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Article

On Vertex-Edge-Degree Topological Descriptors for Certain Crystal Networks

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Abstract: Due to the combinatorial nature of graphs they are used easily in pure sciences and social sciences. The dynamical arrangement of vertices and their associated edges make them flexible (like liquid) to attain the shape of any physical structure or phenomenon easily. In the field of ICT they are used to reflect distributed component and communication among them. Mathematical chemistry is another interesting domain of applied mathematics that endeavors to display the structure of compounds that are formed in result of chemical reactions. This area attracts the researchers due to its applications in theoretical and organic chemistry. It also inspires the mathematicians due to involvement of mathematical structures. Regular or irregular bonding ability of molecules and their formation of chemical compounds can be analyzed using atomic valences (vertex degrees). Pictorial representation of these compounds helps in identifying their properties by computing different graph invariants that is really considered as an application of graph theory. This paper reflects the work on topological indices such as ev-degree Zagreb index, the first ve-degree Zagreb α index, the first ve-degree Zagreb β index, the second ve-degree Zagreb index, ve-degree Randic index, the ev-degree Randic index, the ve-degree atom-bond connectivity index, the ve-degree geometric-arithmetic index, the ve-degree harmonic index and the ve-degree sum-connectivity index for crystal structural networks namely, bismuth tri-iodide and lead chloride. In this article we have determine the exact values of ve-degree and ev-degree based topological descriptors for crystal networks.

Keywords: *ev*-degree; *ve*-degree; topological indices; crystal networks

1 Introduction

Computation of topological indices for large chemical structures becomes very challenging but still useful in depicting the structure and physico-chemical properties that are extremely important in reticular chemistry. Recently reticular Metal-organic frameworks MOFs are evolved as porous conductive solids with great applicability in fuel cells, batteries, capacitors, sensors and electronics. In MOFs covalent fibers of carbon atoms form mesh like crystals [1,2]. In reticular chemistry, the numerically representation of structural characteristics of molecules, are the topological indices, which are obtained by using the graphical methods. These indices play an important role in the area of mathematical chemistry and control theory, mainly in QSAR/QSPR investigations [3,4].

The networks that are topologically equivalent, although they exibit different labelings of distinct atoms but due to topological indices they are invariant. These indices describe the connections among the atoms and in this way they are basic invariants that show a relationship with biological activity and chemical reactivity. Topological study of a MOF means transforming the connectivity of any structure into a unique number representing an index of the metal-organic framework under consideration.

Wiener in his article [5], introduced the concept of topological index while he was studying the structural relationships to identify boiling points of paraffins. Many topological indices are used to reflect the structural arrangement of graphs. In general, they are classified into distance or degree-based topological indices along with these counting related indices of graphs have play a vital role in chemical characterization. Article [6–22] can give more deep insight as literature survey.

2 Preliminaries

Let G be a simple connected graph with vertex sets $V(G)$ and edge sets $E(G)$. The degree of a vertex ε, denoted by $d(\varepsilon)$, is the number of edges that are incident to the ε. The open neighborhood of ε is defined as $N(\varepsilon) = \{\varepsilon \in V(G) : \lambda\varepsilon \in \mathrm{E(G)}\}$ and closed neighborhood $N[\varepsilon] = N(\varepsilon) \cup \{\varepsilon\}$ [23]. The *ve*-degree, denoted by $d_{ve}(\varepsilon)$, of any vertex $\varepsilon \in V$ is the number of different edges that are incident to any vertex from the $N[\varepsilon]$. In [24] defined the *ev*-degree of the edge $e = \lambda\varepsilon \in \mathrm{E}$, denoted by $d_{ev}(e)$, the number of vertices of the union of the closed neighborhoods of λ and ε. For details see [25–30].

The *ve*-degree and *ev*-degree topological indices are defines as: $\sum_{e\in E(G)}(d_{ev}(e))^2$, $\sum_{\varepsilon\in V} d_{ve}(\varepsilon)^2$, $\sum_{\lambda\varepsilon\in E}(d_{ve}(\varepsilon) + d_{ve}(\lambda))$, $\sum_{\lambda\varepsilon\in E}(d_{ve}(\lambda) \times d_{ve}(\varepsilon))$, $\sum_{\lambda\varepsilon\in E}(d_{ve}(\lambda) \times d_{ve}(\varepsilon))^{-\frac{1}{2}}$, $\sum_{e_1\in E} d_{ve}(e_1)^{-\frac{1}{2}}$, $\sum_{\lambda\varepsilon\in E}\left(\frac{d_{ve}(\lambda)+\mathrm{d_{ve}}(\varepsilon)-2}{d_{ve}(\lambda)\times d_{ve}(\varepsilon)}\right)^{\frac{1}{2}}$, $\sum_{\lambda\varepsilon\in E}\frac{2(d_{ve}(\lambda)\times d_{ve}(\varepsilon))^{\frac{1}{2}}}{d_{ve}(\lambda)+\mathrm{d_{ve}}(\varepsilon)}$, $\sum_{\lambda\varepsilon\in E}\frac{2}{d_{ve}(\lambda)+\mathrm{d_{ve}}(\varepsilon)}$ and $\sum_{\lambda\varepsilon\in E}(d_{ve}(\lambda)+\mathrm{d_{ve}}(\varepsilon))^{-\frac{1}{2}}$ are *ev*-degree Zagreb (M_{ev}) index, the first *ve*-degree Zagreb α ($M^1_{\alpha ve}$) index, the first *ve*-degree Zagreb β ($M^1_{\beta ve}$) index, the second *ve*-degree Zagreb (M^2_{ve}) index, *ve*-degree Randic (R_{ve}) index, the *ev*-degree Randic (R_{ev}) index, the *ve*-degree atom-bond connectivity (ABC_{ve}) index, the *ve*-degree geometric-arithmetic (GA_{ve}) index, the *ve*-degree harmonic (H_{ve}) index and the *ve*-degree sum-connectivity (χ_{ve}) index, respectively.

3 Crystal Structures

The physical structure of solid materials is significant for engineering applications. It depends on the arrangements of the atoms, ions, or molecules that becomes the reason for strength of solid materials. The connectivity pattern of ions or atoms in a solid and repetitive patterns in three dimensions is known as crystal structure and material is called crystalline solid or crystalline material. Due to different crystalline structure of a materials their performance and characteristics varies. The unit cell is the basic structure that explains the crystal structure and repetition of this unit cell forms the whole crystal. Some of the examples of crystalline materials are alloys, metals, and some ceramic materials. In this paper topological indices for the bismuth tri-iodide and lead chloride are determined by mapping their crystalline structures in the form of graphs.

4 Graph of Bismuth Tri-Iodide

Bismuth tri-iodide (BiI_3) is an inorganic compound. It is the result of the response of bismuth and iodine, which is important in qualitative inorganic analysis. Layered BiI_3 crystal is considered to be a three-layered stacking structure, where bismuth atom planes are lying between iodide atom planes, which form the sequence I-Bi-I planes. The rhombohedral BiI_3 crystal with R-3 symmetry is formed by the periodic stacking of three layers [31,32]. In 1995, Nason et al. [33] synthesized a unit crystal of BiI_3. The Fig. 1 shows one unit of bismuth tri-iodide.

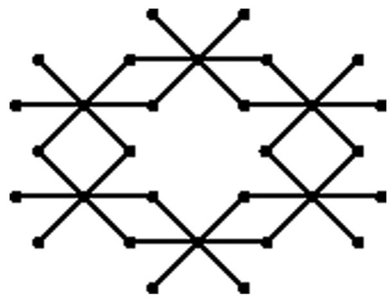

Figure 1: One unit of bismuth tri-iodide

The graph of a single unit of bismuth tri-iodide contains six 4-cycles of which two are at the bottom, two on the top and two in the middle. The unit cells of bismuth tri-iodide can be arranged either linearly or in a sheet form. A linear arrangement with q unit cells is called q-bismuth chain, $p \times q$ bismuth sheet is obtained by arrangements of pq unit cells into p rows and q columns. A $p \times q$ bismuth sheet throughout onward represented by BiI_3. A sheet of BiI_3 contains $11pq + 10p + 7q + 2$ vertices and $18pq + 12p + 6q$ edges, which are shown in Tab. 1. The number of vertices corresponding to their degrees of $BiI3$ are shown in Tab. 2 and the edge partition based on degree of end vertices of each edge is shown in Tab. 3.

Table 1: Vertices and edges of BiI_3

Total vertices	Total edges
$11pq + 10p + 7q + 2$	$18pq + 12p + 6q$

Table 2: Number of vertices corresponding to their degrees of BiI_3

$d(\varepsilon)$	Number of vertices
1	$4p + 4q + 4$
2	$6pq + 4p + 4q - 2$
3	$2pq - 2q$
6	$3pq + 2p + q$
Total	$11pq + 10p + 7q + 2$

Table 3: Edge partition of BiI_3

$(d(\lambda), \mathrm{d}(\varepsilon))$	Number of edges
(1,6)	$4p + 4q + 4$
(2,6)	$12pq + 8p + 8q - 4$
(3,6)	$6pq - 6q$
Total	$18pq + 12p + 6q$

We partitioned the edges of BiI_3, based on *ev*-degree in Tab. 4.

Table 4: Edge partition of BiI_3

Number of edges	$d_{ev}(\varepsilon)$	$(d(\lambda), d(\varepsilon))$
$4p + 4q + 4$	7	(1,6)
$12pq + 8p + 8q - 4$	8	(2,6)
$6pq - 6q$	9	(3,6)

In Tab. 5, we partitioned the vertices of BiI_3, based on *ev*-degree.

Table 5: Vertex partition of BiI_3, based on *ve*-degree

Number of vertices	$d_{ve}(\varepsilon)$	$d(\varepsilon)$
$4p + 4q + 4$	6	1
$6pq + 4p + 4q - 2$	12	2
$2pq - 2q$	18	3
$2q + 4$	10	6
$4p + 2q - 6$	12	6
$3pq - 2p - 3q + 2$	14	6

We partitioned the edge of $BiI3$ with respect to *ve*-degrees.

Now we calculated *ev*-degree and *ve*-degree based indices such as M_{ev} index, $M^1_{\alpha ve}$ index, $M^1_{\beta ve}$ index, M^2_{ve} index, R_{ve} index, R_{ev} index, ABC_{ve} index, GA_{ve} index, H_{ve} index and χ_{ve} index for BiI_3.

4.1 ev-Degree Zagreb Index

By using *ev*-degree of BiI_3 from Tab. 4, we compute the *ev*-degree based Zagreb index:

$$M^{ev}(BiI3) = \sum_{e \in E(BiI3)} (d_{ev}(e))^2$$

$$= (4p + 4q + 4) \times 7^2 + (12pq + 8p + 8q - 4) \times 8^2 + (6pq - 6q) \times 9^2$$

$$= 1254pq + 708p + 222q - 60$$

4.2 The First *ve*-degree Zagreb α Index

Using Tab. 5 we compute the first *ve*-degree Zagreb α index:

$$M^1_{\alpha ve}(BiI_3) = \sum_{\varepsilon \in V} d_{ve}(\varepsilon)^2$$

$$\begin{aligned} M^1_{\alpha ve}(BiI3) = {} & (4p + 4q + 4)(6)^2 + (6pq + 4p + 4q - 2)(12)^2 + (2pq - 2q)(18)^2 \\ & + (2q + 4)(10)^2 + (4p + 2q - 6)(12)^2 + (3pq - 2p - 3q + 2)(14)^2 \end{aligned}$$

$= 2100pq + 904p - 28q - 216.$

4.3 The First ve-degree Zagreb β Index

Using Tab. 6 we compute the first *ve*-degree Zagreb β index:

$$M^1_{\beta ve}(BiI_3) = \sum_{\lambda\varepsilon\in E}(d_{ve}(\lambda) + d_{ve}(\varepsilon))$$

$$\begin{aligned} M^1_{\beta ve}(BiI_3) &= (4q+8)(16) + (4p-4)(18) + (8q+16)(22) + (16p+12q-28)(24) \\ &\quad +(12pq-8p-12q+8)(26) + (4p-4)(30) + (6pq-4p-6q+4)(32) \\ &= 504pq + 240p + 24q - 48. \end{aligned}$$

Table 6: Edge partition of BiI_3, based on *ve*-degree

Number of edges	$d_{ve}(\lambda), d_{ve}(\varepsilon))$	$(d(\lambda), \mathrm{d}(\varepsilon))$
$4q+8$	(6,10)	(1,6)
$4p-4$	(6,12)	(1,6)
$8q+16$	(10,12)	(2,6)
$16p+12q-28$	(12,12)	(2,6)
$12pq-8p-12q+8$	(12,14)	(2,6)
$4p-4$	(12,18)	(3,6)
$6pq-4p-6q+4$	(14,18)	(3,6)

4.4 The second ve-degree Zagreb index

Using Tab. 6 we compute the second *ve*-degree Zagreb index:

$$M^2_{ve}(BiI_3) = \sum_{\lambda\varepsilon\in E}(d_{ve}(\lambda) \times d_{ve}(\varepsilon))$$

$$\begin{aligned} M^2_{ve}(BiI3) &= (4q+8)(60) + (4p-4)(72) + (8q+16)(120) + (16p+12q-28)(144) \\ &\quad + (12pq-8p-12q+8)(168) + (4p-4)(216) + (6pq-4p-6q+4)(252) \\ &= 3528pq + 1104p - 600q - 432. \end{aligned}$$

4.5 ve-degree Randic Index

Using Tab. 6 we compute the *ve*-degree Randic index:

$$R_{ve}(BiI_3) = \sum_{\lambda\varepsilon\in E}(d_{ve}(\lambda) \times d_{ve}(\varepsilon))^{-\frac{1}{2}}$$

$$\begin{aligned} R_{ve}(BiI3) &= (4q+8)(60)^{-\frac{1}{2}} + (4p-4)(72)^{-\frac{1}{2}} + (8q+16)(120)^{-\frac{1}{2}} + (16p+12q-28)(144)^{-\frac{1}{2}} \\ &\quad + (12pq-8p-12q+8)(168)^{-\frac{1}{2}} + (4p-4)(216)^{-\frac{1}{2}} + (6pq-4p-6q+4)(252)^{-\frac{1}{2}} \end{aligned}$$

$$= \left(\frac{\sqrt{42}+\sqrt{7}}{7}\right)pq + \left(\frac{84+21\sqrt{2}-6\sqrt{42}+7\sqrt{6}-6\sqrt{7}}{63}\right)p + \left(\frac{105+14\sqrt{15}-15\sqrt{42}+14\sqrt{30}-15\sqrt{7}}{105}\right)q$$

$$+\frac{-21-3\sqrt{2}-\sqrt{6}}{9}+\frac{4\sqrt{15}+4\sqrt{30}}{15}+\frac{2\sqrt{7}+2\sqrt{42}}{21}$$

4.6 The ev-degree Randic Index

Using Tab. 4 we compute the *ev*-degree Randic index:

$$R_{ev}(BiI_3) = \sum_{e_1 \in E} d_{ve}(e_1)^{-\frac{1}{2}}$$

$$R_{ev}(BiI3) = (4p+4q+4)(7)^{-\frac{1}{2}} + (12pq+8p+8q-4)(8)^{-\frac{1}{2}} + (6pq-6q)(9)^{-\frac{1}{2}}$$

$$= \left(3\sqrt{2}+2\right)pq + \left(\frac{4}{7}\sqrt{7}+2\sqrt{2}\right)p + \left(\frac{4}{7}\sqrt{7}+2\sqrt{2}-2\right)q + \frac{4}{7}\sqrt{7}-\sqrt{2}.$$

4.7 The ve-degree Atom-bond Connectivity Index

Using Tab. 6 we compute the *ve*-degree atom-bond connectivity index:

$$ABC_{ve}(BiI_3) = \sum_{\lambda\varepsilon \in E} \left(\frac{d_{ve}(\lambda)+d_{ve}(\varepsilon)-2}{d_{ve}(\lambda)\times d_{ve}(\varepsilon)}\right)^{\frac{1}{2}}$$

$$ABC_{ve}(BiI3) = (4q+8)\sqrt{\frac{14}{60}} + (4p-4)\sqrt{\frac{16}{72}} + (8q+16)\sqrt{\frac{20}{120}} + (16p+12q-28)\sqrt{\frac{22}{144}}$$

$$+(12pq-8p-12q+8)\sqrt{\frac{24}{168}} + (4p-4)\sqrt{\frac{28}{216}} + (6pq-4p-6q+4)\sqrt{\frac{30}{252}}$$

$$= \left(\frac{12\sqrt{7}+\sqrt{210}}{7}\right)pq + \left(\frac{12\sqrt{22}+2\sqrt{42}+12\sqrt{2}}{9}\right)p + \left(\frac{-24\sqrt{7}-2\sqrt{210}}{21}\right)p$$

$$+\left(\frac{-180\sqrt{7}+140\sqrt{6}+105\sqrt{22}-\sqrt{210}}{105}\right)q + \frac{24\sqrt{6}-12\sqrt{2}-21\sqrt{22}-2\sqrt{42}}{9} + \frac{120\sqrt{7}+38\sqrt{210}}{105}.$$

4.8 The ve-degree Geometric-arithmetic Index

Using Tab. 6 we compute the *ve*-degree geometric-arithmetic index:

$$GA_{ve}(BiI_3) = \sum_{\lambda\varepsilon \in E} \frac{2(d_{ve}(\lambda)\times d_{ve}(\varepsilon))^{\frac{1}{2}}}{d_{ve}(\lambda)+d_{ve}(\varepsilon)}$$

$$GA_{ve}(BiI3) = (4q+8)\frac{(2)\sqrt{60}}{16} + (4p-4)\frac{(2)\sqrt{72}}{18} + (8q+16)\frac{(2)\sqrt{120}}{22} + (16p+12q-28)\frac{(2)\sqrt{144}}{24}$$
$$+(12pq-8p-12q+8)\frac{(2)\sqrt{168}}{26} + (4p-4)\frac{(2)\sqrt{216}}{30} + (6pq-4p-6q+4)\frac{(2)\sqrt{252}}{32}$$

$$= \left(\frac{24}{13}\sqrt{42}+\frac{9}{4}\sqrt{7}\right)pq + \left(16+\frac{8}{3}\sqrt{2}-\frac{16}{13}\sqrt{42}+\frac{8}{5}\sqrt{6}-\frac{3}{2}\sqrt{7}\right)p$$

$$+\left(\sqrt{15}-\frac{24}{13}\sqrt{42}+\frac{16}{11}\sqrt{30}+12-\frac{9}{4}\sqrt{7}\right)q+2\sqrt{15}-\frac{8}{5}\sqrt{6}-\frac{8}{3}\sqrt{2}-28+\frac{32}{11}\sqrt{30}$$

$$+\frac{3}{2}\sqrt{7}+\frac{16}{13}\sqrt{42}.$$

4.9 The ve-degree Harmonic Index

Using Tab. 6 we compute the *ve*-degree harmonic index:

$$H_{ve}(BiI_3)=\sum_{\lambda\varepsilon\in E}\frac{2}{d_{ve}(\lambda)+d_{ve}(\varepsilon)}$$

$$H_{ve}(BiI_3)=(4q+8)\frac{2}{16}+(4p-4)\frac{2}{18}+(8q+16)\frac{2}{22}+(16p+12q-28)\frac{2}{24}$$

$$+(12pq-8p-12q+8)\frac{2}{26}+(4p-4)\frac{2}{30}+(6pq-4p-6q+4)\frac{2}{32}$$

$$=\frac{135}{104}pq+\frac{2759}{2340}p+\frac{1063}{1144}q+\frac{7091}{25740}.$$

4.10 The ve-degree Sum-connectivity Index

Using Tab. 6 we compute the *ve*-degree sum-connectivity index:

$$\chi_{ve}(BiI_3)=\sum_{\lambda\varepsilon\in E}(d_{ve}(\lambda)+d_{ve}(\varepsilon))^{-\frac{1}{2}}$$

$$\begin{aligned}\chi_{ve}(BiI3)&=(4q+8)\frac{1}{\sqrt{16}}+(4p-4)\frac{1}{\sqrt{18}}+(8q+16)\frac{1}{\sqrt{22}}+(16p+12q-28)\frac{1}{\sqrt{24}}\\&+(12pq-8p-12q+8)\frac{1}{\sqrt{26}}+(4p-4)\frac{1}{\sqrt{30}}+(6pq-4p-6q+4)\frac{1}{\sqrt{32}}\\&=\left(\frac{6}{13}\sqrt{26}+\frac{3}{4}\sqrt{2}\right)pq+\left(\frac{4}{3}\sqrt{6}-\frac{4}{13}\sqrt{26}+\frac{2}{15}\sqrt{30}+\frac{1}{6}\sqrt{2}\right)p\\&+\left(1-\frac{6}{13}\sqrt{26}+\frac{4}{11}\sqrt{22}+\sqrt{6}-\frac{3}{4}\sqrt{2}\right)q+2-\frac{1}{6}\sqrt{2}+\frac{4}{13}\sqrt{26}+\frac{8}{11}\sqrt{22}-\frac{7}{3}\sqrt{6}-\frac{2}{15}\sqrt{30}.\end{aligned}$$

5 The Graph of Lead Chloride

Lead chloride is a precious halide stone that usually occurs in mineral cotunnite. The structure of lead chloride is orthorhombic dipyramidal. The diagram of a solitary unit of lead chloride is obtained from bismuth tri-iodide by joining an extra vertex to only one 2-degree vertex of every one of the 4-cycles. Fig. 2 shows one unit of lead chloride.

The unit cells of lead chloride can be arranged either linearly or in a sheet form. A linear arrangement with q unit cells is called q-lead chloride chain, $p \times q$ lead chloride sheet is obtained by arrangements of pq unit cells into p rows and q columns. A $p \times q$ lead chloride sheet throughout onward represented by LC. A sheet of LC contains $12pq + 10p + 7q + 2$ vertices and $24pq + 12p + 6q$ edges, which are shown in Tab. 7. The number of vertices corresponding to their degrees of LC are shown in Tab. 8 and the edge partition based on degree of end vertices of each edge is shown in the Tab. 9.

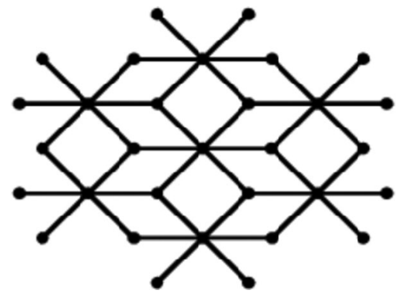

Figure 2: One unit of lead chloride

Table 7: Vertices and edges of *LC*

Total vertices	Total edges
$12pq + 10p + 7q + 2$	$24pq + 12p + 6q$

Table 8: Number of vertices corresponding to their degrees of *LC*

$d(\varepsilon)$	Number of vertices
1	$4p + 4q + 4$
2	$4p + 4q - 2$
3	$8pq - 2q$
6	$4pq + 2p + q$
Total	$12pq + 10p + 7q + 2$

Table 9: Edge partition of *LC*

$(d(\lambda), \mathrm{d}(\varepsilon))$	Number of edges
(1,6)	$4p + 4q + 4$
(2,6)	$8p + 8q - 4$
(3,6)	$24pq - 6q$
Total	$24pq + 12p + 6q$

We partitioned the edges of *LC*, based on *ev*-degree in Tab. 10.

Table 10: Edge partition of *LC*

Number of edges	$d_{ev}(\varepsilon)$	$(d(\lambda), d(\varepsilon))$
$4p + 4q + 4$	7	(1,6)
$8p + 8q - 4$	8	(2,6)
$24pq - 6q$	9	(3,6)

In Tab. 11, we partitioned the vertices of LC, based on ev-degree.

Table 11: Vertex partition of LC, based on ve-degree

Number of vertices	$d_{ve}(\varepsilon)$	$d(\varepsilon)$
$4p+4q+4$	6	1
$4p+4q-2$	12	2
$8pq-2q$	18	3
$2q+4$	12	6
$4p-4$	14	6
$2q-2$	16	6
$4pq-2p-3q+2$	18	6

We partitioned the edge of LC with respect to ve-degrees.

Now we calculated ev-degree and ve-degree based indices such as M_{ev} index, $M^1_{\alpha ve}$ index, $M^1_{\beta ve}$ index, M^2_{ve} index, R_{ve} index, R_{ev} index, ABC_{ve} index, GA_{ve} index, H_{ve} index and χ_{ve} index for LC.

5.1 *ev-Degree Zagreb Index*

By using ev-degree of LC from Tab. 10, we compute the ev-degree based Zagreb index:

$$\mathcal{M}^{ev}(LC) = \sum_{e\in E(LC)} (d_{ev}(e))^2$$

$$= (4p+4q+4)\times 7^2 + (8p+8q-4)\times 8^2 + (24pq-6q)\times 9^2$$

$$= 1944pq + 708p + 222q - 60.$$

5.2 *The First ve-degree Zagreb α Index*

Using Tab. 11 we compute the first ve-degree Zagreb α index:

$$M^1_{\alpha ve}(LC) = \sum_{\varepsilon\in V} d_{ve}(\varepsilon)^2$$

$$M^1_{\alpha ve}(LC) = (4p+4q+4)(6)^2 + (4p+4q-2)(12)^2 + (8pq-2q)(18)^2 + (2q+4)(12)^2$$

$$+(4p-4)(14)^2 + (2q-2)(16)^2 + (4pq-2p-3q+2)(18)^2$$

$$= 3888pq + 856p - 100q - 216.$$

5.3 *The First ve-degree Zagreb β Index*

Using Tab. 12 we compute the first ve-degree Zagreb β index:

$$M^1_{\beta ve}(LC) = \sum_{\lambda\varepsilon\in E} (d_{ve}(\lambda) + d_{ve}(\varepsilon))$$

$$M^1_{\beta ve}(LC) = (4q+8)(18) + (4p-4)(20) + (4q+8)(24) + (8p-8)(26) + (4q-4)(28)$$
$$+(4q+8)(30) + (12p-12)(32) + (8q-8)(34) + (24pq-12p-18q+12)(36)$$
$$= 768pq + 288p + 96q - 96.$$

Table 12: Edge partition of LC, based on ve-degree

Number of edges	$(d_{ve}(\lambda), \mathrm{d}_{\mathrm{ve}}(\varepsilon))$	$(d(\lambda), \mathrm{d}(\varepsilon))$
$4q+8$	(6,12)	(1,6)
$4p-4$	(6,14)	(1,6)
$4q+8$	(12,12)	(2,6)
$8p-8$	(12,14)	(2,6)
$4q-4$	(12,16)	(2,6)
$4q+8$	(12,18)	(3,6)
$12p-12$	(14,18)	(3,6)
$8q-8$	(16,18)	(3,6)
$24pq-12p-18q+12$	(18,18)	(3,6)

5.4 The second ve-degree Zagreb index

Using Tab. 12 we compute the second ve-degree Zagreb index:

$$M^2_{ve}(LC) = \sum_{\lambda\varepsilon\in E}(d_{ve}(\lambda) \times d_{ve}(\varepsilon))$$

$$M^2_{ve}(LC) = (4q+8)(72) + (4p-4)(84) + (4q+8)(144) + (8p-8)(168) + (4q-4)(192)$$
$$+(4q+8)(216) + (12p-12)(252) + (8q-8)(288) + (24pq-12p-18q+12)(324)$$
$$= 6048pq + 1680p + 264q - 1296.$$

5.5 ve-degree Randic Index

Using Tab. 12 we compute the ve-degree Randic index:

$$R_{ve}(LC) = \sum_{\lambda\varepsilon\in E}(d_{ve}(\lambda) \times d_{ve}(\varepsilon))^{-\frac{1}{2}}$$

$$R_{ve}(LC) = (4q+8)(72)^{-\frac{1}{2}} + (4p-4)(84)^{-\frac{1}{2}} + (4q+8)(144)^{-\frac{1}{2}} + (8p-8)(168)^{-\frac{1}{2}}$$
$$+(4q-4)(192)^{-\frac{1}{2}} + (4q+8)(216)^{-\frac{1}{2}} + (12p-12)(252)^{-\frac{1}{2}} + (8q-8)(288)^{-\frac{1}{2}}$$
$$+(24pq-12p-18q+12)(324)^{-\frac{1}{2}}$$
$$= \frac{4}{7}\sqrt{7}pq + \left(\frac{2\sqrt{21}+2\sqrt{42}}{21}\right)p + \left(\frac{1}{3} + \frac{2\sqrt{2}}{3} + \frac{\sqrt{3}}{6} + \frac{\sqrt{6}}{9} - \frac{3\sqrt{7}}{7}\right)q$$

$$+\frac{\sqrt{2}}{3}+\frac{2}{3}-\frac{\sqrt{3}}{6}+\frac{2\sqrt{6}}{9}-\frac{2\sqrt{42}}{21}-\frac{2\sqrt{21}}{21}.$$

5.6 The ev-degree Randic Index

Using Tab. 10 we compute the *ev*-degree Randic index:

$$R_{ev}(LC)=\sum_{e_1\in E}d_{ve}(e_1)^{-\frac{1}{2}}$$

$$R_{ev}(LC)=(4p+4q+4)(7)^{-\frac{1}{2}}+(8p+8q-4)(8)^{-\frac{1}{2}}+(24pq-6q)(9)^{-\frac{1}{2}}$$

$$=8pq+\left(\frac{4\sqrt{7}}{7}+2\sqrt{2}\right)p+\left(\frac{4\sqrt{7}}{7}+2\sqrt{2}-2\right)q+\frac{4\sqrt{7}}{7}-\sqrt{2}.$$

5.7 The ve-degree Atom-bond Connectivity Index

Using Tab. 12 we compute the *ve*-degree atom-bond connectivity index:

$$ABC_{ve}(LC)=\sum_{\lambda\varepsilon\in E}\left(\frac{d_{ve}(\lambda)+d_{ve}(\varepsilon)-2}{d_{ve}(\lambda)\times d_{ve}(\varepsilon)}\right)^{\frac{1}{2}}$$

$$ABC_{ve}(LC)=(4q+8)\sqrt{\frac{16}{72}}+(4p-4)\sqrt{\frac{18}{84}}+(4q+8)\sqrt{\frac{22}{144}}+(8p-8)\sqrt{\frac{24}{168}}$$

$$+(4q-4)\sqrt{\frac{26}{192}}+(4q+8)\sqrt{\frac{28}{216}}+(12p-12)\sqrt{\frac{30}{252}}+(8q-8)\sqrt{\frac{32}{288}}$$

$$+(24pq-12p-18q+12)\sqrt{\frac{34}{324}}$$

$$=\frac{4\sqrt{210}}{7}+\left(\frac{8\sqrt{7}}{7}+\frac{2\sqrt{42}}{7}\right)p+\left(\frac{\sqrt{22}+8+4\sqrt{2}}{3}+\frac{\sqrt{78}}{6}\right)q+\left(\frac{2\sqrt{42}}{9}-\frac{3\sqrt{210}}{7}\right)q$$

$$+\frac{8\sqrt{2}}{3}+\frac{2\sqrt{22}}{3}+\frac{10\sqrt{42}}{63}-\frac{\sqrt{78}}{6}-\frac{8}{3}-\frac{8\sqrt{7}}{7}.$$

5.8 The ve-degree Geometric-arithmetic Index

Using Tab. 12 we compute the *ve*-degree geometric-arithmetic index:

$$GA_{ve}(LC)=\sum_{\lambda\varepsilon\in E}\frac{2(d_{ve}(\lambda)\times d_{ve}(\varepsilon))^{\frac{1}{2}}}{d_{ve}(\lambda)+d_{ve}(\varepsilon)}$$

$$GA_{ve}(LC)=(4q+8)\frac{(2)\sqrt{72}}{18}+(4p-4)\frac{(2)\sqrt{84}}{20}+(4q+8)\frac{(2)\sqrt{144}}{24}+(8p-8)\frac{(2)\sqrt{168}}{26}+(4q-4)\frac{(2)\sqrt{192}}{28}$$

$$+(4q+8)\frac{(2)\sqrt{216}}{30}+(12p-12)\frac{(2)\sqrt{252}}{32}+(8q-8)\frac{(2)\sqrt{288}}{34}$$

$$+(24pq-12p-18q+12)\frac{(2)\sqrt{324}}{36}$$

$$=9\sqrt{7}pq+\left(\frac{4\sqrt{21}}{5}+\frac{16\sqrt{42}}{13}\right)p+\left(4+\frac{424\sqrt{2}}{51}+\frac{16\sqrt{3}}{7}+\frac{8\sqrt{6}}{5}-\frac{27\sqrt{7}}{4}\right)q$$

$$-\frac{16\sqrt{2}}{51}-\frac{16\sqrt{42}}{13}-\frac{4\sqrt{21}}{5}+8-\frac{16\sqrt{3}}{7}+\frac{16\sqrt{6}}{5}.$$

5.9 The ve-degree Harmonic Index

Using Tab. 6 we compute the *ve*-degree harmonic index:

$$H_{ve}(LC)=\sum_{\lambda\varepsilon\in E}\frac{2}{d_{ve}(\lambda)+d_{ve}(\varepsilon)}$$

$$H_{ve}(LC)=(4q+8)\frac{2}{18}+(4p-4)\frac{2}{20}+(4q+8)\frac{2}{24}+(8p-8)\frac{2}{26}+(4q-4)\frac{2}{28}+(4q+8)\frac{2}{30}$$

$$+(12p-12)\frac{2}{32}+(8q-8)\frac{2}{34}+(24pq-12p-18q+12)\frac{2}{34}$$

$$=\frac{3}{2}pq+\frac{66}{65}p+\frac{28949}{42840}q+\frac{22082}{69615}.$$

5.10 The ve-degree Sum-Connectivity Index

Using Tab. 12 we compute the *ve*-degree sum-connectivity index:

$$\chi_{ve}(LC)=\sum_{\lambda\varepsilon\in E}(d_{ve}(\lambda)+d_{ve}(\varepsilon))^{-\frac{1}{2}}$$

$$\chi_{ve}(LC)=(4q+8)\frac{1}{\sqrt{18}}+(4p-4)\frac{1}{\sqrt{20}}+(4q+8)\frac{1}{\sqrt{24}}+(8p-8)\frac{1}{\sqrt{26}}+(4q-4)\frac{1}{\sqrt{28}}$$
$$+(4q+8)\frac{1}{\sqrt{30}}+(12p-12)\frac{1}{\sqrt{32}}+(8q-8)\frac{1}{\sqrt{34}}+(24pq-12p-18q+12)\frac{1}{\sqrt{36}}$$

$$=3\sqrt{2}pq+\left(\frac{4\sqrt{26}}{13}+\frac{2\sqrt{5}}{5}\right)p+\left(-\frac{19\sqrt{2}}{12}+\frac{\sqrt{6}}{3}+\frac{2\sqrt{30}}{15}+\frac{2\sqrt{7}}{7}+\frac{4\sqrt{34}}{17}\right)q$$

$$+\frac{4\sqrt{2}}{3}+\frac{2\sqrt{6}}{3}-\frac{2\sqrt{5}}{5}-\frac{2\sqrt{7}}{7}-\frac{4\sqrt{34}}{17}+\frac{4\sqrt{30}}{15}-\frac{4\sqrt{26}}{13}.$$

6 Graphical Representation and Discussion

Data or information visualization is becoming more popular due to ease of understanding and analysis in the modern scientific field. This section shows the graphical behavior of the above calculated topological descriptors for crystal networks (bismuth tri-iodide and lead chloride) is shown. It can be observed that by increasing the values of parameters values of topological descriptors are also increased. These graphical representations of *ve*-degree based topological descriptors are shown in Figs. 3–6.

In this section, we will discuss the graphical behavior of above calculated topological descriptors for crystal networks namely, bismuth tri-iodide and lead chloride. We observe that with the increase the values of parameters, the values of the defined topological descriptors are increased. The graphical representation of all above *ve*-degree based topological descriptors are shown in Figs. 3–6.

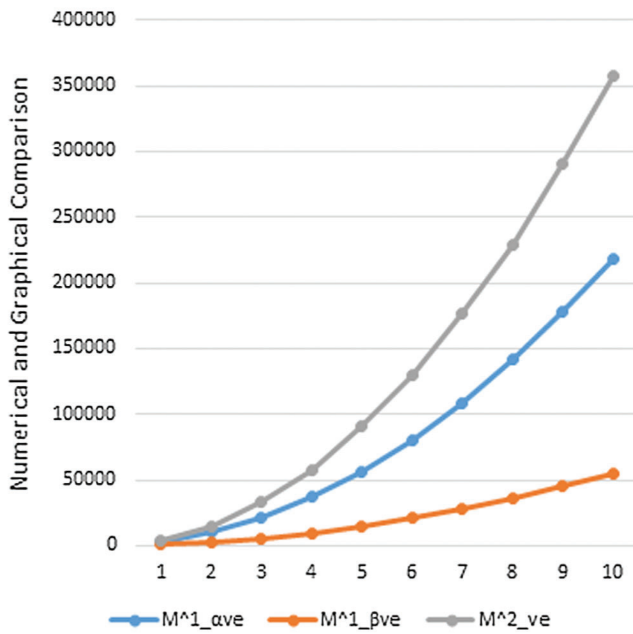

Figure 3: Graphical comparison of $M^1_{\alpha ve}, M^1_{\beta ve}, M^2_{ve}$ for BiI_3

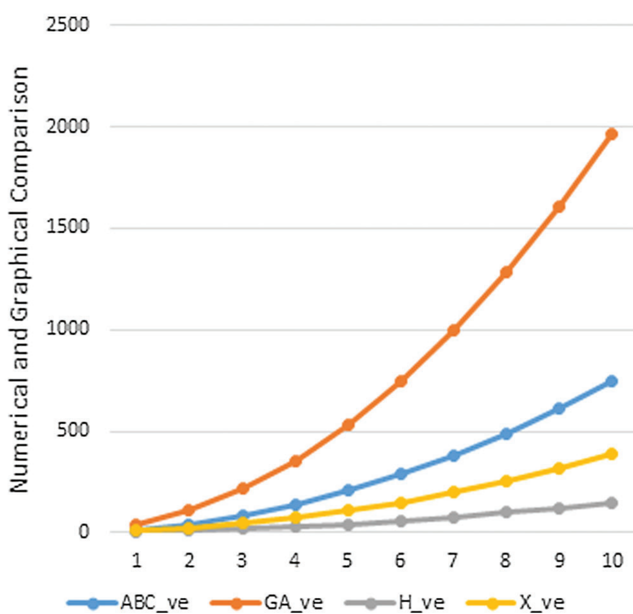

Figure 4: Graphical comparison of $ABC_{ve}, GA_{ve}, H_{ve}, \chi_{ve}$ for BiI_3

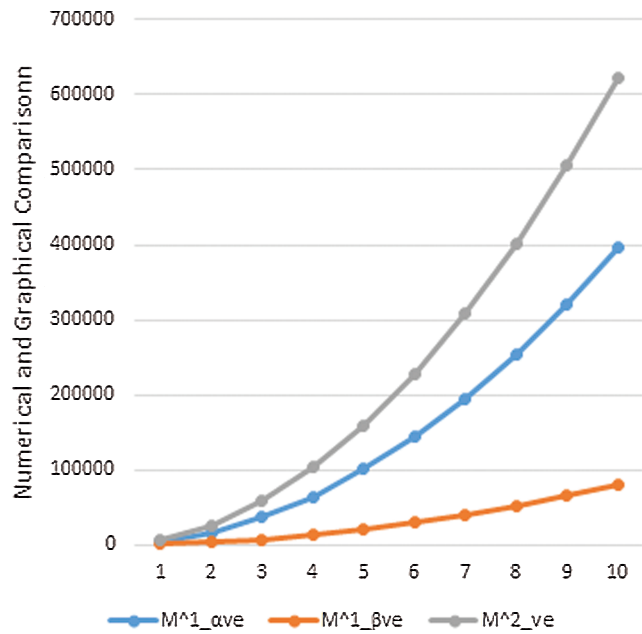

Figure 5: Graphical comparison of $M^1_{\alpha ve}, M^1_{\beta ve}, M^2_{ve}$ for LC

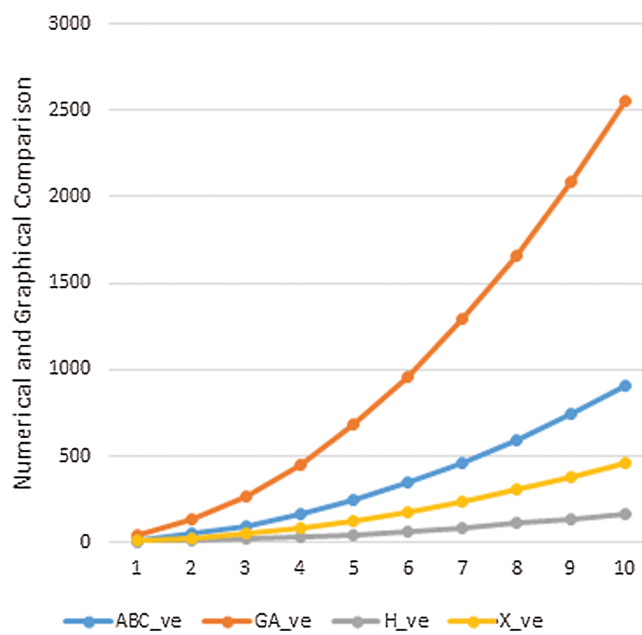

Figure 6: Graphical comparison of $ABC_{ve}, GA_{ve}, H_{ve}, \chi_{ve}$ for LC

7 Conclusion

For numerical representaion of topologies for graphs or netwroks, topological descriptors are most useful invariants. That is why such investigations are widely used in computer applications and mathematical chemistry. Calculated results in this paper for *ev*-degree and *ve*-degree based topological indices for the crystal networks are shown pictorial in form of line chart from Figs. 3–6. In all the line charts it can be seen clearly that by increasing the values of *p* or *q* vlaues of topolgical decsriptors also incraese in a regular manner.

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