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On topological aspects of bilayer Germanium Phosphide

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Abstract

A material having electrical conductivity value falling between conductor and insulator is known as semiconductor. Due to high adaptability of these materials makes them best basic material used in advanced electronics and communications. Some popular semiconductors in periodic table are silicon, germanium and gallium arsenide. Here in this article we will give topological aspects on different structural form of germanium phosphide. A semiconductor used in high frequency communication and diodes.

Keywords: Germanium Phosphide, topological parameters, degree invariants.

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1. Introduction

A presentation of some points (nodes) connected by lines is called graph. In *graph theory*, a graph is consists of two sets, the non empty set of objects having points (nodes) is called vertex set while the set of connected lines which are the unordered pairs of points is called *edge set* [1].

A topology branch of mathematical chemistry which applies theory of graphs to chemical structures or networks for their molding and studying their properties is known as chemical graph theory. In this context, the structure of a chemical compound or network is presented by a graph in which points represents atoms and connected lines represents bonds of the chemical structure[1]. A numeric quantity derived from the graphical representation of a structure is called a topological parameter for that structure. It is used to study physical and chemical properties for the relative structure. In view of graph theory, this numeric parameter is a graph invariant which means that it is irrespective from the presentation of structure graphically.

Simonraj and George [9] have investigated physicochemical properties of dominating silicate networks, later on Baig et al. [2] computed different indices for DSL. One may found a variety of research articles on these parameters, in which authors had produced helpful results on different chemical structures, nano tubes and networks explaining their physicochemical properties (electron negativity, electron

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configuration, enthalpy and stability etc) [4, 5, 8, 9]. Some of them are computed with the help of number of edges connected to a vertex whereas some based on distance of a vertex from a particular point [5]. In the queue of these invariants *weiner index* is the oldest distance based index, which was first introduced by Harry Weiner in 1947. Later on many other indices were made defined and studied to till date. Some very popular indices are Randic index, family of Zagreb indices, Geometric index [4] and Connectivity indices [13] are just few names of them.

1.1. Topological invariants

For a particular atom the numbers of bonds connected to it is known as its *degree*. Here we will define some topological invariants, which are computed with the help of degree of an atom associated to a chemical graph.

Definition 1.1 ([3])**.** For a simply connected graph, the sum of squares of degrees of all its vertices is known as First Zagreb index defined as:

$$M_1 = \sum_{u \sim v} (d_u + d_v). \tag{1.1}$$

Definition 1.2 ([10, 13])**.** For any real value of α, Randic index is defined as:

$$R_\alpha = \sum_{u \sim v} (d_u . d_v)^\alpha, \tag{1.2}$$

where α is a real number.

Definition 1.3 ([5])**.** For any simply connected graph atomic bond Connectivity index is,

$$ABC = \sum_{u \sim v} \sqrt{\frac{d_u + d_v - 2}{d_u . d_v}}. \tag{1.3}$$

Definition 1.4 ([5, 10])**.** We define Geometric Arithmetic and Harmonic indices as,

$$GA = \sum_{u \sim v} \frac{2\sqrt{d_u . d_v}}{d_u + d_v}, \tag{1.4}$$

$$H = \sum_{u \sim v} \frac{2}{d_u + d_v}. \tag{1.5}$$

Definition 1.5 ([13])**.** Another connectivity index is defined as,

$$SCI = \sum_{u \sim v} (d_u + d_v)^{\frac{-1}{2}}. \tag{1.6}$$

For a connected graph G, and any $u \in V(G)$ the set of all edges incident to u is known as its *neighborhood* denoted by $N(u)$. On including u to its neighborhood is called *closed neighborhood* denoted by $N[u]$. In context to these literature definitions of a graph G, we define the sum of degrees of all vertices in a neighborhood of a vertex u as sum degree, i.e.,

$$S_u = \sum_{v \in N(u)} d_v. \tag{1.7}$$

In literal meaning to above definition we defined forth and fifth version of ABC and GA, respectively as follows.

Definition 1.6 ([2])**.** For a connected graph G

$$ABC_4 = \sum_{u \sim v} \sqrt{\frac{S_u + S_v - 2}{S_u . S_v}}. \tag{1.8}$$

Definition 1.7 ([4]). For a connected graph G

$$GA_5 = \sum_{u\sim v} \frac{2\sqrt{S_u.S_v}}{S_u + S_v}. \tag{1.9}$$

2. Germanium Phosphide

After the discovery of graphene, the pedigree of two dimensional 2D crystals has increases, holding a lot of diveristy encompassing all prudent electronic properties required for nano electronics. Dirac semimetals like graphene, silicene, germanene and semiconductors, transition metal dichalcogenide (TMDC) (phosporene) has useful applications in nano technology. In optoelectronics very first application were reported on the basis of TMDC.

All elements of group fourteen in periodic table are semimetallic. Combination of group 14 elements with Phosphorene (an allotropic form of Phosporus P) produced very good results in electronics.

A layered material composed by Phosphorene (P) and Germanene (a single layer material consisting Germanium atoms) (Ge) with stoichiometry called Germanium Phosphide GeP_3 was first reported in 1970. Generally GeP_x found in three phases for $(x = 1, 3, 5)$. Here x is controlled by chemical reaction and a clean phase single layer crystal can be obtained.

Experiments shows that, GeP_3 crystal owns corrugated Arsenic type honeycomb structure in ABC stacking, which is a superconductive material and crystallized in layered structure. The bulk GeP_3 is metal, while monolayer (1L) and bilayer (2L) GeP_3 is a semiconductor. Furthermore bilayer GeP_3 ($2LGeP_3$) have notable high carrier mobility and a conspicuous light absorbtion in solar spectrum [6, 7, 11, 12].

3. Structure of $2LGeP_3$

Here in this article we will explain the structure of GeP_3 in four different ways with the help of geomatrical shapes like triangle, rhombous, rectangle and cocentric circles. Naming to these structures shapes as triangulene, rhombohedral, rectangular (jagged) and circumcoronene, respectively. These structural shapes are very familiar in nano technology.

4. Triangulene $2LGeP_3$

In Triangulene $2LGeP_3$, structure of bilayer germanium phosphide ($2LGeP_3$) is presented with the influence of regular triangle shape. It has total $3n^2 + 9n$ edges for $n \geqslant 2$. Here n counts the number of hexagons in the base of monolayer $1LGeP_3$ structure.

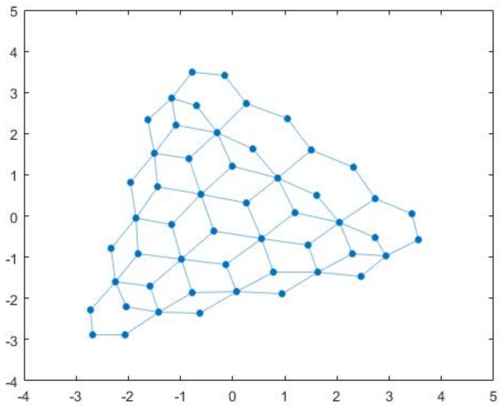

Figure 1: $T2LGeP_3^4$ Triangulene Bilayer Germanium Phosphide for $n = 4$.

4.1. Partioning for the edge set of Triangulene $2LGeP_3$ graph

By using the definition of *degree* of a vetrex in molecular graph, we give a partition to the edge set of $2LGeP_3$ on the basis of degrees of end vertices of the edges. This edge partition consists of total 8 subsets of edge set defined as follows:

$$\begin{aligned}
E_1 &= \{u \sim v \mid d_u = 2 \wedge d_v = 2\}, & E_2 &= \{u \sim v \mid d_u = 2 \wedge d_v = 3\},\\
E_3 &= \{u \sim v \mid d_u = 2 \wedge d_v = 4\}, & E_4 &= \{u \sim v \mid d_u = 2 \wedge d_v = 5\},\\
E_5 &= \{u \sim v \mid d_u = 2 \wedge d_v = 6\}, & E_6 &= \{u \sim v \mid d_u = 3 \wedge d_v = 4\},\\
E_7 &= \{u \sim v \mid d_u = 3 \wedge d_v = 5\}, & E_8 &= \{u \sim v \mid d_u = 3 \wedge d_v = 6\},
\end{aligned}$$

with cardinalities as $|E_1| = 4$, $|E_2| = 2n-2$, $|E_3| = 6$, $|E_4| = 4n-2$, $|E_5| = 2n-2$, $|E_6| = 2$, $|E_7| = 6n-8$, and $|E_8| = 3n^2-5n+2$, respectively $\forall\ n \geqslant 2$.

4.2. Computational Results for Triangulene $2LGeP_3$

Here in this section we will compute some topological parameters based on degrees of connected atoms in Triangulene Bilayer Germanium Phosphide for the appurtenance of a reader we will represent this structure shortly as $T2LGeP_3^n$.

Theorem 4.1. *For $n \geqslant 2$, the first Zagreb index for Triangulene Bilayer Germanium Phosphide ($T2LGeP_3$) is:*

$$M_1(T2LGeP_3^n) = 27n^2 - 57n - 20.$$

Proof. By using (1.1) we have

$$\begin{aligned}
M_1(T2LGeP_3^n) = {} & (4)(2+2) + (2n-2)(2+3) + (6)(2+4) + (4n-2)(2+5)\\
& + (2n-2)(2+6) + (2)(3+4) + (6n-8)(3+5) + (3n^2-5n+2)(3+6),
\end{aligned}$$

after computing we get,

$$M_1(T2LGeP_3^n) = 27n^2 - 57n - 20.$$

□

Theorem 4.2. *For $n \geqslant 2$, the second Zagreb index for Triangulene Bilayer Germanium Phosphide ($T2LGeP_3$) is:*

$$M_2(T2LGeP_3^n) = 54n^2 + 76n - 76.$$

Proof. By using (1.2) and taking $\alpha = 1$ we have

$$\begin{aligned}
M_2(T2LGeP_3^n) = {} & (4)(2.2) + (2n-2)(2.3) + (6)(2.4) + (4n-2)(2.5)\\
& + (2n-2)(2.6) + (2)(3.4) + (6n-8)(3.5) + (3n^2-5n+2)(3.6),
\end{aligned}$$

after computing we get,

$$M_2(T2LGeP_3^n) = 54n^2 + 76n - 76.$$

□

Theorem 4.3. *With $n \geqslant 2$ the General Randic index for Triangulene Bilayer Germanium Phosphide is,*

$$R_\alpha(T2LGeP_3^n) = \begin{cases} 54n^2 + 76n - 76, & \alpha = 1,\\ 3n^2 - (\frac{2}{\sqrt{6}} + \frac{4}{\sqrt{10}} + \frac{2}{\sqrt{12}} + \frac{6}{\sqrt{15}} - \frac{5}{\sqrt{18}})n + (2 - \frac{2}{\sqrt{6}} + \frac{6}{\sqrt{8}} - \frac{2}{\sqrt{10}} - \frac{8}{\sqrt{15}} + \frac{2}{\sqrt{18}}), & \alpha = 1/2,\\ (3\sqrt{18})n^2 + (2\sqrt{6} + 4\sqrt{10} + 4\sqrt{3} + 6\sqrt{15} - 15\sqrt{2})n + (8 + 12\sqrt{2}), & \alpha = -1/2,\\ \frac{1}{6}n^2 + \frac{46}{45}n + \frac{143}{180}, & \alpha = -1. \end{cases}$$

Proof. By using (1.2) and degree based partition in Subsection 4.1 given previously we get the desired results. □

Corollary 4.4. *For $\alpha = 1$ and $\alpha = -1$, the general randic index is also called Second Zagreb index and Second Modified Zagreb index, respectively.*

Theorem 4.5. *Consider the Triangulene Bilayer Germanium Phosphide, then for $n \geqslant 2$ the atomic bond Connectivity index is equal to*

$$ABC(T2LGeP_3^n) = (\frac{\sqrt{14}}{2})n^2 + (\frac{120\sqrt{2}+36\sqrt{10}-25\sqrt{14}}{30})n + (\frac{30\sqrt{2}+5\sqrt{15}-24\sqrt{10}+5\sqrt{14}}{15}).$$

Proof. By using the definition (1.3) of ABC index and degree based partition in Subsection 4.1 given previously we get the desired results. □

Theorem 4.6. *With $n \geqslant 2$ the Geometric Arithmetic index for Triangulene Bilayer Germanium Phosphide is,*

$$GA(T2LGeP_3^n) = 2\sqrt{2}n^2 + (\frac{4\sqrt{6}}{5} + \frac{8\sqrt{10}}{7} + \frac{3\sqrt{15}}{4} - \frac{20\sqrt{2}}{3} + \sqrt{3})n + (\frac{4\sqrt{2}}{3} - \frac{4\sqrt{6}}{5} - \frac{4\sqrt{10}}{7} + \frac{\sqrt{3}}{7} + 4).$$

Proof. By using the definition (1.4) of GA index and degree based partition in Subsection 4.1 given previously we get the desired results. □

Theorem 4.7. *With $n \geqslant 2$ the Sum Connectivity index for Triangulene Bilayer Germanium Phosphide is,*

$$SCI(T2LGeP_3^n) = n^2 + (\frac{2}{\sqrt{5}} + \frac{4}{\sqrt{7}} + \sqrt{8} - \frac{5}{3})n + (\sqrt{6} + \frac{8}{3} - \frac{10}{\sqrt{8}} - \frac{2}{\sqrt{5}}).$$

Proof. By using the definition (1.6) of SCI index and degree based partition in Subsection 4.1 given previously we get the desired results. □

Theorem 4.8. *With $n \geqslant 2$, the Harmonic index for Triangulene Bilayer Germanium Phosphide is*

$$H(T2LGeP_3^n) = \frac{1}{3}n^2 + \frac{892}{315}n + \frac{1081}{630}.$$

Proof. By using the definition (1.5) of Harmonic index and degree based partition in Subsection 4.1 given previously we get the desired results. □

4.3. *neighborhood partition*

Now here by using the definition (1.7) of S_u we give an other different edge partition to the edge set of $T2LGeP_3^n$ on the basis of *sum degree* of neighborhood vertices of all the edges. And this partition consists of total 22 partite subsets of edge set defined as follows:

$$\begin{aligned}
\xi_1 &= \{u \sim v \mid S_u = 4 \wedge S_v = 7\}, & \xi_2 &= \{u \sim v \mid S_u = 10 \wedge S_v = 12\},\\
\xi_3 &= \{u \sim v \mid S_u = 5 \wedge S_v = 6\}, & \xi_4 &= \{u \sim v \mid S_u = 9 \wedge S_v = 13\},\\
\xi_5 &= \{u \sim v \mid S_u = 5 \wedge S_v = 10\}, & \xi_6 &= \{u \sim v \mid S_u = 10 \wedge S_v = 13\},\\
\xi_7 &= \{u \sim v \mid S_u = 6 \wedge S_v = 10\}, & \xi_8 &= \{u \sim v \mid S_u = 10 \wedge S_v = 16\},\\
\xi_9 &= \{u \sim v \mid S_u = 6 \wedge S_v = 9\}, & \xi_{10} &= \{u \sim v \mid S_u = 12 \wedge S_v = 16\},\\
\xi_{11} &= \{u \sim v \mid S_u = 9 \wedge S_v = 9\}, & \xi_{12} &= \{u \sim v \mid S_u = 9 \wedge S_v = 15\},\\
\xi_{13} &= \{u \sim v \mid S_u = 9 \wedge S_v = 10\}, & \xi_{14} &= \{u \sim v \mid S_u = 13 \wedge S_v = 15\},\\
\xi_{15} &= \{u \sim v \mid S_u = 7 \wedge S_v = 12\}, & \xi_{16} &= \{u \sim v \mid S_u = 13 \wedge S_v = 16\},\\
\xi_{17} &= \{u \sim v \mid S_u = 13 \wedge S_v = 17\}, & \xi_{18} &= \{u \sim v \mid S_u = 15 \wedge S_v = 16\},\\
\xi_{19} &= \{u \sim v \mid S_u = 16 \wedge S_v = 17\}, & \xi_{20} &= \{u \sim v \mid S_u = 16 \wedge S_v = 18\},\\
\xi_{21} &= \{u \sim v \mid S_u = 17 \wedge S_v = 18\}, & \xi_{22} &= \{u \sim v \mid S_u = 18 \wedge S_v = 18\},
\end{aligned}$$

with cardinalities as $|\xi_1| = |\xi_3| = |\xi_5| = |\xi_9| = |\xi_{11}| = |\xi_{13}| = |\xi_{15}| = |\xi_{19}| = |\xi_4| = |\xi_{12}| = |\xi_{14}| = |\xi_{18}| = 2$ and $|\xi_7| = |\xi_{17}| = 2n-4$, $|\xi_6| = |\xi_{16}| = |\xi_{21}| = 4n-10$, $|\xi_2| = 4$, $|\xi_8| = n+1$, $|\xi_{10}| = 2n$, $|\xi_{20}| = 5n-10$, $|\xi_{22}| = 3n^2-15n+19$. Fourth version of ABC and fifth version of GA indices will be computed by using above edge partition.

Theorem 4.9. *Consider the Triangulene Bilayer Germanium Phosphide* $T2LGeP_3^n$*, then for* $n \geqslant 3$ *the* ABC_4 *is equal to*

$$\begin{aligned} ABC_4(T2LGeP_3^n) = {} & \left(\frac{\sqrt{34}}{6}\right)n^2 + \left(\frac{\sqrt{210}}{15} + \frac{4\sqrt{21}}{\sqrt{130}} + \frac{\sqrt{15}}{10} + \frac{\sqrt{78}}{12} + \frac{3\sqrt{38}}{13} + \frac{2\sqrt{28}}{\sqrt{221}} + \frac{5}{3} + \frac{4\sqrt{33}}{\sqrt{306}} - \frac{5\sqrt{34}}{6}\right)n \\ & + \left(\frac{3}{\sqrt{7}} + \frac{\sqrt{30}}{3} + \frac{\sqrt{26}}{5} + \frac{\sqrt{78}}{9} + \frac{\sqrt{170}}{15} + \frac{\sqrt{357}}{21} + \frac{4\sqrt{65}}{39} + \frac{2\sqrt{330}}{45} + \frac{\sqrt{435}}{30} + \frac{\sqrt{527}}{34}\right. \\ & \left. - \frac{2\sqrt{210}}{15} - \frac{10\sqrt{21}}{\sqrt{130}} + \frac{\sqrt{15}}{10} - \frac{15\sqrt{39}}{26} - \frac{4\sqrt{28}}{\sqrt{221}} - \frac{10\sqrt{33}}{\sqrt{306}} + \frac{19\sqrt{34}}{18} - \frac{22}{9} + \frac{4}{\sqrt{6}}\right). \end{aligned}$$

Proof. By using the definition (1.8) of ABC_4 index and partition sets in Subsection 4.3 given previously we get the desired results. □

Theorem 4.10. *With* $n \geqslant 3$*, the* GA_5 *for Triangulene Bilayer Germanium Phosphide is:*

$$\begin{aligned} GA_5(T2LGeP_3^n) = {} & 3n^2 + \left(\frac{\sqrt{15}}{2} + \frac{8\sqrt{130}}{23} + \frac{4\sqrt{10}}{13} + \frac{8\sqrt{3}}{7} + \frac{32\sqrt{13}}{29} + \frac{2\sqrt{221}}{15} + \frac{60\sqrt{2}}{7} + \frac{24\sqrt{34}}{35} - 5\right)n \\ & + \left(\frac{8\sqrt{7}}{11} + \frac{12\sqrt{30}}{11} + \frac{4\sqrt{2}}{3} + \frac{4\sqrt{6}}{5} + \frac{12\sqrt{10}}{19} + \frac{8\sqrt{21}}{19}\right. \\ & + \frac{6\sqrt{13}}{11} + \frac{\sqrt{195}}{7} - \frac{63\sqrt{15}}{62} + \frac{16\sqrt{17}}{33} - \frac{20\sqrt{130}}{23} \\ & \left. + \frac{4\sqrt{10}}{13} - \frac{80\sqrt{13}}{29} - \frac{4\sqrt{221}}{15} - \frac{120\sqrt{2}}{7} - \frac{12\sqrt{34}}{7} + 21\right). \end{aligned}$$

Proof. By using the definition (1.9) of GA_5 index and partition sets in Subsection 4.3 given previously we get the desired results. □

5. Rhombohedral $2LGeP_3$

In Rhomboherdal $2LGeP_3$, the structure of bilayer Germanium Phosphide is presented by the influence of rhombus shape. It has total $6n^2+8n-2$ edges for $n \geqslant 2$. Here n counts the number of hexagons from either the side of monolayer $1LGeP_3$ structure.

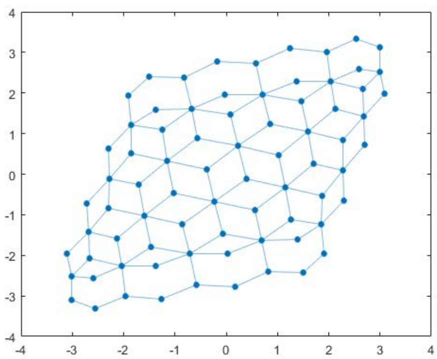

Figure 2: $R2LGeP_3^4$ Rhombohedral Bilayer Germanium Phosphide for $n = 4$.

5.1. *Partioning for the edge set of Rhombohedral 2LGeP$_3$ graph*

By using the definition of *degree* of a vetrex in molecular graph, we give a partition to the edge set of Rhombohedral structure for bilayer Germanium Phosphide after computing degrees of vertices for all the edges. We concluded that for $n \geqslant 2$ the edge set of this structural shape have 8 sub partite edge sets defined as follows:

$$E_1 = \{u \sim v \mid d_u = 2 \wedge d_v = 2\}, \qquad E_2 = \{u \sim v \mid d_u = 2 \wedge d_v = 3\},$$
$$E_3 = \{u \sim v \mid d_u = 2 \wedge d_v = 4\}, \qquad E_4 = \{u \sim v \mid d_u = 2 \wedge d_v = 5\},$$
$$E_5 = \{u \sim v \mid d_u = 2 \wedge d_v = 6\}, \qquad E_6 = \{u \sim v \mid d_u = 3 \wedge d_v = 4\},$$
$$E_7 = \{u \sim v \mid d_u = 3 \wedge d_v = 5\}, \qquad E_8 = \{u \sim v \mid d_u = 3 \wedge d_v = 6\},$$

with cardinalities as $|E_1| = 4$, $|E_2| = 4n - 4$, $|E_3| = 6$, $|E_4| = 4n - 2$, $|E_5| = 4n - 4$, $|E_6| = 2$, $|E_7| = 6n - 8$ and $|E_8| = 6n^2 - 10n + 4$, respectively $\forall\ n \geqslant 2$.

5.2. *Computational results for Rhombohedral 2LGeP$_3$*

Now we will compute some degree based topological parameter for Rhombohedral Bilayer Germanium Phosphide. For the convenience, we will represent this structure shortly as $R2LGeP_3^n$.

Theorem 5.1. *For $n \geqslant 2$, the first Zagreb index for Rhombohedral Bilayer Germanium Phosphide is:*

$$M_1(R2LGeP_3^n) = 54n^2 + 38n - 28.$$

Proof. By using (1.1)

$$\begin{aligned} M_1(R2LGeP_3^n) = {} & (4)(2+2) + (4n-4)(2+3) + (6)(2+4) + (4n-2)(2+5) \\ & + (4n-4)(2+6) + (2)(3+4) + (6n-8)(3+5) + (6n^2 - 10n + 4)(3+6), \end{aligned}$$

after computing we get,

$$M_1(R2LGeP_3^n) = 54n^2 + 38n - 28.$$

□

Theorem 5.2. *For $n \geqslant 2$, the second Zagreb index for Rhombohedral Bilayer Germanium Phosphide is:*

$$M_2(R2LGeP_3^n) = 108n^2 + 22n - 52.$$

Proof. By using (1.2) and taking $\alpha = 1$

$$\begin{aligned} M_2(R2LGeP_3^n) = {} & (4)(2.2) + (4n-4)(2.3) + (6)(2.4) + (4n-2)(2.5) \\ & + (4n-4)(2.6) + (2)(3.4) + (6n-8)(3.5) + (6n^2 - 10n + 4)(3.6), \end{aligned}$$

after computing we get,

$$M_2(R2LGeP_3^n) = 108n^2 + 22n - 52.$$

□

Theorem 5.3. *With $n \geqslant 2$ the General Randic index for Rhombohedral Bilayer Germanium Phosphide is,*

$$R_\alpha(R2LGeP_3^n) = \begin{cases} 108n^2 + 22n - 52, & \alpha = 1, \\ \sqrt{2}n^2 + (\frac{4}{\sqrt{6}} + \frac{4}{\sqrt{10}} + \frac{2}{\sqrt{3}} + \frac{6}{\sqrt{15}} - \frac{10}{\sqrt{18}})n + (\frac{4\sqrt{2}}{3} - \frac{4}{\sqrt{6}} - \frac{2}{\sqrt{10}} - \frac{1}{\sqrt{3}} - \frac{8}{\sqrt{15}} + 2 + \frac{3}{\sqrt{2}}), & \alpha = -1/2, \\ (18\sqrt{2})n^2 + (4\sqrt{10} + 6\sqrt{15} - 30\sqrt{2} + 24)n + (24\sqrt{2} - 4\sqrt{3} - 2\sqrt{10} - 8\sqrt{15} + 8), & \alpha = 1/2, \\ \frac{1}{3}n^2 + \frac{56}{45}n + \frac{73}{180}, & \alpha = -1. \end{cases}$$

Proof. By using the definition (1.2) of Randic index

$$R_{\alpha} = \sum_{u \sim v} (d_u . d_v)^{\alpha},$$

and degree based partition in Subsection 5.1 given previously we get the desired results. □

Corollary 5.4. *For $\alpha = 1$ and $\alpha = -1$, the general randic index is also called Second Zagreb index and Second Modified Zagreb index, respectively.*

Theorem 5.5. *With $n \geqslant 2$, the atomic bond Connectivity index for Rhombohedral Bilayer Germanium Phosphide is:*

$$ABC(R2LGeP_3^n) = \sqrt{14}n^2 + (\frac{12}{\sqrt{2}} + \frac{6\sqrt{10}}{5} - \frac{5\sqrt{14}}{3})n + (\frac{\sqrt{15}}{3} - \frac{8\sqrt{10}}{5} + \frac{2\sqrt{14}}{3}).$$

Proof. By using the definition (1.3) of ABC index and degree based partition in Subsection 5.1 given previously we get the desired results. □

Theorem 5.6. *With $n \geqslant 2$, the Geometric Arithmetic index for Rhombohedral Bilayer Germanium Phosphide is:*

$$GA(R2LGeP_3^n) = (4\sqrt{2})n^2 + (\frac{8\sqrt{6}}{5} + \frac{8\sqrt{10}}{7} + \frac{3\sqrt{15}}{2} - \frac{20\sqrt{2}}{3} + 2\sqrt{3})n + (\frac{20\sqrt{2}}{3} - \frac{8\sqrt{6}}{5} - \frac{4\sqrt{10}}{7} - \frac{8\sqrt{15}}{4} + 4).$$

Proof. By using the definition (1.4) of GA index and degree based partition in Subsection 5.1 given previously we get the desired results. □

Theorem 5.7. *With $n \geqslant 2$, the Sum Connectivity index for Rhombohedral Bilayer Germanium Phosphide is:*

$$SCI(R2LGeP_3^n) = 2n^2 + (\frac{4}{\sqrt{5}} + \frac{4}{\sqrt{7}} + \frac{10}{\sqrt{8}} - \frac{10}{3})n + (\sqrt{6} - \frac{4}{\sqrt{5}} - 3\sqrt{2} + \frac{10}{3}).$$

Proof. By using the definition (1.6) of SCI Index and degree based partition in Subsection 5.1 given previously we get the desired results. □

Theorem 5.8. *With $n \geqslant 2$, the Harmonic index for Rhombohedral Bilayer Germanium Phosphide is:*

$$H(R2LGeP_3^n) = \frac{4}{3}n^2 + \frac{1903}{630}n + \frac{13}{45}.$$

Proof. By using the definition (1.5) of Harmonic index and degree based partition in Subsection 5.1 given previously we get the desired results. □

5.3. *neighborhood prtition*

Now here by using the definition (1.7) of S_u we give an other different edge partition to the edge set of Rhombohedral bilayer Germanium Phosphide on the basis of *Sum degree* of neighborhood vertices of all the edges. We concluded that for $n \geqslant 3$ the neighborhood based edge partition for the edge set of $R2LGeP_3^n$ have 25 sub-partite sets defined as follows:

$$\begin{aligned}
\xi_1 &= \{u \sim v \mid S_u = 5 \wedge S_v = 6\}, & \xi_2 &= \{u \sim v \mid S_u = 5 \wedge S_v = 7\},\\
\xi_3 &= \{u \sim v \mid S_u = 5 \wedge S_v = 10\}, & \xi_4 &= \{u \sim v \mid S_u = 6 \wedge S_v = 10\},\\
\xi_5 &= \{u \sim v \mid S_u = 6 \wedge S_v = 9\}, & \xi_6 &= \{u \sim v \mid S_u = 9 \wedge S_v = 9\},\\
\xi_7 &= \{u \sim v \mid S_u = 9 \wedge S_v = 10\}, & \xi_8 &= \{u \sim v \mid S_u = 7 \wedge S_v = 12\},\\
\xi_9 &= \{u \sim v \mid S_u = 11 \wedge S_v = 12\}, & \xi_{10} &= \{u \sim v \mid S_u = 10 \wedge S_v = 12\},\\
\xi_{11} &= \{u \sim v \mid S_u = 10 \wedge S_v = 16\}, & \xi_{12} &= \{u \sim v \mid S_u = 12 \wedge S_v = 16\},
\end{aligned}$$

$$\xi_{13} = \{u \sim v \mid S_u = 11 \wedge S_v = 16\}, \qquad \xi_{14} = \{u \sim v \mid S_u = 9 \wedge S_v = 15\},$$
$$\xi_{15} = \{u \sim v \mid S_u = 12 \wedge S_v = 17\}, \qquad \xi_{16} = \{u \sim v \mid S_u = 13 \wedge S_v = 15\},$$
$$\xi_{17} = \{u \sim v \mid S_u = 13 \wedge S_v = 16\}, \qquad \xi_{18} = \{u \sim v \mid S_u = 13 \wedge S_v = 17\},$$
$$\xi_{19} = \{u \sim v \mid S_u = 15 \wedge S_v = 16\}, \qquad \xi_{20} = \{u \sim v \mid S_u = 17 \wedge S_v = 16\},$$
$$\xi_{21} = \{u \sim v \mid S_u = 18 \wedge S_v = 16\}, \qquad \xi_{22} = \{u \sim v \mid S_u = 17 \wedge S_v = 18\},$$
$$\xi_{23} = \{u \sim v \mid S_u = 18 \wedge S_v = 18\}, \qquad \xi_{24} = \{u \sim v \mid S_u = 10 \wedge S_v = 13\},$$
$$\xi_{25} = \{u \sim v \mid S_u = 9 \wedge S_v = 13\}.$$

with cardinalities as $|\xi_1| = |\xi_2| = |\xi_5| = |\xi_6| = |\xi_7| = |\xi_8| = |\xi_9| = |\xi_{10}| = |\xi_{13}| = |\xi_{14}| = |\xi_{15}| = |\xi_{16}| = |\xi_{19}| = |\xi_{25}| = 2$ and $|\xi_4| = |\xi_{22}| = 4n-8$, $|\xi_{17}| = |\xi_{24}| = 4n-10$, $|\xi_{11}| = 2n$, $|\xi_{12}| = 4n-6$, $|\xi_{18}| = 2n-4$, $|\xi_{20}| = |\xi_3| = 4$, $|\xi_{21}| = 8n-16$, $|\xi_{23}| = 6n^2-24n+24$. Forth version of ABC and fifth version of GA indices will be computed by using these set cardinalities.

Theorem 5.9. *With $n \geqslant 3$, the ABC_4 for Rhombohedral Bilayer Germanium Phosphide is:*

$$\begin{aligned} ABC_4(R2LGeP_3^n) = {} & (\frac{\sqrt{34}}{3})n^2 + (\frac{2\sqrt{210}}{15} + \frac{\sqrt{15}}{5} + \frac{\sqrt{78}}{6} + \frac{3\sqrt{39}}{13} + \frac{2\sqrt{28}}{\sqrt{221}} + \frac{4\sqrt{33}}{\sqrt{306}} + \frac{8}{3} - \frac{4\sqrt{34}}{18} + \frac{4\sqrt{21}}{\sqrt{130}})n \\ & + (\frac{\sqrt{30}}{5} + \frac{2\sqrt{14}}{7} + \frac{2\sqrt{26}}{5} - \frac{4\sqrt{210}}{15} + \frac{\sqrt{170}}{15} + \frac{\sqrt{357}}{21} + \frac{\sqrt{77}}{11} + \frac{2}{\sqrt{6}} - \frac{5\sqrt{78}}{36} \\ & + \frac{5\sqrt{11}}{22} + \frac{2\sqrt{330}}{45} + \frac{3}{\sqrt{17}} + \frac{2\sqrt{30}}{15} - \frac{15\sqrt{39}}{26} \\ & - \frac{4\sqrt{28}}{\sqrt{221}} + \frac{\sqrt{435}}{30} + \frac{\sqrt{527}}{17} - \frac{8\sqrt{33}}{\sqrt{306}} + \frac{4\sqrt{34}}{3} - \frac{10\sqrt{21}}{130} + \frac{4\sqrt{65}}{39} - \frac{40}{9}). \end{aligned}$$

Proof. By using the definition (1.8) of ABC_4 index and partition sets in Subsection 5.3 given previously we get the desired results. □

Theorem 5.10. *With $n \geqslant 3$, the GA_5 for Rhombohedral Bilayer Germanium Phosphide is:*

$$\begin{aligned} GA_5(R2LGeP_3^n) = {} & 6n^2 + (\sqrt{15} + \frac{8\sqrt{10}}{13} + \frac{16\sqrt{3}}{7} + \frac{32\sqrt{13}}{29} + \frac{2\sqrt{221}}{15} + \frac{96\sqrt{2}}{17} + \frac{24\sqrt{34}}{35} + \frac{8\sqrt{130}}{23} - 24)n \\ & + (\frac{8\sqrt{30}}{11} + \frac{\sqrt{35}}{6} + \frac{8\sqrt{2}}{3} - 2\sqrt{15} + \frac{4\sqrt{6}}{5} + \frac{12\sqrt{10}}{19} + \frac{8\sqrt{21}}{19} + \frac{8\sqrt{33}}{23} - \frac{24\sqrt{3}}{7} + \frac{16\sqrt{11}}{29} + \frac{\sqrt{15}}{2} \\ & + \frac{8\sqrt{51}}{29} + \frac{\sqrt{195}}{7} - \frac{80\sqrt{13}}{29} - \frac{4\sqrt{221}}{15} + \frac{16\sqrt{15}}{31} + \frac{32\sqrt{17}}{33} - \frac{192\sqrt{2}}{17} - \frac{48\sqrt{34}}{35} \\ & - \frac{20\sqrt{130}}{23} + \frac{6\sqrt{13}}{11} + 26). \end{aligned}$$

Proof. By using the definition (1.9) of GA_5 index and partition sets in Subsection 5.3 given previously we get the desired results. □

6. Rectangular $2LGeP_3$

In Rectangular $2LGeP_3$, the structure of bilayer Germanium Phosphide is presented by the influence of rectangle shape. It has total $12n^2$ edges for $n \geqslant 2$. Here n represents the number of hexagons counted from either the side in monolayer $1LGeP_3$ structure.

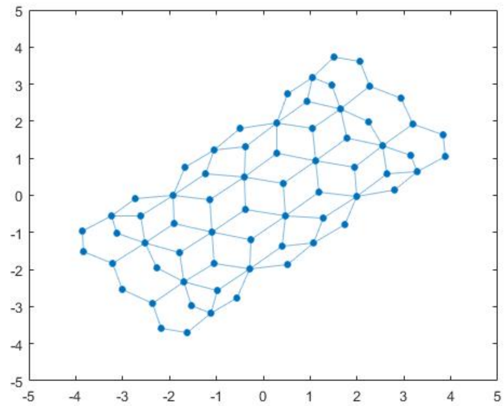

Figure 3: $Rct2LGeP_3^3$ Rectangular Bilayer Germanium Phosphide for $n = 3$.

6.1. Partioning for the edge set of Rectangular $2LGeP_3$ graph

By using the definition of *degree* of a vetrex in molecular graph, we give a partition to the edge set of Rectangular structure for bilayer Germanium Phosphide after computing degrees of end vertices for all the edges. We concluded that for $n \geqslant 2$ the edge set of this structural shape have 6 sub partite edge sets defined as follows:

$$E_1 = \{u \sim v \mid d_u = 2 \wedge d_v = 2\}, \quad E_2 = \{u \sim v \mid d_u = 2 \wedge d_v = 3\}, \quad E_3 = \{u \sim v \mid d_u = 2 \wedge d_v = 4\},$$
$$E_4 = \{u \sim v \mid d_u = 2 \wedge d_v = 6\}, \quad E_5 = \{u \sim v \mid d_u = 3 \wedge d_v = 4\}, \quad E_6 = \{u \sim v \mid d_u = 3 \wedge d_v = 6\},$$

with cardinalities as $|E_1| = 4$, $|E_2| = 4n - 4 = |E_3| = |E_5|$, $|E_4| = 8n - 8$, $|E_6| = 12n^2 - 20n + 8$, $\forall\, n \geqslant 2$.

6.2. Computational results for Rectangular $2LGeP_3$

Now we will compute some degree based topological parameters for Rectangular Bilayer Germanium Phosphide. For the convenience, we will represent this structure shortly by $Rct2LGeP_3^n$.

Theorem 6.1. *With $n \geqslant 2$, the first Zagreb index for Rectangular Bilayer Germanium Phosphide is:*

$$M_1(Rct2LGeP_3^n) = 108n^2 - 44n.$$

Proof. By using (1.1) we have

$$\begin{aligned} M_1(Rct2LGeP_3^n) = (4)(2+2) + (4n-4)(2+3) + (4n+4)(2+4) \\ + (8n-8)(2+6) + (4n-4)(3+4) + (12n^2-20n+8)(3+6), \end{aligned}$$

after computing we get,

$$M_1(Rct2LGeP_3^n) = 108n^2 - 44n.$$

□

Theorem 6.2. *With $n \geqslant 2$, the second Zagreb index for Rectangular Bilayer Germanium Phosphide is:*

$$M_2(Rct2LGeP_3^n) = 216n^2 - 160n + 24.$$

Proof. By using (1.2) and taking $\alpha = 1$

$$\begin{aligned} M_2(Rct2LGeP_3^n) = (4)(2.2) + (4n-4)(2.3) + (4n+4)(2.4) + (8n-8)(2.6) + (4n-4)(3.4) \\ + (12n^2-20n+8)(3.6), \end{aligned}$$

after computing we get,

$$M_2(Rct2LGeP_3^n) = 216n^2 - 160n + 24.$$

□

Theorem 6.3. *With $n \geqslant 2$, the General Randic index for Rectangular Bilayer Germanium Phosphide is:*

$$R_\alpha(Rct2LGeP_3^n) = \begin{cases} 216n^2 - 160n + 24, & \alpha = 1, \\ \frac{4}{\sqrt{2}}n^2 + (\frac{4}{\sqrt{6}} + \frac{6}{\sqrt{3}} - \frac{20}{3\sqrt{2}} + \sqrt{2})n + (2 - \frac{4}{\sqrt{6}} + \sqrt{2} - \frac{6}{\sqrt{3}} + \frac{8}{3\sqrt{2}}), & \alpha = -1/2, \\ (36\sqrt{2})n^2 + (4\sqrt{6} + 4\sqrt{8} + 24\sqrt{3} - 60\sqrt{2})n + (8 - 4\sqrt{6} + 4\sqrt{8} - 24\sqrt{3} + 24\sqrt{2}), & \alpha = 1/2, \\ \frac{2}{3}n^2 + \frac{19}{18}n + \frac{5}{18}, & \alpha = -1. \end{cases}$$

Proof. By using the definition (1.2) of Randic index

$$R_\alpha = \sum_{u \sim v} (d_u.d_v)^\alpha,$$

and degree based partition in Subsection 6.1 given previously we get the desired results. □

Corollary 6.4. *For $\alpha = 1$ and $\alpha = -1$, the general randic index is also called Second Zagreb index and Second Modified Zagreb index, respectively.*

Theorem 6.5. *With $n \geqslant 2$, the atomic bond Connectivity index for Rectangular Bilayer Germanium Phosphide is:*

$$ABC(Rct2LGeP_3^n) = 2\sqrt{14}n^2 + (\frac{16}{\sqrt{2}} + \frac{2\sqrt{15}}{3} - \frac{10\sqrt{14}}{3})n + (\frac{4\sqrt{14}}{3} - \frac{4}{\sqrt{2}} - \frac{2\sqrt{15}}{3}).$$

Proof. By using the definition (1.3) of ABC index and degree based partition in Subsection 6.1 given previously we get the desired results. □

Theorem 6.6. *With $n \geqslant 2$, the Geometric Arithmetic index for Rectangular Bilayer Germanium Phosphide is:*

$$GA(Rct2LGeP_3^n) = (8\sqrt{2})n^2 + (\frac{8\sqrt{6}}{5} + \frac{8\sqrt{2}}{3} + 4\sqrt{3} + \frac{16\sqrt{3}}{7} - 40\frac{\sqrt{2}}{3})n + (4 - \frac{8\sqrt{6}}{5} + 8\sqrt{2} - \frac{44\sqrt{3}}{7}).$$

Proof. By using the definition (1.4) of GA index and degree based partition in Subsection 6.1 given previously we get the desired results. □

Theorem 6.7. *With $n \geqslant 2$, the Sum Connectivity index for Rectangular Bilayer Germanium Phosphide is:*

$$SCI(Rct2LGeP_3^n) = 4n^2 + (\frac{4}{\sqrt{5}} + \frac{4}{\sqrt{6}} + \frac{4}{\sqrt{7}} - \frac{20}{3} + \sqrt{8})n + (\frac{14}{3} - \frac{4}{\sqrt{5}} + \frac{4}{\sqrt{6}} - \sqrt{8} - \frac{4}{\sqrt{7}}).$$

Proof. By using the definition (1.6) of SCI index and degree based partition in Subsection 6.1 given previously we get the desired results. □

Theorem 6.8. *With $n \geqslant 2$, the Harmonic index for Rectangular Bilayer Germanium Phosphide is:*

$$H(Rct2LGeP_3^n) = \frac{8}{3}n^2 + \frac{514}{315}n + \frac{116}{315}.$$

Proof. By using the definition (1.5) of Harmonic index and degree based partition in Subsection 6.1 given previously we get the desired results. □

6.3. neighborhood Partition

Now here by using the definition (1.7) of S_u we give an other different edge partition to the edge set of Rectangular bilayer Germanium Phosphide on the basis of *sum degree* of neighborhood vertices of all the edges. We concluded that for $n \geqslant 3$ the neighborhood based edge partition for the edge set of $Rct2LGeP_3^n$

have 12 sub-partite sets defined as follows:

$$\xi_1 = \{u \sim v \mid S_u = 5 \wedge S_v = 6\}, \qquad \xi_2 = \{u \sim v \mid S_u = 5 \wedge S_v = 10\},$$
$$\xi_3 = \{u \sim v \mid S_u = 6 \wedge S_v = 10\}, \qquad \xi_4 = \{u \sim v \mid S_u = 6 \wedge S_v = 9\},$$
$$\xi_5 = \{u \sim v \mid S_u = 10 \wedge S_v = 9\}, \qquad \xi_6 = \{u \sim v \mid S_u = 10 \wedge S_v = 10\},$$
$$\xi_7 = \{u \sim v \mid S_u = 10 \wedge S_v = 16\}, \qquad \xi_8 = \{u \sim v \mid S_u = 12 \wedge S_v = 16\},$$
$$\xi_9 = \{u \sim v \mid S_u = 9 \wedge S_v = 16\}, \qquad \xi_{10} = \{u \sim v \mid S_u = 16 \wedge S_v = 16\},$$
$$\xi_{11} = \{u \sim v \mid S_u = 16 \wedge S_v = 18\}, \qquad \xi_{12} = \{u \sim v \mid S_u = 18 \wedge S_v = 18\},$$

with cardinalities as $|\xi_1| = |\xi_2| = |\xi_4| = |\xi_9| = 4$ and $|\xi_3| = |\xi_6| = |\xi_8| = 4n-8$, $|\xi_{10}| = 4n$, $|\xi_7| = 10n-10$, $|\xi_5| = 8$, $|\xi_{11}| = 14n-22$, $|\xi_{12}| = 12n^2-40n+32$.

Forth version of ABC and fifth version of GA indices will be computed by using these set cardinalities.

Theorem 6.9. *With $n \geqslant 3$, the ABC_4 for Rectangular Bilayer Germanium Phosphide is:*

$$\begin{aligned}ABC_4(Rct2LGeP_3^n) = {} & (\frac{2\sqrt{34}}{3})n^2 + (\frac{2\sqrt{210}}{15} + \frac{6\sqrt{2}}{5} + \frac{\sqrt{78}}{6} + \frac{\sqrt{30}}{4} + \frac{14}{3} - \frac{20\sqrt{34}}{9} + \sqrt{15})n + (\frac{2\sqrt{30}}{5} + \frac{2\sqrt{26}}{5} \\ & - \frac{4\sqrt{210}}{15} + \frac{2\sqrt{78}}{9} + \frac{4\sqrt{170}}{15} - \frac{12\sqrt{2}}{5} - \frac{\sqrt{78}}{3} + \frac{\sqrt{23}}{3} - \frac{22}{3} + \frac{16\sqrt{34}}{9} - \sqrt{15}).\end{aligned}$$

Proof. By using the definition (1.9) of ABC_4 index and partition sets in Subsection 6.3 given previously we get the desired results. □

Theorem 6.10. *With $n \geqslant 3$, the GA_5 for Rectangular Bilayer Germanium Phosphide is:*

$$\begin{aligned}GA_5(Rct2LGeP_3^n) = {} & 12n^2 + (\sqrt{15} + \frac{40\sqrt{10}}{13} + \frac{16\sqrt{3}}{7} + 24\sqrt{2} - 32)n + (\frac{8\sqrt{30}}{11} + \frac{8\sqrt{2}}{3} - 2\sqrt{15} + \frac{8\sqrt{6}}{5} + \frac{48\sqrt{10}}{19} \\ & - \frac{40\sqrt{10}}{13} - \frac{32\sqrt{3}}{7} - \frac{264\sqrt{2}}{7} + 28).\end{aligned}$$

Proof. By using the definition (1.9) of GA_5 index and partition sets in Subsection 6.3 given previously we get the desired results. □

7. Circumcoronene $2LGeP_3$

In Circumcoronene $2LGeP_3$, the structure of bilayer Germanium Phosphide is presented by the influence of cocentric circles. It has total $18n^2 - 6n$ edges for $n \geqslant 2$. Here n represents the number of hexagons counted from either the side in monolayer $1LGeP_3$ structure.

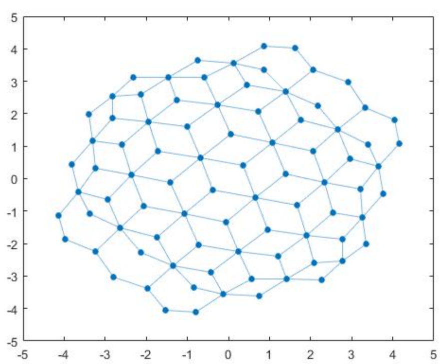

Figure 4: $C2LGeP_3^3$ Circumcoronene Bilayer Germanium Phosphide for $n = 3$.

7.1. Partioning for the edge set of Rectangular $2LGeP_3$ graph

By using the definition of *degree* of a vertex in molecular graph, we give a partition to the edge set of Rectangular structure for bilayer Germanium Phosphide after computing degrees of vertices for all the edges. We concluded that for $n \geqslant 2$ the edge set of this structural shape have 8 sub partite edge sets defined as follows:
$E_1 = \{u \sim v \mid d_u = 2 \wedge d_v = 2\}$
$E_2 = \{u \sim v \mid d_u = 2 \wedge d_v = 3\}$
$E_3 = \{u \sim v \mid d_u = 2 \wedge d_v = 4\}$
$E_4 = \{u \sim v \mid d_u = 2 \wedge d_v = 5\}$
$E_5 = \{u \sim v \mid d_u = 2 \wedge d_v = 6\}$
$E_6 = \{u \sim v \mid d_u = 3 \wedge d_v = 4\}$
$E_7 = \{u \sim v \mid d_u = 3 \wedge d_v = 5\}$
$E_8 = \{u \sim v \mid d_u = 3 \wedge d_v = 6\}$
with cardinalities as $|E_2| = |E_5| = 4n-4$, $|E_1| = 4 = |E_3| = |E_6|$, $|E_4| = 8n-4$, $|E_7| = 12n-16$, $|E_8| = 18n^2-34n+16 \;\forall\; n \geqslant 2$.

7.2. Computational results for Circumcoronene $2LGeP_3$

Now we will compute some degree based topological parameters for Circumcoronene Bilayer Germanium Phosphide. For the convenience, we will represent this structure shortly by $C2LGeP_3^n$.

Theorem 7.1. *With $n \geqslant 2$, the first Zagreb index for Circumcoronene Bilayer Germanium Phosphide is:*

$$M_1(C2LGeP_3^n) = 162n^2 - 102n + 4.$$

Proof. By using (1.1)

$$\begin{aligned} M_1(C2LGeP_3^n) &= (4)(2+2) + (4n-4)(2+3) + (4)(2+4) + (8n-4)(2+5) + (4n-4)(2+6) \\ &\quad + (4)(3+4) + (12n-16)(8) + (18n^2-34n+16)(3+6), \end{aligned}$$

after computing we get,

$$M_1(C2LGeP_3^n) = 162n^2 - 102n + 4.$$

□

Theorem 7.2. *With $n \geqslant 2$, the second Zagreb index for Circumcoronene Bilayer Germanium Phosphide is:*

$$M_2(C2LGeP_3^n) = 324n^2 - 280n + 32.$$

Proof. By using (1.2) and taking $\alpha = 1$

$$\begin{aligned} M_2(C2LGeP_3^n) &= (4)(2.2) + (4n-4)(2.3) + (4)(2.4) + (8n-4)(2.5) \\ &\quad + (4n-4)(2.6) + (4)(3.4) + (12n-16)(3.5) + (18n^2-34n+16)(3.6), \end{aligned}$$

after computing we get,

$$M_2(C2LGeP_3^n) = 324n^2 - 280n + 32.$$

□

Theorem 7.3. *With $n \geqslant 2$, the General Randic index for Circumcoronene Bilayer Germanium Phosphide is:*

$$R_\alpha(C2LGeP_3^n) = \begin{cases} 324n^2 - 280n + 32, & \alpha = 1, \\ \sqrt{18}n^2 + (\frac{4}{\sqrt{6}} + \frac{8}{\sqrt{10}} + \frac{4}{\sqrt{12}} + \frac{12}{\sqrt{15}} - \frac{34}{\sqrt{18}})n + (2 - \frac{4}{\sqrt{6}} + \frac{4}{\sqrt{8}} - \frac{4}{\sqrt{10}} - \frac{16}{\sqrt{15}} + \frac{16}{\sqrt{18}}), & \alpha = -1/2, \\ (18\sqrt{18})n^2 + (4\sqrt{6} + 8\sqrt{10} + 4\sqrt{12} & \\ +12\sqrt{15} - 34\sqrt{18})n + (8 - 4\sqrt{6} + 4\sqrt{8} - 4\sqrt{10} - 16\sqrt{15} + 16\sqrt{18}), & \alpha = 1/2, \\ 4n^2 + \frac{4864}{315}n + \frac{13}{45}, & \alpha = -1. \end{cases}$$

Proof. By using the definition (1.2) of Randic index,

$$R_\alpha = \sum_{u\sim v}(d_u.d_v)^\alpha,$$

and degree based partition in Subsection 7.1 given previously we get the desired results. □

Corollary 7.4. *For $\alpha = 1$ and $\alpha = -1$, the general randic index is also called Second Zagreb index and Second Modified Zagreb index, respectively.*

Theorem 7.5. *With $n \geqslant 2$, the atomic bond Connectivity index for Circumcoronene Bilayer Germanium Phosphide is:*

$$ABC(C2LGeP_3^n) = 3\sqrt{14}n^2 + (\frac{16}{\sqrt{2}} + \frac{12\sqrt{10}}{5} - \frac{17\sqrt{14}}{3})n + (\frac{2\sqrt{15}}{3} - \frac{4}{\sqrt{12}} - \frac{16\sqrt{10}}{5} + \frac{8\sqrt{14}}{3}).$$

Proof. By using the definition (1.3) of ABC index and degree based partition in Subsection 7.1 given previously we get the desired results. □

Theorem 7.6. *With $n \geqslant 2$, the Geometric Arithmetic index for Circumcoronene Bilayer Germanium Phosphide is:*

$$\begin{aligned} GA(C2LGeP_3^n) = (12\sqrt{2})n^2 + (\frac{8\sqrt{6}}{5} + \frac{16\sqrt{10}}{7} + 2\sqrt{3} - \frac{68\sqrt{2}}{3} + 3\sqrt{15})n \\ + (4 - \frac{8\sqrt{6}}{5} + - \frac{8\sqrt{10}}{7} - 4\sqrt{15} + \frac{2\sqrt{3}}{7} + \frac{40\sqrt{2}}{3}). \end{aligned}$$

Proof. By using the definition (1.4) of GA index and degree based partition in Subsection 7.1 given previously we get the desired results. □

Theorem 7.7. *With $n \geqslant 2$, the Sum Connectivity index for Circumcoronene Bilayer Germanium Phosphide is:*

$$SCI(C2LGeP_3^n) = 6n^2 + (\frac{4}{\sqrt{5}} + \frac{8}{\sqrt{7}} - \frac{34}{3} + 4\sqrt{2})n + (\frac{22}{3} - \frac{4}{\sqrt{5}} + \frac{4}{\sqrt{6}} - \frac{20}{\sqrt{8}}).$$

Proof. By using the definition (1.6) of SCI index and degree based partition in Subsection 7.1 given previously we get the desired results. □

Theorem 7.8. *With $n \geqslant 2$, the Harmonic index for Circumcoronene Bilayer Germanium Phosphide is:*

$$H(C2LGeP_3^n) = 4n^2 + \frac{4864}{315}n + \frac{13}{45}.$$

Proof. By using the definition (1.5) of Harmonic index and degree based partition in Subsection 7.1 given previously we get the desired results. □

7.3. neighborhood partition

Now here by using the definition (1.7) of S_u we give an other different edge partition to the edge set of Circumcoronene Bilayer Germanium Phosphide after computing *sum degree* of neighborhood vertices for all the edges. We concluded that for $n \geqslant 3$ the neighborhood based edge partition for the edge set of $C2LGeP_3^n$ have 22 sub-partite sets defined as follows:

$$\begin{aligned} &\xi_1 = \{u \sim v \mid S_u = 5 \wedge S_v = 7\}, && \xi_2 = \{u \sim v \mid S_u = 5 \wedge S_v = 10\}, \\ &\xi_3 = \{u \sim v \mid S_u = 6 \wedge S_v = 10\}, && \xi_4 = \{u \sim v \mid S_u = 9 \wedge S_v = 10\}, \\ &\xi_5 = \{u \sim v \mid S_u = 7 \wedge S_v = 12\}, && \xi_6 = \{u \sim v \mid S_u = 11 \wedge S_v = 12\}, \\ &\xi_7 = \{u \sim v \mid S_u = 10 \wedge S_v = 12\}, && \xi_8 = \{u \sim v \mid S_u = 10 \wedge S_v = 13\}, \end{aligned}$$

$$\xi_9 = \{u \sim v \mid S_u = 9 \wedge S_v = 13\}, \qquad \xi_{10} = \{u \sim v \mid S_u = 11 \wedge S_v = 16\},$$
$$\xi_{11} = \{u \sim v \mid S_u = 12 \wedge S_v = 16\}, \qquad \xi_{12} = \{u \sim v \mid S_u = 10 \wedge S_v = 15\},$$
$$\xi_{13} = \{u \sim v \mid S_u = 12 \wedge S_v = 17\}, \qquad \xi_{14} = \{u \sim v \mid S_u = 13 \wedge S_v = 16\},$$
$$\xi_{15} = \{u \sim v \mid S_u = 13 \wedge S_v = 17\}, \qquad \xi_{16} = \{u \sim v \mid S_u = 13 \wedge S_v = 15\},$$
$$\xi_{17} = \{u \sim v \mid S_u = 15 \wedge S_v = 18\}, \qquad \xi_{18} = \{u \sim v \mid S_u = 17 \wedge S_v = 18\},$$
$$\xi_{19} = \{u \sim v \mid S_u = 18 \wedge S_v = 18\}, \qquad \xi_{20} = \{u \sim v \mid S_u = 16 \wedge S_v = 17\},$$
$$\xi_{21} = \{u \sim v \mid S_u = 10 \wedge S_v = 16\}, \qquad \xi_{22} = \{u \sim v \mid S_u = 16 \wedge S_v = 18\},$$

with cardinalities as $|\xi_1| = |\xi_2| = |\xi_4| = |\xi_5| = |\xi_6| = |\xi_7| = |\xi_9| = |\xi_{10}| = |\xi_{12}| = |\xi_{13}| = |\xi_{16}| = |\xi_{17}| = |\xi_{20}| = 4$ and $|\xi_3| = |\xi_{15}| = 4n-8$, $|\xi_8| = |\xi_{14}| = 8n-20$, $|\xi_{11}| = 4n-4$, $|\xi_{18}| = 8n-12$, $|\xi_{21}| = 2n-2$, $|\xi_{22}| = 10n-18$, $|\xi_{19}| = 18n^2-54n+40$.

Forth version of ABC and fifth version of GA indices will be computed by using these set cardinalities.

Theorem 7.9. *With $n \geqslant 3$, the ABC_4 for Circumcoronene Bilayer Germanium Phosphide is:*

$$\begin{aligned}
ABC_4(C2LGeP_3^n) = (\sqrt{34})n^2 &+ \Big(\frac{2\sqrt{210}}{15} + \frac{8\sqrt{21}}{\sqrt{130}} + \frac{\sqrt{78}}{6} + \frac{6\sqrt{39}}{13} + \frac{8\sqrt{7}}{\sqrt{221}} + \frac{8\sqrt{33}}{\sqrt{306}} - 3\sqrt{34} + \frac{\sqrt{15}}{5} + \frac{10}{3}\Big)n \\
&+ \Big(\frac{4\sqrt{14}}{7} + \frac{2\sqrt{26}}{5} - \frac{4\sqrt{210}}{15} + \frac{2\sqrt{170}}{15} + \frac{2\sqrt{357}}{21} - \frac{2\sqrt{77}}{11} + \frac{4}{\sqrt{6}} - \frac{20\sqrt{21}}{\sqrt{130}} - \frac{8\sqrt{65}}{39} + \frac{5}{\sqrt{11}} \\
&- \frac{\sqrt{78}}{6} + \frac{2\sqrt{138}}{15} + \frac{6}{\sqrt{17}} - \frac{15\sqrt{39}}{13} - \frac{16\sqrt{7}}{221} \\
&+ \frac{4\sqrt{30}}{15} + \frac{2\sqrt{930}}{45} - \frac{12\sqrt{33}}{\sqrt{306}} + \frac{20\sqrt{34}}{9} + \frac{\sqrt{527}}{17} - \frac{\sqrt{15}}{5} - 6\Big).
\end{aligned}$$

Proof. By using the definition (1.8) of ABC_4 index and partition sets in Subsection 7.3 given previously we get the desired results. □

Theorem 7.10. *With $n \geqslant 3$, the GA_5 for Circumcoronene Bilayer Germanium Phosphide is:*

$$\begin{aligned}
GA_5(C2LGeP_3^n) = 18n^2 &+ \Big(\sqrt{15} + \frac{16\sqrt{130}}{23} + \frac{16\sqrt{3}}{7} + \frac{64\sqrt{13}}{29} + \frac{4\sqrt{221}}{15} + \frac{48\sqrt{34}}{35} + \frac{8\sqrt{10}}{13} + \frac{120\sqrt{2}}{7} - 54\Big)n \\
&+ \Big(\frac{2\sqrt{35}}{3} + \frac{8\sqrt{2}}{3} + \frac{24\sqrt{10}}{19} + \frac{16\sqrt{21}}{9} + \frac{16\sqrt{33}}{23} + \frac{8\sqrt{30}}{11} - \frac{40\sqrt{130}}{23} + \frac{12\sqrt{13}}{11} + \frac{32\sqrt{11}}{27} \\
&- \frac{16\sqrt{3}}{7} + \frac{8\sqrt{6}}{5} + \frac{16\sqrt{51}}{29} - \frac{160\sqrt{13}}{29} - \frac{8\sqrt{221}}{15} + \frac{2\sqrt{195}}{7} \\
&+ \frac{8\sqrt{30}}{11} - \frac{72\sqrt{34}}{35} + \frac{32\sqrt{17}}{33} - \frac{2\sqrt{15}}{4} - \frac{8\sqrt{10}}{13} - \frac{216\sqrt{2}}{7} + 40\Big).
\end{aligned}$$

Proof. By using the definition (1.9) of GA_5 index and partition sets in Subsection 7.3 given previously we get the desired results. □

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