symmetry

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# Study of $\theta^{\phi}$ Networks via Zagreb Connection Indices

**Muhammad Asif [1], Bartłomiej Kizielewicz [2], Atiq ur Rehman [1], Muhammad Hussain [1] and Wojciech Sałabun [2,*]**

[1] Department of Mathematics, COMSATS University Islamabad (Lahore Campus), Lahore 53713, Pakistan; sp18-pmt-001@cuilahore.edu.pk (M.A.); atiqurehman@cuilahore.edu.pk (A.u.R.); muhammad.hussain@cuilahore.edu.pk (M.H.)

[2] Research Team on Intelligent Decision Support Systems, Department of Artificial Intelligence and Applied Mathematics, Faculty of Computer Science and Information Technology, West Pomeranian University of Technology in Szczecin, ul. Żołnierska 49, 71-210 Szczecin, Poland; bartlomiej-kizielewicz@zut.edu.pl

* Correspondence: wojciech.salabun@zut.edu.pl; Tel.: +48-91-449-5580

**Abstract:** Graph theory can be used to optimize interconnection network systems. The compatibility of such networks mainly depends on their topology. Topological indices may characterize the topology of such networks. In this work, we studied a symmetric network $\theta^{\phi}$ formed by $\phi$ time repetition of the process of joining $\theta$ copies of a selected graph $\Omega$ in such a way that corresponding vertices of $\Omega$ in all the copies are joined with each other by a new edge. The symmetry of $\theta^{\phi}$ is ensured by the involvement of complete graph $K_{\theta}$ in the construction process. The free hand to choose an initial graph $\Omega$ and formation of chemical graphs using $\theta^{\phi}\Omega$ enhance its importance as a family of graphs which covers all the pre-defined graphs, along with space for new graphs, possibly formed in this way. We used Zagreb connection indices for the characterization of $\theta^{\phi}\Omega$. These indices have gained worth in the field of chemical graph theory in very small duration due to their predictive power for enthalpy, entropy, and acentric factor. These computations are mathematically novel and assist in topological characterization of $\theta^{\phi}\Omega$ to enable its emerging use.

**Keywords:** Zagreb connection indices; graph invariants; interconnection networks; mk graphs; topological index

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## 1. Introduction

Graph theory provides a fundamental tool for designing and analyzing desired networks with accuracy and gives a thorough understanding of the manners by which the parts of a system interconnected through topology of an interconnection network [1]. Along with the other disciplines, graph theory has a special place in the field of chemistry, especially in chemical graph theory [2]. Thus, chemical graph theory is a composition of chemistry, computer science, and graph theory [3–5]. It provides information about organic substances regarding their physicochemical properties with the help of graph invariants using chemical graphs associated with their molecular structure. A chemical graph is a simple connected and hydrogen depleted graph consisting of vertices replacing atoms and edges for the bonds between atoms. A simple graph is comprised of only a single edge between two vertices and no self-loop (an edge with the same initial and final vertex). Graph invariants have strong applications in quantitative structure properties relationship (QSPR) investigation [6]. These invariants reduce the practical work to some extent to study the new chemicals structures using the topology of desired chemical structure. Topological indices are also the graph invariants that map chemical graphs into a numeric value and characterize the underlying structure's topology. Harry Wiener, in 1947, first introduced Wiener index [7]. Later on, the first and second Zagreb indices were proposed in Reference [8,9] as

$$M_1(\Omega) = \sum_{st \in E(\Omega)} (d_s + d_t), \qquad M_2(\Omega) = \sum_{st \in E(\Omega)} (d_s d_t).$$

Zagreb connection indices have been recently introduced, which are based on connection numbers of vertices as $\tau_s, s \in V(\Omega)$. The connection number $\tau_s$ is assigned to the vertex $s \in V(\Omega)$ of a graph calculated as distinct vertices at a distance of two from vertex $s$. Zagreb connection indices studied in Reference [10–13] are defined as

$$ZC_1(\Omega) = \sum_{s \in V(\Omega)} \tau_s^2, \qquad ZC_2(\Omega) = \sum_{st \in E(\Omega)} \tau_s \times \tau_t$$

and

$$ZC_1^*(\Omega) = \sum_{s \in V(\Omega)} (d_s \tau_s) = \sum_{st \in E(\Omega)} (\tau_s + \tau_t).$$

Ali et al. [10,13] and Jakkannavar and Basavanagoud [14] concluded that these indices have a good correlation with entropy, enthalpy, and acentric factors. The published work of Reference [15–18], along with the chemical applicability of these indices and formation of chemical networks using $\theta^\phi\Omega$, provides motivation for the study of $\theta^\phi\Omega$ via Zagreb connection indices. The $\theta^\phi\Omega$ is a symmetric network formed by the Cartesian product of any graph $\Omega$ with complete graph $K_\theta$, then resultant graph with $K_\theta$, and repeat this process $\phi$ times, i.e., $\theta^\phi\Omega = K_\theta \times (K_\theta \times (K_\theta \times (\ldots \times (K_\theta \times \Omega)\ldots)))$. The symmetry of underlying network $\theta^\phi\Omega$ is due to the iterative Cartesian product of $\Omega$ with complete graph $K_\theta$. The Cartesian product $\Omega_H \times \Omega_K$ of any two graphs $\Omega_H$ and $\Omega_K$ is defined in such a way that $V(\Omega_H \times \Omega_K) = V(\Omega_H) \times V(\Omega_K)$ and set of edge $E(\Omega_H \times \Omega_K)$,

$$\begin{aligned} E(\Omega_H \times \Omega_K) \quad &= \quad \{(u_{\Omega_H}, u_{\Omega_K})(v_{\Omega_H}, v_{\Omega_K}) : [u_{\Omega_H} = v_{\Omega_H} \in V(\Omega_H) \wedge u_{\Omega_K} v_{\Omega_K} \in E(\Omega_K)] \\ &\quad \vee [u_{\Omega_H} v_{\Omega_H} \in E(\Omega_H) \wedge u_{\Omega_K} = v_{\Omega_K} \in V(\Omega_K)]\}. \end{aligned}$$

The Cartesian product of path graph $P_3$ and cycle $C_4$ are shown in Figure 1.

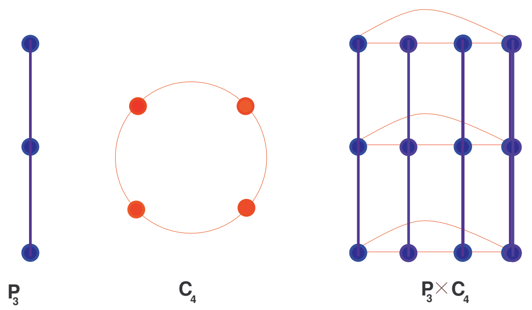


**Figure 1.** Cartesian product of $P_3$ and $C_n$, where $n = 4$.

In this work, we first compute exact results for Zagreb connection indices $ZC_1$, $ZC_2$, and $ZC_1^*$ of $\theta^\phi\Omega$ for arbitrary values of $\theta$ and $\phi$ when $\Omega = N_1$ consists single vertex. Further, we determined closed form formulas and bounds regarding $ZC_1$, $ZC_2$, and $ZC_1^*$ for $\theta^\phi\Omega$ when $\Omega$ is any given graph. At the end, we computed exact results for $\theta^\phi\Omega$ when $\Omega$ belongs to a certain family of graphs as applications of computed results.

## 2. Materials and Methods

We used edges and vertices partition technique based on the connection number assigned to the vertices for desired computation [19–22]. For this purpose, we focused on the construction rules of $\theta^\phi\Omega$ defined in Reference [23,24] and combinatorial enlisting by vertices and edges segment procedure. Throughout this work, $\Omega$ is notation for graph, $V(\Omega)$ for set of vertices, the set of edges $E(\Omega)$, $|V(\Omega)| = n_\Omega$ for order and $|E(\Omega)| = e_\Omega$ size of $\Omega$, $d_s$ for degree of vertex $s \in \Omega$, $P_n$ for path, $C_n$ for cycle, $N_n$ for null graph of order $n$, and $K_\theta$ for complete graph having order $\theta$. The Cartesian product of graphs $\Omega_H$ and $\Omega_K$ is denoted by $\Omega_H \times \Omega_K$. The topological indices computation, along with their mathematical study regarding certain graph or family of graphs, is very rich area of study today.

## 3. $\theta^\phi$ Network

$\theta\Omega$ is a network formed by $\theta$ copies of graph $\Omega$ in such a way that the corresponding vertices of all copies of graphs linked by new edges, i.e., $\theta\Omega = \theta(\Omega) = K_\theta \times \Omega$. $\theta^2(\Omega)$, is the graph formed by $\theta$ copies of $\theta\Omega$, i.e., $\theta^2(\Omega) = \theta(\theta\Omega) = K_\theta \times (K_\theta \times \Omega)$. The $\phi$ times repetition of such a process formed a large network as $\theta^\phi(\Omega) = \theta(\theta^{\phi-1}\Omega) = \theta(\theta(\theta^{\phi-2}\Omega)) = \theta(\theta(\theta((\theta^{\phi-3}\Omega)))) = \ldots = \underbrace{\theta(\theta(\theta(\ldots(\theta}_{(\phi-1)\text{ times}}(\theta\Omega))\ldots))) = \underbrace{\theta(\theta(\theta(\ldots(\theta}_{(\phi)\text{ times}}(\Omega))\ldots))) = \underbrace{K_\theta \times (K_\theta \times (K_\theta \times (\ldots \times (K_\theta}_{(\phi)\text{ times}} \times \Omega)\ldots)))$. The construction of $\theta^\phi\Omega$ implies that the $|V(\theta^\phi\Omega)| = \theta^\phi n_\Omega$, and $|E(\theta^\phi\Omega)| = \theta^\phi e_\Omega + \binom{\theta}{2} n_\Omega \phi \theta^{\phi-1}$.

### *Molecular Networks Formed by $\theta^\phi\Omega$*

The formation of molecular networks by $\theta^\phi\Omega$ encouraged us to study these networks via Zagreb connection indices. Figure 2 presents chemical graphs of organic compounds formed by $\theta^\phi\Omega$ when $\Omega = N_1$ consists of only one vertex.

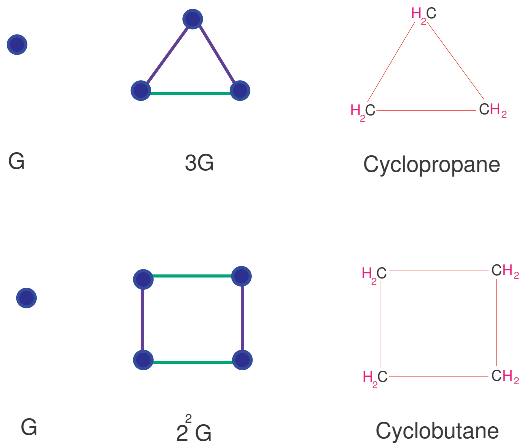


**Figure 2.** $\theta^\phi\Omega$ as organic compounds.

Carbon Nanotube $TUC_4(m,3)$ as $3P_n$

Let $P_n$ be the graph of alkane. The graph formed by $P_n$ as $3P_n$ is a carbon nanotube $TUC_4(m,3)$, as shown in Figure 3.

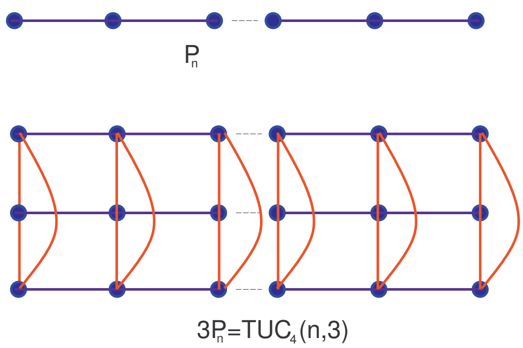


**Figure 3.** $3P_n$ as carbon nanotube $TUC_4(n,3)$.

Cyclobutane can also be formed by $2P_2$.

## 4. Main Results

### *4.1. $\theta^{\phi}\Omega$ When $\Omega$ Consist of Only One Vertex*

In case of one vertex graph $\Omega = N_1$, $\theta\Omega$ must be a complete graph $K_{\theta}$. The total number of vertices of $\theta^{\phi}\Omega$ is $|V(\theta^{\phi}\Omega)| = \theta^{\phi}$, and the number of edges is $|E(\theta^{\phi}\Omega)| = \binom{\theta}{2}\phi\theta^{\phi-1}$. The $\theta^{\phi}N_1$ for $\theta = 2$ is the cube $Q_{\phi}$ of dimension $\phi$. The cube of dimension $\phi = 1,2,3,4$ is shown in Figure 4 as $2N_1 = K_2 \times N_1$, $2^2N_1 = K_2 \times (K_2 \times N_1)$, $2^3N_1 = K_2 \times (K_2 \times (K_2 \times N_1))$, $2^4N_1 = K_2 \times (K_2 \times (K_2 \times (K_2 \times N_1)))$. The $\theta^{\phi}N_1$ for $\theta = 3$ and $\phi = 1,2,3,4$ is shown in Figure 5 as $3N_1 = K_3 \times N_1$, $3^2N_1 = K_3 \times (K_3 \times N_1)$, $3^3N_1 = K_3 \times (K_3 \times (K_3 \times N_1))$.

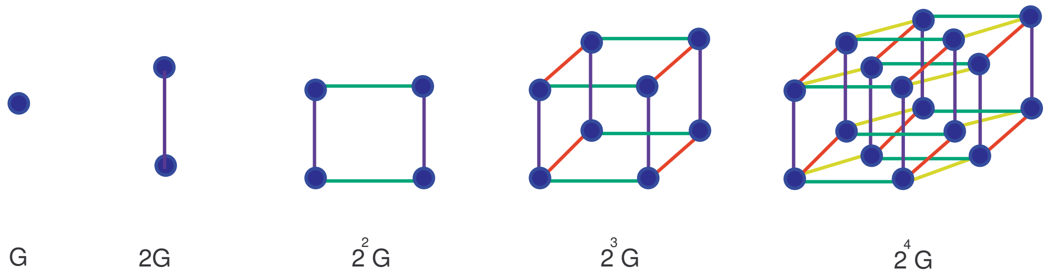


**Figure 4.** $\theta^{\phi}\Omega$ for $\theta = 2$ and $\phi = 1,2,3,4$ when $\Omega = N_1$.

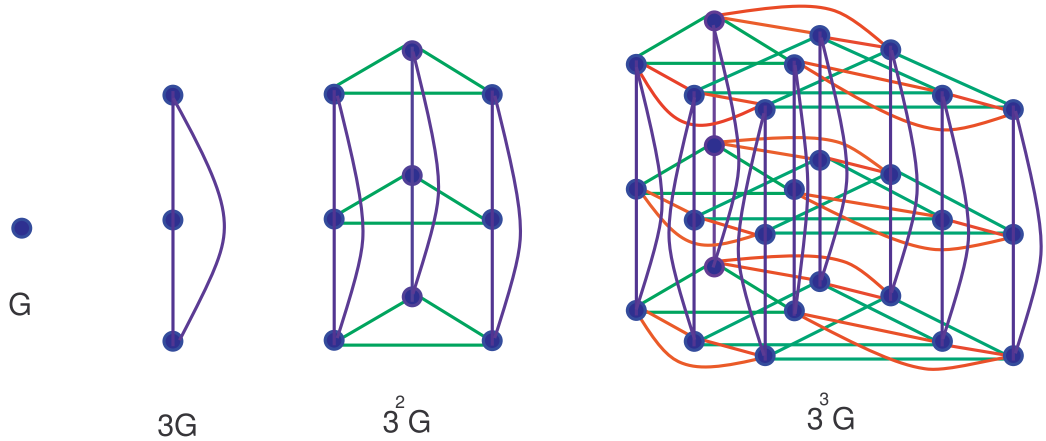


**Figure 5.** $\theta^{\phi}\Omega$ for $\phi = 1,2,3$ when $\Omega$ is a single vertex graph.

**Theorem 1.** *Let $\Omega$ be the graph with $n_{\Omega} = 1$. Then, $ZC_1, ZC_2$, and $ZC_1^*$ of $\theta^{\phi}\Omega$ are*

$$\begin{aligned} ZC_1(\theta^{\phi}\Omega) &= \frac{1}{4}\phi^2(\phi-1)^2(\theta-1)^4\theta^{\phi}, \\ ZC_2(\theta^{\phi}\Omega) &= \frac{1}{4}\binom{\theta}{2}\phi^3(\phi-1)^2(\theta-1)^4\theta^{\phi-1}, \\ ZC_1^*(\theta^{\phi}\Omega) &= \binom{\theta}{2}\phi^2(\phi-1)(\theta-1)^2\theta^{\phi-1}. \end{aligned}$$

**Proof.** Let $\Omega$ be the graph with $n_G = 1$, $|V(\theta^{\phi}\Omega)| = \theta^{\phi}$, and $|E(\theta^{\phi}\Omega)| = \binom{\theta}{2}\phi\theta^{\phi-1}$. For the connection number of each vertex of $\Omega$, we use vertex listing technique. The observation shows that $\theta^1\Omega$ is complete graph $K_{\theta}$, and the degree of each vertex $v \in \theta\Omega$ is $d_v = \theta - 1$. The connection number $\tau_{\theta^{\phi}\Omega}(v)$ of each vertex $v \in \theta^{\phi}\Omega$ is zero for $\phi = 1,2$. The construction of $\theta^{\phi}\Omega$ implies that the complicated network formed for larger value $\phi$. The increase in value of $\phi$ causes an increase in the degree $d_{\theta^{\phi}\Omega}(v)$, as well as connection number $\tau_{\theta^{\phi}\Omega}(v)$

of $v \in \theta^{\phi}(\Omega)$. The connection number of each vertex $v \in \theta^{\phi}(\Omega)$ is $\tau_{\theta^{\phi}\Omega}(v) = \frac{\phi(\phi-1)(\theta-1)^2}{2}$. Using these, we determine first connection Zagreb index $ZC_1(\theta^{\phi}\Omega)$.

$$ZC_1(\theta^{\phi}\Omega) = \sum_{u \in V(\theta^{\phi}\Omega)} (\tau_{\theta^{\phi}\Omega}(v))^2,$$

$$ZC_1(\theta^{\phi}\Omega) = \sum_{u \in V(\theta^{\phi}\Omega)} (\frac{\phi(\phi-1)(\theta-1)^2}{2})^2.$$

In case $n_{\Omega} = 1$, the total number of vertices of $\theta^{\phi}\Omega$ is $\theta^{\phi}$, i.e, $|V(\theta^{\phi}\Omega)| = \theta^{\phi}$.

$$ZC_1(\theta^{\phi}\Omega) = \frac{1}{4}\phi^2(\phi-1)^2(\theta-1)^4\theta^{\phi}. \tag{1}$$

Now, for $ZC_2(\theta^{\phi}\Omega)$,

$$ZC_2(\theta^{\phi}\Omega) = \sum_{uv \in E(\theta^{\phi}\Omega)} \tau_{\theta^{\phi}\Omega}(u)\tau_{\theta^{\phi}\Omega}(v),$$

since the connection number of each vertex $v \in \theta^{\phi}(\Omega)$ is $\tau_{\theta^{\phi}\Omega}(v) = \frac{\phi(\phi-1)(\theta-1)^2}{2}$, and the total number of edges in case $n_{\Omega} = 1$ is $\binom{\theta}{2}\phi\theta^{\phi-1}$. So,

$$ZC_2(\theta^{\phi}\Omega) = \sum_{uv \in E(\theta^{\phi}\Omega)} (\frac{\phi(\phi-1)(\theta-1)^2}{2})(\frac{\phi(\phi-1)(\theta-1)^2}{2}),$$

$$ZC_2(\theta^{\phi}\Omega) = \binom{\theta}{2}\phi\theta^{\phi-1}(\frac{\phi(\phi-1)(\theta-1)^2}{2})^2,$$

$$ZC_2(\theta^{\phi}\Omega) = \frac{1}{4}\binom{\theta}{2}\phi^3(\phi-1)^2(\theta-1)^4\theta^{\phi-1}. \tag{2}$$

Now, for $ZC_1^*(\Omega)$,

$$ZC_1^*(\theta^{\phi}\Omega) = \sum_{uv \in E(\theta^{\phi}\Omega)} (\tau_{\theta^{\phi}\Omega}(u) + \tau_{\theta^{\phi}\Omega}(v)),$$

since the connection number of each vertex $v \in \theta^{\phi}(\Omega)$ is $\tau_{\theta^{\phi}\Omega}(v) = \frac{\phi(\phi-1)(\theta-1)^2}{2}$, and the total number of edges in case $n_{\Omega} = 1$ is $\binom{\theta}{2}\phi\theta^{\phi-1}$. So,

$$ZC_1^*(\theta^{\phi}\Omega) = \sum_{uv \in E(\theta^{\phi}\Omega)} (\frac{\phi(\phi-1)(\theta-1)^2}{2} + \frac{\phi(\phi-1)(\theta-1)^2}{2}),$$

$$ZC_1^*(\theta^{\phi}\Omega) = \binom{\phi}{2}\phi\theta^{\phi-1}(\phi(\phi-1)(\theta-1)^2),$$

$$ZC_1^*(\theta^{\phi}\Omega) = \binom{\phi}{2}\phi^2(\phi-1)(\theta-1)^2\theta^{\phi-1}. \tag{3}$$

Equations (1)–(3) complete the proof. □

### 4.2. $\theta^\phi\Omega$ When $\Omega$ Is Any $n_\Omega$-Vertex Simple Connected Graph

In case of any $n_\Omega$-vertex simple connected graph $\Omega$, $\theta\Omega$ is a complete graph consisting of $\theta$ copies of $\Omega$. The total number of vertices in $\theta^\phi\Omega$ is $|V(\theta^\phi\Omega)| = \theta^\phi|V(\Omega)|$, and the number of edges is $|E(\theta^\phi\Omega)| = \theta^\phi|E(\Omega)| + \binom{\theta}{2}|V(\Omega)|\phi\theta^{\phi-1}$. The connection number associated to the vertex $u \in \theta^\phi\Omega$ is $\tau_u + (\frac{2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2}{2})$. In this section, we determined generalized results for $ZC_1, ZC_2$, and $ZC_1^*$ of $\theta^\phi\Omega$. We also made a more concise approach and find the bonds and extremal for some specific families of graphs using already proven results for connection Zagreb indices. Figure 6 presents the case when $\theta^\phi\Omega$ graphs and $\Omega$ is a simple connected graph with $|V(\Omega)| \geq 1$ for $\phi = 0, 1, 2$. The second example is presented in Figure 7, where $\theta^\phi P_n$ graph for $\phi = 0, 1, 2$ and $n = 3$.

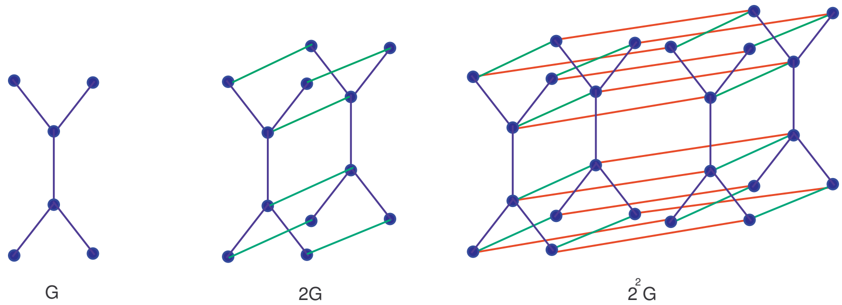


**Figure 6.** $\theta^\phi\Omega$ graphs when $\Omega$ is a simple connected graph with $|V(\Omega)| \geq 1$ for $\phi = 0, 1, 2$.

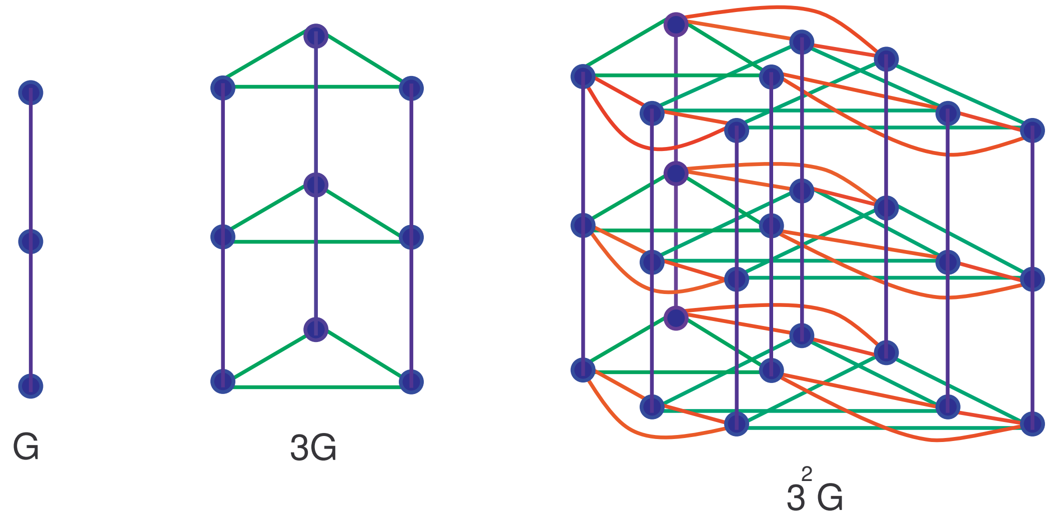


**Figure 7.** $\theta^\phi P_n$ graph for $\phi = 0, 1, 2$ and $n = 3$.

**Theorem 2.** *Let $\Omega$ be a simple connected graph with $|V(\Omega)| = n_\Omega \geq 2$. Then, $ZC_1$ of $\theta^\phi\Omega$ is*

$$\begin{aligned} ZC_1(\theta^\phi\Omega) &= \theta^\phi ZC_1(\Omega) + [2(\theta-1)\phi + \phi(\phi-1)(\theta-1)^2]\theta^\phi ZC_1^*(\Omega) \\ &+ [\frac{2(\theta-1)\phi + \phi(\phi-1)(\theta-1)^2}{2}]^2\theta^\phi M_1(\Omega). \end{aligned}$$

**Proof.** Let $\Omega$ be a simple connected graph. The connection number of each vertex $v \in \theta^\phi(\Omega)$ is $\tau_{\theta^\phi\Omega}(v) = \tau_v + (\frac{2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2}{2})d_v$. The total number of vertices in $\theta^\phi\Omega$ is $|V(\theta^\phi\Omega)| = \theta^\phi n_\Omega$, and the number of edges is $|E(\theta^\phi\Omega)| = \theta^\phi e_\Omega + \binom{\theta}{2}n_\Omega\phi\theta^{(\phi-1)}$. Using these results, we determine first connection Zagreb index $ZC_1(\theta^\phi\Omega)$ as

$$ZC_1(\theta^\phi\Omega) = \sum_{u \in V(\theta^\phi\Omega)} (\tau_{\theta^\phi\Omega}(u))^2,$$

$$ZC_1(\theta^{\phi}\Omega) = \sum_{u \in V(\theta^{\phi}\Omega)} (\tau_u + (\frac{2(\theta-1)\phi + \phi(\phi-1)(\theta-1)^2}{2})d_u)^2,$$

$$\begin{aligned} ZC_1(\theta^{\phi}\Omega) &= \sum_{u \in V(\theta^{\phi}\Omega)} (\tau_u)^2 + \sum_{u \in V(\theta^{\phi}\Omega)} 2[(\frac{2(\theta-1)\phi + \phi(\phi-1)(\theta-1)^2}{2})d_u\tau_u] \\ &+ \sum_{u \in V(\theta^{\phi}\Omega)} [(\frac{2(\theta-1)\phi + \phi(\phi-1)(\theta-1)^2}{2})d_u]^2, \end{aligned}$$

$$\begin{aligned} ZC_1(\theta^{\phi}\Omega) &= \sum_{u \in V(\theta^{\phi}\Omega)} \tau_u^2 + 2[\frac{2(\theta-1)\phi + \phi(\phi-1)(\theta-1)^2}{2}] \sum_{u \in V(\theta^{\phi}\Omega)} d_u\tau_u \\ &+ [\frac{2(\theta-1)\phi + \phi(\phi-1)(\theta-1)^2}{2}]^2 \sum_{u \in V(\theta^{\phi}\Omega)} d_u^2. \end{aligned}$$

As $|V(\Omega)| \geq 1$, the total number of vertices of $\theta^{\phi}\Omega$ is $\theta^{\phi}n_{\Omega}$, i.e, $|V(\theta^{\phi}\Omega)| = \theta^{\phi}|V(\Omega)|$.

$$\begin{aligned} ZC_1(\theta^{\phi}\Omega) &= \theta^{\phi} \sum_{u \in V(\Omega)} \tau_u^2 + 2[\frac{2(\theta-1)\phi + \phi(\phi-1)(\theta-1)^2}{2}]\theta^{\phi} \sum_{u \in V(\Omega)} d_u\tau_u \\ &+ [\frac{2(\theta-1)\phi + \phi(\phi-1)(\theta-1)^2}{2}]^2\theta^{\phi} \sum_{u \in V(\Omega)} d_u^2. \end{aligned}$$

Since $ZC_1(\Omega) = \sum_{u \in V(\Omega)} \tau_u^2, ZC_1^*(\Omega) = \sum_{u \in V(\Omega)} d_u\tau_u$, and $M_1(\Omega) = \sum_{u \in V(\Omega)} d_u^2$. Replacing these formulas, we get

$$\begin{aligned} ZC_1(\theta^{\phi}\Omega) &= \theta^{\phi}ZC_1(\Omega) + [2(\theta-1)\phi + \phi(\phi-1)(\theta-1)^2]\theta^{\phi}ZC_1^*(\Omega) \\ &+ [\frac{2(\theta-1)\phi + \phi(\phi-1)(\theta-1)^2}{2}]^2\theta^{\phi}M_1(\Omega). \end{aligned} \tag{4}$$

□

**Theorem 3.** *Let $\Omega$ be the simple connected graph with $|V(\Omega)| = n_{\Omega} \geq 2$. Then,*

$$\begin{aligned} ZC_2(\theta^{\phi}\Omega) \leq\ & \theta^{\phi}ZC_2(\Omega) + \binom{\theta}{2}\phi\theta^{(\phi-1)}ZC_1(\Omega) + [2(\theta-1)\phi + \phi(\phi-1)(\theta-1)^2][\Delta\theta^{\phi} + \\ & \binom{\theta}{2}\phi\theta^{(\phi-1)}]ZC_1^*(\Omega) + [\frac{2(\theta-1)\phi + \phi(\phi-1)(\theta-1)^2}{2}]^2[\theta^{\phi}M_2(\Omega) + \\ & \binom{\theta}{2}\phi\theta^{(\phi-1)}M_1(\Omega)], \end{aligned}$$

*and*

$$\begin{aligned} ZC_2(\theta^{\phi}\Omega) \geq\ & \theta^{\phi}ZC_2(\Omega) + \binom{\theta}{2}\phi\theta^{(\phi-1)}ZC_1(\Omega) + [2(\theta-1)\phi + \phi(\phi-1)(\theta-1)^2][\delta\theta^{\phi} + \\ & \binom{\theta}{2}\phi\theta^{(\phi-1)}]ZC_1^*(\Omega) + [\frac{2(\theta-1)\phi + \phi(\phi-1)(\theta-1)^2}{2}]^2[\theta^{\phi}M_2(\Omega) + \\ & \binom{\theta}{2}\phi\theta^{(\phi-1)}M_1(\Omega)]. \end{aligned}$$

*Equality holds for regular graph $\Omega$.*

**Proof.** Let $\Omega$ be the simple connected graph with $n_\Omega \geq 2$. The connection number of each vertex $v \in \theta^\phi(\Omega)$ is $\tau_{\theta\phi\Omega}(v) = \tau_v + (\frac{2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2}{2})d_v$. The total number of vertices in $\theta^\phi\Omega$ is $|V(\theta^\phi\Omega)| = \theta^\phi n_\Omega$, and the number of edges is $|E(\theta^\phi\Omega)| = \theta^\phi e_\Omega + \binom{\theta}{2} n_\Omega \phi\theta^{(\phi-1)}$.

$$ZC_2(\theta^\phi\Omega) = \sum_{uv\in E(\theta^\phi\Omega)} \tau_{\theta\phi\Omega}(u)\tau_{\theta\phi\Omega}(v).$$

Let $A = \{u, v : uv \in E(\Omega)\}$.

$$ZC_2(\theta^\phi\Omega) = \sum_{uv\in E(\theta^\phi\Omega)} \Pi_{a\in A}[\tau_a + (\frac{2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2}{2})d_a],$$

$$\begin{aligned} ZC_2(\theta^\phi\Omega) = \sum_{uv\in E(\theta^\phi\Omega)} \tau_u\tau_v &+ [\frac{2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2}{2}] \sum_{uv\in E(\theta^\phi\Omega)} (d_u\tau_v + d_v\tau_u) \\ &+ [\frac{2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2}{2}]^2 \sum_{uv\in E(\theta^\phi\Omega)} d_u d_v. \end{aligned}$$

The edges between corresponding vertices of all the $\theta^\phi$ copies of graph $\Omega$ in $\theta^\phi\Omega$ have the same end vertex connection number $\tau_u + (\frac{2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2}{2})d_u$. These edges are $\binom{\theta}{2} n_\Omega \phi\theta^{(\phi-1)}$ in number. The edges between vertices of all the $\theta^\phi$ copies of graph $\Omega$ have different end vertex connection numbers $\tau_{\theta\phi\Omega}(u) = \tau_u + (\frac{2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2}{2})d_u$ and $\tau_{\theta\phi\Omega}(v) = \tau_v + (\frac{2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2}{2})d_u$ for $uv \in G$. These edges make the total $\theta^\phi e_\Omega$. Using these findings, we get

$$\begin{aligned} ZC_2(\theta^\phi\Omega) \quad = \quad & \theta^\phi \sum_{uv\in E(\Omega)} \tau_u\tau_v + \binom{\theta}{2}\phi\theta^{(\phi-1)} \sum_{u\in V(\Omega)} \tau_u^2 + [\frac{2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2}{2}] \\ & [\theta^\phi \sum_{uv\in E(\Omega)} (d_u\tau_v + d_v\tau_u) + \binom{\theta}{2}\phi\theta^{(\phi-1)} \sum_{u\in V(\Omega)} 2d_u\tau_u] + \\ & [\frac{2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2}{2}]^2[\theta^\phi \sum_{uv\in E(\Omega)} (d_u d_v) + \binom{\theta}{2}\phi\theta^{(\phi-1)} \sum_{u\in V(\Omega)} d_u^2]. \end{aligned}$$

Since $ZC_1(\Omega) = \sum_{u\in V(\Omega)} \tau_u^2, ZC_2(\Omega) = \sum_{uv\in E(\Omega)} \tau_u\tau_v, ZC_1^*(\Omega) = \sum_{u\in V(\Omega)} d_u\tau_u$ $M_1(\Omega) = \sum_{u\in V(\Omega)} d_u^2$, and $M_2(\Omega) = \sum_{uv\in E(\Omega)} d_u d_v$. Replacing these formulas, we get

$$\begin{aligned} ZC_2(\theta^\phi\Omega) \quad = \quad & \theta^\phi ZC_2(\Omega) + \binom{\theta}{2}\phi\theta^{(\phi-1)} ZC_1(\Omega) + [\frac{2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2}{2}][\theta^\phi \\ & \sum_{uv\in E(\Omega)} (d_u\tau_v + d_v\tau_u) + 2\binom{\theta}{2}\phi\theta^{(\phi-1)} ZC_1^*] + [\frac{2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2}{2}]^2 \\ & [\theta^\phi M_2(\Omega) + \binom{\theta}{2}\phi\theta^{(\phi-1)} M_1(\Omega)]. \end{aligned} \tag{5}$$

Replacing $d_u = d_v = \Delta$, we get

$$\begin{aligned} ZC_2(\theta^\phi\Omega) \quad &\leq \quad \theta^\phi ZC_2(\Omega) + \binom{\theta}{2}\phi\theta^{(\phi-1)}ZC_1(\Omega) + [\frac{2(\theta-1)\phi + \phi(\phi-1)(\theta-1)^2}{2}][\theta^\phi \\ &\sum_{uv\in E(\Omega)}(\Delta\tau_v + \Delta\tau_u) + 2\binom{\theta}{2}\phi\theta^{(\phi-1)}ZC_1^*] + [\frac{2(\theta-1)\phi + \phi(\phi-1)(\theta-1)^2}{2}]^2 \\ &[\theta^\phi M_2(\Omega) + \binom{\theta}{2}\phi\theta^{(\phi-1)}M_1(\Omega)]. \end{aligned}$$

$$\begin{aligned} ZC_2(\theta^\phi\Omega) \quad &\leq \quad \theta^\phi ZC_2(\Omega) + \binom{\theta}{2}\phi\theta^{(\phi-1)}ZC_1(\Omega) + [2(\theta-1)\phi + \phi(\phi-1)(\theta-1)^2] \\ &[\Delta\theta^\phi + \binom{\theta}{2}\phi\theta^{(\phi-1)}]ZC_1^*(\Omega) + [\frac{2(\theta-1)\phi + \phi(\phi-1)(\theta-1)^2}{2}]^2 \\ &[\theta^\phi M_2(\Omega) + \binom{\theta}{2}\phi\theta^{(\phi-1)}M_1(\Omega)]. \end{aligned} \tag{6}$$

Now, again, replacing $d_u = d_v = \delta$ in equation (5), we get inequality (7).

$$\begin{aligned} ZC_2(\theta^\phi\Omega) \quad &\geq \quad \theta^\phi ZC_2(\Omega) + \binom{\theta}{2}\phi\theta^{(\phi-1)}ZC_1(\Omega) + [2(\theta-1)\phi + \phi(\phi-1)(\theta-1)^2] \\ &[\delta\theta^\phi + \binom{\theta}{2}\phi\theta^{(\phi-1)}]ZC_1^*(\Omega) + [\frac{2(\theta-1)\phi + \phi(\phi-1)(\theta-1)^2}{2}]^2 \\ &[\theta^\phi M_2(\Omega) + \binom{\theta}{2}\phi\theta^{(\phi-1)}M_1(\Omega)]. \end{aligned} \tag{7}$$

The inequalities (6) and (7) complete the proof. □

**Theorem 4.** *Let $\Omega$ be the simple connected graph with $|V(\Omega)| = n_\Omega \geq 2$. Then,*

$$\begin{aligned} ZC_1^*(\theta^\phi\Omega) \quad &\leq \quad \theta^\phi ZC_1^*(\Omega) + 2\binom{\theta}{2}\theta^{(\phi-1)}(M_1(\Omega) - 2e_\Omega) + (\frac{2(\theta-1)\phi + \phi(\phi-1)(\theta-1)^2}{2}) \\ &[\theta^\phi M_1(\Omega) + 2\binom{\theta}{2}\theta^{(\phi-1)}e_\Omega]. \end{aligned} \tag{8}$$

*Equality holds for $\{C_3, C_4\}-$free network $\Omega$. In addition,*

$$\begin{aligned} ZC_1^*(\theta^\phi\Omega) \quad &\geq \quad \theta^\phi ZC_1^*(\Omega) + (\frac{2(\theta-1)\phi + \phi(\phi-1)(\theta-1)^2}{2}) \\ &[\theta^\phi M_1(\Omega) + 2\binom{\theta}{2}\theta^{(\phi-1)}e_\Omega]. \end{aligned} \tag{9}$$

Equality holds when $\Omega$ is a complete graph.

**Proof.** Let $\Omega$ be the simple connected graph with $n_\Omega \geq 2$. The connection number of each vertex $v \in \theta^\phi(\Omega)$ is $\tau_{\theta^\phi\Omega}(v) = \tau_v + ((\theta-1)\phi + \frac{1}{2}\phi(\phi-1)(\theta-1)^2)d_v$. The total number of vertices in $\theta^\phi\Omega$ is $|V(\theta^\phi\Omega)| = \theta^\phi n_\Omega$, and the number of edges is $|E(\theta^\phi\Omega)| = \theta^\phi e_\Omega + \binom{\theta}{2}n_\Omega\theta^{(\phi-1)}$.

$$ZC_1^*(\theta^\phi\Omega) = \sum_{uv\in E(\theta^\phi\Omega)}(\tau_{\theta^\phi\Omega}(u) + \tau_{\theta^\phi\Omega}(v)),$$

$$ZC_2(\theta^{\phi}\Omega) = \sum_{uv\in E(\theta^{\phi}\Omega)} [(\tau_u + (\frac{2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2}{2})d_u) + (\tau_v + ((\theta-1)\phi + \frac{1}{2}\phi(\phi-1)(\theta-1)^2)d_v)],$$

$$ZC_1^*(\theta^{\phi}\Omega) = \sum_{uv\in E(\theta^{\phi}\Omega)} (\tau_u+\tau_v) + (\frac{2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2}{2}) \sum_{uv\in E(\theta^{\phi}\Omega)} (d_u+d_v).$$

The edges between corresponding vertices of all the $\theta^{\phi}$ copies of graph $\Omega$ in $\theta^{\phi}\Omega$ have the same end vertex connection number $\tau_u + (\frac{2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2}{2})d_u$. These edges are $\binom{\theta}{2}n_{\Omega}\theta^{(\phi-1)}$ in number. The edges between vertices of all the $\theta^{\phi}$ copies of graph $\Omega$ have different end vertex connection numbers $\tau_{\theta^{\phi}\Omega}(u) = \tau_u + (\frac{2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2}{2})d_u$ and $\tau_{\theta^{\phi}\Omega}(v) = \tau_v + (\frac{2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2}{2})d_u$ for $uv \in \Omega$. These edges make the total $\theta^{\phi}e_{\Omega}$. Using these findings, we get

$$ZC_1^*(\theta^{\phi}\Omega) = \theta^{\phi}\sum_{uv\in E(\Omega)}(\tau_u+\tau_v) + 2\binom{\theta}{2}\theta^{(\phi-1)}\sum_{u\in V(\Omega)}\tau_u + [\frac{2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2}{2}] [\theta^{\phi}\sum_{uv\in E(\Omega)}(d_u+d_v) + \binom{\theta}{2}\theta^{(\phi-1)}\sum_{u\in V(\Omega)}2d_u].$$

Since, for a connected graph $\Omega$, $\sum_{u\in V(\Omega)}\tau_u \leq M_1(\Omega) - 2e_{\Omega}$ [15], $0 \leq \sum_{u\in V(\Omega)}\tau_u$, and $\sum_{u\in V(\Omega)} d_u = 2|E(\Omega)|$. Hence,

$$ZC_1^*(\theta^{\phi}\Omega) \leq \theta^{\phi}ZC_1^*(\Omega) + 2\binom{\theta}{2}\theta^{(\phi-1)}(M_1(\Omega)-2e_{\Omega}) + (\frac{2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2}{2}) [\theta^{\phi}M_1(\Omega) + 2\binom{\theta}{2}\theta^{(\phi-1)}e_{\Omega}], \tag{10}$$

and

$$ZC_1^*(\theta^{\phi}\Omega) \geq \theta^{\phi}ZC_1^*(\Omega) + (\frac{2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2}{2})[\theta^{\phi}M_1(\Omega) + 2\binom{\theta}{2}\theta^{(\phi-1)}e_{\Omega}]. \tag{11}$$

Equations (10) and (11) complete the proof. □

### *4.3. Applications of Computed Results as Zagreb Connection Indices of $\theta^{\phi}C_n$ and $\theta^{\phi}K_{\theta_1}$*

Figures 8 and 9 present simple applications of computed results as Zagreb connection indices of $\theta^{\phi}C_n$ and $\theta^{\phi}K_{\theta_1}$.

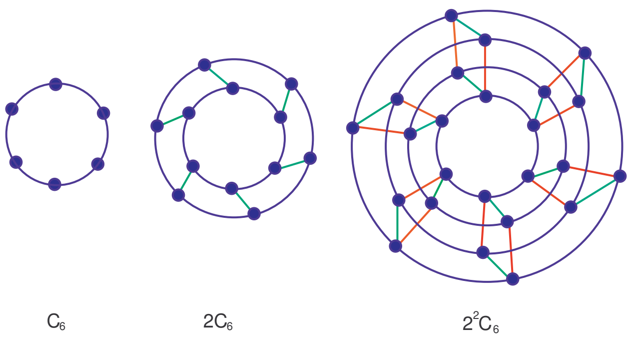


**Figure 8.** $\theta^{\phi}C_n$ for $n = 6$ and $k = 1, 2$.

**Corollary 1.** *Let $\Omega = C_n$ be a uni-cyclic graph of order $n$. Then,*

$$ZC_1(\theta^{\phi}C_n) = 4n\theta^{\phi}[1+2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2+(\frac{2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2}{2})^2].$$

**Proof.** Let $\Omega = C_n$ be a uni-cyclic graph of order $n$. By replacing $ZC_1(C_n) = 4n$, $M_1(C_n) = 4n$, and $ZC_2(C_n) = 4n$ in Theorem 2, we get the required result as

$$ZC_1(\theta^{\phi}C_n) = 4n\theta^{\phi}[1+2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2+(\frac{2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2}{2})^2].$$

□

**Corollary 2.** *Let $\Omega = C_n$ be a uni-cyclic graph of order $n$.*

$$ZC_2(\theta^{\phi}C_n) = 4n\theta^{\phi}[(1+\binom{\theta}{2}\phi\theta)(\frac{2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2}{2})^2+(2\theta^{\phi}+\binom{\theta}{2}\phi\theta)(2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2)].$$

**Proof.** By replacing $ZC_1(C_n) = 4n, ZC_2(C_n) = 4n, ZC_1^*(C_n) = 4n, M_2(\Omega) = 4n$, and $M_1(C_n) = 4n$ in Theorem 3, we get the required result as

$$ZC_2(\theta^{\phi}C_n) = 4n\theta^{\phi}[(1+\binom{\theta}{2}\phi\theta)(\frac{2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2}{2})^2+(2\theta^{\phi}+\binom{\theta}{2}\phi\theta)(2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2)].$$

□

**Corollary 3.** *Let $\Omega = C_n$ be a uni-cyclic graph for $n \geq 5$. Then,*

$$ZC_1^*(\theta^{\phi}C_n) = 4n\theta^{\phi}[(1+\binom{\theta}{2}\phi\theta)(1+\frac{2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2}{2})].$$

**Proof.** Let $\Omega = C_n$ be a uni-cyclic graph for $n \geq 5$. Then, by replacing $ZC_1^*(C_n) = 4n$, $M_1(C_n) = 4n$ and $e_{\Omega} = n$ in Theorem 4, we get the required result as

$$ZC_1^*(\theta^{\phi}C_n) = 4n\theta^{\phi}[(1+\binom{\theta}{2}\phi\theta)(1+\frac{2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2}{2})].$$

□

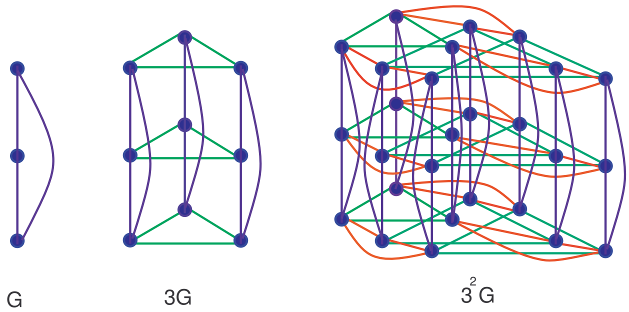


**Figure 9.** $\theta^{\phi}K_{\theta_1}$ graph for $k = 0, 1, 2$ and $\theta_1 = 3$.

**Corollary 4.** *Let $\Omega = K_{\theta_1}$ be a complete graph of order $\theta_1$. Then,*

$$ZC_1(\theta^{\phi}K_{\theta_1}) = 4\theta_1(\theta_1-1)^2[\frac{2(\theta-1)\phi+\phi(\phi-1)(\theta-1)^2}{2}]^2\theta^{\phi}.$$

**Proof.** Let $\Omega = K_{\theta_1}$ be a complete graph of order $\theta_1$. By replacing $ZC_1(K_{\theta_1}) = ZC_1^*(K_{\theta_1}) = 0$ and $M_1(K_{\theta_1}) = \theta_1(\theta_1 - 1)^2$ in Theorem 2, we get the required result as

$$ZC_1(\theta^\phi K_{\theta_1}) = 4\theta_1(\theta_1 - 1)^2 [\frac{2(\theta - 1)\phi + \phi(\phi - 1)(\theta - 1)^2}{2}]^2 \theta^\phi.$$

□

**Corollary 5.** *Let $\Omega = K_{\theta_1}$ be a complete graph of order $\theta_1$. Then,*

$$ZC_2(\theta^\phi \Omega) = [\frac{2(\theta - 1)\phi + \phi(\phi - 1)(\theta - 1)^2}{2}]^2 [\frac{(\theta_1 - 1)}{2} + \binom{\theta}{2}\phi\theta]\theta_1(\theta_1 - 1)^2 \theta^\phi.$$

**Proof.** Let $\Omega = K_{\theta_1}$ be a complete graph of order $\theta_1$ and size $\frac{\theta_1(\theta_1-1)}{2}$. Replacing $ZC_1(K_{\theta_1}) = 0$, $ZC_2(K_{\theta_1}) = 0, ZC_1^*(K_{\theta_1}) = 0, M_2(G) = \frac{\theta_1(\theta_1-1)^3}{2}$, and $M_1(K_{\theta_1}) = \theta_1(\theta_1 - 1)^2$ in Theorem 3, we get the required result as

$$ZC_2(\theta^\phi \Omega) = [\frac{2(\theta - 1)\phi + \phi(\phi - 1)(\theta - 1)^2}{2}]^2 [\frac{(\theta_1 - 1)}{2} + \binom{\theta}{2}\phi\theta]\theta_1(\theta_1 - 1)^2 \theta^\phi.$$

□

**Corollary 6.** *Let $\Omega = K_{\theta_1}$ be a complete graph for $\theta_1 \geq 5$. Then,*

$$ZC_1^*(\theta^\phi \Omega) = [\frac{2(\theta - 1)\phi + \phi(\phi - 1)(\theta - 1)^2}{2}][\theta_1 - 1 + \binom{\theta}{2}\phi\theta]\theta_1(\theta_1 - 1)\theta^\phi. \quad (12)$$

**Proof.** Let $\Omega = K_{\theta_1}$ be a complete graph of order $\theta_1$ and size $\frac{\theta_1(\theta_1-1)}{2}$. Using $ZC_1^*(K_{\theta_1}) = 0$, $M_1(K_{\theta_1}) = \theta_1(\theta_1 - 1)^2$ and Theorem 4, we get the required result as

$$ZC_1^*(\theta^\phi \Omega) = [\frac{2(\theta - 1)\phi + \phi(\phi - 1)(\theta - 1)^2}{2}][\theta_1 - 1 + \binom{\theta}{2}\phi\theta]\theta_1(\theta_1 - 1)\theta^\phi. \quad (13)$$

□

## 5. Conclusions

The applicability of this study can be measured by the published work of refs. [10–15,25–30] on Zagreb connection indices, along with the free hand to choose an initial graph $\Omega$ for $\theta^\phi\Omega$ and formation of chemical graphs by the $\theta^\phi\Omega$ network. In Theorem 1, we computed exact formulas for these indices of $\underbrace{K_\theta \times (K_\theta \times (K_\theta \times ( \ldots \times (K_\theta}_{(\phi)\text{ times}} \times \Omega) \ldots)))$ when $\Omega = N_1$ is a single vertex graph. By setting $\theta = 2$ in Theorem 1, Equations (1)–(3), we get Zagreb connection indices of cube of dimension $\phi$ as $ZC_1(2^\phi N_1) = \frac{1}{4}\phi^2(\phi - 1)^2 2^\phi, ZC_2(2^\phi N_1) = \frac{1}{4}\phi^3(\phi - 1)^2 2^{\phi-1}$, and $ZC_1^*(2^\phi N_1) = \phi^2(\phi - 1)2^{\phi-1}$. In Theorem 2, we determined generalized exact formulas for $ZC_1(\theta^\phi\Omega)$ for any connected graph $\Omega$ and determined exact results for $ZC_1(\theta^\phi C_n)$ in Corollary 1 and $ZC_1(\theta^\phi K_{\theta_1})$ in Corollary 4. Further, in Theorem 3, we established bounds for $ZC_2(\theta^\phi\Omega)$ regarding generalized graph $\Omega$ with equality for regular graph $\Omega$ and determined the exact formula in Corollary 2 and Corollary 5 for $\Omega = C_n$ and $\Omega = K_{\theta_1}$, respectively. In Theorem 4, we established bounds for $ZC_1^*(\theta^\phi\Omega)$ with equality over $\{C_3, C_4\}-$free graph $\Omega$. The computed results in Corollary 3 for $ZC_1^*(\theta^\phi K_m)$ and Corollary 6 for $ZC_1^*(\theta^\phi C_n), n \geq 5$ are the application of Theorem 4.

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