

## Zagreb Polynomials and Redefined Zagreb Indices of silicon-carbon $Si_2C_3-I[p,q]$ and $Si_2C_3-II[p,q]$

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### Abstract

The application of graph theory in chemical and molecular structure research far exceeds people's expectations, and it has recently grown exponentially. In the molecular graph, atoms are represented by vertices and bonded by edges. In this report, we study the silicon-carbon  $Si_2C_3-I[p,q]$  and  $Si_2C_3-II[p,q]$ . We compute several Zagreb polynomials and Redefined Zagreb indices of these silicon-carbons.

**Keywords:** Silicon, Zagreb index, Zagreb polynomial.

### 1. Introduction

Silicon has many advantages over other semiconductor materials: it is minimal effort, it is non-toxic, basically its accessibility is unlimited, and it is involved in purging, development for many years behind it. It is used for all cutting-edge electronics badget

The most reliable structures of two-dimensional (2D) silicon-carbon monolayer mixes with different stoichiometric blends were expected in [1] which in light of the molecule swarm streamlining signified as (PSO) method joined with thickness utilitarian hypothesis optimization.

Graphene sheets are effectively limited to [2,3], and from this point on, this honeycomb structure's 2D material is very much due to its surprising mechanical, electronic and optical properties (including its anomalous quantum effect). To a large extent, it aroused a strong interest in research lobby, overwhelming electronic conductivity and

high mechanical quality. In particular, the intriguing electronic properties of graphene make this 2D material potentially useful for faster, smaller electronic products.

Like carbon, silicon also has a honeycomb structure of two-dimensional allotropes, particularly siliconene. So far, a series of efforts have been made to open a band gap on the sheets of silicene. In addition, a two-dimensional silicon-carbon (Si-C) monolayer can be viewed as an undoped two-dimensional carbon monolayer - graphene and an undoped two-dimensional monolayer of silicon - between the siliconene Tuning material. A great deal of effort has been read [4,5] to predict the most stable structure of SiC sheet for more data.

In this paper we study Zagreb polynomials and Redefined Zagreb indices of Silicon Carbide structures.

## 2. Basic Definitions

Many studies have shown that there is a strong intrinsic link between the chemical properties of chemical compounds and drugs (such as boiling point and melting point) and their molecular structure. The topological index defined on the structure of these chemical molecules can help researchers better understand the physical characteristics, chemical reactivity and biological activity. Therefore, the study of topological indices of chemical substances and chemical structures of drugs can make up for the lack of chemical experiments and provide theoretical basis for the preparation of drugs and chemical substances.

In the past two decades, a large number of digital map invariants (topological indices) have been defined and used for correlation analysis in theoretical chemistry, pharmacology, toxicology and environmental chemistry.

The first and second Zagreb indices are one of the oldest and most well-known topological indices defined by Gutman in 1972 and are given different names in the literature, such as the Zagreb group index, Sag. Loeb group parameters and the most common Zagreb index. The Zagreb index is one of the first indices introduced and has been used to study molecular complexity, chirality, ZE isomers and heterogeneous systems. The Zagreb index shows the potential applicability of deriving multiple linear regression models.

The first and the second Zagreb indices [6] are defined as

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)$$

and

$$M_2(G) = \sum_{uv \in E(G)} (d_u \times d_v).$$

For details see [7]. Considering the Zagreb indices, Fath-Tabar ([8]) defined first and the second Zagreb polynomials as

$$M_1(G, x) = \sum_{uv \in E(G)} x^{d_u + d_v}$$

and

$$M_2(G, x) = \sum_{uv \in E(G)} x^{d_u \cdot d_v}.$$

The properties of  $M_1(G, x)$ ,  $M_2(G, x)$  polynomials for some chemical structures have been studied in the literature [9,10].

After that, in [11], the authors defined the third Zagreb index

$$M_3(G) = \sum_{uv \in E(G)} (d_u - d_v).$$

and the polynomial

$$M_3(G, x) = \sum_{uv \in E(G)} x^{d_u - d_v}.$$

In the year 2016, [12] following Zagreb type polynomials were defined

$$M_4(G, x) = \sum_{uv \in E(G)} x^{d_u(d_u + d_v)}$$

$$M_5(G, x) = \sum_{uv \in E(G)} x^{d_v(d_u + d_v)}$$

$$M_{a,b}(G, x) = \sum_{uv \in E(G)} x^{ad_u + bd_v}$$

$$M'_{a,b}(G, x) = \sum_{uv \in E(G)} x^{(d_u+a)(d_v+b)}.$$

Ranjini et al. [13] redefines the Zagreb index, ie, the redefined first, second and third Zagreb indices of graph  $G$ . These indicators appear as

$$\text{Re}ZG_1(G) = \sum_{uv \in E(PD_1)} \frac{d_u + d_v}{d_u \cdot d_v}$$

$$\text{Re}ZG_2(G) = \sum_{uv \in E(PD_1)} \frac{d_u \cdot d_v}{d_u + d_v}$$

$$\text{Re}ZG_3(G) = \sum_{uv \in E(PD_1)} (d_u \cdot d_v)(d_u + d_v).$$

For details about topological indices and its applications we refer [15-22].

### 3. Silicon Carbide $Si_2C_3-I[p, q]$

Figure 1 and Figure 2 show two-dimensional molecular diagrams of silicon carbide  $Si_2C_3-I$ . In order to describe its molecular graph, we have set this way: we define  $p$  as the number of connected units in a row (chain), and  $q$  as the number of connected rows, the number of  $p$  cells per connection. In Figures 3 and 4, we demonstrate how cells are connected in one row (chain) and how one row is connected to another row. We will use  $Si_2C_3-I[p, q]$  to represent this molecular graph.

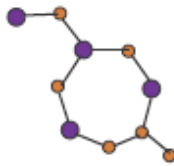


Figure 1. Unit Cell of  $Si_2C_3-I[p, q]$

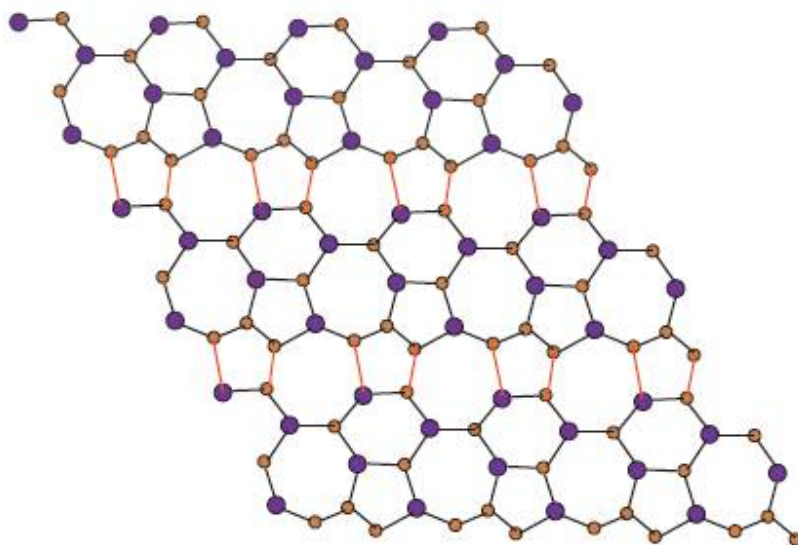


Figure 2. Sheet of  $Si_2C_3-I[p,q]$  for  $p=4$  and  $q=3$

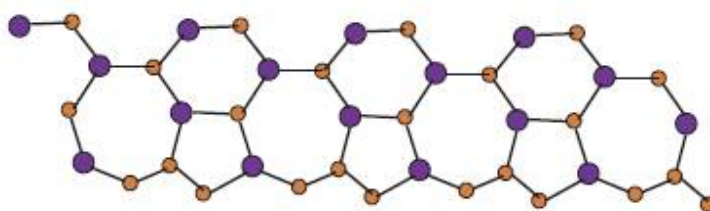


Figure 3. Sheet of  $Si_2C_3-I[p,q]$  for  $p=4$  and  $q=1$

A

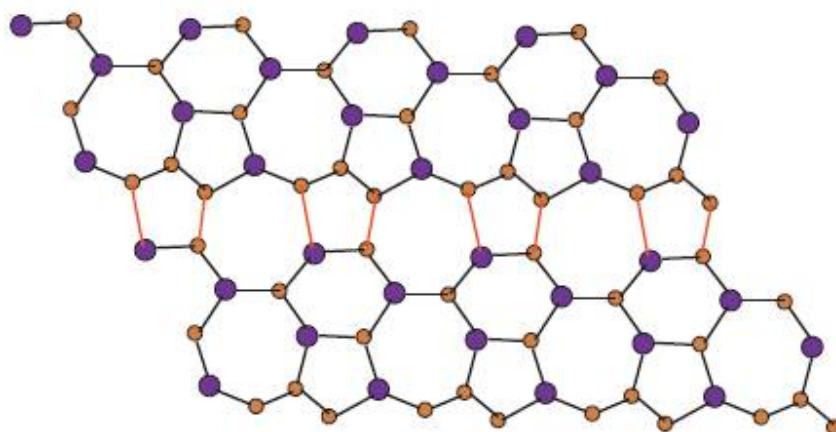


Figure 4. Sheet of  $Si_2C_3-I[p,q]$  for  $p=4$  and  $q=2$

In figures 1-4 Carbon atom C are shown as brown and Silicon atom Si are shown as blue.

**Theorem 1.** Let  $Si_2C_3-I[p,q]$  be the Silicon Carbide. Then

1.  $M_1(Si_2C_3-I, x) = x^3 + (p + 2q + 1)x^4 + (6p + 8q - 9)x^5 + (15pq - 9p - 13q + 7)x^6.$
2.  $M_2(Si_2C_3-I, x) = x^2 + x^3 + (p + 2q)x^4 + (6p + 8q - 9)x^6 + (15pq - 9p - 13q + 7)x^9.$
3.  $M_3(Si_2C_3-I, x) = (15pq - 8p - 11q + 7) + 2(3p + 4q - 4)x + x^2.$
4.  $M_4(Si_2C_3-I, x) = x^3 + x^4 + (p + 2q)x^8 + (6p + 8q - 9)x^{10} + (15pq - 9p - 13q + 7)x^{18}.$
5.  $M_5(Si_2C_3-I, x) = x^6 + x^{12} + (p + 2q)x^8 + (6p + 8q - 9)x^{15} + (15pq - 9p - 13q + 7)x^{18}.$
6.  $M_{a,b}(Si_2C_3-I, x) = 2x^a + (7p + 10q - 9)x^{2a} + (p + 2q + 1)x^{2b} + (15pq - 9p - 13q + 7)x^{3a} + (15pq - 3p - 5q - 1)x^{3b}.$
7.  $M'_{a,b}(Si_2C_3-I, x) = x^{(1+a)(2+b)} + x^{(1+a)(3+b)} + (p + 2q)x^{(2+a)(2+b)} + (6p + 8q - 9)x^{(2+a)(3+b)} + (15pq - 9p - 13q + 7)x^{(3+a)(3+b)}.$

## Proof

We can see from [14] that the total number of vertices are  $10pq$  and total number of edges are  $15pq - 2p - 3q$ .

The edge set of  $Si_2C_3-I[p,q]$  with  $p, q \geq 1$  has following five partitions,

$$\begin{aligned} E_{\{1,2\}} &= \{e = uv \in E(Si_2C_3-I[p,q]) | d_u = 1, d_v = \}, \\ E_{\{1,3\}} &= \{e = uv \in E(Si_2C_3-I[p,q]) | d_u = 1, d_v = \}, \\ E_{\{2,2\}} &= \{e = uv \in E(Si_2C_3-I[p,q]) | d_u = 2, d_v = \}, \\ E_{\{2,3\}} &= \{e = uv \in E(Si_2C_3-I[p,q]) | d_u = 2, d_v = 3\}. \end{aligned}$$

And

$$E_{\{3,3\}} = \{e = uv \in E(Si_2C_3-I[p,q]) | d_u = 3, d_v = \}.$$

Now

$$\begin{aligned} |E_{\{1,2\}}| &= 1, \\ |E_{\{1,3\}}| &= 1, \\ |E_{\{2,2\}}| &= p + 2q, \\ |E_{\{2,3\}}| &= 6p - 1 + 8(q - 1), \end{aligned}$$

And

$$|E_{\{3,3\}}| = 15pq - 9p - 13q + 7.$$

$$\begin{aligned} 1. M_1(Si_2C_3-I[p,q],x) &= \sum_{uv \in E(Si_2C_3-I[p,q])} x^{d_u+d_v} \\ &= \sum_{uv \in E_{\{1,2\}}(Si_2C_3-I[p,q])} x^{1+2} + \sum_{uv \in E_{\{1,3\}}(Si_2C_3-I[p,q])} x^{1+3} + \sum_{uv \in E_{\{2,2\}}(Si_2C_3-I[p,q])} x^{2+2} \\ &\quad + \sum_{uv \in E_{\{2,3\}}(Si_2C_3-I[p,q])} x^{2+3} + \sum_{uv \in E_{\{3,3\}}(Si_2C_3-I[p,q])} x^{3+3} \\ &= |E_{\{1,2\}}(Si_2C_3-I[p,q])| x^3 + |E_{\{1,3\}}(Si_2C_3-I[p,q])| x^4 + |E_{\{2,2\}}(Si_2C_3-I[p,q])| x^4 \\ &\quad + |E_{\{2,3\}}(Si_2C_3-I[p,q])| x^5 + |E_{\{3,3\}}(Si_2C_3-I[p,q])| x^6 \\ &= x^3 + x^4 + (p+2q)x^4 + (6p-1+8(q-1))x^5 + (15pq-9p-13q+7)x^6 \\ &= x^3 + (p+2q+1)x^4 + (6p+8q-9)x^5 + (15pq-9p-13q+7)x^6. \end{aligned}$$

$$\begin{aligned} 2. M_2(Si_2C_3-I[p,q],x) &= \sum_{uv \in E(Si_2C_3-I[p,q])} x^{d_u \times d_v} \\ &= \sum_{uv \in E_{\{1,2\}}(Si_2C_3-I[p,q])} x^{1 \times 2} + \sum_{uv \in E_{\{1,3\}}(Si_2C_3-I[p,q])} x^{1 \times 3} + \sum_{uv \in E_{\{2,2\}}(Si_2C_3-I[p,q])} x^{2 \times 2} \\ &\quad + \sum_{uv \in E_{\{2,3\}}(Si_2C_3-I[p,q])} x^{2 \times 3} + \sum_{uv \in E_{\{3,3\}}(Si_2C_3-I[p,q])} x^{3 \times 3} \\ &= |E_{\{1,2\}}(Si_2C_3-I[p,q])| x^2 + |E_{\{1,3\}}(Si_2C_3-I[p,q])| x^3 + |E_{\{2,2\}}(Si_2C_3-I[p,q])| x^4 \\ &\quad + |E_{\{2,3\}}(Si_2C_3-I[p,q])| x^6 + |E_{\{3,3\}}(Si_2C_3-I[p,q])| x^9 \\ &= x^2 + x^3 + (p+2q)x^4 + (6p+8q-9)x^6 + (15pq-9p-13q+7)x^9. \end{aligned}$$

$$\begin{aligned}
3. M_3(Si_2C_3-I[p,q],x) &= \sum_{uv \in E(Si_2C_3-I[p,q])} x^{d_v-d_u} \\
&= \sum_{uv \in E_{\{1,2\}}(Si_2C_3-I[p,q])} x^{2-1} + \sum_{uv \in E_{\{1,3\}}(Si_2C_3-I[p,q])} x^{3-1} + \sum_{uv \in E_{\{2,2\}}(Si_2C_3-I[p,q])} x^{2-2} + \\
&+ \sum_{uv \in E_{\{2,3\}}(Si_2C_3-I[p,q])} x^{3-2} + \sum_{uv \in E_{\{3,3\}}(Si_2C_3-I[p,q])} x^{3-3} \\
&= |E_{\{1,2\}}(Si_2C_3-I[p,q])| x^1 + |E_{\{1,3\}}(Si_2C_3-I[p,q])| x^2 + |E_{\{2,2\}}(Si_2C_3-I[p,q])| x^0 \\
&+ |E_{\{2,3\}}(Si_2C_3-I[p,q])| x^1 + |E_{\{3,3\}}(Si_2C_3-I[p,q])| x^0 \\
&= x + x^2 + (p+2q) + (6p+8q-9)x + (15pq-9p-13q+7) \\
&= (15pq-8p-11q+7) + (6p+8q-8)x + x^2 \\
&= (15pq-8p-11q+7) + 2(3p+4q-4)x + x^2.
\end{aligned}$$

$$\begin{aligned}
4. M_4(Si_2C_3-I[p,q],x) &= \sum_{uv \in E(Si_2C_3-I[p,q])} x^{d_u(d_u+d_v)} \\
&= \sum_{uv \in E_{\{1,2\}}(Si_2C_3-I[p,q])} x^3 + \sum_{uv \in E_{\{1,3\}}(Si_2C_3-I[p,q])} x^4 + \sum_{uv \in E_{\{2,2\}}(Si_2C_3-I[p,q])} x^8 \\
&+ \sum_{uv \in E_{\{2,3\}}(Si_2C_3-I[p,q])} x^{10} + \sum_{uv \in E_{\{3,3\}}(Si_2C_3-I[p,q])} x^{18} \\
&= |E_{\{1,2\}}(Si_2C_3-I[p,q])| x^3 + |E_{\{1,3\}}(Si_2C_3-I[p,q])| x^4 + |E_{\{2,2\}}(Si_2C_3-I[p,q])| x^8 \\
&+ |E_{\{2,3\}}(Si_2C_3-I[p,q])| x^{10} + |E_{\{3,3\}}(Si_2C_3-I[p,q])| x^{18} \\
&= x^3 + x^4 + (p+2q)x^8 + (6p+8q-9)x^{10} + (15pq-9p-13q+7)x^{18}.
\end{aligned}$$



$$\begin{aligned}
5. M_5(Si_2C_3-I[p,q],x) &= \sum_{uv \in E(Si_2C_3-I[p,q])} x^{d_u+d_v} \\
&= \sum_{uv \in E_{\{1,2\}}(Si_2C_3-I[p,q])} x^6 + \sum_{uv \in E_{\{1,3\}}(Si_2C_3-I[p,q])} x^{12} + \sum_{uv \in E_{\{2,2\}}(Si_2C_3-I[p,q])} x^8 \\
&+ \sum_{uv \in E_{\{2,3\}}(Si_2C_3-I[p,q])} x^{15} + \sum_{uv \in E_{\{3,3\}}(Si_2C_3-I[p,q])} x^{18} \\
&= |E_{\{1,2\}}(Si_2C_3-I[p,q])| x^6 + |E_{\{1,3\}}(Si_2C_3-I[p,q])| x^{12} + |E_{\{2,2\}}(Si_2C_3-I[p,q])| x^8 \\
&+ |E_{\{2,3\}}(Si_2C_3-I[p,q])| x^{15} + |E_{\{3,3\}}(Si_2C_3-I[p,q])| x^{18} \\
&= x^6 + x^{12} + (p+2q)x^8 + (6p+8q-9)x^{15} + (15pq-9p-13q+7)x^{18}.
\end{aligned}$$

$$\begin{aligned}
6. M_{a,b}(Si_2C_3-I[p,q],x) &= \sum_{uv \in E(Si_2C_3-I[p,q])} x^{ad_u+bd_v} \\
&= \sum_{uv \in E_{\{1,2\}}(Si_2C_3-I[p,q])} x^{a+2b} + \sum_{uv \in E_{\{1,3\}}(Si_2C_3-I[p,q])} x^{a+3b} + \sum_{uv \in E_{\{2,2\}}(Si_2C_3-I[p,q])} x^{2a+2b} \\
&+ \sum_{uv \in E_{\{2,3\}}(Si_2C_3-I[p,q])} x^{2a+3b} + \sum_{uv \in E_{\{3,3\}}(Si_2C_3-I[p,q])} x^{3a+3b} \\
&= |E_{\{1,2\}}(Si_2C_3-I[p,q])| x^{a+2b} + |E_{\{1,3\}}(Si_2C_3-I[p,q])| x^{a+3b} + |E_{\{2,2\}}(Si_2C_3-I[p,q])| x^{2a+2b} \\
&+ |E_{\{2,3\}}(Si_2C_3-I[p,q])| x^{2a+3b} + |E_{\{3,3\}}(Si_2C_3-I[p,q])| x^{3a+3b} \\
&= x^{a+2b} + x^{a+3b} + (p+2q)x^{2a+2b} + (6p+8q-9)x^{2a+3b} + (15pq-9p-13q+7)x^{3a+3b} \\
&= 2x^a + (7p+10q-9)x^{2a} + (p+2q+1)x^{2b} + (15pq-9p-13q+7)x^{3a} \\
&+ (15pq-3p-5q-1)x^{3b}
\end{aligned}$$

$$\begin{aligned}
7. M_{a,b}(Si_2C_3-I, x) &= \sum_{uv \in E(Si_2C_3-I)} x^{(d_u+a)(d_v+b)} \\
&= \sum_{uv \in E_{\{1,2\}}(Si_2C_3-I)} x^{(1+a)(2+b)} + \sum_{uv \in E_{\{1,3\}}(Si_2C_3-I)} x^{(1+a)(3+b)} + \sum_{uv \in E_{\{2,2\}}(Si_2C_3-I)} x^{(2+a)(2+b)} \\
&\quad + \sum_{uv \in E_{\{2,3\}}(Si_2C_3-I)} x^{(2+a)(3+b)} + \sum_{uv \in E_{\{3,3\}}(Si_2C_3-I)} x^{(3+a)(3+b)} \\
&= |E_{\{1,2\}}(Si_2C_3-I)| x^{(1+a)(2+b)} + |E_{\{1,3\}}(Si_2C_3-I)| x^{(1+a)(3+b)} + |E_{\{2,2\}}(Si_2C_3-I)| x^{(2+a)(2+b)} \\
&\quad + |E_{\{2,3\}}(Si_2C_3-I)| x^{(2+a)(3+b)} + |E_{\{3,3\}}(Si_2C_3-I)| x^{(3+a)(3+b)} \\
&= x^{(1+a)(2+b)} + x^{(1+a)(3+b)} + (p+2q)x^{(2+a)(2+b)} + (6p+8q-9)x^{(2+a)(3+b)} + (15pq-9p-13q+7)x^{(3+a)(3+b)}.
\end{aligned}$$

**Theorem 2.** Let  $Si_2C_3-I[p, q]$  be the Silicon Carbide. Then,

1.  $\text{Re } ZG_1(Si_2C_3-I[p, q]) = 15pq.$
2.  $\text{Re } ZG_2(Si_2C_3-I[p, q]) = 15pq - \frac{53}{10}p - \frac{79}{10}q + \frac{67}{60}.$
3.  $\text{Re } ZG_3(Si_2C_3-I[p, q]) = 15pq - 290p - 430q + 126.$

**Proof:**

$$\begin{aligned}
1. \operatorname{Re} ZG_1(Si_2C_3-I[p, q]) &= \sum_{uv \in E(Si_2C_3-I[p, q])} \frac{d_u + d_v}{d_u \cdot d_v} \\
&= \sum_{uv \in E_{\{1,2\}}(Si_2C_3-I[p, q])} \frac{1+2}{1 \cdot 2} + \sum_{uv \in E_{\{1,3\}}(Si_2C_3-I[p, q])} \frac{1+3}{1 \cdot 3} + \sum_{uv \in E_{\{2,2\}}(Si_2C_3-I[p, q])} \frac{2+2}{2 \cdot 2} \\
&\quad + \sum_{uv \in E_{\{2,3\}}(Si_2C_3-I[p, q])} \frac{2+3}{2 \cdot 3} + \sum_{uv \in E_{\{3,3\}}(Si_2C_3-I[p, q])} \frac{3+3}{3 \cdot 3} \\
&= |E_{\{1,2\}}(Si_2C_3-I[p, q])| \frac{3}{2} + |E_{\{1,3\}}(Si_2C_3-I[p, q])| \frac{4}{3} + |E_{\{2,2\}}(Si_2C_3-I[p, q])| \frac{4}{4} \\
&\quad + |E_{\{2,3\}}(Si_2C_3-I[p, q])| \frac{5}{6} + |E_{\{3,3\}}(Si_2C_3-I[p, q])| \frac{6}{9} \\
&= \frac{3}{2} + \frac{4}{3} + (p+2q) + \frac{5}{6}(6p+8q-9) + \frac{2}{3}(15pq-9p-13q+7) \\
&= 15pq + (1+5-6)p + \left(2 + \frac{20}{3} - \frac{26}{3}\right)q + \left(\frac{3}{2} + \frac{4}{3} - \frac{15}{2} + \frac{14}{3}\right) \\
&= 15pq + \left(\frac{6+20-26}{3}\right)q + \left(\frac{9+8-45+28}{6}\right) \\
&= 15pq.
\end{aligned}$$

$$\begin{aligned}
2. \operatorname{Re} ZG_2(Si_2C_3-I[p, q]) &= \sum_{uv \in E(Si_2C_3-I[p, q])} \frac{d_u \cdot d_v}{d_u + d_v} \\
&= \sum_{uv \in E_{\{1,2\}}(Si_2C_3-I[p, q])} \frac{1 \cdot 2}{1+2} + \sum_{uv \in E_{\{1,3\}}(Si_2C_3-I[p, q])} \frac{1 \cdot 3}{1+3} + \sum_{uv \in E_{\{2,2\}}(Si_2C_3-I[p, q])} \frac{2 \cdot 2}{2+2} \\
&\quad + \sum_{uv \in E_{\{2,3\}}(Si_2C_3-I[p, q])} \frac{2 \cdot 3}{2+3} + \sum_{uv \in E_{\{3,3\}}(Si_2C_3-I[p, q])} \frac{3 \cdot 3}{3+3} \\
&= |E_{\{1,2\}}(Si_2C_3-I[p, q])| \frac{2}{3} + |E_{\{1,3\}}(Si_2C_3-I[p, q])| \frac{3}{4} + |E_{\{2,2\}}(Si_2C_3-I[p, q])| \frac{4}{4} \\
&\quad + |E_{\{2,3\}}(Si_2C_3-I[p, q])| \frac{6}{5} + |E_{\{3,3\}}(Si_2C_3-I[p, q])| \frac{9}{6} \\
&= \frac{2}{3} + \frac{3}{4} + (p+2q) + \frac{6}{5}(6p+8q-9) + \frac{3}{2}(15pq-9p-13q+7) \\
&= 15pq + \left(1 + \frac{36}{5} - \frac{27}{2}\right)p + \left(2 + \frac{48}{5} - \frac{39}{2}\right)q + \left(\frac{2}{3} + \frac{3}{4} - \frac{54}{5} + \frac{21}{2}\right) \\
&= 15pq + \left(\frac{10+72-135}{10}\right)p + \left(\frac{20+96-195}{10}\right)q + \left(\frac{40+45-648+630}{60}\right) \\
&= 15pq - \frac{53}{10}p - \frac{79}{10}q + \frac{67}{60}.
\end{aligned}$$

$$\begin{aligned}
3. \operatorname{Re} ZG_3(Si_2C_3-I[p, q]) &= \sum_{uv \in E(Si_2C_3-I[p, q])} (d_u \cdot d_v)(d_u + d_v) \\
&= \sum_{uv \in E_{\{1,2\}}(Si_2C_3-I[p, q])} (1 \cdot 2)(1+2) + \sum_{uv \in E_{\{1,3\}}(Si_2C_3-I[p, q])} (1 \cdot 3)(1+3) + \sum_{uv \in E_{\{2,2\}}(Si_2C_3-I[p, q])} (2 \cdot 2)(2+2) \\
&\quad + \sum_{uv \in E_{\{2,3\}}(Si_2C_3-I[p, q])} (2 \cdot 3)(2+3) + \sum_{uv \in E_{\{3,3\}}(Si_2C_3-I[p, q])} (3 \cdot 3)(3+3) \\
&= 6|E_{\{1,2\}}(Si_2C_3-I[p, q])| + 12|E_{\{1,3\}}(Si_2C_3-I[p, q])| + 16|E_{\{2,2\}}(Si_2C_3-I[p, q])| \\
&\quad + 30|E_{\{2,3\}}(Si_2C_3-I[p, q])| + 54|E_{\{3,3\}}(Si_2C_3-I[p, q])| \\
&= 6+12+16(p+2q)+30(6p+8q-9)+54(15pq-9p-13q+7) \\
&= 15pq - 290p - 430q + 126.
\end{aligned}$$

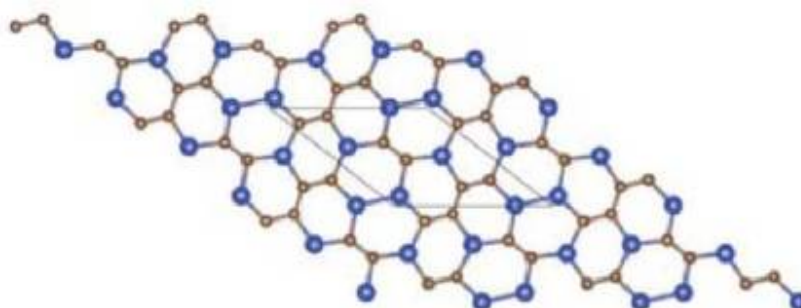
#### 4. Silicon Carbide Si<sub>2</sub>C<sub>3</sub>-I [p, q]

Figure 5-8 shows a two-dimensional molecular map of silicon carbide  $Si_2C_3-II$ . In order to describe its molecular graph, we set this way [14]: we define p as the number of unit

cells connected in a row (chain), and with  $q$ , we represent the number of connected rows, the number of rows per connection It is  $p$  units. In Figures 7 and 8, we demonstrate how cells are connected in a row (chain) and how a row is connected to another row. We will use  $Si_2C_3-II[p,q]$  to represent this molecular graph.



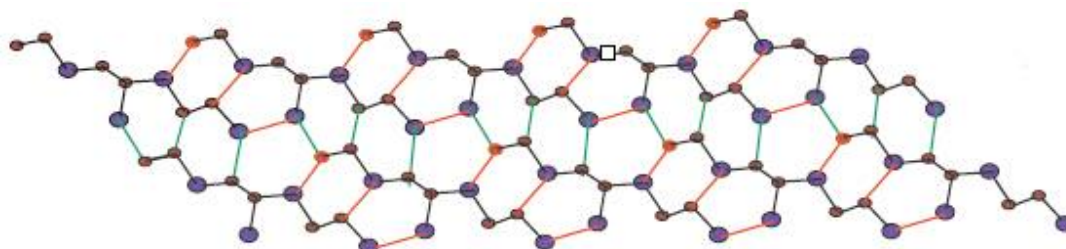
**Figure 5. One Unit of  $Si_2C_3-II[p,q]$**



**Figure 6. Sheet of  $Si_2C_3-II[p,q]$  for  $p=3$  and  $q=3$**



**Figure 7. Sheet of  $Si_2C_3-II[p,q]$  for  $p=5$  and  $q=1$**



**Figure 8. Sheet of  $Si_2C_3-II[p,q]$  for  $p=5$  and  $q=2$**

**Theorem 4** Let  $Si_2C_3-II[p,q]$  be the Silicon Carbide. Then

1.  $M_1(Si_2C_3-II, x) = 2x^3 + (2p + 2q + 1)x^4 + 2(4p + 4q - 7)x^5 + (15pq - 13p - 13q + 11)x^6.$
2.  $M_2(Si_2C_3-II, x) = 2x^2 + x^3 + 2(p + q)x^4 + 2(4p + 4q - 7)x^6 + (15pq - 13p - 13q + 11)x^9.$
3.  $M_3(Si_2C_3-II, x) = (15pq - 11p - 11q + 11) + 4(2p + 2q - 3)x + x^2.$
4.  $M_4(Si_2C_3-II, x) = 2x^3 + x^4 + 2(p + q)x^8 + 2(4p + 4q - 7)x^{10} + (15pq - 13p - 13q + 11)x^{18}.$
5.  $M_5(Si_2C_3-II, x) = 2x^6 + x^{12} + 2(p + q)x^8 + 2(4p + 4q - 7)x^{15} + (15pq - 13p - 13q + 11)x^{18}.$
6.  $M_{a,b}(Si_2C_3-II, x) = 3x^a + 2(5p + 5q - 7)x^{2a} + 2(p + q + 1)x^{2b} + (15pq - 13p - 13q + 11)x^{3a} + (15pq - 5p - 5q - 3)x^{3b}.$
7.  $M'_{a,b}(Si_2C_3-II, x) = 2x^{(1+a)(2+b)} + x^{(1+a)(3+b)} + 2(p + q)x^{(2+a)(2+b)} + 2(4p + 4q - 7)x^{(2+a)(3+b)} + (15pq - 13p - 13q + 11)x^{(3+a)(3+b)}.$

**Proof:** Let  $G$  be the graph of  $Si_2C_3-II[p, q]$  where we define  $p$  as the number of connected unit cells in a row (chain) and by  $q$  we represents the number of connected rows each with  $p$  number of cells. From the graph of  $Si_2C_3-II[p, q]$  we can see that the total number of vertices are  $10pq$  and total number of edges are  $15pq - 3p - 3q$ .

The edge set of  $Si_2C_3-II[p, q]$  with  $p, q \geq 1$  has following five partitions,

$$E_{\{1,2\}} = \{e = uv \in E(Si_2C_3-II[p, q]) | d_u = 1, d_v = \},$$

$$E_{\{1,3\}} = \{e = uv \in E(Si_2C_3-II[p, q]) | d_u = 1, d_v = \},$$

$$E_{\{2,2\}} = \{e = uv \in E(Si_2C_3-II[p, q]) | d_u = 2, d_v = \},$$

$$E_{\{2,3\}} = \{e = uv \in E(Si_2C_3-II[p, q]) | d_u = 2, d_v = 3\}.$$

And

$$E_{\{3,3\}} = \{e = uv \in E(Si_2C_3-II[p, q]) | d_u = 3, d_v = \}.$$

Now

$$|E_{\{1,2\}}| = 2,$$

$$|E_{\{1,3\}}| = 1,$$

$$|E_{\{2,2\}}| = 2p + 2q,$$

$$|E_{\{2,3\}}| = 8p + 8q - 14,$$

And

$$|E_{\{3,3\}}| = 15pq - 13p - 13q + 11.$$

$$\begin{aligned}
 1. M_1(Si_2C_3-II[p, q], x) &= \sum_{uv \in E(Si_2C_3-II[p, q])} x^{d_u + d_v} \\
 &= \sum_{uv \in E_{\{1,2\}}(Si_2C_3-II[p, q])} x^{1+2} + \sum_{uv \in E_{\{1,3\}}(Si_2C_3-II[p, q])} x^{1+3} + \sum_{uv \in E_{\{2,2\}}(Si_2C_3-II[p, q])} x^{2+2} \\
 &\quad + \sum_{uv \in E_{\{2,3\}}(Si_2C_3-II[p, q])} x^{2+3} + \sum_{uv \in E_{\{3,3\}}(Si_2C_3-II[p, q])} x^{3+3} \\
 &= |E_{\{1,2\}}(Si_2C_3-II[p, q])| x^3 + |E_{\{1,3\}}(Si_2C_3-II[p, q])| x^4 + |E_{\{2,2\}}(Si_2C_3-II[p, q])| x^4 \\
 &\quad + |E_{\{2,3\}}(Si_2C_3-II[p, q])| x^5 + |E_{\{3,3\}}(Si_2C_3-II[p, q])| x^6 \\
 &= 2x^3 + x^4 + (2p + 2q)x^4 + (8p + 8q - 14)x^5 + (15pq - 13p - 13q + 11)x^6 \\
 &= 2x^3 + (2p + 2q + 1)x^4 + 2(4p + 4q - 7)x^5 + (15pq - 13p - 13q + 11)x^6.
 \end{aligned}$$

$$\begin{aligned}
 2. M_2(Si_2C_3-II[p, q], x) &= \sum_{uv \in E(Si_2C_3-II[p, q])} x^{d_u \times d_v} \\
 &= \sum_{uv \in E_{\{1,2\}}(Si_2C_3-II[p, q])} x^{1 \times 2} + \sum_{uv \in E_{\{1,3\}}(Si_2C_3-II[p, q])} x^{1 \times 3} + \sum_{uv \in E_{\{2,2\}}(Si_2C_3-II[p, q])} x^{2 \times 2} \\
 &\quad + \sum_{uv \in E_{\{2,3\}}(Si_2C_3-II[p, q])} x^{2 \times 3} + \sum_{uv \in E_{\{3,3\}}(Si_2C_3-II[p, q])} x^{3 \times 3} \\
 &= |E_{\{1,2\}}(Si_2C_3-II[p, q])| x^2 + |E_{\{1,3\}}(Si_2C_3-II[p, q])| x^3 + |E_{\{2,2\}}(Si_2C_3-II[p, q])| x^4 \\
 &\quad + |E_{\{2,3\}}(Si_2C_3-II[p, q])| x^6 + |E_{\{3,3\}}(Si_2C_3-II[p, q])| x^9 \\
 &= 2x^2 + x^3 + (2p + 2q)x^4 + (8p + 8q - 14)x^6 + (15pq - 13p - 13q + 11)x^9 \\
 &= 2x^2 + x^3 + 2(p + q)x^4 + 2(4p + 4q - 7)x^6 + (15pq - 13p - 13q + 11)x^9.
 \end{aligned}$$

$$\begin{aligned}
3. M_3(Si_2C_3-II[p, q], x) &= \sum_{uv \in E(Si_2C_3-II[p, q])} x^{d_v - d_u} \\
&= \sum_{uv \in E_{\{1,2\}}(Si_2C_3-II[p, q])} x^{2-1} + \sum_{uv \in E_{\{1,3\}}(Si_2C_3-II[p, q])} x^{3-1} + \sum_{uv \in E_{\{2,2\}}(Si_2C_3-II[p, q])} x^{2-2} + \\
&+ \sum_{uv \in E_{\{2,3\}}(Si_2C_3-II[p, q])} x^{3-2} + \sum_{uv \in E_{\{3,3\}}(Si_2C_3-II[p, q])} x^{3-3} \\
&= |E_{\{1,2\}}(Si_2C_3-II[p, q])| x^1 + |E_{\{1,3\}}(Si_2C_3-II[p, q])| x^2 + |E_{\{2,2\}}(Si_2C_3-II[p, q])| x^0 \\
&+ |E_{\{2,3\}}(Si_2C_3-II[p, q])| x^1 + |E_{\{3,3\}}(Si_2C_3-II[p, q])| x^0 \\
&= 2x + x^2 + (2p + 2q) + (8p + 8q - 14)x + (15pq - 13p - 13q + 11) \\
&= (15pq - 11p - 11q + 11) + (8p + 8q - 12)x + x^2 \\
&= (15pq - 11p - 11q + 11) + 4(2p + 2q - 3)x + x^2.
\end{aligned}$$

$$\begin{aligned}
4. M_4(Si_2C_3-II[p, q], x) &= \sum_{uv \in E(Si_2C_3-II[p, q])} x^{d_u + d_v} \\
&= \sum_{uv \in E_{\{1,2\}}(Si_2C_3-II[p, q])} x^3 + \sum_{uv \in E_{\{1,3\}}(Si_2C_3-II[p, q])} x^4 + \sum_{uv \in E_{\{2,2\}}(Si_2C_3-II[p, q])} x^8 \\
&+ \sum_{uv \in E_{\{2,3\}}(Si_2C_3-II[p, q])} x^{10} + \sum_{uv \in E_{\{3,3\}}(Si_2C_3-II[p, q])} x^{18} \\
&= |E_{\{1,2\}}(Si_2C_3-II[p, q])| x^3 + |E_{\{1,3\}}(Si_2C_3-II[p, q])| x^4 + |E_{\{2,2\}}(Si_2C_3-II[p, q])| x^8 \\
&+ |E_{\{2,3\}}(Si_2C_3-II[p, q])| x^{10} + |E_{\{3,3\}}(Si_2C_3-II[p, q])| x^{18} \\
&= 2x^3 + x^4 + (2p + 2q)x^8 + (8p + 8q - 14)x^{10} + (15pq - 13p - 13q + 11)x^{18} \\
&= 2x^3 + x^4 + 2(p + q)x^8 + 2(4p + 4q - 7)x^{10} + (15pq - 13p - 13q + 11)x^{18}.
\end{aligned}$$



$$\begin{aligned}
5. M_5(Si_2C_3-II[p,q],x) &= \sum_{uv \in E(Si_2C_3-II[p,q])} x^{d_v(d_u+d_v)} \\
&= \sum_{uv \in E_{\{1,2\}}(Si_2C_3-II[p,q])} x^6 + \sum_{uv \in E_{\{1,3\}}(Si_2C_3-II[p,q])} x^{12} + \sum_{uv \in E_{\{2,2\}}(Si_2C_3-II[p,q])} x^8 \\
&+ \sum_{uv \in E_{\{2,3\}}(Si_2C_3-II[p,q])} x^{15} + \sum_{uv \in E_{\{3,3\}}(Si_2C_3-II[p,q])} x^{18} \\
&= |E_{\{1,2\}}(Si_2C_3-II[p,q])| x^6 + |E_{\{1,3\}}(Si_2C_3-II[p,q])| x^{12} + |E_{\{2,2\}}(Si_2C_3-II[p,q])| x^8 \\
&+ |E_{\{2,3\}}(Si_2C_3-II[p,q])| x^{15} + |E_{\{3,3\}}(Si_2C_3-II[p,q])| x^{18} \\
&= 2x^6 + x^{12} + (2p+2q)x^8 + (8p+8q-14)x^{15} + (15pq-13p-13q+11)x^{18} \\
&= 2x^6 + x^{12} + 2(p+q)x^8 + 2(4p+4q-7)x^{15} + (15pq-13p-13q+11)x^{18}.
\end{aligned}$$

$$\begin{aligned}
6. M_{a,b}(Si_2C_3-II[p,q],x) &= \sum_{uv \in E(Si_2C_3-II[p,q])} x^{(ad_u+bd_v)} \\
&= \sum_{uv \in E_{\{1,2\}}(Si_2C_3-II[p,q])} x^{a+2b} + \sum_{uv \in E_{\{1,3\}}(Si_2C_3-II[p,q])} x^{a+3b} + \sum_{uv \in E_{\{2,2\}}(Si_2C_3-II[p,q])} x^{2a+2b} \\
&+ \sum_{uv \in E_{\{2,3\}}(Si_2C_3-II[p,q])} x^{2a+3b} + \sum_{uv \in E_{\{3,3\}}(Si_2C_3-II[p,q])} x^{3a+3b} \\
&= |E_{\{1,2\}}(Si_2C_3-II[p,q])| x^{a+2b} + |E_{\{1,3\}}(Si_2C_3-II[p,q])| x^{a+3b} + |E_{\{2,2\}}(Si_2C_3-II[p,q])| x^{2a+2b} \\
&+ |E_{\{2,3\}}(Si_2C_3-II[p,q])| x^{2a+3b} + |E_{\{3,3\}}(Si_2C_3-II[p,q])| x^{3a+3b} \\
&= 2x^{a+2b} + x^{a+3b} + (2p+2q)x^{2a+2b} + (8p+8q-14)x^{2a+3b} + (15pq-13p-13q+11)x^{3a+3b} \\
&= 3x^a + (10p+10q-14)x^{2a} + (2p+2q+2)x^{2b} + (15pq-13p-13q+11)x^{3a} \\
&+ (15pq-5p-5q-3)x^{3b} \\
&= 3x^a + 2(5p+5q-7)x^{2a} + 2(p+q+1)x^{2b} + (15pq-13p-13q+11)x^{3a} \\
&+ (15pq-5p-5q-3)x^{3b}.
\end{aligned}$$

$$\begin{aligned}
7. \dot{M}_{a,b}(Si_2C_3-II, x) &= \sum_{w \in E(Si_2C_3-II)} x^{(d_u+a)(d_v+b)} \\
&= \sum_{w \in E_{\{1,2\}}(Si_2C_3-II)} x^{(1+a)(2+b)} + \sum_{w \in E_{\{1,3\}}(Si_2C_3-II)} x^{(1+a)(3+b)} + \sum_{w \in E_{\{2,2\}}(Si_2C_3-II)} x^{(2+a)(2+b)} \\
&+ \sum_{w \in E_{\{2,3\}}(Si_2C_3-II)} x^{(2+a)(3+b)} + \sum_{w \in E_{\{3,3\}}(Si_2C_3-II)} x^{(3+a)(3+b)} \\
&= |E_{\{1,2\}}(Si_2C_3-II)| x^{(1+a)(2+b)} + |E_{\{1,3\}}(Si_2C_3-II)| x^{(1+a)(3+b)} + |E_{\{2,2\}}(Si_2C_3-II)| x^{(2+a)(2+b)} \\
&+ |E_{\{2,3\}}(Si_2C_3-II)| x^{(2+a)(3+b)} + |E_{\{3,3\}}(Si_2C_3-II)| x^{(3+a)(3+b)} \\
&= 2x^{(1+a)(2+b)} + x^{(1+a)(3+b)} + (2p+2q)x^{(2+a)(2+b)} + (8p+8q-14)x^{(2+a)(3+b)} + (15pq-13p-13q+11)x^{(3+a)(3+b)} \\
&= 2x^{(1+a)(2+b)} + x^{(1+a)(3+b)} + 2(p+q)x^{(2+a)(2+b)} + 2(4p+4q-7)x^{(2+a)(3+b)} + (15pq-13p-13q+11)x^{(3+a)(3+b)}.
\end{aligned}$$

**Theorem 2:** Let  $Si_2C_3-II[p, q]$  be the Silicon Carbide. Then,

4.  $\text{Re } ZG_1(Si_2C_3-II[p, q]) = 15pq.$
5.  $\text{Re } ZG_2(Si_2C_3-II[p, q]) = 15pq - \frac{79}{10}p - \frac{79}{10}q + \frac{107}{60}.$
6.  $\text{Re } ZG_3(Si_2C_3-II[p, q]) = 15pq - 430p - 430q + 198.$

**Proof:**

$$\begin{aligned}
1. \operatorname{Re} ZG_1(Si_2C_3-II[p, q]) &= \sum_{uv \in E(Si_2C_3-II[p, q])} \frac{d_u + d_v}{d_u \cdot d_v} \\
&= \sum_{uv \in E_{\{1,2\}}(Si_2C_3-II[p, q])} \frac{1+2}{1 \cdot 2} + \sum_{uv \in E_{\{1,3\}}(Si_2C_3-II[p, q])} \frac{1+3}{1 \cdot 3} + \sum_{uv \in E_{\{2,2\}}(Si_2C_3-II[p, q])} \frac{2+2}{2 \cdot 2} \\
&\quad + \sum_{uv \in E_{\{2,3\}}(Si_2C_3-II[p, q])} \frac{2+3}{2 \cdot 3} + \sum_{uv \in E_{\{3,3\}}(Si_2C_3-II[p, q])} \frac{3+3}{3 \cdot 3} \\
&= |E_{\{1,2\}}(Si_2C_3-II[p, q])| \frac{3}{2} + |E_{\{1,3\}}(Si_2C_3-II[p, q])| \frac{4}{3} + |E_{\{2,2\}}(Si_2C_3-II[p, q])| \frac{4}{4} \\
&\quad + |E_{\{2,3\}}(Si_2C_3-II[p, q])| \frac{5}{6} + |E_{\{3,3\}}(Si_2C_3-II[p, q])| \frac{6}{9} \\
&= 2\left(\frac{3}{2}\right) + \frac{4}{3} + (2p+2q) + \frac{5}{6}(8p+8q-14) + \frac{2}{3}(15pq-13p-13q+11) \\
&= 15pq + \left(2 + \frac{20}{3} - \frac{26}{3}\right)p + \left(2 + \frac{20}{3} - \frac{26}{3}\right)q + \left(3 + \frac{4}{3} - \frac{35}{3} + \frac{22}{3}\right) \\
&= 15pq + \left(\frac{6+20-26}{3}\right)p + \left(\frac{6+20-26}{3}\right)q + \left(\frac{9+4-35+22}{3}\right) \\
&= 15pq.
\end{aligned}$$

$$\begin{aligned}
2. \operatorname{Re} ZG_2(Si_2C_3-II[p, q]) &= \sum_{uv \in E(Si_2C_3-II[p, q])} \frac{d_u \cdot d_v}{d_u + d_v} \\
&= \sum_{uv \in E_{\{1,2\}}(Si_2C_3-II[p, q])} \frac{1 \cdot 2}{1+2} + \sum_{uv \in E_{\{1,3\}}(Si_2C_3-II[p, q])} \frac{1 \cdot 3}{1+3} + \sum_{uv \in E_{\{2,2\}}(Si_2C_3-II[p, q])} \frac{2 \cdot 2}{2+2} \\
&\quad + \sum_{uv \in E_{\{2,3\}}(Si_2C_3-II[p, q])} \frac{2 \cdot 3}{2+3} + \sum_{uv \in E_{\{3,3\}}(Si_2C_3-II[p, q])} \frac{3 \cdot 3}{3+3} \\
&= |E_{\{1,2\}}(Si_2C_3-II[p, q])| \frac{2}{3} + |E_{\{1,3\}}(Si_2C_3-II[p, q])| \frac{3}{4} + |E_{\{2,2\}}(Si_2C_3-II[p, q])| \frac{4}{4} \\
&\quad + |E_{\{2,3\}}(Si_2C_3-II[p, q])| \frac{6}{5} + |E_{\{3,3\}}(Si_2C_3-II[p, q])| \frac{9}{6} \\
&= 2\left(\frac{2}{3}\right) + \frac{3}{4} + (2p+2q) + \frac{6}{5}(8p+8q-14) + \frac{3}{2}(15pq-13p-13q+11) \\
&= 15pq + \left(2 + \frac{48}{5} - \frac{39}{2}\right)p + \left(2 + \frac{48}{5} - \frac{39}{2}\right)q + \left(\frac{4}{3} + \frac{3}{4} - \frac{84}{5} + \frac{33}{2}\right) \\
&= 15pq + \left(\frac{20+96-195}{10}\right)p + \left(\frac{20+96-195}{10}\right)q + \left(\frac{80+45-1008+990}{60}\right) \\
&= 15pq - \frac{79}{10}p - \frac{79}{10}q + \frac{107}{60}.
\end{aligned}$$

$$\begin{aligned}
3. \operatorname{Re} ZG_3(Si_2C_3-II[p, q]) &= \sum_{uv \in E(Si_2C_3-II[p, q])} (d_u \cdot d_v)(d_u + d_v) \\
&= \sum_{uv \in E_{\{1,2\}}(Si_2C_3-II[p, q])} (1 \cdot 2)(1+2) + \sum_{uv \in E_{\{1,3\}}(Si_2C_3-II[p, q])} (1 \cdot 3)(1+3) + \sum_{uv \in E_{\{2,2\}}(Si_2C_3-II[p, q])} (2 \cdot 2)(2+2) \\
&\quad + \sum_{uv \in E_{\{2,3\}}(Si_2C_3-II[p, q])} (2 \cdot 3)(2+3) + \sum_{uv \in E_{\{3,3\}}(Si_2C_3-II[p, q])} (3 \cdot 3)(3+3) \\
&= 6|E_{\{1,2\}}(Si_2C_3-II[p, q])| + 12|E_{\{1,3\}}(Si_2C_3-II[p, q])| + 16|E_{\{2,2\}}(Si_2C_3-II[p, q])| \\
&\quad + 30|E_{\{2,3\}}(Si_2C_3-II[p, q])| + 54|E_{\{3,3\}}(Si_2C_3-II[p, q])| \\
&= 2(6) + 12 + 16(2p+2q) + 30(8p+8q-14) + 54(15pq-13p-13q+11) \\
&= 15pq - 430p - 430q + 198.
\end{aligned}$$

### Concluding Remarks

In this paper, we have computed several algebraic Zagreb type polynomials and first, second and third Zagreb indices for the **silicon-carbon**  $Si_2C_3-I[p,q]$  and  $Si_2C_3-II[p,q]$ .

Our results are important for the researcher working in this area of research and applicable in many areas of applied sciences, for example, chemistry, physics, electronics, etc.

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