge partition of cuboctahedral bi-metallic structure.

Deg of end nodes	Total no. of edges
$d_s = 1$, $d_t = 4$	$36n$
$d_s = 2$, $d_t = 2$	$16n$
$d_s = 2$, $d_t = 3$	$120n$
$d_s = 2$, $d_t = 4$	$42n$
$d_s = 3$, $d_t = 3$	$24n$
$d_s = 3$, $d_t = 4$	$16n$

$$\begin{aligned}
M(H;a,b) &= \sum_{i\leq j} m_{ij}\left(H;a^i b^j\right),\\
&= \sum_{1\leq 4} m_{14}(H)a^1b^4 + \sum_{2\leq 2} m_{22}(H)a^2b^2 + \sum_{2\leq 3} m_{23}(H)a^2b^3 + \sum_{2\leq 4} m_{24}(H)a^2b^4\\
&\quad + \sum_{3\leq 3} m_{33}(H)a^3b^3 + \sum_{3\leq 4} m_{34}(H)a^3b^4,\\
&= \sum_{uv\in E_{\{1,4\}}} m_{14}(H)a^1b^4 + \sum_{uv\in E_{\{2,2\}}} m_{22}(H)a^2b^2 + \sum_{uv\in E_{\{2,3\}}} m_{23}(H)a^2b^3 + \sum_{uv\in E_{\{2,4\}}} m_{24}(H)a^2b^4\\
&\quad + \sum_{uv\in E_{\{3,3\}}} m_{33}(H)a^3b^3 + \sum_{uv\in E_{\{3,4\}}} m_{34}(H)a^3b^4,\\
&= \left|E_{\{1,4\}}\right|a^1b^4 + \left|E_{\{2,2\}}\right|a^2b^2 + \left|E_{\{2,3\}}\right|a^2b^3 + \left|E_{\{2,4\}}\right|a^2b^4 + \left|E_{\{3,3\}}\right|a^3b^3 + \left|E_{\{3,4\}}\right|a^3b^4,\\
&= 36na^1b^4 + 16na^2b^2 + 120na^2b^3 + 42na^2b^4 + 24na^3b^3 + 16na^3b^4.
\end{aligned} \tag{10}$$

□

Theorem 2. *Let H be a cuboctahedral bi-metallic. Then, first Zagreb index is*

$$M_1(H) = 1352n. \tag{11}$$

Proof 2. The M-polynomial is constructed from Figure 1 and by the use of Table 1 and Table 2 as

$$\begin{aligned}
\frac{\partial f}{\partial a} &= \frac{\partial}{\partial a}\left\{36na^1b^4 + 16na^2b^2 + 120na^2b^3 + 42na^2b^4 + 24na^3b^3 + 16na^3b^4\right\},\\
a\frac{\partial f}{\partial a} &= 36na^1b^4 + 32na^2b^2 + 240na^2b^3 + 84na^2b^4 + 72na^3b^3 + 48na^3b^4;\ D_b f(a,b) = b\frac{\partial f}{\partial b},\\
\frac{\partial f}{\partial b} &= \frac{\partial}{\partial b}\left\{36na^1b^4 + 16na^2b^2 + 120na^2b^3 + 42na^2b^4 + 24na^3b^3 + 16na^3b^4\right\},\\
b\frac{\partial f}{\partial b} &= 144na^1b^4 + 32na^2b^2 + 360na^2b^3 + 168na^2b^4 + 72na^3b^3 + 64na^3b^4,\\
M_1(H) &= \left(D_a + D_b\right)\left(f(a,b)\right|_{(a=b=1)} = 1352n.
\end{aligned} \tag{12}$$

□

Theorem 3. *Let H be a cuboctahedral bi-metallic. Then, second Zagreb index is*

$$M_2(H) = 1672n. \tag{13}$$

Proof 3. The M-polynomial is constructed from Figure 1 and by the use of Table 1 and Table 2 as

$$\begin{aligned}
M(H,a,b) &= 36na^1b^4 + 16na^2b^2 + 120na^2b^3 + 42na^2b^4 + 24na^3b^3 + 16na^3b^4,\\
D_a f(a,b) &= 36na^1b^4 + 32na^2b^2 + 240na^2b^3 + 84na^2b^4 + 72na^3b^3 + 48na^3b^4,\\
D_bD_a f(a,b) &= 144na^1b^4 + 64na^2b^2 + 720na^2b^3 + 336na^2b^4 + 216na^3b^3 + 192na^3b^4,\\
M_2(H) &= D_bD_a f(a,b)|_{(a=b=1)} = 144n + 64n + 720n + 336n + 216n + 192n,\\
M_2(H) &= 1672n.
\end{aligned} \tag{14}$$

□

Theorem 4. *Let H be a cuboctahedral bi-metallic. Then, the modified Second Zagreb Index is*

$${}^{m}M_2(H) = \frac{169}{4}n. \tag{15}$$

Proof 4. The M-polynomial is constructed from Figure 1 and by the use of Table 1 and Table 2 as

$$\begin{aligned}
\frac{f(x,b)}{x} &= 36nx^0b^4 + 16nx^1b^2 + 120nx^1b^3 + 42nx^1b^4 + 24nx^2b^3 + 16nx^2b^4,\\
S_a(a,b) &= 36na^1b^4 + 8na^2b^2 + 60na^2b^3 + 21na^2b^4 + 8na^3b^3 + \frac{16}{3}na^3b^4,\\
S_b\left(S_a(a,b)\right) &= b\int_0^b \frac{S_a(a,x)}{x}\,dx;\\
{}^{m}M_2(H) &= S_bS_a f(a,b)|_{(a=b=1)} = 9n + 4n + 20n + \frac{21}{4}n + \frac{8}{3}n + \frac{4}{3}n,\\
{}^{m}M_2(H) &= \frac{169}{4}n.
\end{aligned} \tag{16}$$

□

Theorem 5. *Let H be a cuboctahedral bi-metallic. Then, the general Randic index is*

$$R_\alpha(H) = n\left(2^\alpha\left(52 + 16(3)^\alpha(2)^\alpha\right) + 3^\alpha\left(120(2)^\alpha + 66(3)^\alpha\right)\right). \tag{17}$$

Proof 5. The M-polynomial is constructed from Figure 1 and by the use of Table 1 and Table 2 as

$$\begin{aligned}
M(H;a,b) &= 36na^1b^4 + 16na^2b^2 + 120na^2b^3 + 42na^2b^4 + 24na^3b^3 + 16na^3b^4,\\
R_\alpha(H) &= D_a^\alpha D_b^\alpha f(a,b)|_{(a=b=1)};\ R_\alpha(H) = D_a^\alpha D_b^\alpha f(a,b)|_{(a=b=1)},\\
D_b^\alpha f(a,b) &= 36(4)^\alpha na^1b^4 + 16(2)^\alpha na^2b^2 + 120(3)^\alpha na^2b^3 + 42(4)^\alpha na^2b^4 + 24(3)^\alpha na^3b^3 + 16(4)^\alpha na^3b^4,\\
D_a^\alpha D_b^\alpha f(a,b) &= 36(4)^\alpha na^1b^4 + 16(2)^{2\alpha} na^2b^2 + 120(2)^\alpha(3)^\alpha na^2b^3 + 42(2)^{3\alpha} na^2b^4 + 24(3)^{2\alpha} na^3b^3 + 16(3)^\alpha(4)^\alpha na^3b^4,\\
&= 36(2)^{2\alpha}n + 16(2)^{2\alpha}n + 120(2)^\alpha(3)^\alpha n + 42(2)^{3\alpha}n + 24(3)^{2\alpha}n + 16(3)^\alpha(4)^\alpha n,\\
R_\alpha(H) &= n\left(2^\alpha\left(52 + 16(3)^\alpha(2)^\alpha\right) + 3^\alpha\left(120(2)^\alpha + 66(3)^\alpha\right)\right).
\end{aligned} \tag{18}$$

□

Theorem 6. *Let H be a cuboctahedral bi-metallic. Then, inverse Randic index is*

$$RR_\alpha(H) = n(2)^{1-2\alpha}\left(26 + 29(3)^{-\alpha}\right) + n(3)^{-\alpha}\left(15(2)^{3-\alpha} + 24\right). \tag{19}$$

Proof 6. The M-polynomial is constructed from Figure 1 and by the use of Table 1 and Table 2 as

$$\begin{aligned}
M(H;a,b) &= 36na^1b^4 + 16na^2b^2 + 120na^2b^3 + 42na^2b^4 + 24na^3b^3 + 16na^3b^4,\\
RR_\alpha(H) &= S_a^\alpha S_b^\alpha f(a,b)|_{(a=b=1)};\ S_b = b\int_0^b \frac{f(a,x)}{x}\mathrm{d}x\\
&= 9na^1b^4 + 8na^2b^2 + 40na^2b^3 + \frac{21}{2}na^2b^4 + 8na^3b^3 + 4na^3b^4,\\
S_b^\alpha(a,b) &= \frac{36}{(4)^\alpha}nab^4 + \frac{16}{(2)^\alpha}na^2b^2 + \frac{120}{(3)^\alpha}na^2b^3 + \frac{42}{(4)^\alpha}na^2b^4 + \frac{24}{(3)^\alpha}na^3b^3 + \frac{16}{(4)^\alpha}na^3b^4,\\
\frac{S_b^\alpha(x,b)}{x} &= \frac{36}{(4)^\alpha}nb^4 + \frac{16}{(2)^\alpha}nxb^2 + \frac{120}{(3)^\alpha}nxb^3 + \frac{42}{(4)^\alpha}nx^2b^4 + \frac{24}{(3)^\alpha}nx^2b^3 + \frac{16}{(4)^\alpha}nx^2b^4,\\
S_a^\alpha S_b^\alpha(a,b) &= a\int_0^a \frac{S_b^\alpha(x,b)}{x}\mathrm{d}x = \frac{36}{(4)^\alpha}nab^4 + \frac{16}{(2)^{2\alpha}}na^2b^2 + \frac{120}{(2)^\alpha(3)^\alpha}na^2b^3\\
&\quad + \frac{42}{(3)^\alpha(4)^\alpha}na^2b^4 + \frac{24}{(3)^{2\alpha}}na^3b^3 + \frac{16}{(3)^\alpha(4)^\alpha}na^3b^4;\ RR_\alpha(H) = S_a^\alpha S_b^\alpha f(a,b)|_{(a=b=1)},\\
RR_\alpha(H) &= \frac{36}{(2)^{2\alpha}}n + \frac{16}{(2)^{2\alpha}}n + \frac{120}{(2)^\alpha(3)^\alpha}n + \frac{42}{(3)^\alpha(2)^{2\alpha}}n + \frac{24}{(3)^{2\alpha}}n + \frac{16}{(3)^\alpha(2)^{2\alpha}}n,\\
RR_\alpha(H) &= n(2)^{1-2\alpha}\left(26 + 29(3)^{-\alpha}\right) + n(3)^{-\alpha}\left(15(2)^{3-\alpha} + 24\right).
\end{aligned} \tag{20}$$

□

Theorem 7. *Let H be a cuboctahedral bi-metallic. Then, symmetric division index is*

$$SSD(H) = \frac{1862}{3}n. \tag{21}$$

Proof 7. The M-polynomial is constructed from Figure 1 and by the use of Table 1 and Table 2 as

$$
\begin{aligned}
M(H;a,b) &= 36na^1b^4 + 16na^2b^2 + 120na^2b^3 + 42na^2b^4 + 24na^3b^3 + 16na^3b^4,\\
SSD(H) &= (S_bD_a + S_aD_b)f(a,b)|_{(a=b=1)},\\
S_bD_af(a,b) &= 9na^1b^4 + \frac{32}{3}na^2b^2 + 80na^2b^3 + 21na^2b^4 + 24na^3b^3 + 12na^3b^4,\\
S_aD_bf(a,b) &= 144na^1b^4 + 32na^2b^2 + 360na^2b^3 + 168na^2b^4 + 72na^3b^3 + 64na^3b^4;\ (S_bD_a + S_aD_b)f(a,b)\\
&= 144na^1b^4 + 16na^2b^2 + 180na^2b^3 + 84na^2b^4 + 24na^3b^3 + 16na^3b^4,\\
SSD(H) &= (S_bD_a + S_aD_b)f(a,b)|_{(a=b=1)} = 9n + \frac{32}{3}n + 80n + 21n + 24n + 12n\\
&+ 144n + 16n + 180n + 84n + 24n + 16n.;\ SSD(H) = \frac{1862}{3}n.
\end{aligned}
\tag{22}
$$

□

Theorem 8. *Let H be a cuboctahedral bi-metallic. Then, the harmonic index is*

$$\mathbb{H}(H) = \frac{830}{3}n. \tag{23}$$

Proof 8. The M-polynomial is constructed from Figure 1 and by the use of Table 1 and Table 2 as

$$
\begin{aligned}
M(H;a;b) &= 36na^1b^4 + 16na^2b^2 + 120na^2b^3 + 42na^2b^4 + 24na^3b^3 + 16na^3b^4,\\
H(H) &= 2S_ajf(a,b)|_{a=1};\ S_a(a,b) = 36na^1b^4 + 8na^2b^2 + 60na^2b^3 + 21na^2b^4 + 8na^3b^3 + \frac{16}{3}na^3b^4,\\
2jS_a(a,b) &= 72na^5 + 16na^4 + 120na^5 + 42na^6 + 16na^6 + \frac{32}{3}na^7,\\
2S_ajf(a,b)|_{a=1} &= 72n + 16n + 120n + 42n + 16n + \frac{32}{3}n,\\
H(H) &= \frac{830}{3}n.
\end{aligned}
\tag{24}
$$

□

Theorem 9. *Let H be a cuboctahedral bi-metallic. Then, the inverse sum index is*

$$I(H) = \frac{10788}{35}n. \tag{25}$$

Proof 9. The M-polynomial is constructed from Figure 1 and by the use of Table 1 and Table 2 as

$$\begin{aligned}
M(H;a;b) &= 36na^1b^4 + 16na^2b^2 + 120na^2b^3 + 42na^2b^4 + 24na^3b^3 + 16na^3b^4,\\
I(H) &= S_a jD_aD_b f(a,b)|_{a=1};\ D_aD_b f(a,b)\\
&= 144na^1b^4 + 64na^2b^2 + 720na^2b^3 + 336na^2b^4 + 216na^3b^3 + 192na^3b^4,\\
jD_aD_b f(a,b) &= 144na^5 + 64na^4 + 720na^5 + 336na^6 + 216na^6 + 192na^7;\ S_a jD_aD_b f(a,b)\\
&= \frac{144}{5}na^5 + 16na^4 + 144na^5 + 56na^6 + 36na^6 + \frac{192}{7}na^7;\ S_a jD_aD_b f(a,b)|_{a=1},\\
I(H) &= \frac{144}{5}n + 16n + 144n + 56n + 36n + \frac{192}{7}n,\\
I(H) &= \frac{10788}{35}n.
\end{aligned} \tag{26}$$

□

Theorem 10. *Let H be a cuboctahedral bi-metallic. Then, the augmented Zagreb index is*

$$A(H) = 2003.89n. \tag{27}$$

Proof 10. The M-polynomial is constructed from Figure 1 and by the use of Table 1 and Table 2 as

$$\begin{aligned}
M(H;a,b) &= 36na^1b^4 + 16na^2b^2 + 120na^2b^3 + 42na^2b^4 + 24na^3b^3 + 16na^3b^4,\\
A(H) &= S_a^3Q_{-2}jD_a^3D_b^3 f(a,b)|_{a=1},\\
D_a^{\alpha}D_b^{\alpha} f(a,b) &= 36(4)^{\alpha}na^1b^4 + 16(2)^{2\alpha}na^2b^2 + 120(2)^{\alpha}(3)^{\alpha}na^2b^3 + 42(2)^{3\alpha}na^2b^4 + 24(3)^{2\alpha}na^3b^3,\\
+16(3)^{\alpha}(4)^{\alpha}na^3b^4;\ D_a^3D_b^3 f(a,b) &= 36(4)^3na^1b^4 + 16(2)^6na^2b^2 + 120(2)^3(3)^3na^2b^3 + 42(2)^9na^2b^4\\
&\quad + 24(3)^6na^3b^3 + 16(3)^3(4)^3na^3b^4\\
&= 2304na^1b^4 + 1024na^2b^2 + 25920na^2b^3 + 21504na^2b^4 + 17496na^3b^3 + 27648na^3b^4,\\
JD_a^3D_b^3 f(a,b) &= 2304na^5 + 1024na^4 + 25920na^5 + 21504na^6 + 17496na^6 + 27648na^7,\\
Q_{-2}jD_a^3D_b^3 f(a,b) &= 2304na^3 + 1024na^2 + 25920na^3 + 21504na^4 + 17496na^4 + 27648na,^5\\
S_a^3Q_{-2}jD_a^3D_b^3 f(a,b) &= \frac{2304}{27}na^3 + 128na^2 + 960na^3 + 336na^4 + \frac{17496}{64}na^4 + \frac{27648}{125}na^5,\\
S_a^3Q_{-2}jD_a^3D_b^3 f(a,b)|_{a=1} &= \frac{2304}{27}n + 128n + 960n + 336n + \frac{17496}{64}n + \frac{27648}{125}n,\\
A(H) &= 2003.89n.
\end{aligned} \tag{28}$$

□

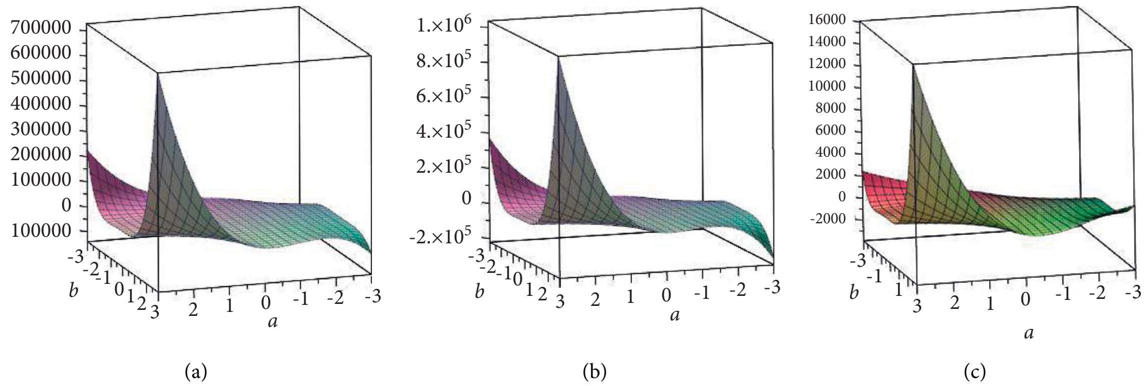

Figure 2: (a) $M_1(H)$ for $n = 1$, (b) $M_2(H)$ for $n = 1$, and (c) ${}^{m}M_2(H)$ for $n = 1$.

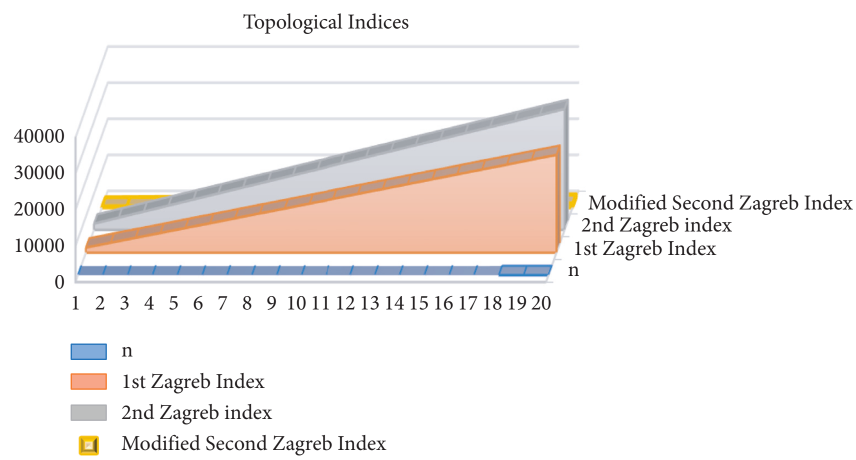

Figure 3: Comparison of $M_1(G), M_2(G), {}^{m}M_2(G)$ for $n = 1$.

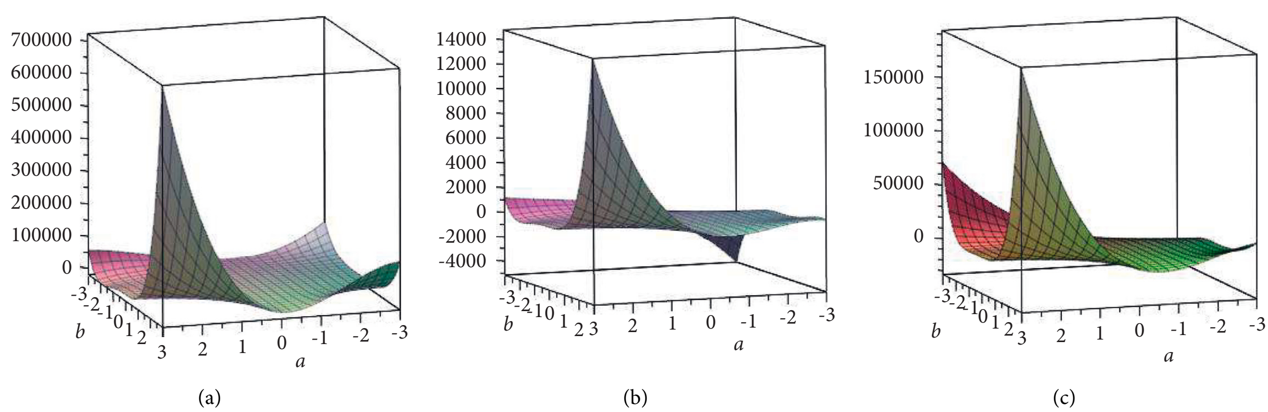

Figure 4: (a) $R_{\alpha}(H)$ for $n = 1, \alpha = 1$, (b) $RR_{\alpha}(H)$ for $n = 1, \alpha = 1$, and (c) $SDD(H)$ for $n = 1$.

4. Graphical Results and Their Discussion

The present section consists of graphical discussion on the results of topological indices which have constructed on the M-polynomial of cuboctahedral bi-metallic structure. From Figure 2, it can be observed that the value of first and second Zagreb index increases with the increase of n with a constant ratio, while the value of modified Zagreb index remains almost constant as the value of n increases or decreases. Also, from Figure 3, it can be seen directly that, for different values of α, the behavior of general Randic index and inverse Randic index decreases with the increase in the value of n. $\alpha = 3$; the change in the values of indices is more as compared with the value for $\alpha = 2$.

The graphical representation of these results can also be observed in Figures 2–6.

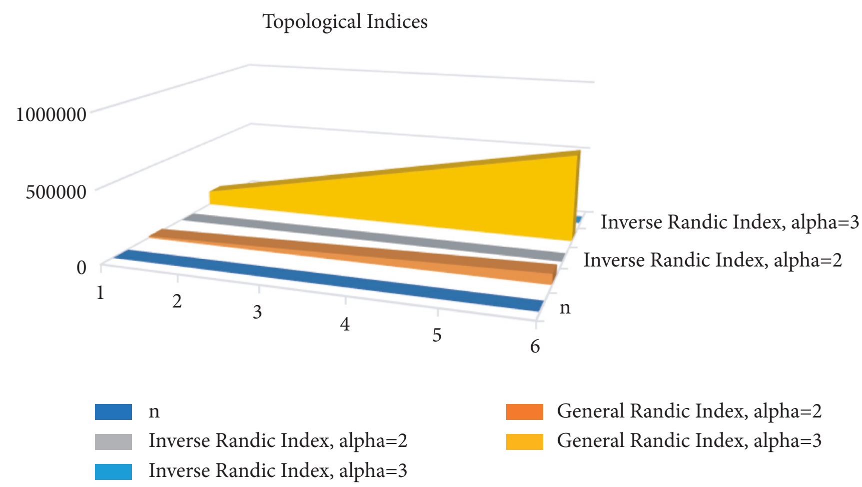

FIGURE 5: Comparison of $R_\alpha(H), RR_\alpha(H)$, for $n = 1$ and $\alpha = 2, 3$.

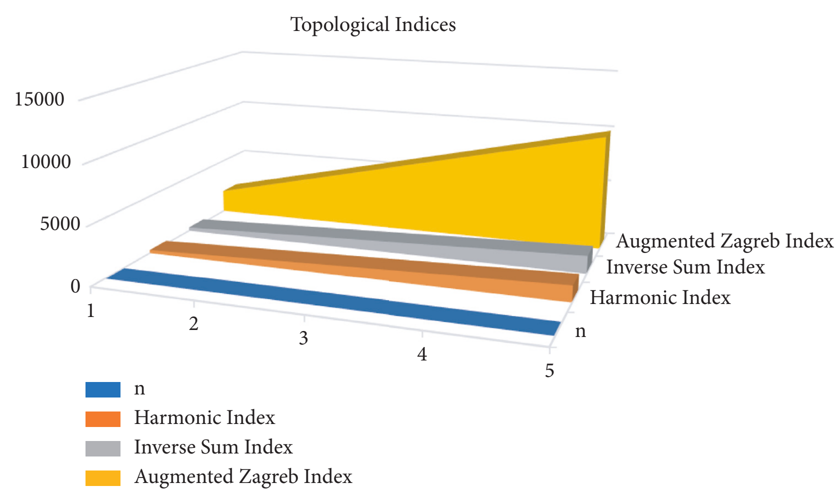

FIGURE 6: Comparison of $H(H), I(H)$, and $A(H)$ for $n = 1$.

5. Conclusion

The use of topological indices is very important to know the behavior of a graph or network. The research of networks through topological indices is important for understanding the basic topology of structure. The method of M-polynomial degree-based indices is applied to examine the unit cell of cubactohedral bi-mettallic which has been illustrated where the hydrogen bond structure was advanced, and it was evaluated for potential energy surface having zero negative eigenvalues of the Hessian, and this value usually increases with the increase of *n*.

Data Availability

The data used to support the findings are cited as references within the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Authors' Contributions

This work was equally contributed by all writers.

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