Advanced Studies in Contemporary Mathematics
34 (2024), No. 2, pp. 87 - 101

www.jangjeon.or.kr
http://dx.doi.org/10.17777/ascm2024.34.2.87

# $M$-POLYNOMIAL AND TOPOLOGICAL INDICES OF PTHALOCYANINE BASED METAL ORGANIC FRAMEWORKS

JOSÉ LUIS LÓPEZ-BONILLA, TAEKYUN KIM, E. LAVANYA, M. A. SRIRAJ, AND P. SIVA KOTA REDDY

Abstract. Metal-organic frameworks (MOF's) are organic-inorganic hybrid materials with crystalline pores that are made up of a predictable arrangement of positively charged metal ions encircled by organic "linker" molecules. Although the structure of MOF can be considered as a chemical graph, there have been very few works on dealing with topological indices on MOF's. In this article, we investigate the degree-based structural indices of pthalocyanine-based metal organic frameworks.

2020 Mathematics Subject Classification. 05C92

Keywords and phrases. $M$-Polynomial, Topological indices, Pthalocyanine based MOF.

## 1. Introduction

Topological Indices are molecular descriptors emanated from its structure of chemical compound. In chemistry, topology helps as a tool to analyse and study the molecular structures. One of the prominent explored TI's in chemical graph theory is degree based TI's, which are used to study different physio chemical properties and biological activities of several chemical compounds/drugs.

Metal-organic frameworks (MOF's) are emerging class of two or three dimensional (2D or 3D) materials manufactured by assembling inorganic and organic connectors via coordination bonds. MOF's are potential candidates for gas storage, separation, detection and sensing, catalysis and drug delivery applications owing to their flexibility, porosity, high surface area and functionality surface. MOF's show an extraordinarily high porosity with up to 9.000 $m^2/g$ combined with a high crystallinity has not been surpassed by any other porous material till date. They have recently been used as heterogeneous catalysts in Friedel Craft reactions, condensation reactions, oxidation reactions, coupling reactions, etc. However, due to its low thermal stability and moisture sensitivity, its catalyst application is limited. Although the first 3D coordination polymer was published by Saito and co-workers in 1959 [8], the first MOF constructed by organic linkers and metal-ions with potential voids was introduced in the late 1990s [12]. Since then, thousands of MOF structures have been reported with a variety of constituents, geometry, size and functionality.

Over the past few decades, the design, synthesis, characterization, properties, and application of MOF's have grown rapidly. Transition metals, alkaline earth metals, $p$-block elements, actynides, and even mixed metals are used to synthesize MOF's. Unlike conventional inorganic materials, such as zeolites and silicates, MOF's ensure that they tightly control their composition, shape, pores and functions by carefully selecting building units and incorporating intelligent functions.

Porphyrins are fascinating building blocks for creating useful porous materials, along with their related derivatives like phthalocyanines. Although porphyrin-based MOF's have been produced three decades ago, the area is still emerging and chemically strong frameworks, which are required for better applications, have just realised recently. The discovery of porphyrins and phthalocyanines with different coordinating groups (phosphonate, azolates, phenolates, etc.) has contributed to this advancement in part because it has enabled the associated MOF's to move beyond metal-carboxylates and achieve novel topologies and characteristics. Combining MOF's with materials that include carbon structures, such as graphene, porphyrin, and carbon nanotubes is an effective method for increasing the properties of MOF's for example; conductivity. Metal ion moieties can be added to MOF materials to improve their catalytic characteristics.

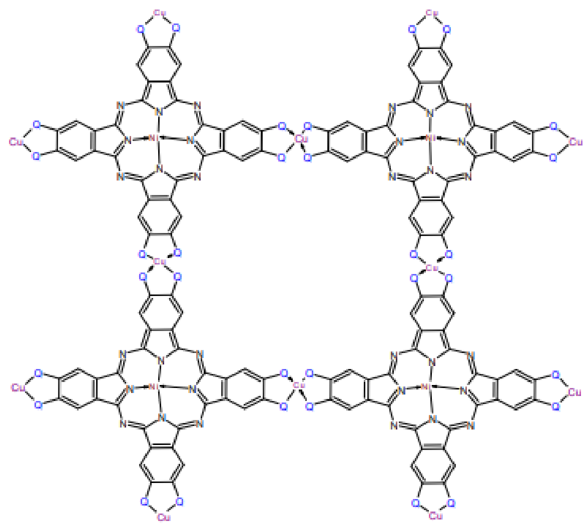

FIGURE 1. Structure of Pthalocyanine based Metal Organic Frameworks

In this article, we study on the structure of some phthalocyanine based MOF's and calculated degree based topological indices by using $M$-polynomial. A python program is written to get the numerical values of topological indices derived for various $m$ and $n$ values. At the end Comparative study and graphical representation of the computed topological indices is done.

## 2. Degree Based Topological Indices

The First Zagreb index was introduced by Gutman and Trinajstic [6] given as:

$$M_1 = \sum_{pq \in E(G)} (d_p + d_q).$$

Gutman [1] proposed the Second Zagreb index in 1972, which is given as:

$$M_2 = \sum_{pq \in E(G)} (d_p \times d_q).$$

The Second Modified Zagreb [15] index is defined as:

$${}^mM_2 = \sum_{pq \in E(G)} \frac{1}{d_p d_q}.$$

In 1987, Fajtlowicz [5] in proposed the Harmonic index and stated as:

$$H(G) = \sum_{pq \in E(G)} \frac{2}{d_p + d_q}.$$

The Inverse sum index [13] is defined as:

$$I(G) = \sum_{pq \in E(G)} \frac{d_p d_q}{d_p + d_q}.$$

The Atom bond connectivity index is contributed by Estrada et al. [3]. It is exemplified as:

$$ABC(G) = \sum_{pq \in E(G)} \sqrt{\frac{d_p + d_q - 2}{d_p \cdot d_q}}.$$

The Geometric-arithmetic index of a graph is established by Vukicevic et al. [14]. It is defined as:

$$GA(G) = \sum_{pq \in E(G)} \frac{2\sqrt{d_p \cdot d_q}}{d_p + d_q}.$$

Symmetric division index is proposed as:

$$SSD(G) = \sum_{pq \in E(G)} \frac{min(d_p, d_q)}{max(d_p, d_q)} + \frac{max(d_p, d_q)}{min(d_p, d_q)}$$

First $K$ Banhatti index [9] is proposed as:

$$B_1(G) = \sum_{pq \in E(G)} (d_p + d_{pq}).$$

Second $K$ Banhatti index is given as:

$$B_2(G) = \sum_{pq \in E(G)} (d_p . d_{pq}).$$

First $K$ Hyper Banhatti index [10] is defined as:

$$HB_1(G) = \sum_{pq \in E(G)} (d_p + d_{pq})^2.$$

Second $K$ Hyper Banhatti index is given as:

$$HB_2(G) = \sum_{pq \in E(G)} (d_p.d_{pq})^2.$$

Modified First $K$ Banhatti index [11] is proposed as:

$$^mB_1(G) = \sum_{pq \in E(G)} \frac{1}{d_p + d_{pq}}.$$

Modified Second $K$ Banhatti index is defined as:

$$^mB_2(G) = \sum_{pq \in E(G)} \frac{1}{d_p.d_{pq}}.$$

Harmonic $K$ Banhatti index is defined as:

$$H_a(G) = \sum_{pq \in E(G)} \frac{2}{d_p + d_{pq}}.$$

## 3. $M$-polynomial and TI's of MOF

$M$-Polynomial helps in the study of behaviour of molecular struct Topological indices are calculated by some derivatives and integration' $M$-Polynomial. In this section we computed many degree based topolog indices mentioned in above section via $M$-Polynomial.

$M$-Polynomial is introduced by Deutsch and Klavzar [2] in 2015 and fined as:

$$M(G; x, y) = \sum_{\delta \leq i \leq j \leq \triangle} m_{ij}(G) x^i y^j$$

where $\delta = min\{d_p | p \in V(G)\}$, $\triangle = max\{d_p | p \in V(G)\}$ and $m_{ij}(G)$ is the number of edges $pq \in E(G)$ such that $\{d_p; d_q\} = \{i : j\}$.

Considering $M(G; x, y) = f(x, y)$, where the operators are defined as

$D_x = x\dfrac{\partial(f(x, y))}{\partial x}$,

$D_y = y\dfrac{\partial(f(x, y))}{\partial y}$,

$L_x(f(x, y)) = f(x^2, y)$,

$L_y(f(x, y)) = f(x, y^2)$,

$S_x(f(x, y)) = \int_0^x \dfrac{f(t, y)}{t} dt$, $S_y(f(x, y)) = \int_0^y \dfrac{f(x, t)}{t} dt$,

$J(f(x, y)) = f(x, x), Q_\alpha(f(x, y)) = x^\alpha f(x, y)$,

$D_x^{\frac{1}{2}}(f(x, y)) = \sqrt{x\dfrac{\partial(f(x, y))}{\partial x}}.\sqrt{f(x, y)}$,

$D_y^{\frac{1}{2}}(f(x, y)) = \sqrt{y\dfrac{\partial(f(x, y))}{\partial y}}.\sqrt{f(x, y)}$,

$S_x^{\frac{1}{2}}(f(x, y)) = \sqrt{\int_0^x \dfrac{f(t, y)}{t} dt}.\sqrt{f(x, y)}$, and

$S_y^{\frac{1}{2}} f(x, y) = \sqrt{\int_0^y \dfrac{f(x, t)}{t} dt}.\sqrt{f(x, y)}$.

TABLE 1. Derivation of some degree based topological indices from M-polynomial.

| Topological index | Derivation from M-Polynomial |
|---|---|
| $M_1[f(x,y)]$ | $(D_x + D_y)[f(x,y)]_{x=y=1}$ |
| $M_2[f(x,y)]$ | $D_xD_y[f(x,y)]_{x=y=1}$ |
| ${}^mM_2[f(x,y)]$ | $S_xS_y[f(x,y)]_{x=y=1}$ |
| $H[f(x,y)]$ | $2S_xJ[f(x,y)]_{x=1}$ |
| $I[f(x,y)]$ | $S_xJD_xD_y[f(x,y)]_{x=1}$ |
| $SSD[f(x,y)]$ | $(D_xS_y + S_xD_y)[f(x,y)]_{x=y=1}$ |
| $ABC[f(x,y)]$ | $D_x^{\frac{1}{2}}Q_{-2}JS_x^{\frac{1}{2}}S_y^{\frac{1}{2}}[f(x,y)]_{x=1}$ |
| $GA[f(x,y)]$ | $2S_xJD_x^{\frac{1}{2}}D_y^{\frac{1}{2}}[f(x,y)]_{x=1}$ |
| $B_1[f(x,y)]$ | $(D_x + D_y + 2D_xQ_{-2}J)[f(x,y)]_{x=y=1}$ |
| $B_2[f(x,y)]$ | $D_xQ_{-2}J(D_x + D_y)[f(x,y)]_{x=1}$ |
| $HB_1[f(x,y)]$ | $(D_x^2 + D_y^2 + 2D_x^2Q_{-2}J + 2D_xQ_{-2}J(D_x + D_y))[f(x,y)]_{x=y=1}$ |
| $HB_2[f(x,y)]$ | $D_x^2Q_{-2}J(D_x^2 + D_y^2)[f(x,y)]_{x=1}^m$ |
| ${}^mB_1[f(x,y)]$ | $S_xQ_{-2}J(L_x + L_y)[f(x,y)]_{x=1}^m$ |
| ${}^mB_2[f(x,y)]$ | $S_xQ_{-2}J(S_x + S_y)[f(x,y)]_{x=1}$ |
| $H_b[f(x,y)]$ | $2S_xQ_{-2}J(L_x + L_y)[f(x,y)]_{x=1}$ |

## 4. COMPUTING $M$-POLYNOMIAL OF PHTHALOCYANINE BASED MOF

Let $G$ be the molecular graph of the Phthalocyacine based MOF, then $M$-polynomial of it is,

$$M[G;x,y] = 4(m+n)x^2y^2 + 32mnx^2y^3 + (8mn - 4m - 4n)x^2y^4 + 24mnx^3y^3 + 4mnx^3y^4.$$

Let $G$ be the graph of Phthalocyanine based MOF, from Figure 1 it can be observed that the number of vertices in $G$ is $51mn + m + n$, in which $20mn + 2m + 2n$ vertices are of degree 2, $28mn$ vertices are of degree 3 and $3mn - m - n$ vertices are of degree 4. The total number of edges in $G$ are $68mn$, based on the degree of end vertices of each edge we have five partitions as :
$E_1(G) = \{pq \in E(G); d_p = 2 \textit{ and } d_q = 2\}$,
$E_2(G) = \{pq \in E(G); d_p = 2 \textit{ and } d_q = 3\}$,
$E_3(G) = \{pq \in E(G); d_p = 2 \textit{ and } d_q = 4\}$,
$E_4(G) = \{pq \in E(G); d_p = 3 \textit{ and } d_q = 3\}$,
$E_5(G) = \{pq \in E(G); d_p = 3 \textit{ and } d_q = 4\}$.
Then $|E_1(G)| = 4(m+n)$, $|E_2(G)| = 32mn$, $|E_3(G)| = 8mn - 4m - 4n$, $|E_4(G)| = 24mn$, $|E_5(G)| = 4mn$.

Now, by using the definition of $M$-polynomial we compute the $M$-polynomial of Phthalocyanine based MOF as:

$$M(G,x,y) = \sum_{\delta \le i \le j \le \triangle} m_{ij} x^i y^j,$$

$$= \sum_{2 \le i \le j \le 4} m_{ij} x^i y^j,$$

$$= \sum_{2\le 2} m_{22}x^2y^2 + \sum_{2\le 3} m_{23}x^2y^3 + \sum_{2\le 4} m_{24}x^2y^4 + \sum_{3\le 3} m_{33}x^3y^3 + \sum_{3\le 4} m_{34}x^3y^4,$$

$$= 4(m+n)x^2y^2 + 32mnx^2y^3 + (8mn-4m-4n)x^2y^4 + 24mnx^3y^3 + 4mnx^3y^4.$$

**Theorem 4.1.** *Let $G$ be the graph representing the molecular structure of Phthalocyanine based MOF's where, $M[G;x,y] = 4(m+n)x^2y^2+32mnx^2y^3+(8mn-4m-4n)x^2y^4+24mnx^3y^3+4mnx^3y^4$.*
*Then,*

(1) $M_1(G) = 380mn - 8m - 8n$.
(2) $M_2(G) = 520mn - 16m - 16n$.
(3) ${}^mM_2(G) = \frac{28}{3}mn + \frac{1}{2}m + \frac{1}{2}n$.
(4) $H(G) = 24.3mn + 1.33m + 1.33n$.
(5) $SSD(G) = 145.66mn - 2m - 2n$.
(6) $I(G) = 325.25mn - 28m - 28n$.
(7) $ABC(G) = [\frac{32}{\sqrt{6}} + 4\sqrt{2} + \frac{16}{3} + 2\sqrt{5}]mn + (2-2\sqrt{2})m + (2-2\sqrt{2})n$.
(8) $GA(G) = [\frac{64\sqrt{6}}{5} + \frac{16\sqrt{2}}{3} + \frac{16\sqrt{3}}{7} + 72]mn + [4 - \frac{8\sqrt{2}}{3}]m + [4 - \frac{8\sqrt{2}}{3}]n$.
(9) $B_1(G) = 868mn - 24m - 24n$.
(10) $B_2(G) = 1244mn - 64m - 64n$.
(11) $HB_1(G) = 5236mn - 276m - 276n$.
(12) $HB_2(G) = 14276mn - 1152m - 1152n$.
(13) ${}^mB_1(G) = \frac{41311}{1890}mn - \frac{m}{6} - \frac{n}{6}$.
(14) ${}^mB_2(G) = \frac{2614}{180}mn + \frac{5}{4}m + \frac{5}{4}n$.
(15) $H_b(G) = \frac{14449}{315}mn + \frac{5}{3}m + \frac{5}{3}n$.

*Proof.* ***Proof:*** Let $M[G;x,y] = f(x,y)$, then

(1) ***First Zagreb Index***
$(D_x + D_y)f(x,y) = 16(m+n)x^2y^2 + 160mnx^2y^3 + (48mn - 24m - 24n)x^2y^4 + 144mnx^3y^3 + 28mnx^3y^4$,
$M_1(G) = (D_x + D_y)[f(x,y)]_{x=y=1} = 380mn - 8m - 8n$.

(2) ***Second Zagreb Index***
$(D_xD_y)f(x,y) = 16(m+n)x^2y^2 + 192mnx^2y^3 + (64mn - 32m - 32n)x^2y^4 + 216mnx^3y^3 + 48mnx^3y^4$
$M_2(G) = (D_xD_y)[f(x,y)]_{x=y=1} = 520mn - 16m - 16n$.

(3) ***Second Modified Zagreb Index***
$S_y f(x,y) = 2(m+n)x^2y^2 + \frac{32}{3}mnx^2y^3 + (2mn-m-n)x^2y^4 + 8mnx^3y^3 + mnx^3y^4$,
$S_xS_y f(x,y) = (m+n)x^2y^2 + \frac{16}{3}mnx^2y^3 + \frac{1}{2}(2mn-m-n)x^2y^4 + \frac{8}{3}mnx^3y^3 + \frac{1}{3}mnx^3y^4$,
${}^mM_2(G) = S_xS_y[f(x,y)]_{x=y=1} = \frac{28}{3}mn + \frac{1}{2}m + \frac{1}{2}n.$

(4) ***Harmonic Index***
$Jf(x,y) = 4(m+n)x^4 + 32mnx^5 + (32mn-4m-4n)x^6 + 4mnx^7$,
$S_xJf(x,y) = (m+n)x^4 + \frac{32}{5}mnx^5 + \frac{1}{6}(32mn-4m-4n)x^6 + \frac{4}{7}mnx^7$,
$H(G) = 2S_xJ[f(x,y)]_{x=1} = 24.3mn + 1.33m + 1.33n.$

(5) ***Symmetric Division Index***
$D_xS_y f(x,y) = 4(m+n)x^2y^2 + \frac{64}{3}mnx^2y^3 + (4mn-2m-2n)x^2y^4 + 24mnx^3y^3 + 3mnx^3y^4$,
$S_xD_y f(x,y) = 4(m+n)x^2y^2 + 48mnx^2y^3 + (16mn-8m-8n)x^2y^4 + 24mnx^3y^3 + \frac{16}{3}mnx^3y^4$,
$(D_xS_y + S_xD_y)f(x,y) = 8(m+n)x^2y^2 + \frac{208}{3}mnx^2y^3 + (20mn - 10m - 10n)x^2y^4 + 48mnx^3y^3 + \frac{34}{3}mnx^3y^4$,
$SSD(G) = (D_xS_y + S_xD_y)[f(x,y)]_{x=y=1} = 145.66mn - 2m - 2n.$

(6) ***Inverse Sum Index***
$JD_xD_y f(x,y) = 16(m+n)x^4 + 192mnx^5 + (280mn-32m-32n)x^6 + 48mnx^7$,

$S_xJD_xD_yf(x,y) = 4(m+n)x^4 + \dfrac{192}{5}mnx^5 + \dfrac{1}{6}(280mn - 32m - 32n)x^6 + \dfrac{48}{7}mnx^7,$
$I(G) = S_xJD_xD_y[f(x,y)]_{x=1} = 325.25mn - 28m - 28n.$

(7) ***Atom-Bond Connectivity Index***
$S_y^{\frac{1}{2}}f(x,y) = \frac{4}{\sqrt{2}}(m+n)x^2y^2 + \frac{32}{\sqrt{3}}mnx^2y^3 + (4mn-2m-2n)x^2y^4 + \frac{24}{\sqrt{3}}mnx^3y^3 + 2mnx^3y^4,$
$S_x^{\frac{1}{2}}S_y^{\frac{1}{2}}f(x,y) = (m+n)x^2y^2 + \frac{32}{3\sqrt{2}}mnx^2y^3 + \frac{1}{\sqrt{2}}(4mn-2m-2n)x^2y^4 + \frac{8}{3}mnx^3y^3 + 2mnx^3y^4,$
$JS_x^{\frac{1}{2}}S_y^{\frac{1}{2}}f(x,y) = (m+n)x^6 + \frac{32}{3\sqrt{2}}mnx^5 + \frac{1}{\sqrt{2}}(4mn-2m-2n)x^6 + \frac{8}{3}mnx^6 + 2mnx^7,$
$Q_{-2}JS_x^{\frac{1}{2}}S_y^{\frac{1}{2}}f(x,y) = (m+n)x^4 + \frac{32}{3\sqrt{2}}mnx^3 + \frac{1}{\sqrt{2}}(4mn-2m-2n)x^4 + \frac{8}{3}mnx^4 + 2mnx^5,$
$D_x^{\frac{1}{2}}Q_{-2}JS_x^{\frac{1}{2}}S_y^{\frac{1}{2}}f(x,y) = 2(m+n)x^4 + \frac{32}{3\sqrt{2}}mnx^3 + \sqrt{2}(4mn-2m-2n)x^4 + \frac{16}{3}mnx^4 + 2\sqrt{5}mnx^5,$
$ABC(G) = D_x^{\frac{1}{2}}Q_{-2}JS_x^{\frac{1}{2}}S_y^{\frac{1}{2}}[f(x,y)]_{x=1} = [\frac{32}{\sqrt{6}} + 4\sqrt{2} + \frac{16}{3} + 2\sqrt{5}]mn + (2-2\sqrt{2})m + (2-2\sqrt{2})n.$

(8) ***Geometric Arithmetic Index***
$D_y^{\frac{1}{2}}f(x,y) = 4\sqrt{2}(m+n)x^2y^2 + 32\sqrt{3}mnx^2y^3 + (16mn-8m-8n)x^2y^4 + 24\sqrt{3}mnx^3y^3 + 8mnx^3y^4,$
$D_x^{\frac{1}{2}}D_y^{\frac{1}{2}}f(x,y) = 8(m+n)x^2y^2 + 32\sqrt{6}mnx^2y^3 + (16mn-8m-8n)\sqrt{2}x^2y^4 + 216mnx^3y^3 + 8\sqrt{3}mnx^3y^4,$
$JD_x^{\frac{1}{2}}D_y^{\frac{1}{2}}f(x,y) = 8(m+n)x^4 + 32\sqrt{6}mnx^5 + (16mn-8m-8n)\sqrt{2}x^6 + 216mnx^6 + 8\sqrt{3}mnx^7,$
$S_xJD_x^{\frac{1}{2}}D_y^{\frac{1}{2}}f(x,y) = 2(m+n)x^4 + \frac{32\sqrt{6}}{5}mnx^5 + (\frac{8}{3}mn - \frac{4}{3}m - \frac{4}{3}n)\sqrt{2}x^6 + 36mnx^6 + \frac{8\sqrt{3}}{7}mnx^7,$
$2S_xJD_x^{\frac{1}{2}}D_y^{\frac{1}{2}}f(x,y) = 4(m+n)x^4 + \frac{64\sqrt{6}}{5}mnx^5 + (\frac{16}{3}mn - \frac{8}{3}m - \dfrac{8}{3}n)\sqrt{2}x^6 + 72mnx^6 + \frac{16\sqrt{3}}{7}mnx^7,$
$GA(G) = 2S_xJD_x^{\frac{1}{2}}D_y^{\frac{1}{2}}[f(x,y)]_{x=1} = [\frac{64\sqrt{6}}{5} + \frac{16\sqrt{2}}{3} + \frac{16\sqrt{3}}{7} + 72]mn + [4 - \frac{8\sqrt{2}}{3}]m + [4 - \frac{8\sqrt{2}}{3}]n.$

(9) ***The First K Banhatti Index***
$(D_x + D_y)[f(x,y)]_{x=y=1} = 380mn - 8m - 8n,$
$Jf(x,y) = 4(m+n)x^4 + 32mnx^5 + (32mn-4m-4n)x^6 + 4mnx^7,$
$Q_{-2}Jf(x,y) = 4(m+n)x^2 + 32mnx^3 + (32mn-4m-4n)x^4 + 4mnx^5,$
$D_xQ_{-2}Jf(x,y) = 8(m+n)x^2 + 96mnx^3 + (128mn-16m-16n)x^4 + 20mnx^5,$

$2D_xQ_{-2}Jf(x,y) = 16(m+n)x^2 + 192mnx^3 + (256mn - 32m - 32n)x^4 + 40mnx^5$,
$2D_xQ_{-2}J[f(x,y)]_{x=1} = 588mn - 16m - 16n$,
$B_1(G) = (D_x + D_y + 2D_xQ_{-2}J)[f(x,y)]_{x=y=1} = 868mn - 24m - 24n$.

(10) ***The Second K Banhatti Index***
$J(D_x + D_y)f(x,y) = 16(m+n)x^4 + 306mnx^5 + (48mn - 24m - 24n)x^6 + 28mnx^7$,
$Q_{-2}J(D_x + D_y)f(x,y) = 16(m+n)x^2 + 306mnx^3 + (48mn - 24m - 24n)x^4 + 28mnx^5$,
$D_xQ_{-2}J(D_x + D_y)f(x,y) = 32(m+n)x^2 + 912mnx^3 + (192mn - 96m - 96n)x^4 + 140mnx^5$,
$B_2(G) = 1244mn - 64m - 64n$.

(11) ***The First K hyper Banhatti Index***
$D_x^2 f(x,y) = 16(m+n)x^2y^2 + 128mnx^2y^3 + (32mn - 16m - 16n)x^2y^4 + 216mnx^3y^3 + 36mnx^3y^4$,
$D_y^2 f(x,y) = 16(m+n)x^2y^2 + 128mnx^2y^3 + (128mn - 64m - 64n)x^2y^4 + 216mnx^3y^3 + 64mnx^3y^4$,
$Q_{-2}Jf(x,y) = 4(m+n)x^2 + 32mnx^3 + (32mn - 4m - 4n)x^4 + 4mnx^5$,
$4(m+n)x^2 + 32mnx^3 + (32mn - 4m - 4n)x^4 + 4mnx^5$,
$D_x^2Q_{-2}Jf(x,y) = 16(m+n)x^2 + 288mnx^3 + (512mn - 64m - 64n)x^4 + 100mnx^5$,
$2D_x^2Q_{-2}J[f(x,y)]_{x=1} = 1800mn - 96m - 96n$,
$D_xQ_{-2}J(D_x + D_y)f(x,y) = 32(m+n)x^2 + 912mnx^3 + (192mn - 96m - 96n)x^4 + 140mnx^5$,
$2D_xQ_{-2}J(D_x + D_y)[f(x,y)]_{x=1} = 2488mn - 128m - 128n$,
$HB(G) = (D_x^2 + D_y^2 + 2D_x^2Q_{-2}J + 2D_xQ_{-2}J(D_x + D_y))[f(x,y)]_{x=y=1} = 5236mn - 276m - 276n$.

(12) ***The Second K hyper Banhatti Index***
$(D_x^2 + D_y^2)f(x,y) = 32(m+n)x^2y^2 + 256mnx^2y^3 + (160mn - 80m - 80n)x^2y^4 + 432mnx^3y^3 + 100mnx^3y^4$,
$J(D_x^2 + D_y^2)f(x,y) = 32(m+n)x^4 + 256mnx^5 + (160mn - 80m - 80n)x^6 + 432mnx^6 + 100mnx^7$,
$Q_{-2}J(D_x^2 + D_y^2)f(x,y) = 32(m+n)x^2 + 256mnx^3 + (160mn - 80m - 80n)x^4 + 432mnx^4 + 100mnx^5$,
$D_x^2Q_{-2}J(D_x^2 + D_y^2)f(x,y) = 128(m+n)x^2 + 2304mnx^3 + (2560mn - 1280m - 1280n)x^4 + 6912mnx^4 + 2500mnx^5$,
$HB_2(G) = D_x^2Q_{-2}J(D_x^2 + D_y^2)[f(x,y)]_{x=1} = 14276mn - 1152m - 1152n$.

(13) ***Modified First K Banhatti Index***
$L_xf(x,y) = 4(m+n)x^4y^2 + 32mnx^4y^3 + (8mn - 4m - 4n)x^4y^4 + 24mnx^6y^3 + 4mnx^6y^4$,
$L_yf(x,y) = 4(m+n)x^2y^4 + 32mnx^2y^6 + (8mn - 4m - 4n)x^2y^8 + 24mnx^3y^6 + 4mnx^3y^8$,
$J(L_x + L_y)f(x,y) = 4(m+n)x^6 + 32mnx^7 + (8mn - 4m - 4n)x^8 +$

$24mnx^9 + 4mnx^{10} + 4(m+n)x^6 + 32mnx^8 + (8mn-4m-4n)x^{10} + 24mnx^9 + 4mnx^{11}$,
$Q_{-2}J(L_x+L_y)f(x,y) = 4(m+n)x^4+32mnx^5+(8mn-4m-4n)x^6+24mnx^7 + 4mnx^8 + 4(m+n)x^4 + 32mnx^6 + (8mn-4m-4n)x^8 + 24mnx^7 + 4mnx^9$,
$S_xQ_{-2}J(L_x+L_y)f(x,y) = 2(m+n)x^4 + \frac{32}{5}mnx^5 + \frac{1}{6}(8mn-4m-4n)x^6 + \frac{24}{7}mnx^7 + \frac{1}{2}mnx^8 + \frac{16}{3}mnx^6 + (mn-\frac{1}{2}m-\frac{1}{2}n)x^8 + \frac{24}{7}mnx^7 + \frac{4}{9}mnx^9$,
${}^mB_1(G) = S_xQ_{-2}J(L_x+L_y)[f(x,y)]_{x=1} = \frac{41311}{1890}mn - \frac{m}{6} - \frac{n}{6}$.

(14) ***Modified Second K Banhatti Index***
$(S_x+S_y)f(x,y) = 4(m+n)x^2y^2+\frac{80}{3}mnx^2y^3+(6mn-3m-3n)x^2y^4+16mnx^3y^3 + \frac{7}{3}mnx^3y^4$,
$J(S_x+S_y)f(x,y) = 4(m+n)x^4 + \frac{80}{3}mnx^5 + (6mn-3m-3n)x^6 + 16mnx^6 + \frac{7}{3}mnx^7$,
$Q_{-2}J(S_x+S_y)f(x,y) = 4(m+n)x^2+\frac{80}{3}mnx^3+(6mn-3m-3n)x^4+16mnx^4 + \frac{7}{3}mnx^5$,
$S_xQ_{-2}J(S_x+S_y)f(x,y) = 2(m+n)x^2 + \frac{80}{9}mnx^3 + \frac{1}{4}(6mn-3m-3n)x^4 + 4mnx^4 + \frac{7}{15}mnx^5$,
${}^mB_2(G) = S_xQ_{-2}J(S_x+S_y)[f(x,y)]_{x=1} = \frac{2614}{180}mn + \frac{5}{4}m + \frac{5}{4}n$.

(15) ***Harmonic K Banhatti Index***
$2S_xQ_{-2}J(L_x+L_y)f(x,y) = 4(m+n)x^4 + \frac{64}{5}mnx^5 + \frac{1}{3}(8mn-4m-4n)x^6 + \frac{48}{7}mnx^7 + mnx^8 + \frac{32}{3}mnx^6 + (2mn-m-n)x^8 + \frac{48}{7}mnx^7 + \frac{8}{9}mnx^9$,
$H_b(G) = 2S_xQ_{-2}J(L_x+L_y)[f(x,y)]_{x=1} = \frac{14449}{315}mn + \frac{5}{3}m + \frac{5}{3}n$.
□

## 5. Program to Generate the Values of the Derived Indices for any Value of $m$ and $n$

print("Numerical Comparision of Derived Degree Based Indices")
print (" $'m=n', 'a', 'b', 'c', 'd', 'e', 'f'$")
for $m$ in range(1,11):
$n = m$
$mn = int(m*n)$
$M_1 = (380mn) - (8m) - (8n)$
$M_2 = (520mn) - (16m) - (16n)$
${}^mM_2 = \frac{28}{3}mn + \frac{1}{2}m + \frac{1}{2}n$
$H = 24.3mn + 1.33m + 1.33n$
$SSD = 145.66mn - 2m - 2n$
$I = 325.25mn - 28m - 28n$
$ABC = [\frac{32}{\sqrt{6}} + 4\sqrt{2} + \frac{16}{3} + 2\sqrt{5}]mn + (2-2\sqrt{2})m + (2-2\sqrt{2})n$
$GA = [\frac{64\sqrt{6}}{5} + \frac{16\sqrt{2}}{3} + \frac{16\sqrt{3}}{7} + 72]mn + [4 - \frac{8\sqrt{2}}{3}]m + [4 - \frac{8\sqrt{2}}{3}]n$
$B_1 = 868mn - 24m - 24n$
$B_2 = 1244mn - 64m - 64n$
$HB_1 = 5236mn - 276m - 276n$

$HB_2 = 14276mn - 1152m - 1152n$
${}^{m}B_1 = \frac{41311}{1890}mn - \frac{m}{6} - \frac{n}{6}$
${}^{m}B_2 = \frac{2614}{180}mn + \frac{5}{4}m + \frac{5}{4}n$
$H_b = \frac{14449}{315}mn + \frac{5}{3}m + \frac{5}{3}n$
$print("m, M_1, M_2, {}^{m}M_2, round(H, 2), SSD, I, ABC, GA, B_1,$
$B_2, HB_1, HB_2, {}^{m}B_1, {}^{m}B_2, H_b").$

## Conclusion

We compute $M(G; x, y)$ in this study, and we use this polynomial to find the different degree-based topological invariants that are included in Figure 2. The graph's encrypted storage is decoded by these topological indices. The aforementioned findings indicate the significant function of topological indices in the fields of wireless communication, electronics, and cryptography. We further employ visual representations to demonstrate the behavior of topological and $M$-polynomial invariants. We are able to comprehend findings in relation to parameters owing to this graphical depiction (See Figures 3, 4, 5, 6 & 7).

## References

[1] K. C. Das and I. Gutman, Some properties of the second Zagreb index, *MATCH Commun. Math. Comput. Chem.*, 52 (2004), 103–112.
[2] E. Deutsch and S. Klavžar, $M$-polynomial and Degree-based Topological Indices, *Iranian Journal of Mathematical Chemistry*, 6(2) (2015), 93–102.
[3] E. Estrada, L. Torres, L. Rodriguez and I. Gutman, An atom-bond connectivity index: modelling the enthalpy of formation of alkanes, *Indian Journal of Chemistry*, 37 (1998), 849–855.
[4] O. Favaron, M. Mahéo, J. F. Saclé, Some eigenvalue properties in graphs (conjectures of Graffiti—II), *Discrete Mathematics*, 111 (1993), 197–220.
[5] S. Fajtlowicz, On conjectures of Graffiti-II, *Congr. Numer.*, 60 (1987), 189–197.
[6] I. Gutman and K. C. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.*, 50 (2004), 83–92.
[7] I. Gutman and N. Trinajstić, Graph theory and molecular orbitals. Total $\varphi$-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.*, 17(4) (1972), 535–538.
[8] Y. Kinoshita, I. Matsubara, T. Higuchi and Y. Saito, The Crystal Structure of Bis(adiponitrilo)copper(I) Nitrate, *Bulletin of the Chemical Society of Japan*, 32(11) (1959), 1221–1226.
[9] V. R. Kulli, On $K$ Banhatti indices of graphs, *J. Comput. Math. Sci.*, 7 (4) (2016), 213–218.
[10] V. R. Kulli, On $K$ hyper-Banhatti indices and coindices of graphs, *Int. Res. J. Pure Algebra*, 6 (5) (2016), 300–304.
[11] V. R. Kulli, New $K$-Banhatti Topological Indices, *Intern. J. Fuzzy Mathematical Archive*, 12(1) (2017), 29–37.

[12] A. Milicević, S. Nikolić and N. Trinajstić, On reformulated Zagreb indices, *Mol Divers.*, 8(4) (2004), 393–399.
[13] K. Pattabiraman, Inverse sum indeg index of graphs, *AKCE Int. J. Graphs Comb.*, 15(2) (2018), 155–167.
[14] D. Vukičević and B. Furtula, Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges, *J. Math. Chem.*, 46(4) (2009), 1369–1376.
[15] O. M. Yaghi and H. Li, Hydrothermal Synthesis of a Metal-Organic Framework Containing Large Rectangular Channels, *J. Am. Chem. Soc.*, 117(41) (1995), 10401—10402.

ESIME-Zacatenco, Instituto Politécnico Nacional, Edif. 4, 1er. Piso, Col. Lindavista CP 07738, CDMX, MÉXICO.
*Email address*: jlopezb@ipn.mx; joseluis.lopezbonilla@gmail.com

Department of Mathematics, Kwangwoon University, Seoul-139-701, REPUBLIC OF KOREA.
*Email address*: tkkim@kw.ac.kr

Department of Mathematics, Acharya Institute of Graduate Studies, Bengaluru-560 107, INDIA.
*Email address*: lavanya.hup@gmail.com

Department of Mathematics, Vidyavardhaka College of Engineering, Mysuru-570 002, Affiliated to Visvesvaraya Technological University, Belagavi-590 018, INDIA.
*Email address*: masriraj@gmail.com

Department of Mathematics, JSS Science and Technology University, Mysuru-570 006, INDIA.
*Email address*: pskreddy@jssstuniv.in

Numerical Comparison of Derived Degree Based Indices

| m=n | M1 | M2 | mM2 | H | SSD | I | ABC | GA | B1 | B2 | HB1 | HB2 | mB1 | mB2 | Hb |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 364 | 488 | 10.33 | 26.96 | 141.66 | 269.25 | 26.87 | 115.31 | 820 | 1116 | 4684 | 11972 | 21.52 | 17.02 | 49.2 |
| 2 | 1488 | 2016 | 39.32 | 102.52 | 574.64 | 1189.0 | 110.79 | 460.33 | 3376 | 4720 | 19840 | 52496 | 86.76 | 63.09 | 190.15 |
| 3 | 3372 | 4584 | 86.97 | 226.68 | 1298.94 | 2759.25 | 251.77 | 1035.07 | 7668 | 10812 | 45468 | 121572 | 195.72 | 138.2 | 422.83 |
| 4 | 6016 | 8192 | 153.28 | 399.44 | 2314.56 | 4980.0 | 449.79 | 1839.51 | 13696 | 19392 | 81568 | 219200 | 348.39 | 242.36 | 747.25 |
| 5 | 9420 | 12840 | 238.25 | 620.8 | 3621.5 | 7851.25 | 704.87 | 2873.66 | 21460 | 30460 | 128140 | 345380 | 544.78 | 375.56 | 1163.41 |
| 6 | 13584 | 18528 | 341.88 | 890.76 | 5219.76 | 11373.0 | 1017.0 | 4137.52 | 30960 | 44016 | 185184 | 500112 | 784.88 | 537.8 | 1671.31 |
| 7 | 18508 | 25256 | 464.17 | 1209.32 | 7109.34 | 15545.25 | 1386.19 | 5631.09 | 42196 | 60060 | 252700 | 683396 | 1068.69 | 729.09 | 2270.96 |
| 8 | 24192 | 33024 | 605.12 | 1576.48 | 9290.24 | 20368.0 | 1812.43 | 7354.37 | 55168 | 78592 | 330688 | 895232 | 1396.22 | 949.42 | 2962.34 |
| 9 | 30636 | 41832 | 764.73 | 1992.24 | 11762.46 | 25841.25 | 2295.72 | 9307.37 | 69876 | 99612 | 419148 | 1135620 | 1767.47 | 1198.8 | 3745.46 |
| 10 | 37840 | 51680 | 943.0 | 2456.6 | 14526.0 | 31965.0 | 2836.06 | 11490.07 | 86320 | 123120 | 518080 | 1404560 | 2182.43 | 1477.22 | 4620.32 |

FIGURE 2. Numerical comparision of derived degree based indices of Pthalocyanine based MOF.

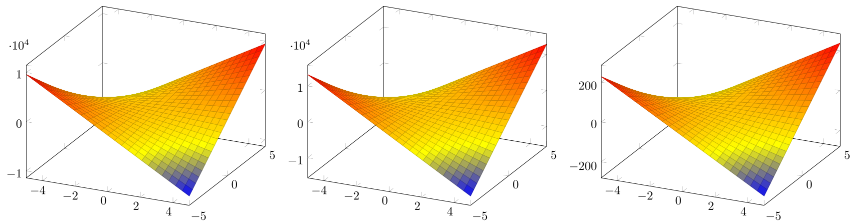


FIGURE 3. 3D plot of First, Second Zagreb index and Second modifies Zagreb index of Pthalocyanine based MOF.

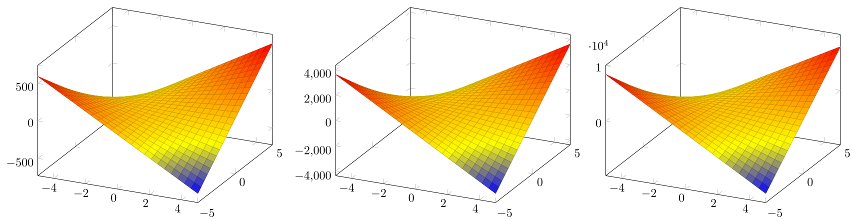


FIGURE 4. 3D plot of Harmonic, Symmetric Division and Inverse sum index of Pthalocyanine based MOF.

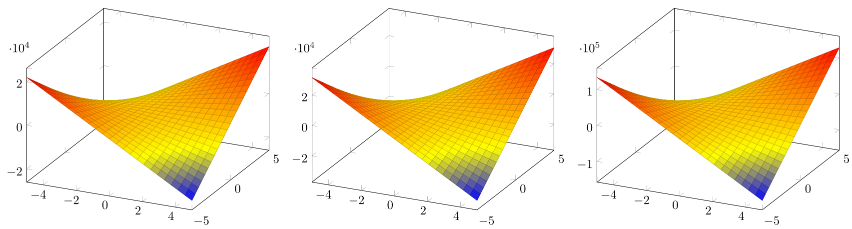


FIGURE 5. 3D plot of Atom-Bond connectivity, Geometric Arithmetic and First $K$ Banhatti of Pthalocyanine based MOF

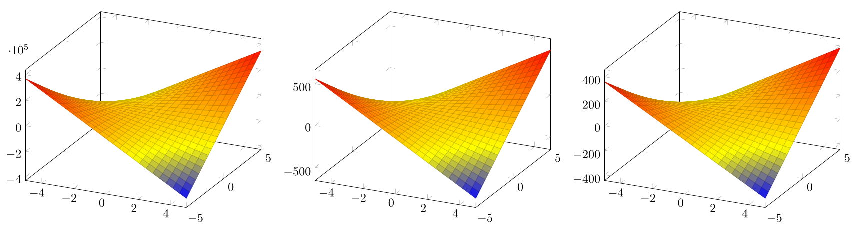


FIGURE 6. 3D plot of Second K Banhatti, First $K$ hyper Banhatti and Second $K$ hyper Banhatti index of Pthalocyanine based MOF.

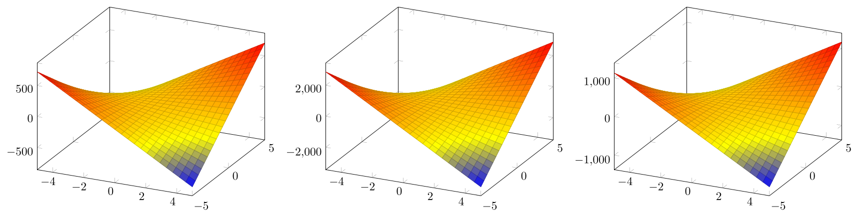


FIGURE 7. 3D plot of Modified First $K$ Banhatti, Modified Second $K$ Banhatti and Harmonic $K$ Banhatti index of Pthalocyanine based MOF