

Penta Beryllium Phosphate: A novel two dimensional network with its topological aspects

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Abstract

It is an important subject to design new materials to attain new applications with distinctive topological properties such as minimum dimension, high piability and thermal stability. In this work, we have created a novel two dimensional (2D) network derived from the natural structure of Penta Beryllium Phosphate (PBP). It is a 2D semi-conductor material with strain tunable energy, visible light sensitivity and propitious applications in optical devices. Here we will represent it's topology with two different dimensions and will explain its topological aspects via different topological invariants including zagreb invariant, Randic invariants, Geometric and connectivity invariant.

Keywords: Penta Beryllium Phosphate; Mathematical Chemistry; Chemical Graph Theory; Topological Invariants; Topological and structural properties; Optical Properties.

Mathematics Subject Classification: 05C09 : 05C92

1. Introduction

In bio science and control system engineering, Quantitative Structural Activity relationship (QSAR) are used to model chemical structures and properties. Predicting the boiling point of a material was the first application of QSAR models. To approach this prediction a numerical quantity is used which is a direct relation between a structure and its property. To transform a structure with in a numerical quantity, a structure is visualized as a graph from the classical definition of discrete mathematics. In discrete mathematics, a graph is a pictorial display of some dots (vertices) connected by some line segments (edges). Drawing a chemical structure as a graph, with presenting its atoms as vertices and bonds as edges, termed as *chemical graph* [3].

Applying classical concepts and definitions from graph theory to field of mathematical chemistry leads to new branch of discrete mathematics termed as *chemical graph theory*. This theory apply mathematical models to understand chemical phenomenon. A theoratical representation of a chemical compound, network or structure as a graph does not change its physical or chemical properties inspite of that it gives deep insight to a chemical phenomenon. To develop a co-relation between a chemical structure and its graphical presentation an invariant mathematical tool is used which is termed as Topological Invariant

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(TI). It has invariant property under the graph transformation of a structure and free from the graph isomorphism that's why it is very helpful to understand topological, physical and chemical properties. Graph theorists invented many different kind of topological invariants based on different results which explains topological properties of different structures and networks [13] [14].

With the passage of time, the theory of graphs growing rapidly in different fields of sciences with respect to theory and applications. Its applications includes computer networking in field of network topologies, mathematical chemistry for modelling chemical structures, social sciences, biological sciences and linguistics is one of the latest application of graph theory [6] [23]. Specifically in field of mathematical chemistry, it has vast applications via TI's. It is very helpful to analyse physical properties for the structure by these invariants. These invariants are highly used in field of chemical graph theory for analysing and modelling of a chemical compound and very much praised in field of chemistry by chemists.

Below we will cite some similar work done in the past. An embedded form of benzene ring in p-type surface is topologically discussed in [1]. Recently a swapped network for interconnection system was explained by Ali et al. [2]. Some topological aspects for bi-layer germanium phosphide network are discussed in [7]. Dominating analysis and comparison for cellular neural network is discussed in [8]. New kind of these parameters based on valency of an atom in a structure for star network is discussed in [15]. Some Zagreb and co-index polynomials for kth level generalized graphs are studied by Maji and Ghorai in [17]. A novel graph invariant named as third leap Zagreb for some operations of graphs defined by Maji in [18]. Some physicochemical properties for dominating silicate network have been done by Simonraj and George [24]. Many counts of research articles can be found with similar work done which includes different indices and properties such as electronic configuration, electron negativity, enthalpy and stability of different structures and nano tubes [11] [19] [20] [26].

From several decades nano science and nano technology have attracted many attentions. Many nano materials including two dimensional structures i.e. crystalline materials made up of single layer atoms plays an important role in new technologies like semi-conductor devices, photo voltaic devices and water purification system. That's why investigating new materials with minimum dimension is always attractive. Graphene was the first 2D single layer material introduced in 2004. After that many 2D materials were developed and predicted through different properties. Two dimensional materials are basically made up of two elements, which may be elemental or compound (consisting more than two elements) [17].

In recent years, many two dimension materials with mono-layer and bi-layer structures are developed having graphyne, germanene, silicene and antimonene. It has been noticed that different configurations of materials provides the results in different properties. This technique helps in to investigate new materials with new properties. Here, in this article a novel two dimensional monolayer network with pentagonal structure named as Penta Beryllium Phosphate (PBP) is presented theoretically. It is compound semi-conductor material comprised of Beryllium (Be) and Phosphorus (P) elements. Experiments shows that this material is dynamically energetic and thermal stable. This property made it very helpful in low range electromagnetic spectrum also in ultra violet range electromagnetic spectrum.[4]

2. Preliminaries

A numerical parameter/invariant computed from graphical presentation of a structure is a map " Γ " from " $\mathcal{Y}$ " to set of real number " $\mathcal{R}$ ", for that relative structure. Here " $\mathcal{Y}$ " is the family of finite simple graphs under the mapping of a family of different topological invariants. Many of the TI's are defined by using the above mapping by counting the edges joined to a vertex whereas few are defined by finding distance between any two vertices. Harry Wiener firstly defined the distance based *wiener index* in 1947 which one is the oldest one in all of these. Later on many others parameters come in to study by different graph theorist which are studied to till date. General family of Zagreb indices, General Randic indices group, connectivity indices, and geometric index are some few popular indices [3].

According to theoretical concept of graphs, this numeric parameter has invariant property and is free from the topology of a graph. This topological property of the invariant attracted many researcher to take advantage from these invariants to explain different topological and geometrical aspects of structures.

This invariant property of the parameter also motivated us, so we decided to implement its mathematical analysis via topological invariants on a novel 2D network structure obtained from a naturally existing compound of Penta Beryllium Phosphate.

2.1. Topological Invariants

The number of connections to a vertex is called the *degree* of the vertex in a graph. Under the transformation for a *molecular graph*, the number of attached bonds to an atom is its valency. So under this graphical symmetry, here we will define some valency (degree) dependent invariants for a structure. For characterization of molecular branching Milan Randic [21] defined Randic invariant computed as:

$$R = \sum_{p \sim q} \frac{1}{\sqrt{\zeta_p \cdot \zeta_q}} \quad (2.1)$$

After that for improvising the Randic invariant, Bollobas [5] redefined and generalized it for any real value of α .

$$R_\alpha = \sum_{p \sim q} (\zeta_p \cdot \zeta_q)^\alpha \quad (2.2)$$

Working for π -electron energy for hydrocarbons Gutman et al. [10] proposed following zagreb invariants, termed as first zagreb and second zagreb.

$$M_1 = \sum_{p \sim q} (\zeta_p + \zeta_q) \quad (2.3)$$

$$M_2 = \sum_{p \sim q} (\zeta_p \cdot \zeta_q) \quad (2.4)$$

One can note that in generalized Randic invariant for $\alpha = 1$, we have Second Zagreb invariant where as for $\alpha = -1$ it is termed as modified second zagreb invariant.

For checking stability of alkanes and for modling the strain energy of cyclo-alkanes Estrada proposed a connectivity invariant which as termed as Atomic Bond Connectivity Invariant [9].

$$ABC = \sum_{p \sim q} \sqrt{\frac{\zeta_p + \zeta_q - 2}{\zeta_p \cdot \zeta_q}} \quad (2.5)$$

Vukicevic et al. [25] proposed another valency based invariant which have better predicting ability than general Randic invariant for some physico-chemical properties. It is computed as follows:

$$GA = \sum_{p \sim q} \frac{2\sqrt{\zeta_p \cdot \zeta_q}}{\zeta_p + \zeta_q} \quad (2.6)$$

Zhou et al. [28] proposed another connectivity invariant termed as Sum Connectivity Invariant. It is highly co-related with general Randic Invariant with a co-relation coefficient of 0.99088 for alkanes.

$$SCI = \sum_{p \sim q} (\zeta_p + \zeta_q)^{-\frac{1}{2}} \quad (2.7)$$

Harmonic Invariant [12] [27] is computed by the arithmetic mean which is as follows:

$$H = \sum_{p \sim q} \left(\frac{2}{\zeta_p + \zeta_q} \right) \quad (2.8)$$

Inverse degree invariant attracted many numerous conjectures generated by computer algorithm and computed as follows:

$$ID = \sum_{p \sim q} \frac{\varsigma_p^2 + \varsigma_q^2}{\varsigma_p^2 \varsigma_q^2} \quad (2.9)$$

Reti et. al referred neighbourhood based topological invariants for first Zagreb and second Zagreb termed as neighbourhood first Zagreb index NM_1 and neighbourhood second Zagreb index NM_2 respectively [22]. Here in above equations ς_p is the degree for a vertex p whereas $p \sim q$ represent two directly connected vertices in a graph or network.

3. Penta Beryllium Phosphate Network

In 2014 Zhang et al. proposed a 2D monolayer carbon allotrope called penta graphene. After developing graphene many different 2D material including C_2Si , CN_2 , penta- CdS_2 and penta- SiC_5 have been proposed which have semi-conductor nature. Recently, Azarmi et al. proposed a novel theoretical 2D monolayer material with pentagonal atomic structure termed as Penta Beryllium Phosphate (PBP). They found that it is energetically dynamic as well as thermally stable. Moreover, it has semi-conductor nature with minimum dimension as compared to all other materials produced so far. [16]

A unit cell 3.1 for Penta Beryllium Phosphate (PBP) includes four "x" and two "y" atoms. Each y atom make bonds with four x atoms, where as each x atom bonds with two y atoms and one y atom form atomic pentagon in the network. Its molecular graph is shown in figure 3.2 which is in 2×2 dimension. A 3×3 super cell for PBP is shown in following figure 3.3. It's structural form have two types of bonds between the atoms. The Be-P bond and P-P bond with bond length 2.16 and 2.07 respectively. Also, in a pentagon of PBP there are three different types of angles between bond and atoms, the P-P-Be has a value of 112.26, Be-p-Be has a value of 117.83 whereas P-Be-P has a value of 97.06 dgrees [4]

Here in this article we are presenting the structure of 2D PBP as a network sheet as described in 3×3 super cell. We are presenting its structure as a two dimensional network in a generalize structure of $n \times m$ dimension, here n and m represents the number of Beryllium atoms in horizontal direction and vertical direction respectively. We have categorized our generalization for two cases, first one is for $n = m$ and second one is for $n \neq m$.

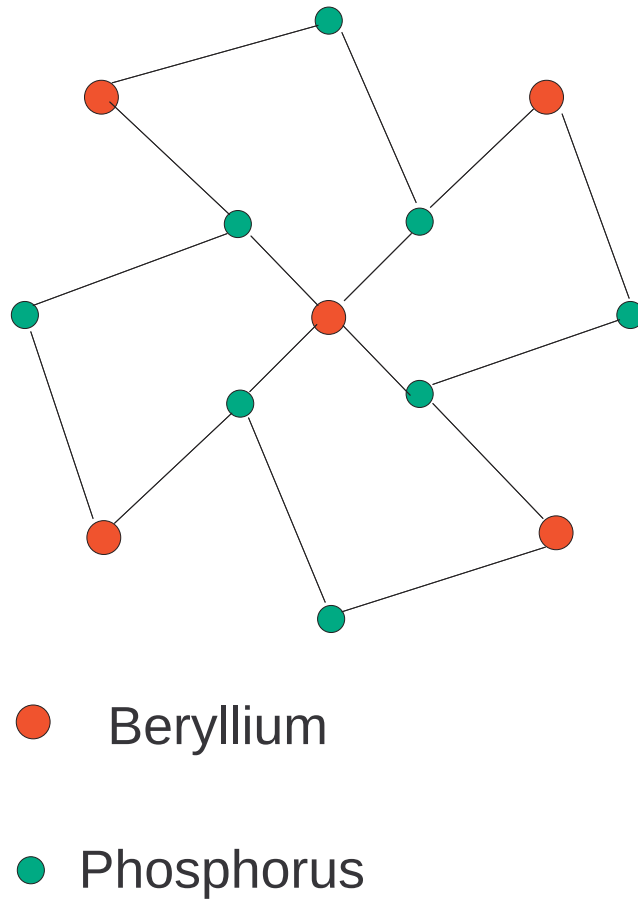


Figure 3.1: A unit cell for Penta Beryllium Phosphate

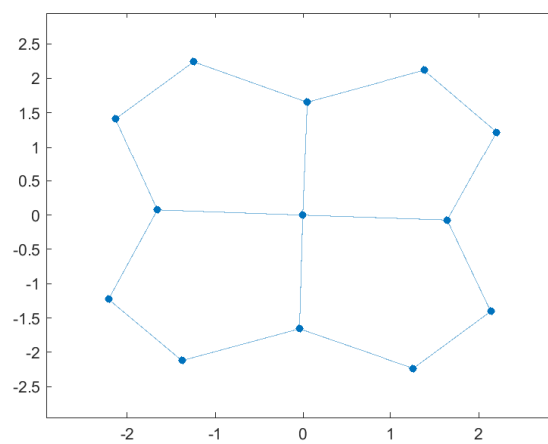


Figure 3.2: Molecular Graph Depiction for 2×2 unit cell of PBP

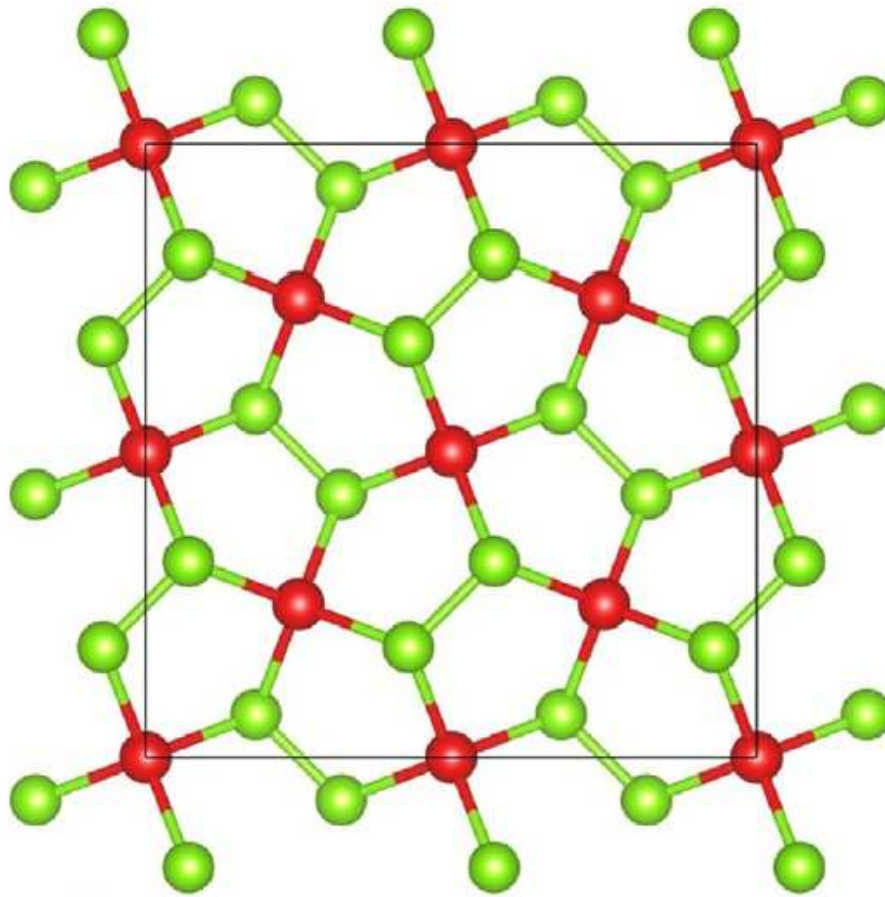


Figure 3.3: A 3×3 supercell in a 2D network sheet of Penta Beryllium Phosphate

4. Penta Beryllium Phosphate (PBP) $Be_2P_3(n \times n)$

Here in this section, we will present the 2D crystal structure of PBP for $n \times n$ dimension. In this dimension the number of Beryllium (Be) atoms in x and y direction is same. A graphical depiction of 5×5 dimensional network is shown in the figure 4.1. As described in previous section in a pentagon for PBP structure there are three atoms for Phosphorus (P) and two atoms for Beryllium (Be). So a mathematical expression for graphical representation for this structural topology is proposed as $Be_2P_3(n \times n)$.

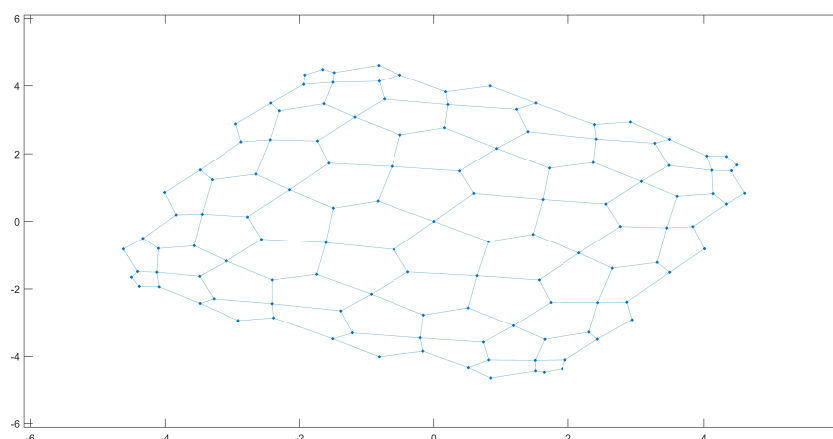


Figure 4.1: A graphical presentation 5×5 2D network sheet of Penta Beryllium Phosphate

Lemma 4.1. For all $n \geq 2$, Penta Beryllium Phosphate $Be_2P_3(n \times n)$ structure has $10n^2 - 14n + 4$ edges (bonds) and $6n^2 - 6n + 1$ vertices (atoms) in a 2D structure for $(n \times n)$ dimension.

Working from the above lemma and generalizing the $n \times n$ dimension of graphical representation for Be_2P_3 we have found there are four different types of edges (bonds) depending on the degree of the two adjacent vertices. We have subdivided the total number of edges into sub-sets of edges differing in degrees of directly connected adjacent vertices which are as follows:

$$|E_{22}| = |\{pq \in E \mid \varsigma_p = 2, \varsigma_q = 2\}| = 4$$

$$|E_{23}| = |\{pq \in E \mid \varsigma_p = 2, \varsigma_q = 3\}| = 8n - 8$$

$$|E_{33}| = |\{pq \in E \mid \varsigma_p = 3, \varsigma_q = 3\}| = 2n^2 + 2n - 12$$

$$|E_{34}| = |\{pq \in E \mid \varsigma_p = 3, \varsigma_q = 4\}| = 8n^2 - 24n + 20$$

Here

$$E_{22} \cup E_{23} \cup E_{33} \cup E_{34} = E(Be_2P_3(n \times n))$$

such that

$$|E(Be_2P_3(n \times n))| = 10n^2 - 14n + 4$$

4.1. Result for $Be_2P_3(n \times n)$

This section will cover some computational results of topological invariants for Penta Beryllium Phosphate (PBP) on $n \times n$ dimension. For our convenience we will represent this chemical graph as $Be_2P_3(n \times n)$.

Theorem 4.1. For all $n \geq 2$, the $n \times n$ dimension topology of Penta Beryllium Phosphate have topological invariants $M_1, M_2, R_{-1}, R_{\frac{1}{2}}, R_{\frac{-1}{2}}$ are as follow:

$$M_1 = 68n^2 - 116n + 44$$

$$M_2 = 114n^2 - 222n + 100$$

$$R_{-1} = \frac{8}{9}n^2 - \frac{4}{9}n$$

$$R_{\frac{1}{2}} = (6 + 16\sqrt{3})n^2 + (8\sqrt{6} - 48\sqrt{3} + 6)n + (40\sqrt{3} - 8\sqrt{6} - 28)$$

$$R_{\frac{-1}{2}} = (\frac{4}{\sqrt{3}} + \frac{2}{3})n^2 + (\frac{4\sqrt{6}}{3} - 4\sqrt{3} + \frac{2}{3})n + (\frac{10}{\sqrt{3}} - \frac{4\sqrt{6}}{3} - 2)$$

Proof. We will provide a general proof for all the topological invariants which will be applicable for further results in next sections. Let $Be_2P_3(n \times n)$ be the $n \times n$ dimensional graph for Penta Beryllium Phosphate structure and $f(\varsigma_p, \varsigma_q)$ be the two variables function with the arguments ς_p and ς_q such that the function $f(\varsigma_p, \varsigma_q)$ will belong to the following set Λ .

$$\Lambda = \{\varsigma_p + \varsigma_q, \varsigma_p \varsigma_q, (\varsigma_p \varsigma_q)^{-1}, (\varsigma_p \varsigma_q)^{\frac{1}{2}}, (\varsigma_p \varsigma_q)^{\frac{-1}{2}}\}$$

and suppose that $\tau = \{M_1, M_2, R_{\frac{1}{2}}, R_{-1}, R_{\frac{-1}{2}}\}$. Then for any $TI \in \tau$ we have,

$$TI = \sum_{p \sim q} f(\varsigma_p, \varsigma_q)$$

By using cardinality of edge sub-sets in 4.1 we have for each TI we obtained;

$$TI = 4(f(\varsigma_p, \varsigma_q)) + (8n - 8)(f(\varsigma_p, \varsigma_q)) + (2n^2 + 2n - 12)(f(\varsigma_p, \varsigma_q)) + (8n^2 - 24n + 20)(f(\varsigma_p, \varsigma_q))$$

From above equation we obtained our desired results. □

Theorem 4.2. For all $n \geq 2$, the $n \times n$ dimension topology of Penta Beryllium Phosphate have topological invariants ABC , GA , H , SCI and ID are as follow:

$$ABC = \left(\frac{4}{3}(\sqrt{15} + 1)\right)n^2 + (4\sqrt{2} - 4\sqrt{15} + \frac{4}{3})n + \left(\frac{10\sqrt{15}}{3} - 2\sqrt{2} - 8\right)$$

$$GA = \left(\frac{32\sqrt{3}}{7} + 2\right)n^2 + \left(\frac{16\sqrt{6}}{5} - \frac{96\sqrt{3}}{7} + 2\right)n + \left(\frac{80\sqrt{3}}{7} - \frac{16\sqrt{6}}{5} - 8\right)$$

$$H = \frac{62}{21}n^2 - \frac{314}{105}n + \frac{18}{35}$$

$$SCI = \left(\frac{8}{\sqrt{7}} + \frac{\sqrt{2}}{\sqrt{3}}\right)n^2 + \left(\frac{8}{\sqrt{5}} - \frac{24}{\sqrt{7}} + \frac{\sqrt{2}}{\sqrt{3}}\right)n + \left(2 - \frac{8}{\sqrt{5}} - 2\sqrt{6} + \frac{20}{\sqrt{7}}\right)$$

$$ID = \frac{11}{6}n^2 - \frac{5}{6}n - \frac{1}{12}$$

Proof. We will provide a general proof for all the topological invariants which will be applicable for further results in next sections. Let $Be_2P_3(n \times n)$ be the $n \times n$ dimensional graph for Penta Beryllium Phosphate structure and $f(\varsigma_p, \varsigma_q)$ be the two variables function with the arguments ς_p and ς_q such that the function $f(\varsigma_p, \varsigma_q)$ will belong to the following set Λ .

$$\Lambda = \left\{ \sqrt{\frac{\varsigma_p + \varsigma_q - 2}{\varsigma_p \cdot \varsigma_q}}, \frac{2\sqrt{\varsigma_p \cdot \varsigma_q}}{\varsigma_p + \varsigma_q}, (\varsigma_p + \varsigma_q)^{\frac{-1}{2}}, \frac{2}{\varsigma_p + \varsigma_q}, \frac{\varsigma_p^2 + \varsigma_q^2}{\varsigma_p^2 \varsigma_q^2} \right\}$$

and suppose that $\tau = \{ABC, GA, SCI, H, ID\}$. Then for any $TI \in \tau$ we have,

$$TI = \sum_{p \sim q} f(\varsigma_p, \varsigma_q)$$

By using cardinality of edge sub-sets in 4.1 we have for each TI we obtained;

$$TI = 4(f(\varsigma_p, \varsigma_q)) + (8n - 8)(f(\varsigma_p, \varsigma_q)) + (2n^2 + 2n - 12)(f(\varsigma_p, \varsigma_q)) + (8n^2 - 24n + 20)(f(\varsigma_p, \varsigma_q))$$

From above equation we obtained our desired results. □

5. Penta Beryllium Phosphate (PBP) $Be_2P_3(n \times m)$

Here in this section we will present the 2D crystal structure of PBP for $n \times m$ dimension. In this dimension the number of beryllium atoms in x direction (horizontal) and y direction (vertical) are not equal and is presented by n and m respectively. This two dimensional topology for Be_2P_3 network has symmetric property over the dimension for $n \times m$ and $m \times n$. A graphical depiction of super cell for 6×4 dimension is shown in the figure 5.1. As described in previous section in a pentagon for PBP structure there are three atoms for Phosphorus (P) and two atoms for Beryllium (Be). So a mathematical expression for graphical representation for this structural topology is proposed as $Be_2P_3(n \times m)$.

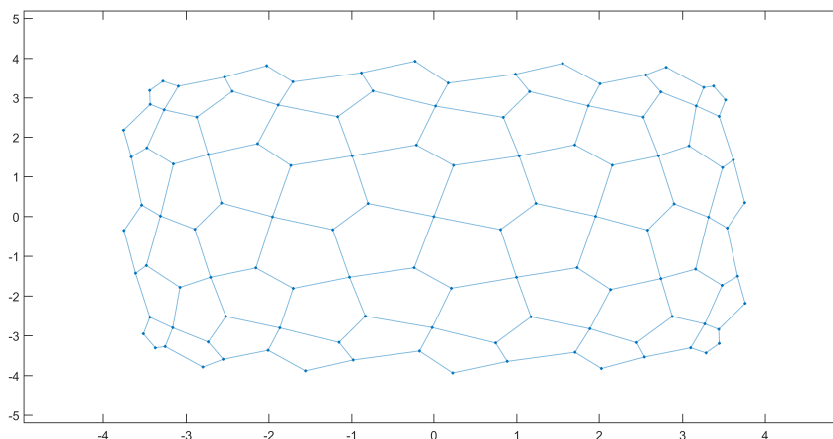


Figure 5.1: A graphical presentation of 4×6 2D network sheet of Penta Beryllium Phosphate

Lemma 5.1. For all $m, n \geq 2$, Penta Beryllium Phosphate $Be_2P_3(m \times n)$ structure has $10mn - 7(m + n) + 4$ edges (bonds) and $6mn - 3(m + n) + 1$ vertices (atoms) in a 2D structure for $(n \times m)$ dimension.

Working from the above lemma and generalizing the $n \times m$ dimension of graphical representation for Be_2P_3 we have found there are four different types of edges (bonds) depending on the degree of the two adjacent vertices. We will subdivide the total number of edges into sub-sets of edges differing in degrees of directly connected adjacent vertices which are as follows:

$$\begin{aligned} |E_{22}| &= |\{pq \in E \mid \varsigma_p = 2, \varsigma_q = 2\}| = 4 \\ |E_{23}| &= |\{pq \in E \mid \varsigma_p = 2, \varsigma_q = 3\}| = 4(m + n) - 8 \\ |E_{33}| &= |\{pq \in E \mid \varsigma_p = 3, \varsigma_q = 3\}| = 2mn + (m + n) - 12 \\ |E_{34}| &= |\{pq \in E \mid \varsigma_p = 3, \varsigma_q = 4\}| = 8mn - 12(m + n) + 20 \end{aligned}$$

Here

$$E_{22} \cup E_{23} \cup E_{33} \cup E_{34} = E(Be_2P_3(n \times m))$$

such that

$$|E(Be_2P_3(n \times m))| = 10mn - 7(m + n) + 4$$

5.1. Result for $Be_2P_3(n \times m)$

This section will cover some computational results of topological invariants for Penta Beryllium Phosphate (PBP) on $n \times m$ dimension. For our convenience we will represent this chemical graph as $Be_2P_3(n \times m)$.

Theorem 5.1. For all $m, n \geq 2$, the $n \times m$ dimension topology of Penta Beryllium Phosphate have topological invariants M_1 , M_2 , $R_{\frac{1}{2}}$, R_{-1} , $R_{-\frac{1}{2}}$ are as follow:

$$\begin{aligned} M_1 &= 68mn - 58(m + n) + 44 \\ M_2 &= 114mn - 111(m + n) + 100 \\ R_{-1} &= \frac{8}{9}mn - \frac{2}{9}(m + n) \\ R_{\frac{1}{2}} &= (6 + 16\sqrt{3})mn + (4\sqrt{6} - 24\sqrt{3} + 3)n + (40\sqrt{3} - 8\sqrt{6} - 28) \\ R_{-\frac{1}{2}} &= \left(\frac{4}{\sqrt{3}} + \frac{2}{3}\right)mn + \left(\frac{1}{3}(2\sqrt{6} - 2\sqrt{3} + 1)\right)(m + n) + \left(\frac{10}{\sqrt{3}} - \frac{4\sqrt{6}}{3} - 2\right) \end{aligned}$$

Proof. We will provide a general proof for all the topological invariants which will be applicable for further results in next sections. Let $Be_2P_3(n \times n)$ be the $n \times n$ dimensional graph for Penta Beryllium Phosphate structure and $f(\zeta_p, \zeta_q)$ be the two variables function with the arguments ζ_p and ζ_q such that the function $f(\zeta_p, \zeta_q)$ will belong to the following set Λ .

$$\Lambda = \{\zeta_p + \zeta_q, \zeta_p \zeta_q, (\zeta_p \zeta_q)^{-1}, (\zeta_p \zeta_q)^{\frac{1}{2}}, (\zeta_p \zeta_q)^{-\frac{1}{2}}\}$$

and suppose that $\tau = \{M_1, M_2, R_{\frac{1}{2}}, R_{-\frac{1}{2}}, R_{-\frac{1}{2}}\}$. Then for any $TI \in \tau$ we have,

$$T = \sum_{p \sim q} f(\zeta_p, \zeta_q)$$

By using cardinality of edge sub-sets in section we have for each TI we obtained;

$$TI = 4(f(\zeta_p, \zeta_q)) + (4(m+n) - 8)(f(\zeta_p, \zeta_q)) + (2mn + (m+n) - 12)(f(\zeta_p, \zeta_q)) \\ + (8mn - 12(m+n) + 20)(f(\zeta_p, \zeta_q))$$

From above equation we obtained our desired results. □

Theorem 5.2. For all $m, n \geq 2$, the $n \times m$ dimension topology of Penta Beryllium Phosphate have topological invariants ABC , GA , SCI , H and ID are as follow:

$$ABC = (\frac{4}{3}(\sqrt{15} + 1))mn + (2\sqrt{2} - 2\sqrt{15} + \frac{2}{3})(m+n) + (\frac{10\sqrt{15}}{3} - 2\sqrt{2} - 8) \\ GA = (\frac{32\sqrt{3}}{7} + 2)mn + (\frac{8\sqrt{6}}{5} - \frac{48\sqrt{3}}{7} + 1)(m+n) + (\frac{80\sqrt{3}}{7} - \frac{16\sqrt{6}}{5} - 8) \\ SCI = (\frac{8}{\sqrt{7}} + \frac{\sqrt{2}}{\sqrt{3}})mn + (\frac{4}{\sqrt{5}} - \frac{12}{\sqrt{7}} + \frac{1}{\sqrt{6}})(m+n) + (2 - \frac{8}{\sqrt{5}} - 2\sqrt{6} + \frac{20}{\sqrt{7}}) \\ H = \frac{62}{21}mn - \frac{157}{105}(m+n) + \frac{18}{35} \\ ID = \frac{11}{6}mn - \frac{5}{12}(m+n) - \frac{1}{12}$$

Proof. We will provide a general proof for all the topological invariants which will be applicable for further results in next sections. Let $Be_2P_3(n \times n)$ be the $n \times n$ dimensional graph for Penta Beryllium Phosphate structure and $f(\zeta_p, \zeta_q)$ be the two variables function with the arguments ζ_p and ζ_q such that the function $f(\zeta_p, \zeta_q)$ will belong to the following set Λ .

$$\Lambda = \left\{ \sqrt{\frac{\zeta_p + \zeta_q - 2}{\zeta_p \cdot \zeta_q}}, \frac{2\sqrt{\zeta_p \cdot \zeta_q}}{\zeta_p + \zeta_q}, (\zeta_p + \zeta_q)^{-\frac{1}{2}}, \frac{2}{\zeta_p + \zeta_q}, \frac{\zeta_p^2 + \zeta_q^2}{\zeta_p^2 \zeta_q^2} \right\}$$

and suppose that $\tau = \{ABC, GA, SCI, H, ID\}$. Then for any $TI \in \tau$ we have,

$$TI = \sum_{p \sim q} f(\zeta_p, \zeta_q)$$

By using cardinality of edge sub-sets in 4.1 we have for each TI we obtained;

$$TI = 4(f(\zeta_p, \zeta_q)) + (4(m+n) - 8)(f(\zeta_p, \zeta_q)) + (2mn + (m+n) - 12)(f(\zeta_p, \zeta_q)) \\ + (8mn - 12(m+n) + 20)(f(\zeta_p, \zeta_q))$$

From above equation we obtained our desired results. □

Corollary 5.1. Results for $Be_2P_3(n \times n)$ in theorems 4.1 and 4.2 is a direct co-sequence of theorems 5.1 and 5.2 by putting $n = m$ from lemma 5.1.

6. Conclusion

In this section we will conclude our work by a comparison between topological invariants. This comparison shows the predicting ability of TI's over the PBP network. A comparison between M_1 , M_2 , R_{-1} , $R_{\frac{1}{2}}$ and $R_{-\frac{1}{2}}$ is shown in figure 6.1. Graphical result shows that second zagreb invariant (General Randic invariant for $\alpha = 1$) has the better predicting ability over the $Be_2P_3(n \times n)$ network. Whereas figure 6.2 shows a comparison between ABC , GA , H , SCI and ID and we conclude that among all these invariants Geometric Arithmetic (GA) has better predicting ability over the $Be_2P_3(n \times n)$ network. On the other hand, similar comparison is done among these invariants over the $Be_2P_3(n \times m)$ network. In figure 6.3 M_1 , M_2 , R_{-1} , $R_{\frac{1}{2}}$ and $R_{-\frac{1}{2}}$ are compared, whereas in figure 6.4 ABC , GA , H , SCI and ID are compared.

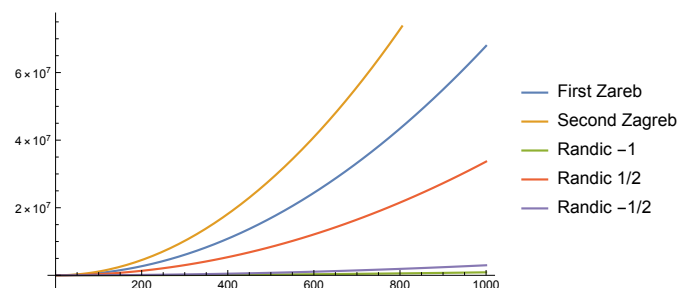


Figure 6.1: Comparison between M_1 , M_2 , R_{-1} , $R_{\frac{1}{2}}$ and $R_{-\frac{1}{2}}$ for $Be_2P_3(n \times n)$

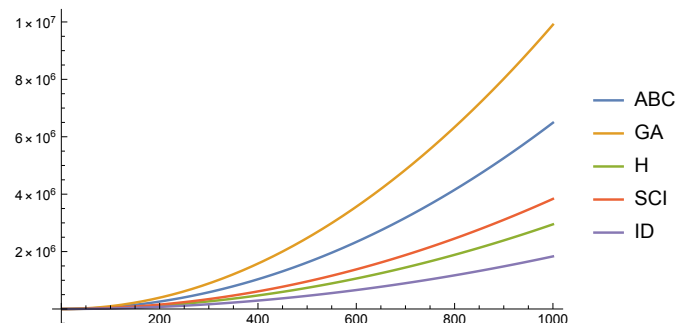


Figure 6.2: Comparison between ABC , GA , H , SCI and ID for $Be_2P_3(n \times n)$

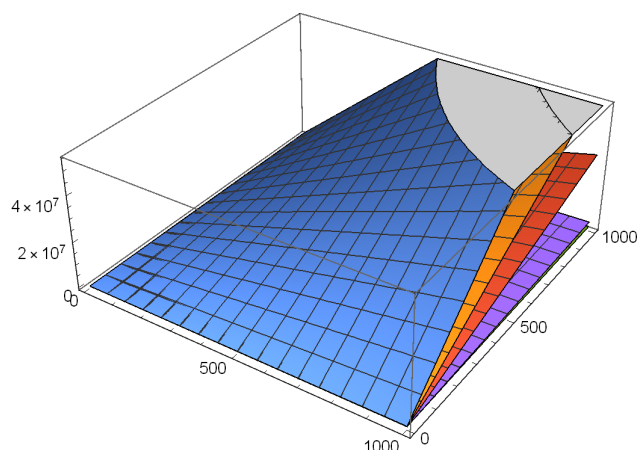


Figure 6.3: Comparison between M_1 (Orange), M_2 (Blue), R_{-1} (Green), $R_{\frac{1}{2}}$ (Red) and $R_{-\frac{1}{2}}$ (Purple) for $Be_2P_3(n \times m)$

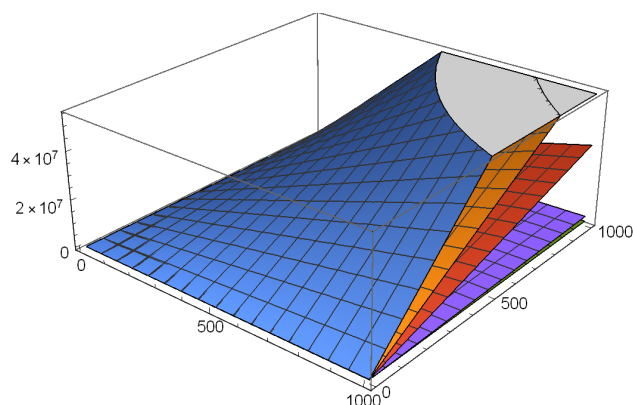


Figure 6.4: Comparison between ABC (Orange) , GA (Blue) , H (Green) , SCI (Red) and ID (Purple) for $Be_2P_3(n \times m)$

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References

- [1] A. Ahmad, "On the degree based topological indices of benzene ring embedded in P-type-surface in 2D network", Hacet. J. Math. Stat, vol. 47, no. 1, 2018.
- [2] A. Ahmad, R. Hasni, K. Elahi and M. A. Asim, "Polynomials of Degree-Based Indices for Swapped Networks Modeled by Optical Transpose Interconnection System", IEEE, Access 8, pp. 214293-214299, 2020.
- [3] H. Ali, H. M. A. Siddiqui and M. K. Shafiq, "On Degree-Based Topological Descriptors of Oxide and Silicate Molecular Structures", MAGNT Res. Rep., vol. 4, pp. 135-142, 2016.
- [4] Z. Azarmi, M. Naseri and S. Parsamehr, "Penta-BeP2 monolayer: A new 2D beryllium phosphate with a narrow band gap", Chemical Physics Letters, vol. 728, pp. 136-141, 2019.
- [5] B. Bollobás and P. Erdos, "Graphs of extremal weights", Ars combinatoria, vol. 50, pp. 225-233, 1998.
- [6] A. H. Dekker and B. D. Colbert, "Network robustness and graph topology", In Proceedings of the 27th Australasian conference on Computer science, Vol. 26, pp. 359-368, 2004.
- [7] F. Ejaz, M. Hussain and R. Hasni, "On topological aspects of bilayer Germanium Phosphide," Journal of Mathematics and Computer Science, vol. 22, no. 4, pp. 347-362, 2021.
- [8] F. Ejaz, M. Hussain, H. Almohamedh, K. M. Alhamed, R. Alabdan and S. Almotairi, "Dominating Topological Analysis and Comparison of the Cellular Neural Network", Mathematical Problems in Engineering, 2021.
- [9] E. Estrada, L. Torres, L. Rodriguez and I. Gutman, "An atom-bond connectivity index: Modelling the enthalpy of formation of alkanes", 1998.
- [10] I. Gutman and N. Trinajstić, "Graph theory and molecular orbitals. Total Φ -electron energy of alternant hydrocarbons", Chemical physics letters, vol. 17, no. 4, pp. 535-538, 1972.
- [11] S. Hayat, S. Wang and J. B. Liu, "Valency-based topological descriptors of chemical networks and their applications" Applied Mathematical Modelling, vol. 60, pp. 164-178, 2018.
- [12] A. Ilic, "Note on the harmonic index of a graph", arXiv preprint arXiv:1204.3313, 2012.
- [13] M. Imran, M. K. Siddiqui, A. Q. Baig, W. Khalid and H. Shaker, "Topological properties of Cellular Neural Networks", Journal of Intelligent and Fuzzy Systems, vol. 37, no. 3, pp. 3605-3614, 2019.
- [14] J. B. Liu, S. Wang, C. Wang and S. Hayat, "Further results on computation of topological indices of certain networks", IET Control Theory and Applications, vol. 11, no. 13, pp. 2065-2071, 2017.
- [15] A. N. A. Koam, A. Ahmad and M. F. Nadeem, "Comparative study of valency-based topological descriptor for hexagon star network", Computer Systems Science and Engineering, Vol. 36, No. 2, pp. 293-306, 2021.
- [16] Y. Li, Y. Liao and Z. Chen, "Be2C monolayer with quasi-planar hexacoordinate carbons: a global minimum structure", Angewandte Chemie, vol. 126, no. 28, pp. 7376-7380, 2014.
- [17] D. Maji and G. Ghorai, "Computing F-index, coindex and Zagreb polynomials of the kth generalized transformation graphs", Heliyon, vol. 6, no. 12, e05781, 2020.
- [18] D. Maji and G. Ghorai, "A novel graph invariant: the third leap Zagreb index under several graph operations", Discrete Mathematics, Algorithms and Applications, vol. 11, no. 05, p. 1950054, 2019.
- [19] M. Paul and I. Rajasingh, "Topological properties of silicate networks", IEEE, In 2009 5th IEEE GCC Conference and Exhibition, pp. 1-5, 2009.
- [20] B. Rajan, A. William, C. Grigorious and S. Stephen, "On certain topological indices of silicate, honeycomb and hexagonal networks", Journal of Computer and Mathematical Sciences, Vol. 3, no. 5, pp. 498-556, 2012.
- [21] M. Randic, "Characterization of molecular branching", Journal of the American Chemical Society, vol. 97, no. 23, pp. 6609-6615, 1975.
- [22] T. Reti, A. Ali, P. Varga and E. Bitay, "Some properties of the neighborhood first Zagreb index", Discrete Mathematics Letters, vol. 2, p. 10-17, 2019.
- [23] Q. A. A. Ruhimat, G. W. Fajariyanto, D. M. Firmansyah and slam, "Optimal computer network based on graph topology model", In Journal of Physics: Conference Series, vol. 1211, no. 1, p. 012007, IOP Publishing, 2019.
- [24] F. Simonraj and A. George, "Topological properties of few poly oxide, poly silicate, DOX and DSL networks", International Journal of future computer and communication, vol. 2, no. 2, pp. 90, 2013.
- [25] D. Vukicevic and B. Furtula, "Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges", Journal of mathematical chemistry, vol. 46, no. 4, pp. 1369-1376, 2009.
- [26] L. Yan, Y. Li, S. Hayat, H. M. A. Siddiqui, M. Imran, S. Ahmad and M. R. Farahani, "On degree-based and frustration related topological indices of single-walled titania nanotubes", Journal of Computational and Theoretical Nanoscience, vol. 13, no. 11, pp. 9027-9032, 2016.
- [27] L. Zhong, "The harmonic index for graphs" Applied Mathematics Letters, vol. 25, no. 3, pp. 561-566, 2012.
- [28] B. Zhou and N. Trinajstić, "On a novel connectivity index", Journal of mathematical chemistry, vol. 46, no. 4, pp. 1252-1270, 2009.