

Research Article

Topological Descriptors and Polynomials for Analysing the Structure of Antimony Telluride

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In a molecular network, molecules are correlated with numerical values, which are referred to as topological indices. The chemical and physical properties of chemical substances can be determined using topological indices. Mathematicians frequently use topological indices to calculate the strain energy, melting point, boiling temperature, distortion, and stability of chemical compounds. Topological indices also serve as a connection between a compound's biological activity and its physical properties. In this research paper, we have computed degree-based topological descriptors and polynomials to analyze the structure of antimony telluride.

1. Introduction

Graph theory is the mathematical theory of the properties and applications of networks or structures that are very useful to help define and visualize relationships between various components. Basically, the graph is a composition of points of departure known as nodes $V(G)$ and the lines formed by joining these vertices called edges $E(G)$ [1]. Each vertex's degree, defined as the number of edges that enter or leave it, is a key parameter. Graphs serve as a model for a broad range of systems whose function and structure are determined by the component elements' connection model. The connectedness of the graphs may be used to filter and condense knowledge [2]. The ideas and concepts of graph theory are widely used in various branches of study. The major role of graph theory in chemical graphs is the mathematical modeling of chemical phenomena. We can generalize the model of a molecule where each vertex represents an atom, and the edges connecting the relevant vertices indicate covalent connections between atoms [3, 4]. Chemists can easily gather details buried in the balance of

the subatomic diagram and anticipate attributes of compounds by assigning numbers and polynomials to chemical compounds. Topological indices have a wide range of applications in theoretical chemistry, particularly in QSPR/QSAR research [5]. Many properties of a molecule are known to be closely linked to its graphical structure, including heat of formation, boiling temperature, potential energy, and stiffness. Researchers can use topological indices defined on chemical molecule architectures to better understand physical features, chemical reactivity, and biological activity [6, 7].

In the current era, research in degree-based topological indices has been rising thoroughly. In recent years, several research papers have been published considering topological indices [8]. Chemical tests are useful to predict the power of topological indices for analyzing the physicochemical properties of molecular structures [9]. While researching on boiling point in 1947, Wiener was the first to develop the notion of the topological index in chemical graph theory [10, 11]. In this research, the structure of antimony telluride is formulated in which a

single atom of antimony makes a bond with six atoms of tellurium, and every tellurium makes a bond with three antimony atoms and three tellurium atoms that make a compound crystallizing in a hexagonal lattice it creates a closed packed structure. We have computed the atom-bond connectivity index, hyper-Zagreb index, geometric arithmetic indexes, redefined first, second, and third Zagreb index, and Randic index of the chemical graph of antimony telluride.

2. Preliminaries

Topological indices are graph invariant, which means they remain the same regardless of how the graph is constructed or named. Giving chemical compound numbers and polynomials makes it easier to explain their physical characteristics [12, 13]. Let G denote a (molecular) graph, with $V(G)$ and $E(G)$ as vertex and edge sets, respectively. The number of edges incident with a vertex p is called the degree of that vertex and denoted by $\Gamma(p)$.

Gutman et al. [14, 15] presented the first Zagreb index (M_1) and second Zagreb index (M_2) almost four decades ago as

$$\begin{aligned} M_1(G) &= \sum_{pt \in E(G)} [\Gamma(p) + \Gamma(t)], \\ M_2(G) &= \sum_{pt \in E(G)} [\Gamma(p) \times \Gamma(t)]. \end{aligned} \quad (1)$$

Shirdel et al. [16] established the “hyper-Zagreb index” as follows:

$$HM(G) = \sum_{pt \in E(G)} [\Gamma(p) + \Gamma(t)]^2. \quad (2)$$

Estrada et al. [17] established the ABC (atom-bond connectivity index), which is extremely important. It is described as

$$ABC(G) = \sum_{pt \in E(G)} \sqrt{\frac{\Gamma(p) + \Gamma(t) - 2}{\Gamma(p) \times \Gamma(t)}}. \quad (3)$$

Vukicevic and Furtula [18] proposed the geometric arithmetic index GA, which is defined as

$$GA(G) = \sum_{pt \in E(G)} \frac{2\sqrt{\Gamma(p) \times \Gamma(t)}}{\Gamma(p) + \Gamma(t)}. \quad (4)$$

The Randic index, created by Randić in 1975 [19], was the first-degree-based topological index, which is written as

$$R_\alpha(G) = \sum_{pt \in E(G)} [\Gamma(p) \times \Gamma(t)]^\alpha, \quad \alpha = 1, -1, \frac{1}{2}, \frac{-1}{2}. \quad (5)$$

The forgotten topological index was introduced by Gutman et al. [20] and was defined as

$$F(G) = \sum_{pt \in E(G)} [\Gamma(p)^2 + \Gamma(t)^2]. \quad (6)$$

Furtula et al. [21] offered the following improved Zagreb index:

$$AZI(G) = \sum_{pt \in E(G)} \left[\frac{\Gamma(p) \times \Gamma(t)}{\Gamma(p) + \Gamma(t) - 2} \right]^3. \quad (7)$$

The redefined 1st, 2nd, and 3rd Zagreb indices for the graph G were established by Ranjini et al. [22] as follows:

$$\begin{aligned} \text{ReZG}_1(G) &= \sum_{pt \in E(G)} \frac{\Gamma(p) + \Gamma(t)}{\Gamma(p) \times \Gamma(t)}, \\ \text{ReZG}_2(G) &= \sum_{pt \in E(G)} \frac{\Gamma(p) \times \Gamma(t)}{\Gamma(p) + \Gamma(t)}, \\ \text{ReZG}_3(G) &= \sum_{pt \in E(G)} [\Gamma(p) \times \Gamma(t)][\Gamma(p) + \Gamma(t)]. \end{aligned} \quad (8)$$

3. Main Results

Antimony telluride is an inorganic chemical compound with molecular formula (Sb_2Te_3) in which a single atom of antimony makes a bond with six atoms of tellurium, and every tellurium makes a bond with three antimony atoms and three tellurium atoms that make a compound crystallizing in a hexagonal lattice it creates a closed packed structure [23]. The 2D molecular structure of antimony telluride (Sb_2Te_3) is given in the figure below. We used the following configuration to characterize its molecular graph: the number of unit cells in a row that is linked is denoted by “ m ”, whereas the total number of linked rows with m cells is denoted by “ n ”. In Figure 1, we showed how cells in a row connect to one another and how one row relates to another.

For the calculation of antimony telluride formulae, we utilize a unit cell initially and then combine it with another unit cell in a horizontal manner, and so on up to m unit cells to compute antimony telluride formulae [23]. After that, we connect the first unit cell with another unit cell in a vertical orientation, and so on up to n unit cells, resulting in the antimony telluride structure shown in Figure 2.

3.1. Antimony Telluride $\text{Sb}_2\text{Te}_3[m, n]$

Theorem 1. Let G represent the structure of antimony telluride $\text{Sb}_2\text{Te}_3[m, n]$ for $m, n \geq 2$, then,

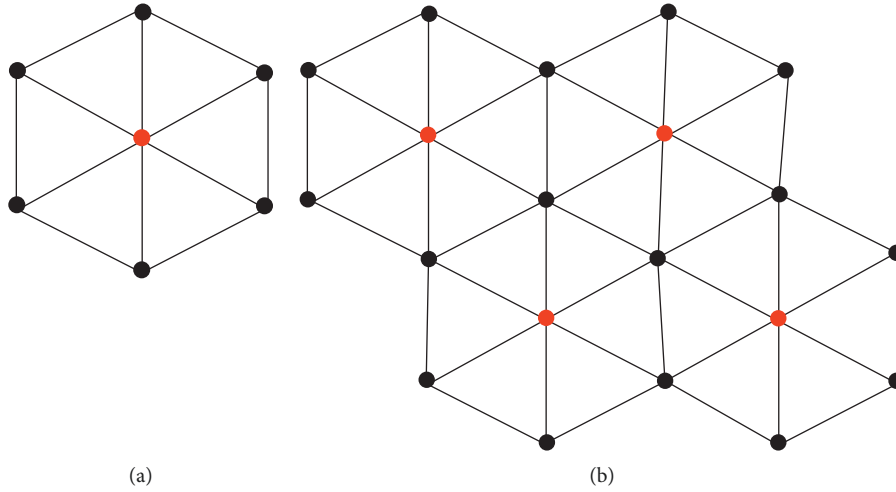


FIGURE 1: Structure of antimony telluride ($\text{Sb}_2\text{Te}_3[m, n]$). (a) Unit cell of antimony telluride $\text{Sb}_2\text{Te}_3[m, n]$. (b) $\text{Sb}_2\text{Te}_3[2, 2]$. Two rows are being connected each with two unit cells. Antimony atoms are red, and telluride atoms are black [23].

$$\text{ABC}(G) = m \left(-\frac{13\sqrt{10}}{15} + \frac{\sqrt{14}}{3} + \frac{3\sqrt{30}}{5} \right) + n \left(-\frac{13\sqrt{10}}{15} + \frac{\sqrt{14}}{3} + \frac{3\sqrt{30}}{5} \right) + mn \left(\frac{3\sqrt{10}}{2} \right) + \left(4 + \frac{7\sqrt{10}}{30} + \frac{\sqrt{14}}{3} - \frac{6\sqrt{30}}{5} \right),$$

$$\text{GA}(G) = m \left(\sqrt{15} + \frac{4\sqrt{2}}{3} + \frac{12\sqrt{30}}{11} - 10 \right) + n \left(\sqrt{15} - \frac{4\sqrt{2}}{3} + \frac{12\sqrt{30}}{11} - 10 \right) + mn(9) + \left(17 - 2\sqrt{15} + \frac{4\sqrt{2}}{3} - \frac{24\sqrt{30}}{11} \right),$$

$$F(G) = 11664mn - 6012m - 6012n + 2790,$$

$$\text{AZI}(G) = \frac{569503793}{12348000} - \frac{22817861}{154350}m - \frac{22817861}{154350}n + \frac{52488}{125}mn,$$

$$\text{ReZG}_1(G) = 2m + 2n + 3mn,$$

$$\text{ReZG}_2(G) = -\frac{19}{11} - \frac{47}{22}m - \frac{47}{22}n + 27mn,$$

$$\text{ReZG}_3(G) = 3888mn - 1536m - 1536n + 480,$$

$$R_1(G) = 6 - 84m - 84n + 324mn, \tag{9}$$

$$R_{-1}(G) = \frac{3}{20} + \frac{3}{10}m + \frac{3}{10}n + \frac{1}{4}mn,$$

$$R_{1/2}(G) = m(4\sqrt{15} + 6\sqrt{2} + 6\sqrt{30} - 60) + n(4\sqrt{15} + 6\sqrt{2} + 6\sqrt{30} - 60) + 54mn + (84 - 8\sqrt{15} + 6\sqrt{2} - 12\sqrt{30}),$$

$$R_{-1/2}(G) = m \left(\frac{4}{\sqrt{15}} + \frac{2}{3\sqrt{2}} + \frac{6}{\sqrt{30}} - \frac{5}{3} \right) + n \left(\frac{4}{\sqrt{15}} + \frac{2}{3\sqrt{2}} + \frac{6}{\sqrt{30}} - \frac{5}{3} \right) + mn \left(\frac{3}{2} \right) + \left(\frac{23}{6} - \frac{8}{\sqrt{15}} + \frac{2}{3\sqrt{2}} - \frac{12}{\sqrt{30}} \right),$$

$$M_1(G) = 108mn - 4m - 4n - 10,$$

$$M_2(G) = 6 - 84m - 84n + 324mn,$$

$$\text{HM}(G) = -2 - 296m - 296n + 1296mn,$$

$$M_1(G, x) = (6)x^6 + (4m + 4n - 8)x^8 + (2m + 2n + 2)x^9 + (6m + 6n - 12)x^{11} + (9mn - 10m - 10n + 11)x^{12},$$

$$M_2(G, x) = (6)x^9 + (4m + 4n - 8)x^{15} + (2m + 2n + 2)x^{18} + (6m + 6n - 12)x^{30} + (9mn - 10m - 10n + 11)x^{36}.$$

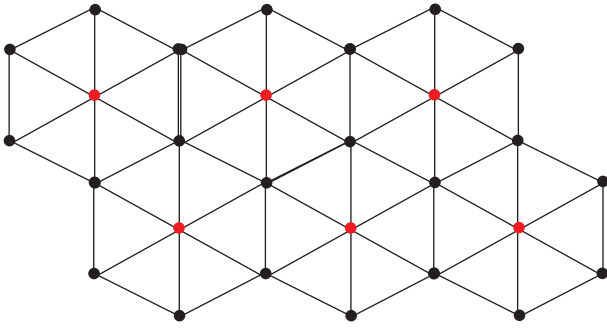


FIGURE 2: Structure of antimony telluride $Sb_2Te_3[m, n]$, $Sb_2Te_3[3, 2]$, two rows are being connected each with three-unit cells [23].

To compute vertices formulae, we now use Table 1. V_3 signifies the set of vertices of degree 3, V_5 the number of

vertices of degree 5, and V_6 the number of vertices of degree 6 in Table 1.

Finally, we discovered that set of vertices of degree 3 are $(2m + 2n + 2)$, set of vertices of degree 5 are $(2m + 2n - 4)$, and set of vertices of degree 6 are $(3mn - 2m - 2n + 2)$. Using the same technique, we will split the Sb_2Te_3 edges to get the abstracted indices. The first edge pack has six edges pt , where $\Gamma(p) = 3$ and $\Gamma(t) = 3$. The second edge pack has $(4m + 4n - 8)$ edges pt , where $\Gamma(p) = 3$ and $\Gamma(t) = 5$. The third edge pack has $(2m + 2n + 2)$ edges pt , where $\Gamma(p) = 3$ and $\Gamma(t) = 6$. The fourth edge pack has $(6m + 6n - 12)$ edges pt , where $\Gamma(p) = 5$ and $\Gamma(t) = 6$. The fifth edge pack has $(9mn - 10m - 10n + 11)$ edges pt , where $\Gamma(p) = 6$ and $\Gamma(t) = 6$. In Table 2, edge partition of $Sb_2Te_3[m, n]$ with $m, n \geq 2$ is shown.

(i) Atom-bond connectivity index

$$\begin{aligned}
 ABC(G) &= \sum_{pt \in E(G)} \sqrt{\frac{\Gamma(p) + \Gamma(t) - 2}{\Gamma(p) \times \Gamma(t)}} = (6) \sqrt{\frac{3+3-2}{3 \times 3}} + (4m+4n-8) \sqrt{\frac{3+5-2}{3 \times 5}} + (2m+2n+2) \sqrt{\frac{3+6-2}{3 \times 6}} \\
 &\quad + (6m+6n-12) \sqrt{\frac{5+6-2}{5 \times 6}} + (9mn-10m-10n+11) \sqrt{\frac{6+6-2}{6 \times 6}}, \\
 ABC(G) &= m \left(-\frac{13\sqrt{10}}{15} + \frac{\sqrt{14}}{3} + \frac{3\sqrt{30}}{5} \right) + n \left(-\frac{13\sqrt{10}}{15} + \frac{\sqrt{14}}{3} + \frac{3\sqrt{30}}{5} \right) + mn \left(\frac{3\sqrt{10}}{2} \right) + \left(4 + \frac{7\sqrt{10}}{30} + \frac{\sqrt{14}}{3} - \frac{6\sqrt{30}}{5} \right).
 \end{aligned} \tag{10}$$

(ii) Geometric arithmetic index

$$\begin{aligned}
 GA(G) &= \sum_{pt \in E(G)} \frac{2\sqrt{\Gamma(p) \times \Gamma(t)}}{\Gamma(p) + \Gamma(t)} = (6) \left(\frac{2\sqrt{3 \times 3}}{3+3} \right) + (4m+4n-8) \left(\frac{2\sqrt{3 \times 5}}{3+5} \right) + (2m+2n+2) \left(\frac{2\sqrt{3 \times 6}}{3+6} \right) \\
 &\quad + (6m+6n-12) \left(\frac{2\sqrt{5 \times 6}}{5+6} \right) + (9mn-10m-10n+11) \left(\frac{2\sqrt{6 \times 6}}{6+6} \right), \\
 GA(G) &= m \left(\sqrt{15} + \frac{4\sqrt{2}}{3} + \frac{12\sqrt{30}}{11} - 10 \right) + n \left(\sqrt{15} - \frac{4\sqrt{2}}{3} + \frac{12\sqrt{30}}{11} - 10 \right) + mn(9) + \left(17 - 2\sqrt{15} + \frac{4\sqrt{2}}{3} - \frac{24\sqrt{30}}{11} \right).
 \end{aligned} \tag{11}$$

The connection between ABC and GA is shown in Table 3 and Figure 3

(iii) Forgotten topological index

$$\begin{aligned}
 F(G) &= \sum_{pt \in E(G)} [\Gamma(p)^2 + \Gamma(t)^2] \\
 &= (6)(3^2 \times 3^2) + (4m+4n-8)(3^2 \times 5^2) + (2m+2n+2)(3^2 \times 6^2) + (6m+6n-12)(5^2 \times 6^2) \\
 &\quad + (9mn-10m-10n+11)(6^2 \times 6^2), \\
 F(G) &= 11664mn - 6012m - 6012n + 2790.
 \end{aligned} \tag{12}$$

TABLE 1: Vertex partition of $Sb_2Te_3[m, n]$.

$[m, n]$	[2, 2]	[2, 3]	[2, 4]	[3, 2]	[3, 3]	[3, 4]	[4, 2]	[4, 3]	[4, 4]
V_3	10	12	14	12	14	16	14	16	18
V_5	4	6	8	6	8	10	8	10	12
V_6	6	10	14	10	17	24	14	24	34

(iv) Augmented Zagreb index

$$\begin{aligned}
 AZI(G) &= \sum_{pt \in E(G)} \left[\frac{\Gamma(p) \times \Gamma(t)}{\Gamma(p) + \Gamma(t) - 2} \right]^3 \\
 &= (6) \left(\frac{3 \times 3}{3 + 3 - 2} \right)^3 + (4m + 4n - 8) \left(\frac{3 \times 5}{3 + 5 - 2} \right)^3 + (2m + 2n + 2) \left(\frac{3 \times 6}{3 + 6 - 2} \right)^3 \\
 &\quad + (6m + 6n - 12) \left(\frac{5 \times 6}{5 + 6 - 2} \right)^3 + (9mn - 10m - 10n + 11) \left(\frac{6 \times 6}{6 + 6 - 2} \right)^3, \\
 AZI(G) &= \frac{569503793}{12348000} - \frac{22817861}{154350}m - \frac{22817861}{154350}n + \frac{52488}{125}mn.
 \end{aligned} \tag{13}$$

The connection between F and AZI is shown in Table 4 and Figure 4.

(v) Redefined 1st Zagreb index

$$\begin{aligned}
 ReZG_1(G) &= \sum_{pt \in E(G)} \frac{\Gamma(p) + \Gamma(t)}{\Gamma(p) \times \Gamma(t)} = (6) \left(\frac{3 + 3}{3 \times 3} \right) + (4m + 4n - 8) \left(\frac{3 + 5}{3 \times 5} \right) + (2m + 2n + 2) \left(\frac{3 + 6}{3 \times 6} \right) \\
 &\quad + (6m + 6n - 12) \left(\frac{5 + 6}{5 \times 6} \right) + (9mn - 10m - 10n + 11) \left(\frac{6 + 6}{6 \times 6} \right), \\
 ReZG_1(G) &= 2m + 2n + 3mn.
 \end{aligned} \tag{14}$$

(vi) Redefined 2nd Zagreb index

$$\begin{aligned}
 ReZG_2(G) &= \sum_{pt \in E(G)} \frac{\Gamma(p) \times \Gamma(t)}{\Gamma(p) + \Gamma(t)} = (6) \left(\frac{3 \times 3}{3 + 3} \right) + (4m + 4n - 8) \left(\frac{3 \times 5}{3 + 5} \right) + (2m + 2n + 2) \left(\frac{3 \times 6}{3 + 6} \right) \\
 &\quad + (6m + 6n - 12) \left(\frac{5 \times 6}{5 + 6} \right) + (9mn - 10m - 10n + 11) \left(\frac{6 \times 6}{6 + 6} \right), \\
 ReZG_2(G) &= \frac{19}{11} - \frac{47}{22}m - \frac{47}{22}n + 27mn.
 \end{aligned} \tag{15}$$

(vii) Redefined 3rd Zagreb index

$$\begin{aligned} \text{ReZG}_3(G) &= \sum_{pt \in E(G)} [\Gamma(p) \times \Gamma(t)] [\Gamma(t) + \Gamma(h)] = (6)[(3 \times 3)(3 + 3)] + (4m + 4n - 8)[(3 \times 5)(3 + 5)] \\ &\quad + (2m + 2n + 2)[(3 \times 6)(3 + 6)] \\ &\quad + (6m + 6n - 12)[(5 \times 6)(5 + 6)] + (9mn - 10m - 10n + 11)[(6 \times 6)(6 + 6)], \end{aligned} \quad (16)$$

$$\text{ReZG}_3(G) = 3888mn - 1536m - 1536n + 480.$$

The connection between ReZG_1 , ReZG_2 , and ReZG_3 is shown in Table 5 and Figure 5.

For $\alpha = 1$,

(viii) General Randic index

$$\begin{aligned} R_1(G) &= \sum_{pt \in E(G)} [\Gamma(p) \times \Gamma(t)]^1 = (6)(3 \times 3) + (4m + 4n - 8)(3 \times 5) + (2m + 2n + 2)(3 \times 6) \\ &\quad + (6m + 6n - 12)(5 \times 6) + (9mn - 10m - 10n + 11)(6 \times 6), \end{aligned} \quad (17)$$

$$R_1(G) = 6 - 84m - 84n + 324mn.$$

For $\alpha = -1$,

$$\begin{aligned} R_{-1}(G) &= \sum_{pt \in E(G)} [\Gamma(p) \times \Gamma(t)]^{-1} = (6)\frac{1}{3 \times 3} + (4m + 4n - 8)\frac{1}{3 \times 5} + (2m + 2n + 2)\frac{1}{3 \times 6} \\ &\quad + (6m + 6n - 12)\frac{1}{5 \times 6} + (9mn - 10m - 10n + 11)\frac{1}{6 \times 6}, \end{aligned} \quad (18)$$

$$R_{-1}(G) = \frac{3}{20} + \frac{3}{10}m + \frac{3}{10}n + \frac{1}{4}mn.$$

For $\alpha = 1/2$,

$$\begin{aligned} R_{1/2}(G) &= \sum_{pt \in E(G)} [\Gamma(p) \times \Gamma(t)]^{1/2} = (6)\sqrt{3 \times 3} + (4m + 4n - 8)\sqrt{3 \times 5} + (2m + 2n + 2)\sqrt{3 \times 6} + (6m + 6n - 12)\sqrt{5 \times 6} \\ &\quad + (9mn - 10m - 10n + 11)\sqrt{6 \times 6}, \end{aligned} \quad (19)$$

$$R_{1/2}(G) = m(4\sqrt{15} + 6\sqrt{2} + 6\sqrt{30} - 60) + n(4\sqrt{15} + 6\sqrt{2} + 6\sqrt{30} - 60) + 54mn + (84 - 8\sqrt{15} + 6\sqrt{2} - 12\sqrt{30}).$$

For $\alpha = -1/2$,

$$\begin{aligned} R_{-1/2}(G) &= \sum_{pt \in E(G)} [\Gamma(p) \times \Gamma(t)]^{-1/2} = \frac{6}{\sqrt{3 \times 3}} + \frac{(4m + 4n - 8)}{\sqrt{3 \times 5}} + \frac{(2m + 2n + 2)}{\sqrt{3 \times 6}} + \frac{(6m + 6n - 12)}{\sqrt{5 \times 6}} + \frac{(9mn - 10m - 10n + 11)}{\sqrt{6 \times 6}}, \end{aligned} \quad (20)$$

$$R_{-1/2}(G) = m\left(\frac{4}{\sqrt{15}} + \frac{2}{3\sqrt{2}} + \frac{6}{\sqrt{30}} - \frac{5}{3}\right) + n\left(\frac{4}{\sqrt{15}} + \frac{2}{3\sqrt{2}} + \frac{6}{\sqrt{30}} - \frac{5}{3}\right) + mn\left(\frac{3}{2}\right) + \left(\frac{23}{6} - \frac{8}{\sqrt{15}} + \frac{2}{3\sqrt{2}} - \frac{12}{\sqrt{30}}\right).$$

The connection between the $R_1(G)$, $R_{-1}(G)$, $R_{1/2}(G)$, and $R_{-1/2}(G)$ is shown in Table 6 and Figure 6.

(ix) First Zagreb index

$$\begin{aligned}
 M_1(G) &= \sum_{pt \in E(G)} [\Gamma(p) + \Gamma(t)] = (6)(6) + (4m + 4n - 8)(8) + (2m + 2n + 2)(9) + (6m + 6n - 12)(11) \\
 &\quad + (9mn - 10m - 10n + 11)(12), \\
 M_1(G) &= 108mn - 4m - 4n - 10.
 \end{aligned}
 \tag{21}$$

(x) Second Zagreb index

$$\begin{aligned}
 M_2(G) &= \sum_{pt \in E(G)} [\Gamma(p) \times \Gamma(t)] = (6)(3 \times 3) + (4m + 4n - 8)(3 \times 5) + (2m + 2n + 2)(3 \times 6) \\
 &\quad + (6m + 6n - 12)(5 \times 6) + (9mn - 10m - 10n + 11)(6 \times 6), \\
 M_2(G) &= 6 - 84m - 84n + 324mn.
 \end{aligned}
 \tag{22}$$

(xi) Hyper-Zagreb index

$$\begin{aligned}
 HM(G) &= \sum_{pt \in E(G)} [\Gamma(p) + \Gamma(t)]^2 = (6)(3 + 3)^2 + (4m + 4n - 8)(3 + 5)^2 + (2m + 2n + 2)(3 + 6)^2 \\
 &\quad + (6m + 6n - 12)(5 + 6)^2 + (9mn - 10m - 10n + 11)(6 + 6)^2, \\
 HM(G) &= -2 - 296m - 296n + 1296mn.
 \end{aligned}
 \tag{23}$$

The connection between $M_1(G)$, $M_2(G)$, and $HM(G)$ is shown in Table 7 and Figure 7.

(xii) First Zagreb polynomial

$$\begin{aligned}
 M_1(G, x) &= \sum_{pt \in E(G)} x^{[\Gamma(p) + \Gamma(t)]} = (6)x^{(3+3)} + (4m + 4n - 8)x^{(3+5)} + (2m + 2n + 2)x^{(3+6)} + (6m + 6n - 12)x^{(5+6)} \\
 &\quad + (9mn - 10m - 10n + 11)x^{(6+6)}, \\
 M_1(G, x) &= (6)x^6 + (4m + 4n - 8)x^8 + (2m + 2n + 2)x^9 + (6m + 6n - 12)x^{11} + (9mn - 10m - 10n + 11)x^{12}.
 \end{aligned}
 \tag{24}$$

(xiii) Second Zagreb polynomial

$$\begin{aligned}
 M_2(G, x) &= \sum_{pt \in E(G)} x^{[\Gamma(p) \times \Gamma(t)]}, \\
 M_2(G, x) &= \sum_{pt \in 33} x^{[\Gamma(p) \times \Gamma(t)]} + \sum_{pt \in 35} x^{[\Gamma(p) \times \Gamma(t)]} + \sum_{pt \in 36} x^{[\Gamma(p) \times \Gamma(t)]} + \sum_{pt \in 56} x^{[\Gamma(p) \times \Gamma(t)]} + \sum_{pt \in 66} x^{[\Gamma(p) \times \Gamma(t)]} \\
 &= (6)x^{(3 \times 3)} + (4m + 4n - 8)x^{(3 \times 5)} + (2m + 2n + 2)x^{(3 \times 6)} + (6m + 6n - 12)x^{(5 \times 6)} + (9mn - 10m - 10n + 11)x^{(6 \times 6)}, \\
 M_2(G, x) &= (6)x^9 + (4m + 4n - 8)x^{15} + (2m + 2n + 2)x^{18} + (6m + 6n - 12)x^{30} + (9mn - 10m - 10n + 11)x^{36}.
 \end{aligned}
 \tag{25}$$

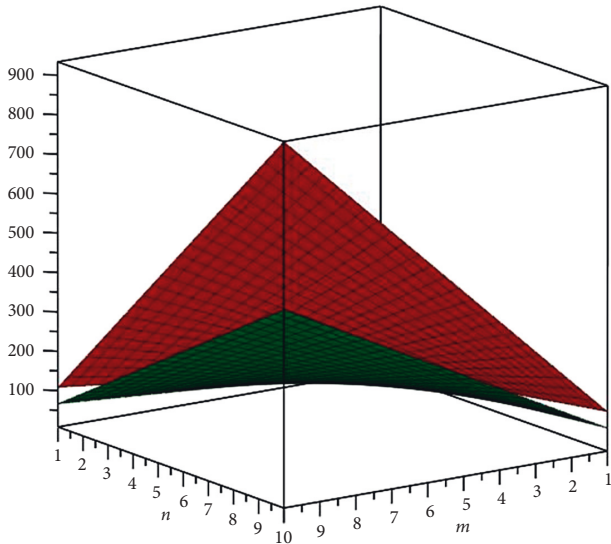


FIGURE 3: Graphical depiction of Table 3.

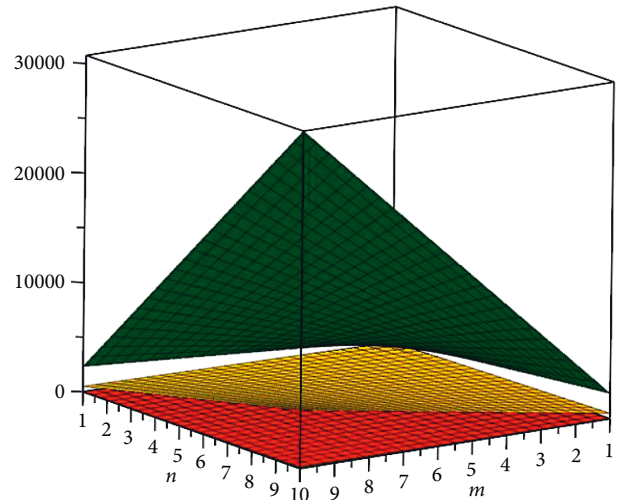


FIGURE 6: Graphical depiction of Table 6.

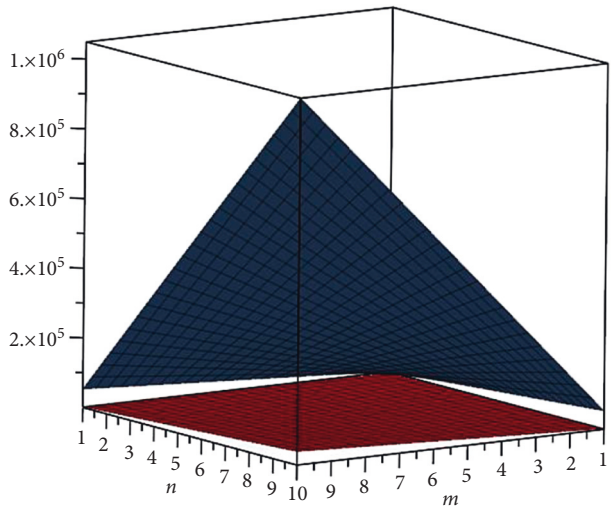


FIGURE 4: Graphical depiction of Table 4.

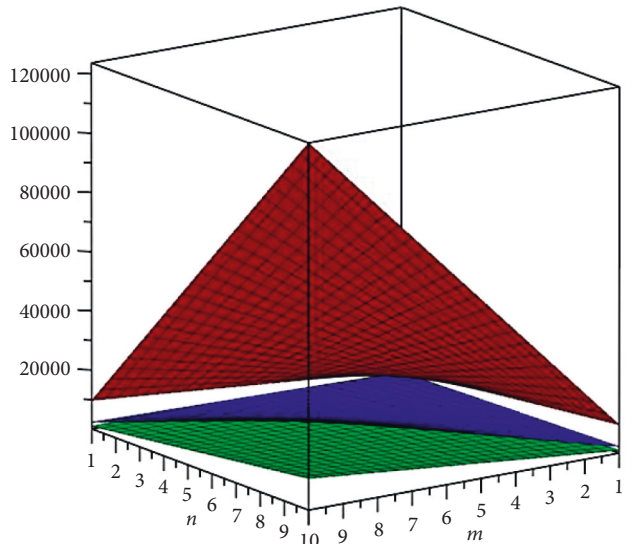


FIGURE 7: Graphical depiction of Table 7.

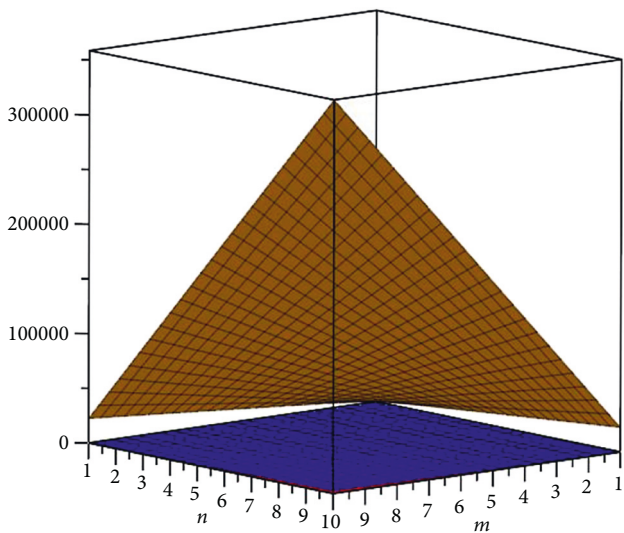


FIGURE 5: Graphical depiction of Table 5.

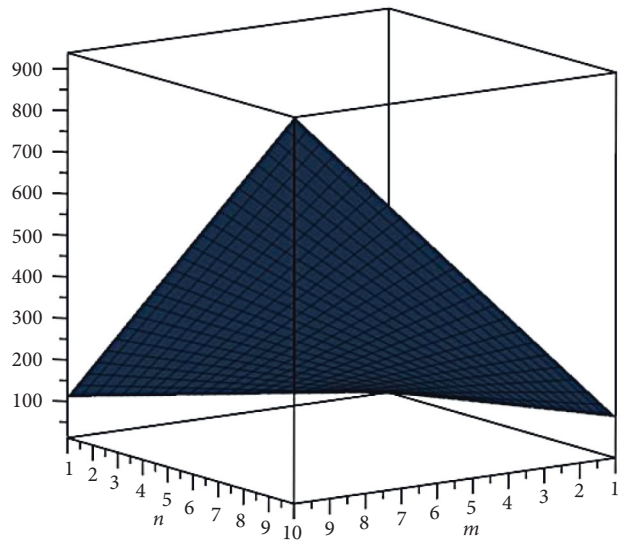


FIGURE 8: Graphical depiction of Table 8.

TABLE 2: Edge partition of $Sb_2Te_3[m, n]$.

$[\Gamma(p), \Gamma(t)]$	Frequency
(3, 3)	6
(3, 5)	$4m + 4n - 8$
(3, 6)	$2m + 2n + 2$
(5, 6)	$6m + 6n - 12$
(6, 6)	$9mn - 10m - 10n + 11$

TABLE 3: Connection between ABC and GA.

(m, n)	ABC(G)	GA(G)
(1, 1)	7.7416	11.6569
(2, 2)	25.5576	42.1245
(3, 3)	52.8604	90.5921
(4, 4)	89.65	157.0597
(5, 5)	135.9264	241.5273
(6, 6)	191.6896	343.9949
(7, 7)	256.9396	464.4625
(8, 8)	331.6764	602.9301
(9, 9)	415.9	759.3977
(10, 10)	509.6104	933.8653

TABLE 4: Connection between F and AZI.

(m, n)	F(G)	AZI(G)
(1, 1)	2430	170.3612
(2, 2)	25398	1134.409
(3, 3)	71694	2938.265
(4, 4)	141318	5581.93
(5, 5)	234270	9065.402
(6, 6)	350550	13388.68
(7, 7)	490158	18551.77
(8, 8)	653094	24554.67
(9, 9)	839358	31397.37
(10, 10)	1048950	39079.88

TABLE 5: Connection between $ReZG_1$, $ReZG_2$, and $ReZG_3$.

(m, n)	$ReZG_1(G)$	$ReZG_2(G)$	$ReZG_3(G)$
(1, 1)	7	21	1296
(2, 2)	20	97.72727	9888
(3, 3)	39	228.4545	26256
(4, 4)	64	413.1818	50400
(5, 5)	95	651.9091	82320
(6, 6)	132	944.6364	122016
(7, 7)	175	1291.364	169488
(8, 8)	224	1692.091	224736
(9, 9)	279	2146.818	287760
(10, 10)	340	2655.545	358560

The connection between the $M_1(G, x)$ and $M_2(G, x)$ is shown in Table 8 and Figure 8.

TABLE 6: Connection between the $R_1(G)$, $R_{-1}(G)$, $R_{1/2}(G)$, and $R_{-1/2}(G)$.

(m, n)	$R_1(G)$	$R_{-1}(G)$	$R_{1/2}(G)$	$R_{-1/2}(G)$
(1, 1)	162	1	43.4559	1.5483
(2, 2)	966	2.35	199.1371	6.0483
(3, 3)	2418	4.2	462.8183	13.5483
(4, 4)	4518	6.55	834.4995	24.0483
(5, 5)	7266	9.4	1314.181	37.5483
(6, 6)	10662	12.75	1901.862	54.0483
(7, 7)	14706	16.6	2597.543	73.5483
(8, 8)	19398	20.95	3401.224	96.0483
(9, 9)	24738	25.8	4312.906	121.5483
(10, 10)	30726	31.15	5332.587	150.0483

TABLE 7: Connection between $M_1(G)$, $M_2(G)$, and $HM(G)$.

(m, n)	$M_1(G)$	$M_2(G)$	$HM(G)$
(1, 1)	90	162	702
(2, 2)	406	966	3998
(3, 3)	938	2418	9886
(4, 4)	1686	4518	18366
(5, 5)	2650	7266	29438
(6, 6)	3830	10662	43102
(7, 7)	5226	14706	59358
(8, 8)	6838	19398	78206
(9, 9)	8666	24738	99646
(10, 10)	10710	30726	123678

TABLE 8: Connection between the $M_1(G, x)$ and $M_2(G, x)$.

(m, n)	x	$M_1(G, x)$	$M_2(G, x)$
(1, 1)	1	12	12
(2, 2)	2	43	43
(3, 3)	3	92	92
(4, 4)	4	159	159
(5, 5)	5	244	244
(6, 6)	6	347	347
(7, 7)	7	468	468
(8, 8)	8	607	607
(9, 9)	9	764	764
(10, 10)	10	939	939

4. Conclusion

In this study, the researcher has computed some topological indices and polynomials of the structure of antimony telluride including the atom-bond connectivity index, hyper-Zagreb index, geometric arithmetic indexes, redefined 1st, 2nd, and 3rd Zagreb index, and Randic index of the chemical graph of antimony telluride. The numerical and visual representations of these indices are also provided. Another intriguing issue for further research is the calculation of various distance-based topological indices and the reverse topological of antimony telluride.

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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