Journal of Prime Research in Mathematics Vol. **16(2)***(2020), 80-88*

MULTIPLICATIVE SHINGALI AND KANABOUR INDICES FOR BISMUTH TRI-IODIDE

ABAID UR REHMAN VIRK

Abstract. Topological indices helps us to collect information about algebraic graphs and gives us mathematical approach to understand the properties of algebraic structures. Here, we will introduce Multiplicative version of Shingali and Kanabour indices and compute these indices for Bismuth Tri-Iodide chain $m - BiI_3$ and sheet $BiI_3(m \times n)$.

Key words: Topological index, Zagreb index, Shingali and Kanabour indices, Bismuth Tri-iodide.
MSC: 11A07, 05C30, 05C25.

1. Introduction

In discrete mathematics, graph theory in general, not only the study of different properties of objects but it also tells us about objects having same properties as investigating object [1, 2]. These properties of different objects if of main interest. In particular, graph polynomials related to graph are rich in information. Mathematical tools like polynomials and topological based numbers have significant importance to collect information about properties of chemical compounds. We can find out many hidden information about compounds through theses tools [3].

Actually, topological indices are numeric quantities that tells us about the whole structure of graph. There are many topological indices that helps us to study physical, chemical reactivities and biological properties [4]. Winner, in 1947, firstly introduce the concept of topological index while working on boiling point [5]. In particular, Hosoya polynomial [6] plays an important in the area of distance-based topological indices, we can find out Winer index, Hyper Wiener index and Tratch-stankevich-zefirove index by Hosoya polynomial [7].

Department of mathematics, University of Sialkot, Sialkot, Pakistan; abaid.math@gmail.com
.

Gutman and Trinajstić introduced first and second Zagreb indices, which are defined as:

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v),$$

$$M_2(G) = \sum_{uv \in E(G)} (d_u \times d_v).$$

respectively.
The modified Randić index is defined as:

$$R'(G) = \sum_{uv \in E(G)} \frac{1}{max\{d_u, d_v\}}.$$

Shigehalli and Kanabur [8] introduced following new degree-based topological indices. Arithmetic-Geometric index is defined as:

$$AG_1 = \sum_{uv \in E(G)} \frac{d_u + d_v}{2\sqrt{d_u \times d_v}}.$$

Shigehalli and Kanabur indices are defined as:

$$SK(G) = \sum_{uv \in E(G)} \frac{d_u + d_v}{2},$$

$$SK_1(G) = \sum_{uv \in E(G)} \frac{d_u \times d_v}{2},$$

$$SK_2(G) = \sum_{uv \in E(G)} \left(\frac{d_u + d_v}{2}\right)^2.$$

We introduce the multiplicative version of Shigehalli and Kanabur indices. The multiplicative modified Randić index is defined as:

$$MR'(G) = \prod_{uv \in E(G)} \frac{1}{max\{d_u, d_v\}}.$$

multiplicative Shigehalli and Kanabur indices and multiplicative Arithmetic-Geometric index are defined as:

$$MAG_1 = \prod_{uv \in E(G)} \frac{d_u + d_v}{2\sqrt{d_u \times d_v}},$$

$$MSK(G) = \prod_{uv \in E(G)} \frac{d_u + d_v}{2},$$

$$MSK_1(G) = \prod_{uv \in E(G)} \frac{d_u \times d_v}{2},$$

$$MSK_2(G) = \prod_{uv \in E(G)} \left(\frac{d_u + d_v}{2} \right)^2.$$

For detailed study about topological indices and their applications, we refer [9, 10] and references therein.

In this paper, we aim to compute the topological indices of Bismuth tri-iodide chains and sheets introduced by Shigehalli and Kanabur. We also plot our results to see the dependence on the involved parameters.

2. Bismuth Tri-Iodide

The BiI_3 is an inorganic compound which is the result of the reaction of iodine and bismuth, which inspired the enthusiasm for subjective inorganic investigations [11]. BiI_3 is an excellent inorganic compound and is very useful in "qualitative inorganic analysis" [11, 12]. It was proved that Bi-doped glass optical strands are one of the most promising dynamic laser media. Different kinds of Bi-doped fiber strands have been created and have been used to construct Bi-doped fiber lasers and optical loudspeakers [13].

Layered BiI_3 gemstones are considered to be a three-layered stack structure in which a plane of bismuth atoms is sandwiched between iodide particle planes to form a continuous I-Bi-I plane [14]. The periodic superposition of the diamond-shaped three layers forms BiI3 crystals with R-3 symmetry [15, 16]. A progressive stack of I-Bi-I layers forms a symmetric hexagonal structure [17] and jewel of BiI_3 was integrated in [18].

3. Computational Results

In this section, we give our main results.

3.1. **Shingali and Kanabour indices for Bismuth Tri-Iodide chain $m-Bil_3$.** Algebraic graph of Bismith Tri-iodide Chain $m-Bil_3$ for $m = 3$ is shown in Figure 1. For Bismith Tri-iodide Chain $|V(m - Bil_3)| = 6(3m + 2)$ and $|E(m - Bil_3)| = 12(2m + 1)$. There are two types of edges in edge set present in Bismith Tri-iodide Chain $m - Bil_3$.

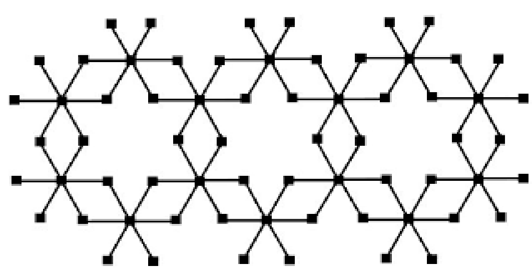

Figure 1. Bismuth Tri-Iodide Chain for $m = 3$ (Bismuth Tri Iodide).

The edge partition of Bismuth Tri-iodide chain $m - Bil_3$ is given in Table 1.

(d_u, d_v)	Frequency
(1,6)	4m+8
(2,6)	20m+4

TABLE 1. Partition of $E(m - Bil_3)$.

Theorem 1. *Let $m - Bil_3$ be Bismith Tri-Iodide chain. Then*

(1) $M\chi(m - Bil_3) = \frac{4}{7}\sqrt{14}(m+2)(5m+1)$.
(2) $MR'(m - Bil_3) = \frac{4}{9}(m+2)(5m+1)$.
(3) $MAG_1(m - Bil_3) = \frac{56}{3}\sqrt{2}(m+2)(5m+1)$.
(4) $MSK(m - Bil_3) = 224(m+2)(5m+1)$.
(5) $MSK_1(m - Bil_3) = 288(m+2)(5m+1)$.
(6) $MSK_2(m - Bil_3) = 3136(m+2)(5m+1)$.

Proof.

$$\begin{aligned} M\chi(m - Bil_3) &= \prod_{uv\in E(m-Bil_3)} \frac{1}{\sqrt{d_u + d_v}} \\ &= \left(\frac{1}{\sqrt{1+6}}\right)(4m+8) \times \left(\frac{1}{\sqrt{2+6}}\right)(20m+4) \\ &= \frac{4}{7}\sqrt{14}(m+2)(5m+1). \end{aligned}$$

$$\begin{aligned} MR'(m - Bil_3) &= \prod_{uv\in E(m-Bil_3)} \frac{1}{max\{d_u, d_v\}} \\ &= \left(\frac{1}{max\{1,6\}}\right)(4m+8) \times \left(\frac{1}{max\{2,6\}}\right)(20m+4) \\ &= \frac{56}{3}\sqrt{2}(m+2)(5m+1). \end{aligned}$$

$$\begin{aligned} MAG_1(m - Bil_3) &= \prod_{uv\in E(m-Bil_3)} \frac{d_u + d_v}{2\sqrt{d_u \times d_v}} \\ &= \left(\frac{1+6}{2\sqrt{1\times 6}}\right)(4m+8) \times \left(\frac{2+6}{2\sqrt{2\times 6}}\right)(20m+4) \\ &= . \end{aligned}$$

$$
\begin{aligned}
MSK(m-Bil_3) &= \prod_{uv\in E(m-Bil_3)} \frac{d_u+d_v}{2} \\
&= \left(\frac{1+6}{2}\right)(4m+8) \times \left(\frac{2+6}{2}\right)(20m+4) \\
&= 224(m+2)(5m+1).
\end{aligned}
$$

$$
\begin{aligned}
MSK_1(m-Bil_3) &= \prod_{uv\in E(m-Bil_3)} \frac{d_u\times d_v}{2} \\
&= \left(\frac{1\times 6}{2}\right)(4m+8) \times \left(\frac{2\times 6}{2}\right)(20m+4) \\
&= 288(m+2)(5m+1).
\end{aligned}
$$

$$
\begin{aligned}
MSK_2(m-Bil_3) &= \prod_{uv\in E(m-Bil_3)} \left(\frac{d_u+d_v}{2}\right)^2 \\
&= \left(\frac{1+6}{2}\right)^2(4m+8) \times \left(\frac{2+6}{2}\right)^2(20m+4) \\
&= 3136(m+2)(5m+1).
\end{aligned}
$$

□

3.2. **Shingali and Kanabour indices for Bismuth Tri-Iodide sheet $Bil_3(m \times n)$.** The algebraic graph of Bismith Tri-iodide sheet $Bil_3(m \times n)$ for $m = 2$ and $n = 3$, is shown in Figure 2. For Bismith Tri-iodide sheet $|V(Bil_3(m \times n))| = 11mn + 10m + 7n + 2$ and $|E(Bil_3(m \times n))| = 18mn + 12m + 6n$. There are two types of edges in edge set present in Bismith Tri-iodide sheet $Bil_3(m \times n)$

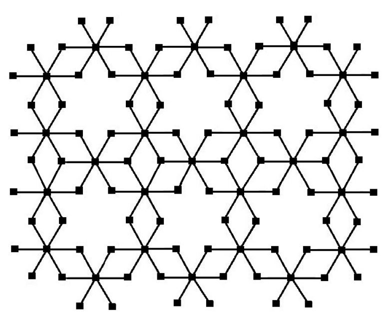

FIGURE 2. Bismuth Tri-Iodide Sheet for $m = 2$ and $n = 3$ (Bismuth Tri Iodide).

The edge partition of Bismuth Tri-iodide sheet $Bil_3(m \times n)$ is given in Table 2.

(d_u, d_v)	Frequency
(1,6)	4(m+n+1)
(2,6)	4(3mn+2m+2n-1)
(3,6)	6n(m-1)

TABLE 2. Partition of $E(Bil_3(m \times n))$.

Theorem 2. *Let $Bil_3(m \times n)$ be Bismith Tri-Iodide sheet. Then*

(1) $M\chi(Bil_3(m \times n)) = \frac{8}{7}\sqrt{14}n(3mn + 2m + 2n - 1)(m + n + 1)(m - 1)$.
(2) $MR'(Bil_3(m \times n)) = \frac{4}{9}n(3mn + 2m + 2n - 1)(m + n + 1)(m - 1)$.
(3) $MAG_1(Bil_3(m \times n)) = \frac{448}{3}n(3mn + 2m + 2n - 1)(m + n + 1)(m - 1)$.
(4) $MSK(Bil_3(m \times n)) = 5376n(3mn + 2m + 2n - 1)(m + n + 1)(m - 1)$.
(5) $MSK_1(Bil_3(m \times n)) = 15552n(3mn + 2m + 2n - 1)(m + n + 1)(m - 1)$.
(6) $MSK_2(Bil_3(m \times n)) = 301056n(3mn + 2m + 2n - 1)(m + n + 1)(m - 1)$.

Proof.

$$\begin{aligned} M\chi(Bil_3(m \times n)) &= \prod_{uv \in E(Bil_3(m \times n))} \frac{1}{\sqrt{d_u + d_v}} \\ &= \left(\frac{1}{\sqrt{1+6}}\right)(4m + 4n + 4) \times \left(\frac{1}{\sqrt{3+6}}\right)(6mn - 6n) \\ &\quad \times \left(\frac{1}{\sqrt{2+6}}\right)(12mn + 8m + 8n - 4) \\ &= \frac{8}{7}\sqrt{14}n(3mn + 2m + 2n - 1)(m + n + 1)(m - 1). \end{aligned}$$

$$\begin{aligned} MR'(Bil_3(m \times n)) &= \prod_{uv \in E(Bil_3(m \times n))} \frac{1}{max\{d_u, d_v\}} \\ &= \left(\frac{1}{max\{1,6\}}\right)(4m + 4n + 4) \times \left(\frac{1}{max\{3,6\}}\right)(6mn - 6n) \\ &\quad \times \left(\frac{1}{max\{2,6\}}\right)(12mn + 8m + 8n - 4) \\ &= \frac{4}{9}n(3mn + 2m + 2n - 1)(m + n + 1)(m - 1). \end{aligned}$$

$$\begin{aligned} MAG_1(Bil_3(m\times n)) &= \prod_{uv\in E(Bil_3(m\times n))} \frac{d_u+d_v}{2\sqrt{d_u\times d_v}} \\ &= \left(\frac{1+6}{2\sqrt{1\times 6}}\right)(4m+4n+4)\times\left(\frac{3+6}{2\sqrt{3\times 6}}\right)(6mn-6n) \\ &\quad \times\left(\frac{2+6}{2\sqrt{2\times 6}}\right)(12mn+8m+8n-4) \\ &= \frac{448}{3}n(3mn+2m+2n-1)(m+n+1)(m-1). \end{aligned}$$

$$\begin{aligned} MSK(Bil_3(m\times n)) &= \prod_{uv\in E(Bil_3(m\times n))} \frac{d_u+d_v}{2} \\ &= \left(\frac{1+6}{2}\right)(4m+4n+4)\times\left(\frac{3+6}{2}\right)(6mn-6n) \\ &\quad \times\left(\frac{2+6}{2}\right)(12mn+8m+8n-4) \\ &\quad = 5376n(3mn+2m+2n-1)(m+n+1)(m-1). \end{aligned}$$

$$\begin{aligned} MSK_1(Bil_3(m\times n)) &= \prod_{uv\in E(Bil_3(m\times n))} \frac{d_u\times d_v}{2} \\ &= \left(\frac{1.6}{2}\right)(4m+4n+4)\times\left(\frac{3.6}{2}\right)(6mn-6n) \\ &\quad \times\left(\frac{2.6}{2}\right)(12mn+8m+8n-4) \\ &= 15552n(3mn+2m+2n-1)(m+n+1)(m-1). \end{aligned}$$

$$\begin{aligned} MSK_2(Bil_3(m\times n)) &= \prod_{uv\in E(Bil_3(m\times n))} \left(\frac{d_u+d_v}{2}\right)^2 \\ &= \left(\frac{1+6}{2}\right)^2(4m+4n+4)\times\left(\frac{3+6}{2}\right)^2(6mn-6n) \\ &\quad \times\left(\frac{2+6}{2}\right)^2(12mn+8m+8n-4) \\ &= 301056n(3mn+2m+2n-1)(m+n+1)(m-1). \end{aligned}$$

$\square$

Conclusion

In this paper, we have computed several degree-based topological indices of Bismuth tri-iodide chains and sheets. Our results are applicable in chemistry, physics and other applied sciences. It is proved fact that topological indices help to predict many properties without going to the wet lab. For example, the first and second Zagreb indices were found to happen for the calculation of the π-electron energy of dendrimers, the Randić index corresponds with boiling point, the atomic bond connectivity (ABC) index gives an exceptionally decent relationship to figuring the strain energy of dendrimers. Therefore there is always room to define and study new topological indices. Redefined Zagreb indices are one step in this direction and are very close to Zagreb indices. Zagreb indices are very well studied by chemists and mathematician due to its huge applications in chemistry.

References

[1] Ali, N., Umar, M. A., Tabassum, A., & Raheem, A. (2018). Super (a,d)-C3-antimagicness of a Corona Graph. *Open Journal of Mathematical Sciences, 2*(1), 371 - 278.

[2] Liu, G., Jia, Z., & Gao, W., (2018). Ontology Similarity Computing Based on Stochastic Primal Dual Coordinate Technique. *Open Journal of Mathematical Sciences, 2*(1), 221-227.

[3] Alaeiyan, M., Farahani, M. R., & Jamil, M. K. (2016). Computation of the fifth geometric-arithmetic index for polycyclic aromatic hydrocarbons pahk. *Applied Mathematics and Nonlinear Sciences, 1*(1), 283-290.

[4] Amić, D., Bešlo, D., Lucic, B., Nikolic, S., & Trinajstic, N. (1998). The vertex-connectivity index revisited. *Journal of Chemical Information and Computer sciences, 38(5)*, 819-822.

[5] Wiener, H. (1947). Structural determination of paraffin boiling points. *Journal of the American Chemical Society, 69*(1), 17-20.

[6] Hosoya, H. (1988). On some counting polynomials in chemistry. *Discrete Applied Mathematics, 19*(1-3), 239-257.

[7] Kier, L. (2012). Molecular connectivity in chemistry and drug research (Vol. 14). *Elsevier.*

[8] Shigehalli V. S., & Kanabur R., Computation of new degree-based topological indices of graphene., *Journal of Nanomaterials,* 4341919.

[9] Anjum, M. S., & Safdar, M. U. (2019). K Banhatti and K hyper-Banhatti indices of nanotubes. *Engineering and Applied Science Letters, 2* (1), 19 - 37.

[10] Shao, Z,Virk, A. R., Javed, M. S., Rehman, M. A., & Farahani, M. R. (2019). Degree based graph invariants for the molecular graph of Bismuth Tri-Iodide. *Engineering and Applied Science Letters, 2*(1), 01-11.

[11] Imran, M., Ali, M., Ahmad, S., Siddiqui, M., & Baig, A. (2018). Topological characterization of the symmetrical structure of bismuth tri-iodide. *Symmetry, 10*(6), 201.

[12] Parker, S. P. (1989). McGraw-Hill dictionary of scientific and technical terms. *McGraw-Hill Book Co.*

[13] Liu, J. B., Siddiqui, M., Zahid, M., Naeem, M., & Baig, A. (2018). Topological Properties of Crystallographic Structure of Molecules. *Symmetry,10*(7), 265.

[14] Smart, L. E., & Moore, E. A. (2016).Solid state chemistry: an introduction. *CRC Press*. Boca Raton, FL, USA, 2005;p.40, ISBN0-7487-7516-1.

[15] Watanabe, K., Karasawa, T., Komatsu, T., & Kaifu, Y. (1986). Optical properties of extrinsic two-dimensional excitons in BiI3 single crystals. *Journal of the Physical Society of Japan, 55*(3), 897-907.

[16] Glusker, J. P., Lewis, M., & Rossi, M. (1994). Crystal structure analysis for chemists and biologists (Vol. 16). *John Wiley & Sons*.

[17] Yorikawa, H., & Muramatsu, S. (2008). Theoretical study of crystal and electronic structures of BiI3. *Journal of Physics: Condensed Matter, 20*(32), 325220.

[18] Nason, D., & Keller, L. (1995). The growth and crystallography of bismuth tri-iodide crystals grown by vapor transport. *Journal of Crystal Growth,156*(3), 221-226.