

## A Study on Topological Graphs in Certain Characterization and Other Graphs

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### Abstract:

There are a few synthetic records that have been acquainted in hypothetical science with measure the properties of sub-atomic geography, for example, distance-based topological lists, degree-based topological files and counting-related topological files. Among the degree-based topological files, the molecule bond availability (ABC) record and mathematical number juggling (GA) file are the most significant, due to their synthetic importance. Certain physicochemical properties, for example, the limit, steadiness and strain energy, of substance compounds are related by these topological lists. In this paper, we concentrate on the atomic topological properties of some unique charts. The files (ABC), (ABC4), (GA) and (GA5) of these uncommon charts are processed.

**Keywords:** atom-bond connectivity (ABC) index; geometric–arithmetic (GA) index; edge partition.

**Introduction:**

Diagram hypothesis, as applied in the investigation of sub-atomic constructions, addresses an interdisciplinary science called compound chart hypothesis or sub-atomic geography. By utilizing instruments taken from chart hypothesis, set hypothesis and measurements, we endeavor to distinguish primary elements engaged with structure–property movement connections. Atoms and displaying obscure constructions can be grouped by the topological portrayal of compound designs with wanted properties. Much exploration has been directed around here over the most recent couple of many years. The topological list is a numeric amount related with synthetic constitutions implying the connection of compound constructions with numerous physicochemical properties, substance reactivity or natural action. Topological records are planned on the grounds of the change of a sub-atomic chart into a number that portrays the geography of the sub-atomic diagram. We concentrate on the connection between the construction, properties, and movement of substance compounds in atomic displaying. Atoms and sub-atomic mixtures are frequently demonstrated by sub-atomic charts. A substance chart is a model used to portray a synthetic compound. A sub-atomic chart is a straightforward diagram whose vertices compare to the molecules and whose edges relate to the bonds. It very well may be portrayed in various ways, for example, by a drawing, a polynomial, an arrangement of numbers, a lattice or by an inferred number called a topological list. The topological record is a numeric amount related with a diagram, which portrays the geography of the chart and is invariant under a diagram automorphism. Some significant sorts of topological records of diagrams are degree-based topological lists, distance-based topological lists and counting-related topological files. The degree-based topological records, the molecule bond network (ABC) and mathematical number juggling (GA) files, are vital, with a huge job in substance chart hypothesis, especially in science. Unequivocally, a topological list  $Top(G)$  of a chart is a number with the end goal that, in case  $H$  is isomorphic to

$G$ , then, at that point,  $Top(H) = Top(G)$ . Obviously the quantity of edges and vertices of a chart are topological records [1–7]. We let  $G = (V, E)$  be a basic diagram, where  $V(G)$  signifies its vertex set and  $E(G)$  means its edge set. For any vertex  $u \in V(G)$ , we call the set  $NG(u) = \{v \in V(G) \mid uv \in E(G)\}$  the open neighborhood of  $u$ ; we signify by  $d_u$  the level of vertex  $u$  and by  $S_u = \sum_{v \in NG(u)} d(v)$  the degree amount of the neighbors of  $u$ . The quantity of vertices and number of edges of the diagram  $G$  are indicated by  $|V(G)|$  and  $|E(G)|$ , individually. A basic chart of request  $n$  in which each pair of particular vertices is contiguous is known as a total

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$G$ , then, at that point,  $Top(H)$

$= Top(G)$ . Obviously the quantity of edges and vertices of a diagram are topological lists [1–7]. We let  $G$

$= (V, E)$  be a straightforward diagram, where  $V(G)$  signifies its vertex set and

$E(G)$  indicates its edge set. For any vertex  $u \in V(G)$ , we call the set  $N_G(u)$

$= \{v \in V(G) \mid uv \in E(G)\}$  the open neighborhood of  $u$ ; we indicate by  $d_u$  the level of vertex  $u$  and by  $S_z$

$= \sum_{v \in N_G(u)} d(v)$  the degree amount of the neighbors of  $u$ . The quantity of vertices and number of edges of the chart  $G$  are denoted by  $|V(G)|$  and  $|E(G)|$ , separately.

A straightforward chart of order  $n$  in which each pair of particular vertices is adjoining is known as a total diagram and is meant by  $K_\pi$ . The documentation in this paper is taken from the books [3,8 – 10]

In this paper, we study the molecular topological properties of some special graphs: Cayley trees,  $\Gamma_m^2$ ; square lattices,  $SL_\pi$ ; a graph  $G_n$ ; and a complete bipartite graph,  $K_{m,\pi}$ . Additionally, the indices  $(ABC)$ ,  $(ABC_4)$ ,  $(GA)$  and  $(GA_5)$  of these special graphs, whose definitions are discussed in the materials and methods section, are computed.

Definition 1. [11] The oldest degree-based topological index, the Randić index, denoted by  $R_{-\frac{1}{2}}(G)$ , is defined as

$$R_{-\frac{1}{2}}(G) = \sum_{x \in E(G)} \frac{1}{\sqrt{d_x d_y}}$$

Definition 2. [12] For any real number  $a \in \mathbb{R}$ , the general Randić index,  $R_a(G)$ , is defined as

$$R_a(G) = \sum_{x \in E(G)} (d_x d_y)^a$$

Definition 3. [13]. The degree-based topological  $ABC$  index is defined as

$$ABC(G) = \sum_{a \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$$

Definition 4. [2]. The degree-based topological  $GA$  index is defined as

$$GA(G) = \sum_{x \in E(G)} \frac{2\sqrt{d_x d_y}}{d_x + d_y}$$

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Recently, several authors have introduced new versions of the  $ABC$  and  $GA$  indices, which we derive in the two definitions below.

Definition 5. [14]. The fourth version ( $ABC_4$ ) of the  $ABC$  index is defined as

$$ABC_4(G) = \sum_{x \in D \in E(G)} \sqrt{\frac{S_x + S_v - 2}{S_x S_v}}$$

Definition 6. [15]. The fifth version ( $GA_5$ ) of the  $GA$  index is defined as

$$GA_5(G) = \sum_{x \in V \in E\{G\}} \frac{2\sqrt{S_x S_v}}{S_x + S_v}$$

The idea of topological indices came from Wiener [16] when he was dealing with the limit of paraffin and was named the record way number. Afterward, the way number was renamed as the Wiener index [17]. Hayat et al. [1] concentrated on different degree-based topological indices for certain types of organizations, like silicates, hexagonal, honeycombs and oxides. Imran et al [7] concentrated on the atomic topological index in stone the insightful shut equation of the  $ABC, ABC_4, ABC_5, GA,$

$GA_4$  and  $GA_5$  records of Sierpinski organizations. M. Darafsheh [18] created various techniques to ascertain the Wiener index, Szeged index and Padmakar-Ivan index for different charts utilizing the gathering of automorphisms of  $G$ . He additionally tracked down the Wiener index of a couple of charts utilizing inductive techniques. A. Ayache and A. Alameri [19] gave some topological indices of  $m^k$ -diagrams, for example, the Wiener index, the hyper-Wiener index, the Wiener extremity, Zagreb indices, Schultz and changed Schultz records and the Wiener-type invariant. Wei Gao et al [20] acquired specific erraticism rendition topological indices of the group of cycloalkanes  $C_n(K_4)$ . As of late, there has been broad investigation into  $ABC$  and  $GA$  indices, just as into their variations. For additional investigations of topological indices of different charts and substance structures, see [21-26].

## 2. Materials and Methods

### 2.1. The Cayley Tree $\Gamma^k$

The Cayley tree  $\Gamma^k$  of order  $k \geq 1$  is an infinite and symmetric regular tree, that is, a graph without cycles, from each vertex of which exactly  $k + 1$  edges are issued. In this paper, we consider the Cayley tree  $\Gamma_n^2 = (V, E, i)$  of order 2 and with  $n$  levels from the root  $x_0$ , where  $V$  is the set of vertices of  $\Gamma_n^2$ ,  $E$  is the set of edges of  $\Gamma_n^2$ , and  $i$  is the incidence function associating each edge  $E \in E$  with its end vertices. If  $i(e) = \{x, y\}$ , then  $x$  and  $y$  are adjacent vertices, and we write  $e = \langle x, y \rangle$ . For any  $x, y \in V$ , the distance  $d(x, y)$  is defined as

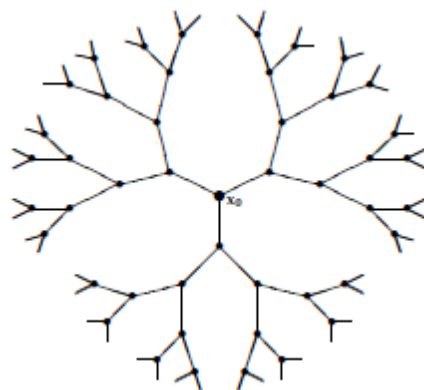
$$d(x, y) = m \{d \mid x = x_1, x_1, x_2, \dots, x_{d-1}, x_d = y \in V\}$$

such that the pairs  $\langle x_0, x_1 \rangle, \langle x_1, x_2 \rangle, \dots, \langle x_{d-1}, x_d \rangle$  are adjacent vertices [27].

For the root  $x_0$  of the Cayley tree, we have

$$\begin{aligned} W_\pi &= \{x \in V \mid d(x_0, x) = n\} \\ V_\pi &= \{x \in V \mid d(x_0, x) \leq n\} \\ E_n &= \{e = \langle x, y \rangle \in E \mid x, y \in V_\pi\} \end{aligned}$$

It is easy to compute the number of vertices reachable in step  $n$  or in level  $n$  starting from the root  $x_0$ , which is  $|W_n| = 3 \times 2^{(n-1)}$ . The number of vertices of  $\Gamma_n^2$  is  $|V_\pi| = 1 + 3 \times (2^n - 1)$ , and the number of edges of  $\Gamma_n^2$  is  $|E_\pi| = 3 \times (2^n - 1)$ , as is shown in Figure 1 below.



**Figure 1 Cayley tree  $\Gamma_n^2$  of order 2 with  $n$  levels where  $n \geq 1$**

## 2.2 The Square Lattice Graph $SL_\pi$

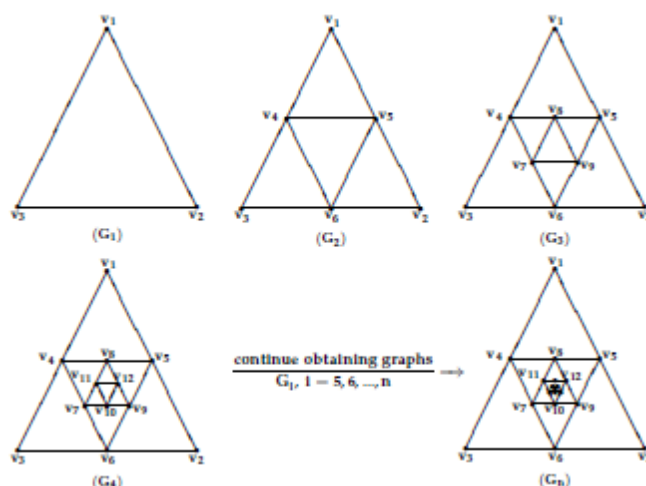
Lattice networks are widely used, for example, in distributed parallel computation, distributed control, wired circuits, and so forth. They are also known as grid or mesh networks. We choose a simple structure of lattice networks called a square lattice because this allows for a theoretical analysis [28].

We consider a square graph  $SL_\pi(V, E)$  of size  $n \times n$  vertices, where  $V$  denotes the set of vertices of  $SL_\pi$  and  $E$  denotes the set of edges of  $SL_\pi$ , such that the number of vertices is  $|V| = n^2$ , and the number of edges is  $|E| = 2n(n - 1)$ , as is shown in Figure 2 below.

Figure 1 Square lattice ( $SL_n$ ) with  $n \geq 1$ .

## 2.3. The Special Graph $G_K$

Other kinds of special graphs, denoted by  $G_\pi$ , can be obtained from other subgraphs. The structures in Figure 3 show how to obtain a graph  $G_\pi$ .



**Figure 3 Structures of graphs  $G_1, G_2, G_3, G_4, \dots, G_n$  of orders 3, 6, 9, 12, ...,  $3n$ .**

In Figure 3, we have obtained the graph sequence  $G_1, G_2, G_3, G_4, \dots, G_n$ . We let  $G_1$  be a complete graph of order 3 ( $G_1 \equiv K_3$ ) and let  $V(G_1) = \{v_1, v_2, v_3\}$ ; we have subdivided the three edges of  $G_1$ . The new vertices are denoted by  $\{v_4, v_5, v_6\}$ , and  $G_2[v_4, v_5, v_6] \equiv K_3$ . Thus,

$$\begin{aligned}
 V(G_2) &= V(G_1) \cup \{v_4, v_5, v_6\} \\
 E(G_2) &= \{v_1v_5, v_5v_2, v_2v_6, v_6v_3, v_3v_4, v_4v_1, v_4v_5, v_5v_6, v_6v_4\} \\
 G_2 &= G_1 - \{v_1v_2, v_2v_3, v_3v_1\} + \{v_1v_5, v_5v_2, v_2v_6, v_6v_3, v_3v_4, v_4v_1, v_4v_5, v_5v_6, v_6v_4\}
 \end{aligned}$$

Now, for  $G_n$ , we have subdivided the edges  $\{v_{3\pi-5}v_{3\pi-4}, v_{3\pi-4}v_{3\pi-3}, v_3 - 3^{v_{3\pi-5}}\}$ . The new vertices are denoted by  $\{v_{3\pi-2}, v_{3\pi-1}, v_{3\pi}\}$  and  $G_n[v_{3\pi-2}, v_{3\pi-1}, v_{3\pi}] \equiv K_3$ . Thus,

$$\begin{aligned}
 V(G_m) &= V(G_{n-1}) \cup \{v_{3m-2}, v_{3m-1}, v_3\} \\
 G_n &= G_{m-1} - \{v_{3\pi-5}v_{3\pi-4}, v_{3\pi-4}v_{3\pi-3}, v_{3\pi-3}v_{3\pi-5}\} + \{v_{3\pi-5}v_{3\pi}, v_{3\pi}v_{3\pi-4}, v_{3\pi-4}v_{3\pi-2}, v_{3\pi-2}v_{3\pi-3}, \\
 &\quad v_{3\pi-3}v_{3\pi-1}, v_{3\pi-1}v_{3\pi-5}, v_{3\pi-2}v_{3\pi-1}, v_{3\pi-1}v_3, v_{3\pi}v_{3\pi-2}\}
 \end{aligned}$$

It can be observed that the number of vertices of a graph  $G_n$  is  $3n$  and that the number of edges is  $6n - 3$  or, mathematically,  $|V(G_m)| = 3n$ , and  $|E(G_m)| = 6n - 3$ , respectively, where  $n \geq 1$

#### 2.4. The Camplede Biportite Grapli $K_{m\pi}$

A graph  $K_{m,\pi}$  is a complete bipartite graph if its vertex set can be partitioned into two subsets  $X$  and  $Y$ , such that one of the two endpoints of each edge in  $X$  and the other in  $Y$ , as well as each vertex  $v \in X$ , is adjacent to all vertices of  $Y$ , as is shown in Figure 4 below. Clearly, if  $|X| = m$  and  $|Y| = n$ , then  $|V(K_{m,\pi})| = m + n$  and  $|E(K_{m,\pi})| = mn$ . For more details, see [10].

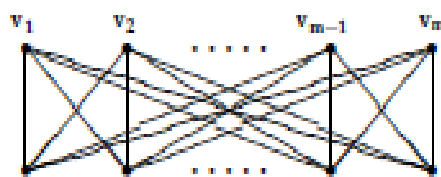


Figure 4 Complete bipartite graph  $K_{m1} \pi$  –

### 3. Results and Discussion

Prior to presenting our main results, the edge partitions of the Cayley tree, lattice square,  $G_n$  and complete bipartite graph, on the basis of the degrees of end vertices of each edge and the degree sum of the neighbors of end vertices of each edge, are discussed below.

Referring to Figure 1, there are two types of edges in  $\Gamma_\pi^2$  on the basis of the degrees of the end vertices of each edge, as follows: the first type, for  $e = uv \in E(\Gamma_\pi^2)$ , is such that  $d_x = 1$  and  $d_v = 3$ ; the other type is for  $E = uv \in E(\Gamma_\pi^2)$  such that  $d_x = d_v = 3$ . In the first type, there are  $3 \times 2^{\pi-1}$  edges, and in the other type, because  $|E(\Gamma_\pi^2)| = 3 \times (2^\pi - 1)$ , there are  $3 \times (2^\pi - 1) - 3 \times 2^{\pi-1} = 3 \times (2^\pi - 2^{\pi-1} - 1) = 3 \times (2^{\pi-1} - 1)$  edges, as is shown in Table 1. Similarly, from Figure 1, there are three types of edges in  $\Gamma_n^2$  on the basis of the degree sum of vertices lying at a unit distance from the end vertices of each edge, as follows: the first type, for  $e = uv \in E(\Gamma_n^2)$ , is such that  $S_x = 3$  and  $S_v = 5$ ; the second type, for  $\varepsilon = uv \in E(\Gamma_n^2)$ , is such that  $S_x = 5$  and  $S_v = 9$ ; the third type, for  $e = uv \in E(\Gamma_n^2)$ , is such that  $S_x = S_v = 9$ . There are  $3 \times 2^{\pi-1}$ ,  $3 \times 2^{\pi-2}$ , and  $3 \times (2^\pi - 1) - 3 \times 2^{\pi-1} - 3 \times 2^{\pi-2} = 3(2^\pi - 2^{\pi-1} - 2^{\pi-2} - 1) = 3 \times 2^{\pi-2}$  edges in the first, second and third types of  $\Gamma_n^2$ , respectively, as is shown in Table 2.

Table 1 Edge partition of  $\Gamma_\pi^2$  on the basis of degrees of end vertices of each edge.

$(d_x, d_v)$ Where $u \cap \in E$	Number of Edges
(1,3)	$3 \times 2^{\pi-1}$
(3,3)	$3 \times (2^{(\pi-1)} - 1)$

### 4. Conclusions

The Randić record has been firmly associated with numerous substance properties of particles and has been found to resemble the edge of boiling over and Kovats constants. The ABC file gives a decent model to the soundness of direct and extended alkanes just as for the strain energy of cycloalkanes. For certain physiochemical properties, the prescient force of the

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GA file is to some degree better than the prescient force of the Randić availability file. In this paper, specific degree-based topological records, specifically, the ABC and GA lists, are contemplated. Still up in the air and registered the shut recipes of the ABC<sub>4</sub> and GA<sub>5</sub> records for these extraordinary charts and organizations. We have likewise registered their ABC and GA records. These outcomes are novel and critical commitments in chart hypothesis and organization science, and they give a decent premise to comprehend the geography of these diagrams and organizations. Later on, we are keen on contemplating and figuring topological records of a tree with breadth  $d$ .

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