Combinatorial Counting Relations of C_3, C_4–Free Graphs

G.Britto Antony Xavier
Department of Mathematics, Sacred Heart College,
Tirupattur-635601, Tamil Nadu, India.
shcbritto@yahoo.co.in
E.Suresh
Department of Mathematics, Velammal Engineering College,
Surapet, Chennai-600066, Tamil Nadu, India.
sureshkako@gmail.com

Abstract

In this paper, we have calculated the combinatorial counting relations varying over the 3–vertex paths of a simple graph G, by restricting our attention to C_3, C_4– free graphs.

1 Introduction

Mathematical chemistry is a branch of theoretical chemistry using mathematical methods to discuss and predict molecular properties without necessarily referring to quantum mechanics [2, 16, 23]. Chemical graph theory is a branch of mathematical chemistry which applies graph theory in mathematical modeling of chemical phenomena [7].

A molecular graph is a representation of the structural formula of a chemical compound such that its vertices correspond to the atoms and the edges to the bonds. Topological indices are the numerical values associated with chemical structures which are used to study and predict the structure-property correlations of organic compounds.

The topological indices $M_1(G)$ and $M_2(G)$ are among the oldest and most thoroughly examined graph-based molecular structure descriptors and has been closely correlated with many chemical properties [3, 17]. Recently, the Zagreb indices and their variants have been used to study molecular complexity, chirality, ZE-isomerism and heterosystems etc. The Zagreb indices are also used by various researchers in their QSPR and QSAR studies. Thus, it attracted more and more attention from chemists and mathematicians. They were defined in 1972 by Ivan Gutman [3, 4] and are given different names in the literature, such as the Zagreb group indices, the Zagreb group parameters and most often, the Zagreb indices. They were eventually named first and second Zagreb indices [1].

Let $G = (V, E)$ be a simple graph with $|V|$ vertices and $|E|$ edges. The degree of v, denoted by $d(v)$ in G. Then

$$M_1 = M_1(G) = \sum_{v \in V(G)} d(v)^2 \tag{1}$$

$$M_2 = M_2(G) = \sum_{uv \in E(G)} d(u)d(v). \tag{2}$$

A numerous amount of research articles were published in various scientic publications on the Zagreb indices. For details of their chemical applications and mathematical theory see the surveys [6, 8, 12, 13, 24] and the references cited therein.
Li and Zheng in [9] defined the first general Zagreb index, defined by

$$M_1^{\alpha} = M_1^{\alpha}(G) = \sum_{v \in V(G)} d(v)^{\alpha}. \tag{3}$$

The present author's defined the second general Zagreb index and their counting relations are established [5] in which, it is defined as

$$M_2^{\alpha} = M_2^{\alpha}(G) = \sum_{uv \in E(G)} [d(u)d(v)]^{\alpha} \tag{4}$$

where $\alpha \in \mathbb{R}$. In [14, 11, 15, 18, 5] various properties and relations of the first general Zagreb index are discussed.

In analogy with Eqs. (3) and (4) the first and second general path Zagreb indices are defined by

$$P_l M_1^{\alpha} = P_l M_1^{\alpha}(G) = \sum_{d(u,v)=l-1} \left[d(u)^{\alpha-1} + d(v)^{\alpha-1}\right] \tag{5}$$

$$P_l M_2^{\alpha} = P_l M_2^{\alpha}(G) = \sum_{d(u,v)=l-1} [d(u)d(v)]^{\alpha} \tag{6}$$

where $l \in N - 1$. Notice that for $l = 2$ is simply the first and second general Zagreb indices [5]. This paper deals with the combinatorial counting relations of general path Zagreb indices in C_3, C_4- free graphs.

2 Preliminaries

Throughout the paper we consider $e \sim f$, where $e(= uw)$ and $f(= wv)$ are edges which are adjacent, i.e., they share a common end-vertex in G. In what $d(e)$ denotes the degree of the edge e in G, which is defined by $d(e) = d(u) + d(w) - 2$. We denote by P_n and C_n the $n-$vertex graph equals to the path and cycle, respectively. For $u, v \in V(G)$, the path length between u and v are denoted by $d(u, v)$ in G.

Let G and H be graphs. We denote by $\sigma_G(H)$ the number of distinct subgraphs of the graph G which are isomorphic to H. Let α, β and γ be positive integers. $D_{\alpha,\beta}$ and $D_{\alpha,\gamma,\beta}$ are the double and triple star trees on $\alpha+\beta+2$, $\alpha+\gamma+\beta+3$ vertices respectively. $D_{\alpha,\beta}$ is obtained from P_2, by attaching α pendent vertices to its one of the vertex and β pendent vertices to its other vertex. $D_{\alpha,\gamma,\beta}$ is obtained from P_3, by attaching α, β pendent vertices to its end vertices and γ pendent vertices to its middle vertex.
It is easy to see that for $\alpha \neq \beta$,

$$\sigma_G(D_{\alpha,\beta}) = \sum_{uv \in E(G)} \left[\begin{array}{l} \binom{d(u)-1}{\alpha}\binom{d(v)-1}{\beta} \\ +\binom{d(u)-1}{\beta}\binom{d(v)-1}{\alpha} \end{array} \right] \tag{7}$$

$$\sigma_G(D_{\alpha,\gamma,\beta}) = \sum_{e \sim f} \left[\begin{array}{l} \binom{d(u)-1}{\alpha}\binom{d(w)-2}{\gamma}\binom{d(v)-1}{\beta} \\ +\binom{d(u)-1}{\beta}\binom{d(w)-2}{\gamma}\binom{d(v)-1}{\alpha} \end{array} \right] \tag{8}$$

whereas

$$\sigma_G(D_{\alpha,\alpha}) = \sum_{uv \in E(G)} \binom{d(u)-1}{\alpha}\binom{d(v)-1}{\alpha} \tag{9}$$

$$\sigma_G(D_{\alpha,\gamma,\alpha}) = \sum_{e \sim f} \binom{d(u)-1}{\alpha}\binom{d(w)-2}{\gamma}\binom{d(v)-1}{\alpha} \tag{10}$$

For $l, \alpha = 2$ in (5) is the well known relation for the ordinary first Zagreb index

$$P_2M_1^2 = 2\sigma_G(P_3) + 2|E| \tag{11}$$

whereas, $\alpha = 1$ in (6) yields the second Zagreb index

$$P_2M_2^1 = P_2M_1^2 + \sigma_G(P_4) - |E|, \tag{12}$$

obtained from

$$\sigma_T(P_4) = \sum_{uv \in E(T)} [d_T(u) - 1][d_T(v) - 1],$$

which was first established in 2009 [19] and later also in [20, 21, 22]. It is easy to see that it is a special case for $m = 3$, of theorem 1 [5].

Theorem 1 *Let G be a C_i- free graph* ($2 < i \leq m$). *Then*

$$\sigma_G(P_{m+1}) = \sum_{d(u,v)=m-2} [d(u) - 1][d(v) - 1] \quad (13)$$

$$= \frac{1}{2} \sum_{d(u,v)=m-1} [(d(u) - 1) + (d(v) - 1)]. \quad (14)$$

In addition, the extension for triangle containing graphs is also given in [25], as

$$\sigma_G(P_4) + 3\sigma(C_3) = \sum_{uv \in E(G)} [d(u) - 1][d(v) - 1] \quad (15)$$

Eq. (15) can be rewritten as

$$P_2M_2^1 = \sigma_G(P_4) + 2\sigma_G(P_3) + 3\sigma(C_3) + |E|. \quad (16)$$

In [5], the authors have obtained the identities for $l = 2$ and $\alpha \geq 2$ in (5) and (6) in which the subgraphs are depicted in Fig.1 as follows,

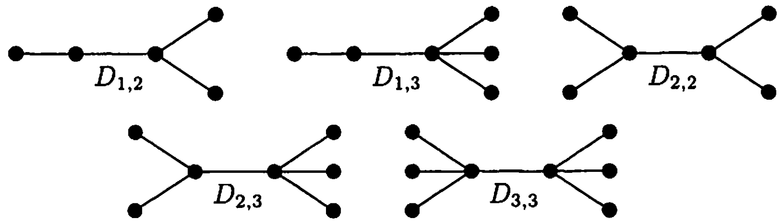

Figure 1: The subgraphs encounterd in Theorems 2 and 3

Theorem 2 *Let G be a simple graph. Then*

$$P_2M_1^3 = 3!\sigma_G(K_{1,3}) + 3P_2M_1^2 - 4|E| \quad (17)$$

$$P_2M_1^4 = 4!\sigma_G(K_{1,4}) + 6P_2M_1^3 - 11P_2M_1^2 + 12|E| \quad (18)$$

$$P_2M_1^5 = 5!\sigma_G(K_{1,5}) + 10P_2M_1^4 - 35P_2M_1^3 + 50P_2M_1^2 - 48|E|. \quad (19)$$

Theorem 3 *Let G be a triangle - free graph. Then*

$$P_2M_2^2 = 4\sigma_G(D_{2,2}) + 6\sigma_G(D_{1,2}) + 9M_2^1 + M_1^3 - 9M_1^2 + 8|E|$$

$$P_2M_2^3 = 36\sigma_G(D_{3,3}) + 144\sigma_G(D_{2,2}) + 72\sigma_G(D_{2,3}) + 42\sigma_G(D_{1,3}) + 84\sigma_G(D_{1,2}) + 49M_2^1 + M_1^4 - 49M_1^2 + 48|E|.$$

3 Main Results

We now give some significant results relating general path Zagreb indices in C_3, C_4- free graphs.

Lemma 4 *Let G be a simple graph. Then*

$$P_3M_1^2 = 2\sigma_G(P_4) + 2\sigma_G(P_3) + 6\sigma_G(C_3) \tag{20}$$

Proof. Comparing, for $m = 3$ in (14) and (16) yields the identity.

Theorem 5 *Let G be a C_3 - free graph. Then*

$$\begin{aligned}
P_3M_1^3 &= 2!\sigma_G(D_{1,2}) + 6\sigma_G(P_4) + 2\sigma_G(P_3) && (21)\\
P_3M_1^4 &= 3!\sigma_G(D_{1,3}) + 12\sigma_G(D_{1,2}) + 14\sigma_G(P_4) + 2\sigma_G(P_3) && (22)\\
P_3M_1^5 &= 4!\sigma_G(D_{1,4}) + 60\sigma_G(D_{1,3}) + 50\sigma_G(D_{1,2}) && (23)\\
&\quad +30\sigma_G(P_4) + 2\sigma_G(P_3)\\
P_3M_1^6 &= 5!\sigma_G(D_{1,5}) + 360\sigma_G(D_{1,4}) + 390\sigma_G(D_{1,3}) + 180\sigma_G(D_{1,2})\\
&\quad +62\sigma_G(P_4) + 2\sigma_G(P_3)\\
P_3M_1^7 &= 6!\sigma_G(D_{1,6}) + 2520\sigma_G(D_{1,5}) + 3360\sigma_G(D_{1,4}) + 2100\sigma_G(D_{1,3})\\
&\quad +602\sigma_G(D_{1,2}) + 126\sigma_G(P_4) + 2\sigma_G(P_3)\\
P_3M_1^8 &= 7!\sigma_G(D_{1,7}) + 37360\sigma_G(D_{1,6}) + 21000\sigma_G(D_{1,5}) + \sigma_G(D_{1,4})\\
&\quad +10206\sigma_G(D_{1,3}) + 1932\sigma_G(D_{1,2}) + 254\sigma_G(P_4) + 2\sigma_G(P_3)\\
P_3M_1^9 &= 8!\sigma_G(D_{1,8}) + 181440\sigma_G(D_{1,7}) + 332640\sigma_G(D_{1,6})\\
&\quad +317520\sigma_G(D_{1,5}) + 166824\sigma_G(D_{1,4}) + 46620\sigma_G(D_{1,3})\\
&\quad +6050\sigma_G(D_{1,2}) + 510\sigma_G(P_4) + 2\sigma_G(P_3)\\
P_3M_1^{10} &= 9!\sigma_G(D_{1,9}) + 1814400\sigma_G(D_{1,8}) + 3780000\sigma_G(D_{1,7})\\
&\quad +4233600\sigma_G(D_{1,6}) + 2739240\sigma_G(D_{1,5}) + 1020600\sigma_G(D_{1,4})\\
&\quad +204630\sigma_G(D_{1,3}) + 18660\sigma_G(D_{1,2}) + 1022\sigma_G(P_4) + 2\sigma_G(P_3)
\end{aligned}$$

Proof. By applying Eqs. (8), (5) and (20) we get

$$\begin{aligned}
\sigma_G(D_{0,0,2}) &= \sum_{e\sim f}\left[\binom{d(u)-1}{2} + \binom{d(v)-1}{2}\right]\\
&= \frac{1}{2!}\left[\sum_{e\sim f}\left[d(u)^2 + d(v)^2\right] - 3\sum_{e\sim f}\left[d(u)+d(v)\right] + 4\sigma_G(P_3)\right]
\end{aligned}$$

obviously $\sigma_G(D_{0,0,\beta}) = \sigma_G(D_{1,\beta})$ and $\sigma_G(D_{0,\gamma,\beta}) = \sigma_G(D_{1+\gamma,\beta})$ and using (5)

$$\begin{aligned}
\sigma_G(D_{1,2}) &= \frac{1}{2!}\left[P_3M_1^3 - 3P_3M_1^2 + 4\sigma_G(P_3)\right]\\
&= \frac{1}{2!}\left[P_3M_1^3 - 3\left(2\sigma_G(P_4) + 2\sigma_G(P_3)\right) + 4\sigma_G(P_3)\right]
\end{aligned}$$

from which Eq.(21) straightforwardly follows. The remaining equalities are obtained recursively in a fully analogous manner.

Corollary 5.1 *Let G be a C_3 - free graph. Then*

$$\begin{aligned}
P_3M_1^3(G) &= 2!\sigma_G(D_{1,2}) + 3P_3M_1^2(G) - 4\sigma_G(P_3)\\
P_3M_1^4(G) &= 3!\sigma_G(D_{1,3}) + 6P_3M_1^3(G) - 11P_3M_1^2(G) + 12\sigma_G(P_3)\\
P_3M_1^5(G) &= 4!\sigma_G(D_{1,4}) + 10M_1^4(G) - 35M_1^3(G)\\
&\quad +50M_1^2(G) - 48\sigma_G(P_3)\\
P_3M_1^6(G) &= 5!\sigma_G(D_{1,5}) + 15P_3M_1^5(G) - 85P_3M_1^4(G)\\
&\quad +225P_3M_1^3(G) - 274P_3M_1^2(G) + 240\sigma_G(P_3)\\
P_3M_1^7(G) &= 6!\sigma_G(D_{1,6}) + 21P_3M_1^6(G) - 175P_3M_1^5(G)\\
&\quad +735P_3M_1^4(G) - 1624P_3M_1^3(G)\\
&\quad +1764P_3M_1^2(G) - 1440\sigma_G(P_3)\\
P_3M_1^8(G) &= 7!\sigma_G(D_{1,7}) + 28P_3M_1^7(G) - 322P_3M_1^6(G)\\
&\quad +1960P_3M_1^5(G) - 6769P_3M_1^4(G) + 13132P_3M_1^3(G)\\
&\quad -13068P_3M_1^2(G) + 10080\sigma_G(P_3)\\
P_3M_1^9(G) &= 8!\sigma_G(D_{1,8}) + 36M_1^8(G) - 546M_1^7(G)\\
&\quad +4536P_3M_1^6(G) - 22449P_3M_1^5(G) + 67284P_3M_1^4(G)\\
&\quad -118124P_3M_1^3(G) + 109584P_3M_1^2(G) - 80640\sigma_G(P_3)\\
P_3M_1^{10}(G) &= 9!\sigma_G(D_{1,9}) + 45P_3M_1^9(G) - 870P_3M_1^8(G)\\
&\quad +9450P_3M_1^7(G) - 63273P_3M_1^6(G) + 269325P_3M_1^5(G)\\
&\quad -723680P_3M_1^4(G) + 1172700P_3M_1^3(G)\\
&\quad -1026576P_3M_1^2(G) + 725760\sigma_G(P_3).
\end{aligned}$$

Combining Eq.(12) and Theorem 1, we get

Corollary 5.2 *Let G be a simple graph. Then*

$$P_3M_1^2 = 2P_2M_2^1 - P_2M_1^2.$$

Lemma 6 *Let G be a C_3, C_4- free graph. Then*

$$P_3M_2^1 = \sigma_G(P_5) + 2\sigma_G(P_4) + \sigma_G(P_3)$$

Proof. For $m = 4$ in (13) implies,

$$\sigma_G(P_5) = \sum_{e\sim f}[d(u)-1][d(v)-1] = P_3M_2{}^1 - P_3M_1^2 + \sigma_G(P_3).$$

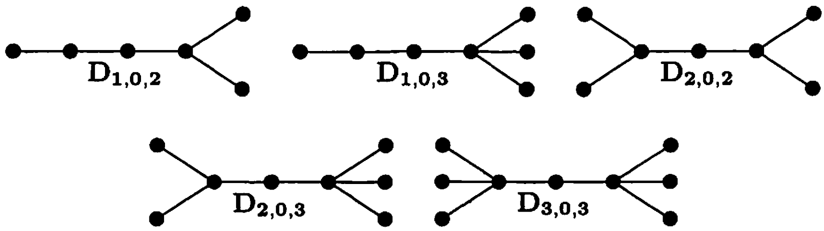

Figure 2: The subgraphs encounterd in Theorem 7.

Theorem 7 *Let G be a C_3, C_4-free graph. Then*

$$\begin{aligned} P_3M_2^2 &= 4\sigma_G(D_{2,0,2}) + 6\sigma_G(D_{1,0,2}) + 2\sigma_G(D_{1,2}) \\ &\quad +9\sigma_G(P_5) + 6\sigma_G(P_4) + \sigma_G(P_3) \end{aligned} \tag{24}$$

$$\begin{aligned} P_3M_2^3 &= 36\sigma_G(D_{3,0,3}) + 72\sigma_G(D_{2,0,3}) + 144\sigma_G(D_{2,0,2}) \\ &\quad +42\sigma_G(D_{1,0,3}) + 84\sigma_G(D_{1,0,2}) + 6\sigma_G(D_{1,3}) + 12\sigma_G(D_{1,2}) \\ &\quad +49\sigma_G(P_5) + 14\sigma_G(P_4) + \sigma_G(P_3) \end{aligned} \tag{25}$$

Proof. Using $\alpha, \beta = 2$ and $\gamma = 0$ in (10), we get

$$\begin{aligned} \sigma_G(D_{2,0,2}) &= \sum_{e\sim f} \binom{d(u)-1}{2}\binom{d(v)-1}{2} \\ 4\sigma_G(D_{2,0,2}) &= \sum_{e\sim f} d(u)^2 d(v)^2 - 3\sum_{e\sim f}\left[d(u)^2 d(v) + d(u)d(v)^2\right] \\ &\quad +2\sum_{e\sim f}\left[d(u)^2 + d(v)^2\right] - 6\sum_{e\sim f}\left[d(u)+d(v)\right] \\ &\quad +9\sum_{e\sim f} d(u)d(v) + 4\sigma_G(P_3) \\ P_3M_2^2 &= 4\sigma_G(D_{2,0,2}) + 3\sum_{e\sim f}\left[d(u)^2 d(v) + d(u)d(v)^2\right] \\ &\quad -2P_3M_1^3 + 6P_3M_1^2 - 9P_3M_2^1 - 4\sigma_G(P_3) \end{aligned}$$

$$\text{i.e.,} \sum_{e\sim f}\left[d(u)^2 d(v) + d(u)d(v)^2\right] = 2\sigma_G(D_{1,0,2}) + 6P_3M_2^1 + P_3M_1^3 - 5P_3M_1^2 + 4\sigma_G(P_3) \tag{26}$$

where we used Eq. (21) and lemma 4, 6.

Using the similar arguments for $\alpha, \beta = 3$ and $\gamma = 0$, we obtain

$$\begin{aligned}
\sigma_G(D_{2,0,2}) &= \sum_{e\sim f}\binom{d(u)-1}{3}\binom{d(v)-1}{3} \\
36\sigma_G(D_{3,0,3}) &= P_3M_2^3 + 36P_3M_2^2 + 121P_3M_2^1 \\
&\quad +11\sum_{e\sim f}\left[d(u)^3d(v) + d(u)d(v)^3\right] \\
&\quad -66\sum_{e\sim f}\left[d(u)^2d(v) + d(u)d(v)^2\right] \\
&\quad -6\sum_{e\sim f}\left[d(u)^3d(v)^2 + d(u)^2d(v)^3\right] \\
&\quad -6P_3M_1^4 + 36P_3M_1^3 - 66P_3M_1^2 + 36\sigma_G(P_3)
\end{aligned}$$

using Eq.(8) we obtain

$$\begin{aligned}
\sum_{e\sim f}\left[d(u)^3d(v)^2 + d(u)^2d(v)^3\right] &= 12\sigma_G(D_{2,0,3}) + 12P_3M_2^2 + 66P_3M_2^1 \\
&\quad +3\sum_{e\sim f}\left[d(u)^3d(v) + d(u)d(v)^3\right] \\
&\quad -29\sum_{e\sim f}\left[d(u)^2d(v) + d(u)d(v)^2\right] \\
&\quad -2P_3M_1^4 + 18P_3M_1^3 - 40P_3M_1^2 + 24\sigma_G(P_3)
\end{aligned} \tag{27}$$

$$\begin{aligned}
\sum_{e\sim f}\left[d(u)^3d(v) + d(u)d(v)^3\right] &= 6\sigma_G(D_{1,0,3}) - 22P_3M_2^1 \\
&\quad +6\sum_{e\sim f}\left[d(u)^2d(v) + d(u)d(v)^2\right] \\
&\quad +P_3M_1^4 - 6P_3M_1^3 + 17P_3M_1^2 - 12\sigma_G(P_3)
\end{aligned} \tag{28}$$

where we used Eq. (21) and combining Eqs. (21), (22), (24), (26), (27), (28) with lemma 4, 6 yields (25).

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