Topological Properties of Bismuth tri-iodide Using Neighborhood M-Polynomial

A.Verma[1], S.Mondal[*2], N.De[3], A.Pal[4]

[1,2]*Research Scholar,* [3,4]*AssociateProfessor,*

[1,2,4]*Department of Mathematics, NIT Durgapur, India.*

[3]*Department of Basic Sciences and Humanities (Mathematics), Calcutta Institute of Engineering and Management, Kolkata, India.*

Abstract — *Anoutstanding way of findingneighborhood degree sum based topological indices is neighborhood M-polynomial. The bismuth tri-iodide BiI_3 is a wide band gap layered semiconductor with several optical properties.In this paper, the neighborhood M-polynomial of bismuth tri-iodide chain and sheet are obtained. Some topological indices based on neighbourhood degree sum are recovered from the neighbourhood M-polynomial. Also, the findings are interpreted graphically.*

Keywords — *Graph,Bismuth tri-iodide,Neighborhood M-polynomial, Topological index.*

I. INTRODUCTION

Chemical graph theory (CGT) creates link between the discrete mathematics and chemical graph theory. A graph G is an ordered pair of vertex and edge sets $(V(G), E(G))$. In chemical graph theory, a graph is used to represent a molecule by considering the atoms as vertices and the chemical bonds as edges. CGT gives an important tool named as topological index to predict different properties and activity. A topological index is a mapping $I: \Theta \to \mathbb{R}$ such that $I(G) = I(H)$ if and only if G, H are isomorphic, where Θ is the collection ofall molecular graphs and $\mathbb{R}$ is the set of real numbers.The idea of topological index was introduced by H. Wiener [1] in 1947 when he was working on boiling point of alkanes. A large number of topological indices were developed afterwards. Researchers have currently concentrated on topological indices based on neighborhood degree sum of vertex [2]-[8]. By neighborhood degree sumδ_u of a vertex$u$, we mean the sum of degrees of all vertices that are adjacent to the vertex. The degree of a vertex is the total number of edges incident to the vertex. To make the computation of topological indices easy, many algebraic polynomials [9]-[11] are used instead their usual definitions. For degree based topological indices M-polynomial [12]-[14] is very effective tool. For the computation of neighborhood degree sum based topological indices, present authors introduced neighborhood M-polynomial [15] whose role for neighborhood degree sum based indices is parallel to the role of the M-polynomial for degree based indices.

The neighborhood M-polynomial [15] of a graph G is defined as,

$$NM(G; x, y) = \sum_{i \le j} m_{(i,j)} x^i y^j.$$

Where $m_{(i,j)}$ is the total number of edges $uv \in E(G)$ such that $\{\delta_u, \delta_v\} = \{i, j\}$. We use $NM(G)$ for $NM(G; x, y)$ for the rest of the article. The Neighborhood degree sum based topological indices defined on edge set of a graph G can be expressed as

$$I(G) = \sum_{uv \in E(G)} f(\delta_u, \delta_v),$$

where$f(\delta_u, \delta_v)$ is the function of δ_u, δ_v used in the definition of indices. The above result can also be written as,

$$I(G) = \sum_{i \le j} m_{(i,j)} f(i, j).$$

We describe some neighborhood degree sum based topological indices in Table I.

The bismuth tri-iodide BiI_3 is an excellent inorganic compound. This wide-band-gap material, which is made up of heavy atoms, is useful as gamma-ray detector at room temperature or an electronic x-ray imaging sensor[16],[17]. Over the years, bi-doped optical glass strings have been shown to be among the most promising dynamic laser media. The layered BiI_3 is a three layered stacking structure. Each of the three layers consists of three atomic planes: one basis plane of bismuth atoms, and two iodine planes above and below it.The rhombohedral crystal of BiI_3 with the R-3 symmetry is formed by stacking three layers periodically [18],[19]. The gradual stacking of one I − Bi – I layer forms the hexagonal structure with symmetry [20]. There are six 4-cycles in the unit BiI_3 graph, two of which are on the main, two in the middle, and two at the bottom. As per arrangement of unit BiI_3, two types of BiI_3 structures (chain and sheet) are considered here. The purpose of this work is to compute some exact expressions of topological indices for bismuth tri-iodide chain and sheet using NM-polynomial approach.

TABLE I

FORMULAE OF SOME NEIGHBORHOOD DEGREE BASED TOPOLOGICAL INDICES

Topological index	**Formulation $(f(x,y))$**
The third version of Zagreb index (M_1') [3]	$x+y$
The neighborhood second Zagreb index (M_2^*) [7]	xy
The neighborhood forgotten topological index (F_N^*) [7]	x^2+y^2
The neighborhood second modified Zagreb index (M_2^{nm}) [15]	$\frac{1}{xy}$
The neighborhood general Randic(NR_α) [15]	$(xy)^\alpha$
The third NDe index (ND_3) [8]	xy(x+y)
The third NDe index (ND_5) [8]	$\frac{x^2+y^2}{xy}$
The neighborhood Harmonic index (NH) [15]	$\frac{2}{x+y}$
The neighborhood inverse sum index (NI) [15]	$\frac{xy}{x+y}$
The Sanskruti index (S) [2]	$\frac{xy}{(x+y-2)^3}$

The relations of some neighborhood degree-based topological indices with the NM-polynomial are shown in the Table II.

TABLE II

DERIVATION OF SOME NEIGHBORHOOD DEGREE BASED TOPOLOGICAL INDICES

Topological index	**Derivation from $NM(G)$**
M_1'	$(D_x+D_y)(NM(G))\|_{x=y=1}$
M_2^*	$(D_xD_y)(NM(G))\|_{x=y=1}$
F_N^*	$({D_x}^2+{D_y}^2)(NM(G))\|_{x=y=1}$
M_2^{nm}	$(S_xS_y)(NM(G))\|_{x=y=1}$
NR_α	$({D_x}^\alpha {D_y}^\alpha)(NM(G))\|_{x=y=1}$
ND_3	$D_xD_y(D_x+D_y)(NM(G))\|_{x=y=1}$
ND_5	$(D_xS_y+S_xD_y)(NM(G))\|_{x=y=1}$
NH	$2S_xJ(NM(G))\|_{x=y=1}$
NI	$S_xJD_xD_y(NM(G))\|_{x=y=1}$
S	${S_x}^3Q_{-2}J{D_x}^3{D_y}^3(NM(G))\|_{x=y=1}$

Where,

$D_x\big(f(x,y)\big)=x\frac{\partial(f(x,y))}{\partial x}$, $D_y\big(f(x,y)\big)=y\frac{\partial(f(x,y))}{\partial y}$,$S_x\big(f(x,y)\big)=\int_0^x\frac{f(t,y)}{t}dt$,

$$S_y\big(f(x,y)\big)=\int_0^y\frac{f(x,t)}{t}dt,\qquad J\big(f(x,y)\big)=f(x,x),\ \ Q_\alpha\big(f(x,y)\big)=x^\alpha f(x,y).$$

II. MAIN RESULTS

In this section, we obtain NM-polynomial of bismuth tri-iodide chain and sheet using edge partition technique. From NM-polynomial, some topological indices are recovered. Results are interpreted graphically using Maple and Matlab software.

A. *Bismuth tri-iodide chain*

The linear arrangement of m unit BiI_3 is known as $m-BiI_3$chain. The unit BiI_3 is depicted in Figure 1(a). The structure of $3-BiI_3$ is shaped by combining three unit cells of BiI_3 linearly as shown in Figure 1(b).

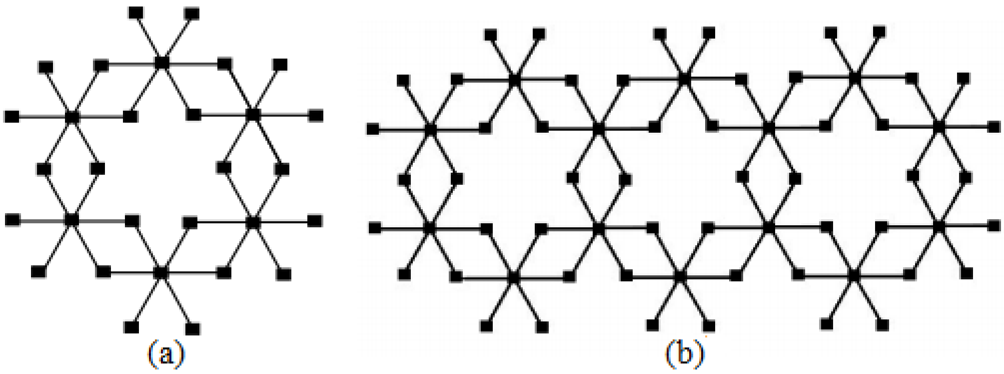

Fig.1. (a)The unit cell and (b) The chain of bismuth tri-iodide for m =3.

Theorem 1. Let G be the bismuth tri-iodide chain**.** Then we have

$$NM(G) = (4m + 8)x^6y^{10} + (8m + 16)x^{10}y^{12} + (12m - 12)x^{12}y^{12}.$$

Proof: The bismuth tri-iodide chainhas 12(2m + 1) number of edges. Its edge set can be partitioned as follows:

TABLE III
THE EDGE PARTITION OF BISMUTH TRI-IODIDE CHAIN

$(\boldsymbol{\delta_u}, \boldsymbol{\delta_v})$	**Cardinality**
(6,10)	$4m + 8$
(10,12)	$8m + 16$
(12,12)	$12m - 12$

Now using the definition of NM-polynomial, we get

$$NM(G) = m_{(6,10)}x^6y^{10} + m_{(10,12)}x^{10}y^{12} + m_{(12,12)}x^{12}y^{12}.$$

After putting the values of $m_{(i,j)}$'s, the required result can be obtained easily. Hence the proof is done.

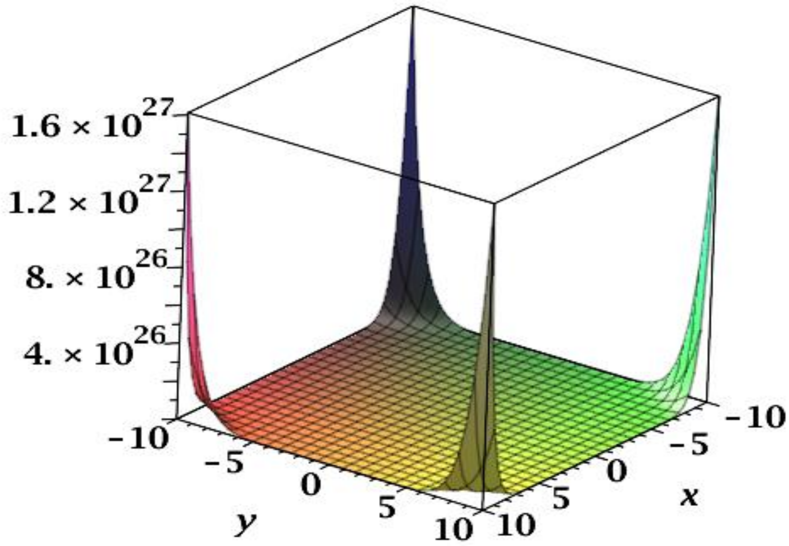

Fig. 2TheNM-polynomial of the bismuth tri-iodidechain for m = 2.

Now using this NM-polynomial, we calculate some neighborhood degree based topological indices of the bismuth tri-iodide chain**.**

Theorem 2. Let$G$be the bismuth tri-iodide chain.Then we have

(i) $M_1'(G) = 528\text{m} + 192,$

(ii) $M_2^*(G) = 2928\text{m} + 672,$
(iii) $F_N^*(G) = 5952\text{m} + 1536,$
(iv) $M_2^{nm}(G) = 0.216\text{m} + 0.183,$
(v) $NR_\alpha(G) = 4[60^\alpha + 2(120)^\alpha + 3(144)^\alpha]\text{m} + 4[2(60)^\alpha + 4(120)^\alpha - 3(144)^\alpha],$
(vi) $ND_3(G) = 70272\text{m} + 8448,$
(vii) $ND_5(G) = 44.166\text{m} + 26.661,$
(viii) $NH(G) = 2.2272m + 1.4545,$
(ix) $NI(G) = 130.63\text{m} + 45.26,$
(x) $S(G) = 5407.88\text{m} + 720.64.$

Proof: Let $NM(G) = (4m+8)x^6y^{10} + (8m+16)x^{10}y^{12} + (12m-12)x^{12}y^{12}$.
Then we have

$$(D_x + D_y)(f(x,y)) = 16(4m+8)x^6y^{10} + 22(8m+16)x^{10}y^{12} + 24(12m-12)x^{12}y^{12},$$
$$(D_xD_y)(f(x,y)) = 60(4m+8)x^6y^{10} + 120(8m+16)x^{10}y^{12} + 144(12m-12)x^{12}y^{12},$$
$$(D_x^2 + D_y^2)(f(x,y)) = 136(4m+8)x^6y^{10} + 244(8m+16)x^{10}y^{12} + 288(12m-12)x^{12}y^{12},$$
$$(S_xS_y)(f(x,y)) = \frac{(m+2)}{15}x^6y^{10} + \frac{(m+2)}{15}x^{10}y^{12} + \frac{(m-1)}{12}x^{12}y^{12},$$
$$D_x^\alpha D_y^\alpha(f(x,y)) = 60^\alpha(4m+8)x^6y^{10} + 120^\alpha(8m+16)x^{10}y^{12} + 144^\alpha(12m-12)x^{12}y^{12},$$
$$D_xD_y(D_x+D_y)(f(x,y)) = 960(4m+8)x^6y^{10} + 2640(8m+16)x^{10}y^{12} + 3456(12m-12)x^{12}y^{12},$$
$$(D_xS_y + S_xD_y)(f(x,y)) = \frac{136(m+2)}{15}x^6y^{10} + \frac{244(m+2)}{15}x^{10}y^{12} + 2(12m-12)x^{12}y^{12},$$
$$S_xJ(f(x,y)) = \frac{(m+2)}{4}x^{16} + \frac{(4m+8)}{11}x^{22} + \frac{(m-1)}{2}x^{24},$$
$$S_xJD_xD_y(f(x,y)) = 15(m+2)x^{16} + \frac{120(4m+8)}{11}x^{22} + 72(m-1)x^{24},$$
$$S_x^3Q_{-2}JD_x^3D_y^3(f(x,y)) = 78.71(4\text{m}+8)x^{14} + 216\,(8\text{m}+16)x^{20} + 280.42(12\text{m}-12)x^{22}.$$

Using Table II, we get

$$M_1'(G) = 16(4m+8)x^6y^{10} + 22(8m+16)x^{10}y^{12} + 24(12m-12)x^{12}y^{12}|_{x=y=1} = 528\text{m} + 192,$$
$$M_2^*(G) = 60(4m+8)x^6y^{10} + 120(8m+16)x^{10}y^{12} + 144(12m-12)x^{12}y^{12}|_{x=y=1} = 2928\text{m} + 672,$$
$$F_N^*(G) = 136(4m+8)x^6y^{10} + 244(8m+16)x^{10}y^{12} + 288(12m-12)x^{12}y^{12}|_{x=y=1} = 5952\text{m} + 1536,$$
$$M_2^{nm}(G) = \frac{(m+2)}{15}x^6y^{10} + \frac{(m+2)}{15}x^{10}y^{12} + \frac{(m-1)}{12}x^{12}y^{12}|_{x=y=1} = 0.216\text{m} + 0.183,$$
$$NR_\alpha(G) = 60^\alpha(4m+8)x^6y^{10} + 120^\alpha(8m+16)x^{10}y^{12} + 144^\alpha(12m-12)x^{12}y^{12}|_{x=y=1}$$
$$= 4[60^\alpha + 2(120)^\alpha + 3(144)^\alpha]\text{m} + 4[2(60)^\alpha + 4(120)^\alpha - 3(144)^\alpha],$$
$$ND_3(G) = 960(4m+8)x^6y^{10} + 2640(8m+16)x^{10}y^{12} + 3456(12m-12)x^{12}y^{12}|_{x=y=1}$$
$$= 70272\text{m} + 8448,$$
$$ND_5(G) = \frac{136(m+2)}{15}x^6y^{10} + \frac{244(m+2)}{15}x^{10}y^{12} + 2(12m-12)x^{12}y^{12}|_{x=y=1} = 44.166\text{m} + 26.661,$$
$$NH(G) = \frac{2(m+2)}{4}x^{16} + \frac{2(4m+8)}{11}x^{22} + \frac{2(m-1)}{2}x^{24}|_{x=1} = 2.2272m + 1.4545,$$
$$NI(G) = 15(m+2)x^{16} + \frac{120(4m+8)}{11}x^{22} + 72(m-1)x^{24}|_{x=1} = 130.63\text{m} + 45.26,$$
$$S(G) = 78.71(4\text{m}+8)x^{14} + 216\,(8\text{m}+16)x^{20} + 280.42(12\text{m}-12)x^{22}|_{x=1} = 5407.88\text{m} + 720.64.$$

Hence the proof is done.

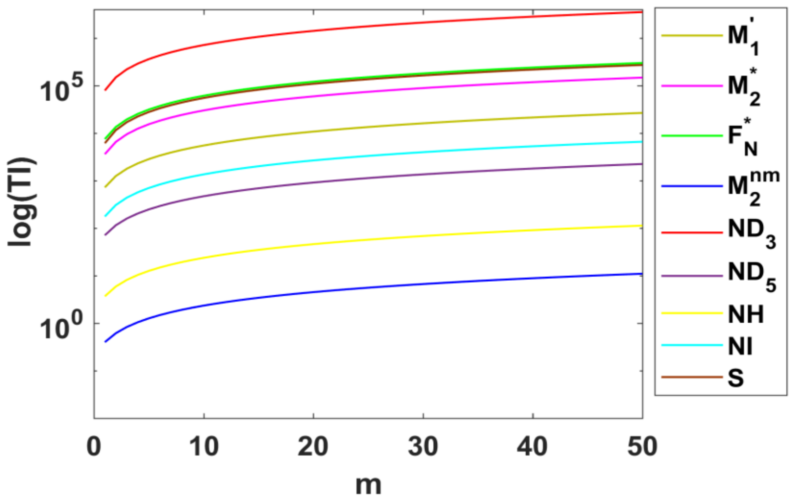

Fig. 3The neighborhood degree based indices of the bismuth tri-iodide chain. By log(TI), we mean logarithm of topological indices.

B. ***Bismuth tri-iodide sheet***

The rectangular arrangement mn unit BiI_3in m rows and n columns is known as $m \times n$ bismuth tri-iodide sheet. The 2×3 bismuth tri-iodide sheet is shown in Figure 4. The bismuth tri-iodide sheethas $18mn + 12m + 6n$ number of edges. Its edge set can be partitioned as follows:

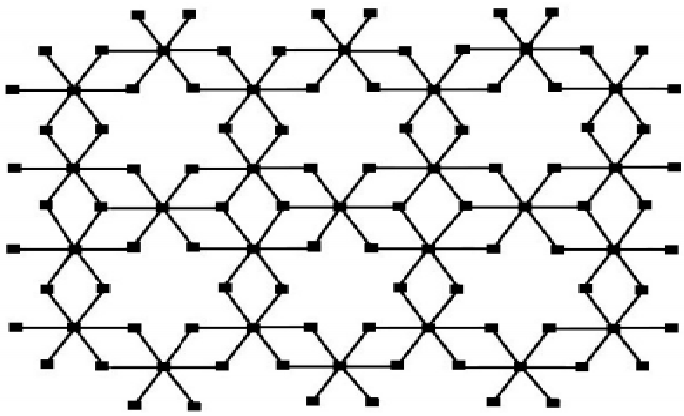

Fig.4The bismuth tri-iodide sheet $BiI_3(m \times n)$ for m = 2 and n = 3.

TABLE 4
THE EDGE PARTITION OF BISMUTH TRI-IODIDE SHEET$BII_3(m \times n)$**.**

(δ_u, δ_v)	**Cardinality**
(6,10)	$4n + 8$
(6,12)	$4m - 4$
(10,12)	$8n + 16$
(12,12)	$16m + 12n - 28$
(12,14)	$12mn - 8m - 12n + 8$
(12,18)	$4m - 4$
(14,18)	$6mn - 4m - 6n + 4$

Using this edge partition we obtain the following theorem like previous.

Theorem 3. Let G bethe bismuth tri-iodidesheet$BiI_3(m \times n)$. Then we have
$NM(G) = (4n+8)x^6y^{10} + (4m-4)x^6y^{12} + (8n+16)x^{10}y^{12} + (16m+12n-28)x^{12}y^{12} + (12mn-8m-12n)x^{12}y^{14} + (4m-4)x^{12}y^{18} + (6mn-4m-6n+4)x^{14}y^{18}$.

Applying Theorem 3 and Table II, we compute the neighborhood degree sum based indices forthe bismuth tri-iodide sheet in the following theorem**.**

Theorem 4. Let$G$be thebismuth tri-iodide sheet$BiI_3(m \times n)$.Then we have

(i) $M_1'(G) = 28n + 240m + 504mn - 256$,
(ii) $M_2^*(G) = 1140m - 600n + 3528mn - 1776$,
(iii) $F_N^*(G) = 2400m - 1248n + 7200mn - 3584$,
(iv) $M_2^{nm}(G) = 0.1216m + 0.1214n + 0.0952mn + 0.0140$,
(v) $NR_\alpha(G) = 4[72^\alpha + 4(144)^\alpha - 2(168)^\alpha + 216^\alpha - 252^\alpha]m + 2[2(60)^\alpha + 4(120)^\alpha + 6(144)^\alpha - 6(168)^\alpha - 3(252)^\alpha] + 4[2(60)^\alpha - 72^\alpha + 4(120)^\alpha - 7(144)^\alpha - 216^\alpha + 252^\alpha]$,
(vi) $ND_3(G) = 19200m - 34368n + 100800mn - 45696$,
(vii) $ND_5(G) = 26.22m + 12.66n + 36.66mn - 7.74$,
(viii) $NH(G) = 0.589m + 0.465n + 0.649mn + 0.137$,
(ix) $NI(G) = 57.62m + 5.83n + 124.788mn - 12.34$,
(x) $S(G) = 1572.7m - 2264.32n + 7672.2mn - 5596.06$.

Proof:Let$NM(G) = (4n+8)x^6y^{10} + (4m-4)x^6y^{12} + (8n+16)x^{10}y^{12} + (16m+12n-28)x^{12}y^{12} + (12mn-8m-12n)x^{12}y^{14} + (4m-4)x^{12}y^{18} + (6mn-4m-6n+4)x^{14}y^{18}$.

Then we have,

$(D_x + D_y)(f(x,y)) = 16(4n+8)x^6y^{10} + 18(4m-4)x^6y^{12} + 22(8n+16)x^{10}y^{12} + 24(16m+12n-28)x^{12}y^{12} + 26(12mn-8m-12n)x^{12}y^{14} + 30(4m-4)x^{12}y^{18} + 32(6mn-4m-6n+4)x^{14}y^{18}$,

$(D_xD_y)(f(x,y)) = 60(4n+8)x^6y^{10} + 72(4m-4)x^6y^{12} + 120(8n+16)x^{10}y^{12} + 144(16m+12n-28)x^{12}y^{12} + 168(12mn-8m-12n)x^{12}y^{14} + 216(4m-4)x^{12}y^{18} + 252(6mn-4m-6n+4)x^{14}y^{18}$,

$(D_x^2 + D_y^2)(f(x,y)) = 136(4n+8)x^6y^{10} + 180(4m-4)x^6y^{12} + 244(8n+16)x^{10}y^{12} + 288(16m+12n-28)x^{12}y^{12} + 340(12mn-8m-12n)x^{12}y^{14} + 468(4m-4)x^{12}y^{18} + 520(6mn-4m-6n+4)x^{14}y^{18}$,

$(S_xS_y)(f(x,y)) = \frac{(n+2)}{15}x^6y^{10} + \frac{(m-1)}{18}x^6y^{12} + \frac{(n+2)}{15}x^{10}y^{12} + \frac{(4m+3n-7)}{36}x^{12}y^{12} + \frac{(3mn-2m-3n)}{42}x^{12}y^{14} + \frac{(m-1)}{54}x^{12}y^{18} + \frac{(3mn-2m-3n+2)}{126}x^{14}y^{18}$,

$D_x^\alpha D_y^\alpha(f(x,y)) = 60^\alpha(4n+8)x^6y^{10} + 72^\alpha(4m-4)x^6y^{12} + 120^\alpha(8n+16)x^{10}y^{12} + 144^\alpha(16m+12n-28)x^{12}y^{12} + 168^\alpha(12mn-8m-12n)x^{12}y^{14} + 216^\alpha(4m-4)x^{12}y^{18} + 252^\alpha(6mn-4m-6n+4)x^{14}y^{18}$,

$D_xD_y(D_x+D_y)(f(x,y)) = 960(4n+8)x^6y^{10} + 1296(4m-4)x^6y^{12} + 2640(8n+16)x^{10}y^{12} + 3456(16m+12n-28)x^{12}y^{12} + 4368(12mn-8m-12n)x^{12}y^{14} + 6480(4m-4)x^{12}y^{18} + 8064(6mn-4m-6n+4)x^{14}y^{18}$,

$(D_xS_y + S_xD_y)(f(x,y)) = \frac{136(n+2)}{15}x^6y^{10} + 10(m-1)x^6y^{12} + \frac{122(2n+4)}{15}x^{10}y^{12} + 2(16m+12n-28)x^{12}y^{12} + \frac{170(3mn-2m-3n)}{21}x^{12}y^{14} + \frac{78(m-1)}{9}x^{12}y^{18} + \frac{130(6mn-4m-6n+4)}{63}x^{14}y^{18}$,

$S_xJ(f(x,y)) = \frac{(n+2)}{4}x^{16} + \frac{(2m-2)}{9}x^{18} + \frac{(4n+8)}{11}x^{22} + \frac{(4m+3n-7)}{6}x^{24} + \frac{(6mn-4m-6n)}{13}x^{26} + \frac{(2m-2)}{15}x^{30} + \frac{(3mn-2m-3n+2)}{16}x^{32}$,

$S_xJD_xD_y(f(x,y)) = 15(n+2)x^{16} + 4(4m-4)x^{18} + \frac{60(8n+16)}{11}x^{22} + 6(16m+12n-28)x^{24} + \frac{84(12mn-8m-12n)}{13}x^{26} + \frac{36(4m-4)}{5}x^{30} + \frac{63(3mn-2m-3n+2)}{4}x^{32}$,

$S_x^3Q_{-2}JD_x^3D_y^3(f(x,y)) = \frac{54000(2n+4)}{343}x^{14} + \frac{729(m-1)}{2}x^{16} + 216(8n+16)x^{20} + \frac{373248(16m+12n-28)}{1331}x^{22} + 343(12mn-8m-12n)x^{24} + \frac{157464(4m-4)}{343}x^{28} + 592.704(6mn-4m-6n+4)x^{30}$.

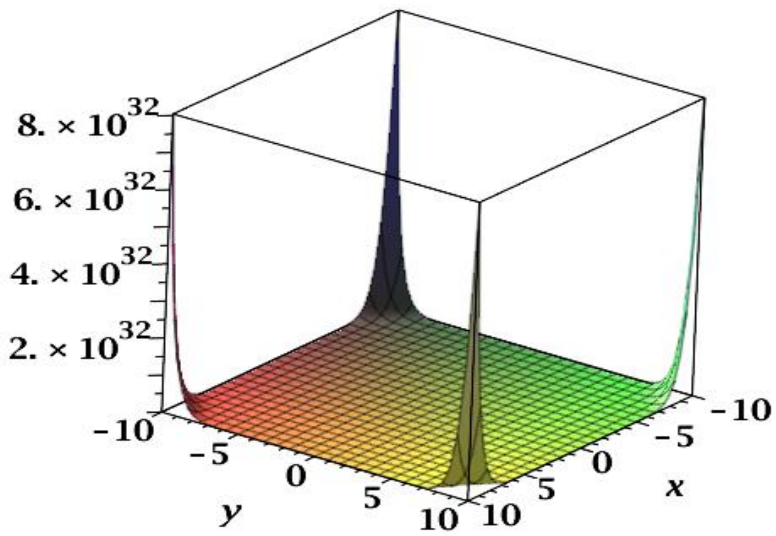

Fig. 5TheNM-polynomial for bismuth tri-iodide sheet.

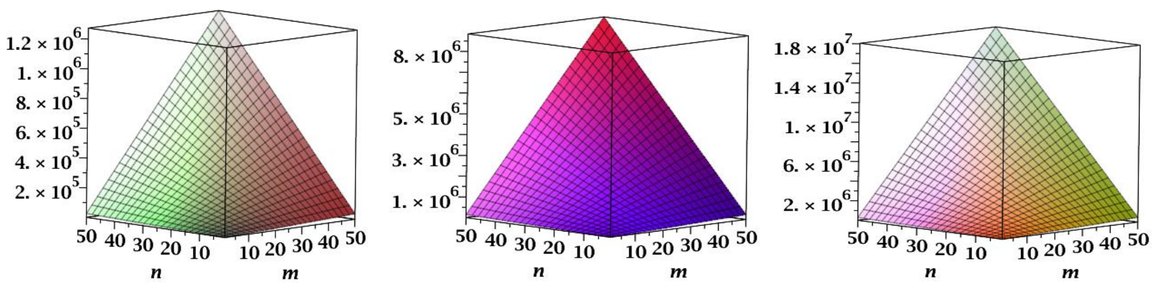

Fig. 6The plotting of M_1', M_2^*, and F_N^*indicesforthe bismuth tri- iodide sheet from left to right respectively.

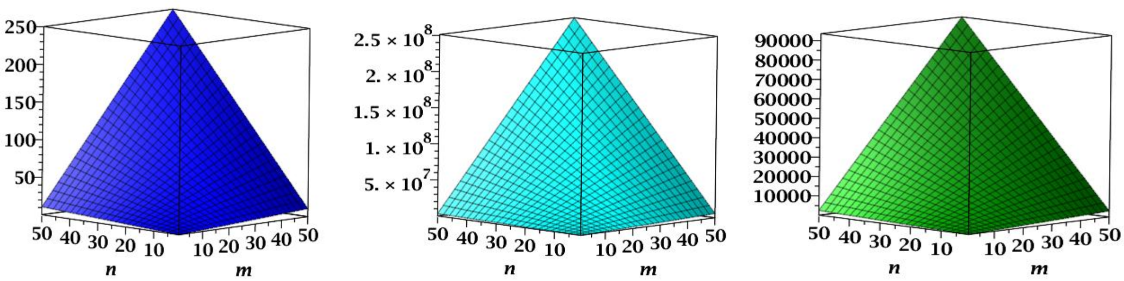

Fig. 7The plotting of M_2^{nm}, ND_3, and ND_5 indicesfor the bismuth tri- iodide sheet from left to right respectively.

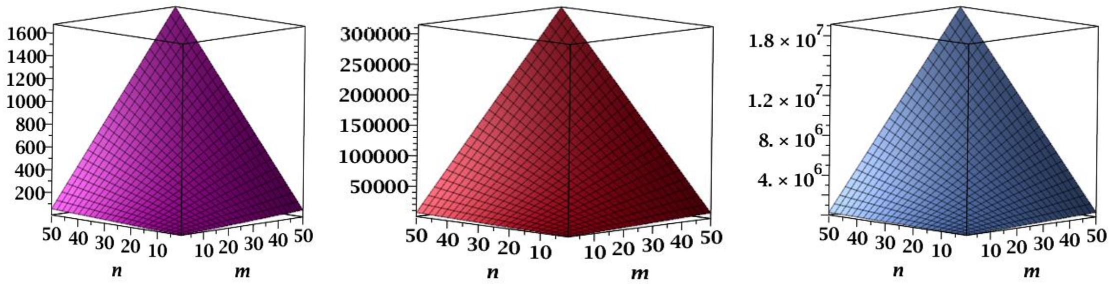

Fig. 8The plotting of NH, NI, and S indicesfor the bismuth tri- iodide sheet from left to right respectively.

III. REMARKS ANDCONCLUSIONS

In this work we have considered two types of bismuth tri- iodide structures: bismuth tri- iodide chain $m - \mathrm{BiI}_3$ and bismuth tri- iodide sheet $\mathrm{BiI}_3(m \times n)$.Firstly we have obtained NM-polynomial of the aforesaid structures. Later some neighborhood degree some based topological indices for the structures under consideration have been derived using NM-polynomial. The results are depicted in Figure 2, Figure 3, and Figures 5-8. From the figures, a comparison can be made. In comparison with other indices, ND_3 has most dominating nature whereas M_2^{nm} grows slowly. The behavior of F_N^* and S are very closed. The indices have the following order

$$M_2^{nm} < NH < ND_5 < NI < M_1' < M_2^* < F_N^* < S < ND_3,$$

i.e., all the indices behave differently in each structure discussed above. This work is helpful to get the underlying topology of the aforesaid structures.

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