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Research Paper

Degree based topological indices and M-polynomials of metal complexes

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Abstract
In chemical graph theory degree based topological indices $M_1(G)$,$M_2(G)$,${}^mM_2(G)$,$R_\alpha(G)$,$RR_\alpha(G)$,SDD(G),H(G),I(G),and A(G) from M-polynomial are generally studied.In this paper degree based topological indices such as-atom bond connectivity index,fourth atom bond connectivity index,forgotten index,redefined third Zagreb index,fifth Zagreb index,SK(G) index,$SK_1(G)$ index,and $SK_2(G)$ index are investigated from M-polynomials for metal complexes of Zinc(II),Manganese(II),Cobalt(II) and Copper(II).

***Keywords**: Degree, differential operator,F-index, metal complex,M-polynomial,molecular graph, topological index,Zagreb index.*

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I. INTRODUCTION

A molecular graph is a representation of the structural formula of a chemical compound in terms of graph theory,whose vertices correspond to the atoms and edges correspond to chemical bonds [1].A topological index is a numerical parameter mathematically derived from the graph structure. All graphs considered in this paper are finite, connected, loop less, and without multiple edges. The topological indices has huge appilcaions in pharmacy, theoretical chemistry and especially in QSPR/QSAR [2].Topological invariant of graphis a single number descriptor which is correlated to certain chemical,thermodynamical and biological behaviour of the chemical compounds. Let

G(V,E) be a graph with vertex set V and edge set E. The degree of a vertex u belong to E(G) is denoted by d_u and is the number of vertices that are adjacent to u. The edge connecting the vertices u and v is denoted by uv.In the study of M-polynomials based topological indices the formulas of topological indices in the form of degree are taken as standard and formation of new formulasin differential operators are done in such away that yields almost close value of the obtained value of toplogical indices.Generally first Zagreb index, second modifed Zagreb index, Randic index, inverse Randic index, symmetric division index, inverse sum index and augmented Zagreb index are investigated from M-polynomials [3-14].

$ABC_4(G)$and $GA_5(G)$ of certain nanotubes are studied by S.Hayat et al. [15].F-indices and F-polynomials of the carbon nanocones are studied by N.K.Raut et al. [16].M-polynomials of drugs used in the treatment of COVID-19 are studied by R.H.Khan et al. [17].Topological indices of vitamin D_3 are studied by M.R.R.Kanna et al. [18].Zagreb polynomials and redefined Zagreb indices of nanostar dendrimers are studied by S.M.Kang et al. [19].Redefined Zagreb indices of rhombic, triangular, hourglass and jagged-rectangle benzenoid systems are studied by M.A.Mohammed et al. [20].Predicting anticancer activity of marine pyridoacridine alkaloids-Computation approach using topological indices study is done by J.Senbagamalar et al. [21].Application of topological indices of Tenofovir chemical structures for the cure of HIV/AIDS patients is discussed by B.K.Shree et al. wherein two new degree based topological indices from M-polynomials-forgotten index and redefined third Zagreb index are introduced [22].M-polynomials and entropy of para-line graph of naphthalene are studied by T.U.Islam et al. [11].In the study of molecular properties of symmetrical networks using topological polynomials X.L.Wang [13] has intoduced the formula for computation of forgotten index in terms of forgotten polynomial.F index is vertex degree based topological index and is studied byFurtula and Gutmandefined F index as the sum of cubes of vertex degrees [23].The forgotten index can be studied by three approaches for graph G(V,E) as

F(G) $= \sum_{uv\in E(G)} d_u^{\,3} = \sum_{uv\in E(G)} (d_u^{\,3} + d_v^{\,3})$,from forgotten polynomial of graph,
F(G,x) $=\sum_{uv\in E(G)} x^{(d_u^2 + d_v^2)}$ and in M-polynomial asF(G) = $(D_x^2 + D_y^2)$ M(G;x,y))$|_{x=y=1}$.

Chemical,physical and biological properties of Zinc(II) and Manganese(II) are studied by S.N.Ipper[24,25] and Cobalt(II),Copper(II) are prepared and investigated by S.N.Ipper [26].The chemical formulas of these metal complexes of Zn(II),Mn(II),Co(II) and Cu(II) are $C_{28}H_{20}O_6N_2Zn$,$C_{26}H_{22}O_{10}Mn$,$C_{28}H_{26}O_6Co$ and $C_{28}H_{26}O_6Cu$ respectively.A chalcone is a simple scaffold of many naturally occuring compounds and has widespread distribution in vegetables, fruits and plants. Many chalcone derivatives have been prepared due to their convenient synthesis.These natural and synthetic compounds have shown numerous interesting biological activities with clinical potentials against various diseases [27].M-polynomial,eccentricity and degree based topological indices of chalconeare studied by N K.Raut et al. [28].Schultz indices and Schultz polynomials of alkanes are studied by H.K.Aljanabi [29].The ABC index is described as

ABC(G) = $\sum_{uv\in E(G)} \sqrt{\frac{d_u+d_v-2}{d_u d_v}}$by M.Ghorbani et al. in [30] and [31,32,33] have introduced the fourth version of atom bond connectivity index asABC$_4$(G) = $\sum_{uv\in E(G)} \sqrt{\frac{S_u+S_v-2}{S_u S_v}}$,

where $S_u = \sum_{uv\in E(G)} d_v$ and $S_v = \sum_{uv\in E(G)} d_u$.

The M-polynomial is quite similar to the Hosoya polynomial except the fact that it produces degree based topological indices.The main advantage of M-polynomial is the information it contains about the degree basedgraph invariants.It is intersting to investigate other degree based topological indices by using differential operators from M-polynomials. The notations used in this paper are mainly taken from books [34--36].The M-polynomial of graph G is defined as,M(G;x,y) = $\sum_{\delta\le i\le j\le\Delta} m_{ij}(G)\, x^i y^j$,

where $\delta = \min\{d_v | v \in V(G)\}$,$\Delta = \max\{d_v | v\in V(G)\}$,and $m_{ij}(G)$ is the edge vu ∈ E(G) such that i ≤ j, with $D_x = x\frac{\partial f(x,y)}{\partial x}$, $D_y = y\frac{\partial f(x,y)}{\partial y}$, $S_x = \int_0^x \frac{f(t,y)}{t}dt$,$S_y = \int_0^y \frac{f(x,t)}{t}dt$, J(f(x,y)) = f(x,x), $Q_\alpha(f(x,y)) = x^\alpha f(x,y)$.

In this paper we study the atom bond connectivity index,fourth atom bond connectivity index,forgotten index,redefined third Zagreb index,fifth Zagreb index,SK index,SK$_1$ index, and

SK$_2$ index from M-polynomials using differential operators for metal complexes of Zinc(II),Manganese(II),Cobalt(II) and Copper(II).

II. MATERIALS AND METHODS

Let G be agraph with vertex set V(G) and edge set E(G).The degree of a vertex u∈(E) is denoted by $d_u$and is the number ofvertices that areadjacent to u.The edge connecting u and v is denoted by uv.Molecular graphs are actually a graphical representation of molecular structure through vertices and edges so that each vertex correspond to atoms and theedges represents the bondsbetween them.The structures of the metal complexes of Zinc(II),Manganese(II),Cobalt(II) and Copper(II) are shown in the figures 1-3.From the 2-dimensional graphs of complexes of Zn (II), Mn (II),Co (II) and Cu (II) the number of vertices and edges are decided. From figure of molecular graph of complex of Zn (II) we get |V(G)| = 37 and |E(G)| = 42.We have five partitions of the edge E(G) of graph G represented in table 2.There are $|E_{\{2,2\}}|$=14,$|E_{\{2,3\}}|$= 16,$|E_{\{2,4\}}|$= 4, $|E_{\{3,3\}}|$= 6, and $|E_{\{1,3\}}|$= 2 edges,for complex of Zinc(II)represented as:$E_{\{2,2\}}$= {uv∈E(G)|d_u=2,d_v=2},$E_{\{2,3\}}$ = {uv∈E(G)|d_u=2,d_v=3},$E_{\{2,4\}}$= {uv∈E(G)|d_u=2,d_v=4},$E_{\{3,3\}}$= {uv∈E(G)|d_u=3,d_v=3},and$E_{\{1,3\}}$= {uv∈E(G)|d_u=1,d_v=3}.

The edge partition of complex of Zinc(II) graph based on the degree sum of neighbor vertices of end vertices of each edge is decided.Using the differential operators given in table 1 the topological indices-atom bond connectivity index,fourth atom bond connectivity index,forgotten index,redefined third Zagreb index, fifth Zagreb index,SK index,SK$_1$ index,and SK$_2$ index are computed.The structure of complexes of Manganese(II) (figure 2) and Cobalt(II) and Copper(II) is given in figure 3.From the molecular graphs of complexes of Manganese(II),Cobalt(II) and Copper(II) the values of |V(G)| and |E(G)| and edge partition of graph Gbased on the degree sum of neighbor vertices of end vertices of each edge are observed and used in thecomputation of topological indices.This is done in the following section.

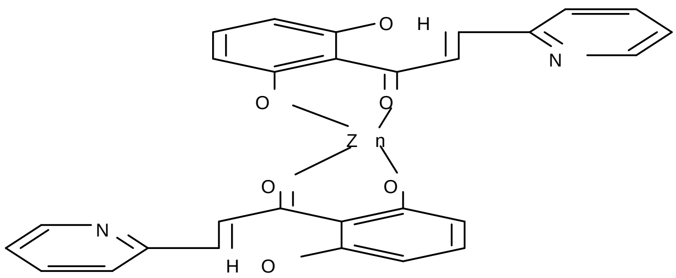

Figure 1. Metal complex of Zinc (II) with chalcone of pyridine-2-carbaldehyde.

III. RESULTS AND DISCUSSION

In the study of M-polynomials based topological indices the formulas of topological indices in degrees are taken as standard and formation of new formulas in terms of differential operators are done in such away that yields almost close value of the obtained value of toplogical indices.Generally first Zagreb index, second modifed Zagreb index, Randic index, inverse Randic index, symmetric division index,inverse sum index and augmented Zagreb index are investigated from M-polynomials.It is interesting to investigate other degree based topological indices by using differential operators from M-polynomials. We have discussed the forgotten index in degree based formula, forgotten polynomial,M-polynomial.We have the close values for the metal complexes of Zn (II), Mn (II), Co (II) and Cu (II) from degree based formulas and differential operator form M-polynomial formulas.In the study of fourth atom bond connectivity indexthe formula of atom bond connectivity index in the form of M-polynomial can be tried for

$ABC_4(G) = \sum_{\mathbf{uv\in E(G)}} \sqrt{\frac{\mathbf{S_u+S_v-2}}{\mathbf{S_uS_v}}}$, where$S_u = \sum_{uv\in E(G)} d_v$,and $S_v=\sum_{uv\in E(G)} d_u$.

The formula for atom bond connectivity index is $S_x^{-½} Q_{-2}J D_x^{-½} D_y^{-½}(M(G;x,y))|_{x = y = 1}$.Ifin place of degree of u and v the sum of degree of neighbouring vertices are used.The result is the same indicating the usability of the formula ABC index in M-polynomial for ABC_4.The edge pattition and degree sum of vetices for complex of Zinc (II) are placed in table 2-3.The edge partition and vertices degree sum of Mn(II),Co(II) and Cu(II) are given table 4-9.The topological indices are computed from M-polynomials by taking thefunction as f(x,y) = M(G;x,y).The topological indices-atom bond connectivity index,fourth atom bond connectivity index,forgotten index,redefined third Zagreb index,fifth Zagreb index,SK index,SK_1 index, and SK_2 index are computed from M-polynomials using differential operators for metal complexes of Manganese(II),Cobalt(II) and Copper(II) and are represented in table 10-11.

Topological indices of complex of Zinc (II)

Theorem 3.1. LetG be the graph of complex of Zinc (II) then its atom bondconnectivity index isABC(G)= 29.65.

Proof. The graph of the complex of Zinc (II) contains 37vertices and 42 edges.From figure 1 we notice that there five separate cases and the number of edges are different:namely $E_{\{2,2\}}$,$E_{\{2,3\}}$, $E_{\{2,4\}}$, $E_{\{3,3\}}$,and $E_{\{1,3\}}$.

$E_{\{2,2\}}$= {uv∈E(G)|d_u=2,d_v=2},$E_{(2,3\}}$ = {uv∈E(G)|d_u=2,d_v=3},$E_{\{2,4\}}$= {uv∈E(G)|d_u=2,d_v=4},

$E_{\{3,3\}}$= {uv∈E(G)|d_u=3,d_v=3},and $E_{(1,3\}}$ = {uv∈E(G)|d_u=1,d_v=3}.

The number of edges $E_{(2,2\}}$,$E_{2,3\}}$,$E_{\{2,4\}}$,$E_{\{3,3\}}$,and $E_{(1,3\}}$ are 14,16,4,6,and 2respectively.

The atom bond connectivity index$ABC(G) = \sum_{\boldsymbol{uv\in E(G)}} \sqrt{\frac{\boldsymbol{d_u+d_v-2}}{\boldsymbol{d_ud_v}}}$.

$=14\sqrt{\frac{\mathbf{2+2-2}}{\mathbf{2*2}}}+16\sqrt{\frac{\mathbf{2+3-2}}{\mathbf{2*3}}}+4\sqrt{\frac{\mathbf{2+4-2}}{\mathbf{2*4}}}+ 6\sqrt{\frac{\mathbf{3+3\ \ -2}}{\mathbf{3*3}}}+ 2\sqrt{\frac{\mathbf{1+3-2}}{\mathbf{1*3}}}$.

= 29.65.

In order to find ABC index from M-polynomials we need the following:

The M-polynomial of complex of Zinc (II) graph G

M(G;x,y) =
$\sum_{\delta\le i\le j\le\Delta} m_{ij}(G)\, x^i y^j$=$\sum_{2\le 2} m_{22}(G)\, x^2 y^2$+$\sum_{2\le 3} m_{23}(G)\, x^2 y^3$ +
$\sum_{2\le 4} m_{24}(G)\, x^2 y^4$+$\sum_{3\le 3} m_{33}(G)\, x^3 y^3$+$\sum_{1\le 3} m_{13}(G)\, x^1 y^3$.

$= |E_{\{2,2\}}|x^2y^2 + |E_{\{2,3\}}|x^2y^3 + |E_{\{2,4\}}|x^2y^4 + |E_{\{3,3\}}|x^3y^3 + |E_{\{1,3\}}|x^1y^3.$

$=14 x^2 y^2 + 16 x^2y^3 + 4 x^2 y^4 + 6x^3y^3 + 2x^1 y^3.$

$M(G;x,y) = 14 x^2 y^2 + 16 x^2y^3 + 4 x^2 y^4 + 6x^3y^3 + 2x^1 y^3.$

$ABC(G) = S_x^{-½} Q_{-2} J D_x^{-½} D_y^{-½}(M(G;x,y))|_{x=y=1}.$

$D_y^{-1/2}(f(x,y)) = 2^{-1/2}\, 14x^2 y^2 + 3^{-1/2}\, 16 x^2 y^3 + 4^{-1/2}\, 4x^2 y^4 + 3^{-1/2}\, 6 x^3 y^3 + 3^{-1/2}\, 2x^1 y^3.$

$D_x^{-1/2}D_y^{-1/2}(f(x,y)) = 2^{-1/2}\, 2^{-1/2}\, 14x^2 y^2 + 2^{-1/2}\, 3^{-1/2}\, 16 x^2 y^3 + 2^{-1/2}\, 4^{-1/2}\, 4x^2 y^4 + 3^{-1/2}\, 3^{-1/2}\, 6 x^3 y^3 + 3^{-1/2}\, 2 x^1 y^3.$

$J D_x^{-1/2}D_y^{-1/2}(f(x,y)) = 2^{-1/2}\, 2^{-1/2}\, 14x^4 + 2^{-1/2}\, 3^{-1/2}\, 16 x^5 + 2^{-1/2}\, 4^{-1/2}\, 4x^6 + 3^{-1/2}\, 3^{-1/2}\, 6 x^6 + 3^{-1/2}\, 2 x^4.$

$Q_{-2} J D_x^{-1/2}D_y^{-1/2}(f(x,y)) = 2^{-1/2}\, 2^{-1/2}\, 14x^2 + 2^{-1/2}\, 3^{-1/2}\, 16 x^3 + 2^{-1/2}\, 4^{-1/2}\, 4x^4 + 3^{-1/2}\, 3^{-1/2}\, 6 x^4 + 3^{-1/2}\, 2 x^2.$

$S_x^{-1/2}Q_{-2} J D_x^{-1/2}D_y^{-1/2}(f(x,y)) = 2^{-1/2}\, 2^{-1/2}\, 14x^2 * (1/ 2^{-1/2}) + 2^{-1/2}\, 3^{-1/2}\, 16 x^3 * (1/3^{-1/2}) + 2^{-1/2}\, 4^{-1/2}\, 4x^4 * (1/4^{-1/2}) + 3^{-1/2}\, 3^{-1/2}\, 6 x^4 * (1/4^{-1/2}) + 3^{-1/2}\, 2 x^2 * (1/2^{-1/2}).$

$ABC(G) = S_x^{-1/2}Q_{-2} J D_x^{-1/2}D_y^{-1/2}(f(x,y))|_{x=y=1} = 29.68.$

Theorem 3.2. Let G be the graph of complex of Zinc(II) then its fourth atom bond connectivity index is $ABC_4(G) = 29.68$.

Proof. The partition based on the degree sum of neighbor vertices of G is obtained (table 3).From figure 1 we notice that there eleven separate cases and the number of edges are different based on degree sum of neighbor vertices of G: namely $E_{\{4,4\}}, E_{\{4,5\}}, E_{\{5,6\}}, E_{\{5,5\}}, E_{\{5,7\}}, E_{\{7,9\}}, E_{\{6,9\}}, E_{\{7,7\}}, E_{\{3,6\}}, E_{\{7,28\}}$, and $E_{\{4,6\}}$.

Using degree sum of neighbors of end vertices of each edge, we have

$E_{\{4,4\}} = \{uv\in E(G)|S_u=4, S_v=4\}, E_{(4,5\}} = \{uv\in E(G)|S_u=4, S_v=5\}, E_{\{5,6\}} = \{uv\in E(G)|S_u=5, S_v=6\},$

$E_{(5,5\}} = \{uv\in E(G)|S_u=5, S_v=5\}, E_{\{5,7\}} = \{uv\in E(G)|S_u=5, S_v=7\}, E_{\{7,9\}} = \{uv\in E(G)|S_u=7, S_v=9\},$

$E_{\{6,9\}} = \{uv\in E(G)|S_u=6, S_v=9\}, E_{\{7,7\}} = \{uv\in E(G)|S_u=7, S_v=7\}, E_{\{3,6\}} = \{uv\in E(G)|S_u=3, S_v=6\},$

$E_{\{7,28\}} = \{uv\in E(G)|S_u=7, S_v=28\}$, and $E_{\{4,6\}} = \{uv\in E(G)|S_u=4, S_v=6\}$.

The fourth atom bond connectivity index is computed as

$$ABC_4(G) = \sum_{uv\in E(G)} \sqrt{\frac{S_u+S_v-2}{S_uS_v}}.$$

$$=E_{\{4,4\}}\sqrt{\frac{4+4-2}{4*4}}+E_{\{4,5\}}\sqrt{\frac{4+5-2}{4*5}}+E_{\{5,6\}}\sqrt{\frac{5+6-2}{5*6}}+E_{\{5,5\}}\sqrt{\frac{5+5-2}{5*5}}+E_{\{5,7\}}\sqrt{\frac{5+7-2}{5*7}}+E_{\{7,9\}}\sqrt{\frac{7+9-2}{7*9}}+$$

$$E_{\{6,9\}}\sqrt{\frac{6+9-2}{6*9}}+E_{\{7,7\}}\sqrt{\frac{7+7-2}{7*7}}+E_{\{3,6\}}\sqrt{\frac{3+6-2}{3*6}}+E_{\{7,28\}}\sqrt{\frac{7+28-2}{7*28}}+E_{\{4,6\}}\sqrt{\frac{4+6-2}{4*6}}.$$

$= 29.68.$

In the application of the degree based formula of ABC index for computation of ABC_4 index in M-polynomial we use S_u and S_v in place of D_x and D_y and follow the same procedure for computation of ABC_4, and the result we obsevedisas follows.

In order to to find ABC_4 index from M-polynomial we need the following:

The M-polynomial of complex of Zinc (II) graph (G) is

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

$\sum_{4\le4} m_{44}(G)\, x^4y^4 + \sum_{4\le5} m_{45}(G)\, x^4y^5 \sum_{5\le6} m_{56}(G)\, x^5y^6 + \sum_{5\le5} m_{55}(G)\, x^5y^5 + \sum_{5\le7} m_{57}(G)\, x^5y^7 + + \sum_{7\le9} m_{79}(G)\, x^7y^9 + \sum_{6\le9} m_{69}(G)\, x^6y^9 \sum_{7\le7} m_{77}(G)\, x^7y^7 + \sum_{3\le6} m_{36}(G)\, x^3y^6 + \sum_{7\le28} m_{728}(G)\, x^7y^{28} + \sum_{4\le6} m_{46}(G)\, x^4y^6.$

$= |E_{\{4,4\}}|x^4y^4 + |E_{\{4,5\}}|x^4y^5 + |E_{\{5,6\}}|x^5y^6 + |E_{\{5,5\}}|x^5y^5 + |E_{\{5,7\}}|x^5y^7 + |E_{\{7,9\}}|x^7y^9 + |E_{\{6,9\}}|x^6y^9 + |E_{\{7,7\}}|x^7y^7 + |E_{\{3,6\}}|x^3y^6 + |E_{\{7,28\}}|x^7y^{28} + |E_{\{4,6\}}|x^4y^6.$

$=5x^4 y^4 + 7x^4y^5 + 7x^5 y^6 + 2x^5y^5 + 4x^5 y^7 + 4 x^7 y^9 + 2x^6y^9 + 4 x^7 y^7 + 2x^3y^6 + 4x^7 y^{28} + x^4 y^6.$

$M(G;x,y) = 5 x^4 y^4 + 7 x^4y^5 + 7 x^5 y^6 + 2x^5y^5 + 4x^5 y^7 + 4 x^7 y^9 + 2 x^6y^9 + 4 x^7 y^7 + 2x^3y^6 + 4x^7 y^{28} + x^4 y^6.$

Fourthatom bond connectivity index $= S_x^{-½} Q_{-2} J D_x^{-½} D_y^{-½}(M(G;x,y))|_{x=y=1}$.

Using S_u and S_v in place of D_x and D_y in the formula of ABC index,we have

$D_y^{-1/2}(f(x,y)) = 5 * 4^{-1/2} x^4 y^4 + 7 * 5^{-1/2} x^4 y^5 + 7 * 6^{-1/2} x^5 y^6 + 2 * 5^{-1/2} x^5 y^5 + 4 * 7^{-1/2} x^5 y^7 + 4 * 9^{-1/2} x^7 y^9 + 2 * 9^{-1/2} x^6 y^9 + 4 * 7^{-1/2} x^7 y^7 + 2 * 6^{-1/2} x^3 y^6 + 4 * 28^{-1/2} x^7 y^{28} + 6^{-1/2} x^4 y^6.$

$D_x^{-1/2} D_y^{-1/2}(f(x,y)) = 5 * 4^{-1/2}\ 4^{-1/2} x^4 y^4 + 7 * 4^{-1/2}\ 5^{-1/2} x^4 y^5 + 7 * 5^{-1/2}\ 6^{-1/2} x^5 y^6 + 2 * 5^{-1/2}\ 5^{-1/2} x^5 y^5 + 4 * 5^{-1/2}\ 7^{-1/2} x^5 y^7 + 4 * 7^{-1/2}\ 9^{-1/2} x^7 y^9 + 2 * 6^{-1/2}\ 9^{-1/2} x^6 y^9 + 4 * 7^{-1/2}\ 7^{-1/2} x^7 y^7 + 2 * 3^{-1/2}\ 6^{-1/2} x^3 y^6 + 4 * 7^{-1/2}\ 28^{-1/2} x^7 y^{28} + 4^{-1/2}\ 6^{-1/2} x^4 y^6.$

$J D_x^{-1/2} D_y^{-1/2}(f(x,y)) = 5 * 4^{-1/2}\ 4^{-1/2} x^8 + 7 * 4^{-1/2}\ 5^{-1/2} x^9 + 7 * 5^{-1/2}\ 6^{-1/2} x^{11} + 2 * 5^{-1/2}\ 5^{-1/2} x^{10} + 4 * 5^{-1/2}\ 7^{-1/2} x^{12} + 4 * 7^{-1/2}\ 9^{-1/2} x^{16} + 2 * 6^{1/2}\ 9^{-1/2} x^{15} + 4 * 7^{-1/2}\ 7^{-1/2} x^{14} + 2 * 3^{-1/2}\ 6^{-1/2} x^9 + 4 * 7^{-1/2}\ 28^{-1/2} x^{35} + 4^{-1/2}\ 6^{-1/2} x^{10}.$

$Q_{-2} J D_x^{-1/2} D_y^{-1/2}(f(x,y)) = 5 * 4^{-1/2}\ 4^{-1/2} x^6 + 7 * 4^{-1/2}\ 5^{-1/2} x^7 + 7 * 5^{-1/2}\ 6^{-1/2} x^9 + 2 * 5^{-1/2}\ 5^{-1/2} x^8 + 4 * 5^{-1/2}\ 7^{-1/2} x^{10} + 4 * 7^{-1/2}\ 9^{-1/2} x^{14} + 2 * 6^{1/2}\ 9^{-1/2} x^{13} + 4 * 7^{-1/2}\ 7^{-1/2} x^{12} + 2 * 3^{-1/2}\ 6^{-1/2} x^7 + 4 * 7^{-1/2}\ 28^{-1/2} x^{33} + 4^{-1/2}\ 6^{-1/2} x^8.$

$S_x^{-1/2} Q_{-2} J D_x^{-1/2} D_y^{-1/2}(f(x,y)) = 5 * 4^{-1/2}\ 4^{-1/2} x^6 (1/6^{-1/2}) + 7 * 4^{-1/2}\ 5^{-1/2} x^7 (1/7^{-1/2}) + 7 * 5^{-1/2}\ 6^{-1/2} x^9 (1/9^{-1/2}) + 2 * 5^{-1/2}\ 5^{-1/2} x^8 (1/8^{-1/2}) + 4 * 5^{-1/2}\ 7^{-1/2} x^{10} (1/10^{-1/2}) + 4 * 7^{-1/2}\ 9^{-1/2} x^{14} (1/14^{-1/2}) + 2 * 6^{1/2}\ 9^{-1/2} x^{13} (1/13^{-1/2}) + 4 * 7^{-1/2}\ 7^{-1/2} x^{12} (1/12^{-1/2}) + 2 * 3^{-1/2}\ 6^{-1/2} x^7 (1/7^{-1/2}) + 4 * 7^{-1/2}\ 28^{-1/2} x^{33} (1/33^{-1/2}) + 4^{-1/2}\ 6^{-1/2} x^8 (1/8^{-1/2}).$

$ABC_4(G) = S_x^{-1/2} Q_{-2} J D_x^{-1/2} D_y^{-1/2}(f(x,y))|_{x=y=1} = 29.68.$

Theorem 3.3. Let G be the graph of complex of Zinc (II) then its fogotten index is

$F(G) = 528.$

Proof. The forgotten index is computed from degree based formula, forgotten polynomial and M-polynomial.

1) Forgotten index: degree based formula

$F(G) = \sum_{uv \in E(G)} (d_u^2 + d_v^2)$

$= 14(2^2+2^2) + 16(2^2+3^2) + 4(2^2+4^2) + 6(3^2+3^2) + 2(1^2+3^2).$

$= 528.$

2) Forgotten index based on forgotten polynomial

$F(G;x,y) = \sum_{uv \in E(G)} x^{[(d_u)^2+(d_v)^2]}.$

$= 14x^{[(2)^2+(2)^2]} + 16x^{[(2)^2+(3)^2]} + 4x^{[(2)^2+(4)^2]} + 6x^{[(3)^2+(3)^2]} + 2x^{[(1)^2+(3)^2]}.$

$= 14x^8 + 16x^{13} + 4x^{20} + 6x^{18} + 2x^{10}.$

$F(G;x,y) = 14x^8 + 16x^{13} + 4x^{20} + 6x^{18} + 2x^{10}.$

$D_x, F(G;x,y) = 14*8x^8 + 16*13x^{13} + 4*20x^{20} + 6*18x^{18} + 2*10x^{10}.$

$F(G) = D_x, F(G;x,y)|_{x=y=1} = 528.$

3) Forgotten index based on M-polynomial

Let $f(x,y) = M(G;x,y) = 14x^2y^2 + 16x^2y^3 + 4x^2y^4 + 6x^3y^3 + 2x^1y^3.$

$D_x(f(x,y)) = 28x^2y^2 + 32x^2y^3 + 8x^2y^4 + 18x^3y^3 + 2x^1y^3.$

$D_y(f(x,y)) = 28x^2y^2 + 48x^2y^3 + 16x^2y^4 + 18x^3y^3 + 6x^1y^3.$

$D_x^2(f(x,y)) = 56x^2y^2 + 64x^2y^3 + 16x^2y^4 + 54x^3y^3 + 2x^1y^3.$

$D_y^2(f(x,y)) = 56x^2y^2 + 144x^2y^3 + 64x^2y^4 + 54x^3y^3 + 18x^1y^3.$

$[D_x^2 + D_y^2](f(x,y)) = 112x^2y^2 + 208x^2y^3 + 80x^2y^4 + 108x^3y^3 + 20x^1y^3.$

$F(G) = [D_x^2 + D_y^2](f(x,y))|_{x=y=1} = 528.$

Theorem 3.4. Let G be the graph of complex of Zinc(II) then its redefined third Zagreb index is $ReZG_3(G) = 1244$.

Proof. The redefined third Zagreb index

$ReZG_3(G) = \sum_{uv \in E(G)} (d_u * d_V)(d_u + d_V) =$

$14(2*2)(2+2) + 16(2*3)(2+3) + 4(2*4)(2+4) + 6(3*3)(3+3) + 2(1*3)(1+3).$

$= 1244.$

The M-polynomial

Let $f(x,y) = M(G;x,y) = 14x^2y^2 + 16x^2y^3 + 4x^2y^4 + 6x^3y^3 + 2x^1y^3.$

$D_x(f(x,y)) = 28x^2y^2 + 32x^2y^3 + 8x^2y^4 + 18x^3y^3 + 2x^1y^3.$

$D_y(f(x,y)) = 28x^2y^2 + 48x^2y^3 + 16x^2y^4 + 18x^3y^3 + 6x^1y^3.$

$(D_x + D_y)(f(x,y)) = 56x^2y^2 + 80x^2y^3 + 24x^2y^4 + 36x^3y^3 + 8x^1y^3.$

$D_y(D_x+D_y)(f(x,y)) = 112x^2 y^2 +240x^2y^3+96x^2 y^4 + 108x^3 y^3 + 24x^1y^3$.

$D_xD_y(D_x+D_y)(f(x,y)) = 224 x^2 y^2 + 480x^2y^3+192x^2 y^4 + 324 x^3 y^3 + 24x^1y^3$.

$ReZG_3(G)(f(x,y)) =D_xD_y(D_x+D_y)|_{x = y =1} = 1244$.

Theorem 3.5. Let G be the graph of complex of Zinc(II) then its fifth Zagreb index is$M_5(G) = 580$.

Proof. The fifth Zagreb index of complex of Zinc (II)

$M_5(G) = \sum_{uv\in E(G)} d_V(d_u + d_V)$.

= 14*2 (2+2) + 16*3 (2+3)+4*4 (2+4)+6*2 (3+3)+2*3 (1+3).

= 580.

The M-polynomial

Let $f(x,y) = M(G;x,y) = 14 x^2 y^2 + 16 x^2y^3+ 4 x^2 y^4 + 6x^3y^3+2x^1 y^3$.

$D_x(f(x,y)) = 28 x^2 y^2 + 32x^2y^3+8 x^2 y^4 + 18 x^3 y^3 + 2x^1y^3$.

$D_y(f(x,y)) = 28 x^2 y^2 + 48x^2y^3+16 x^2 y^4 + 18 x^3 y^3 + 6x^1y^3$.

$(D_x+D_y) (f(x,y)) = 56 x^2 y^2 + 80x^2y^3+24x^2 y^4 + 36 x^3 y^3 + 8x^1y^3$.

$D_y(D_x+D_y) (f(x,y)) = 112 x^2 y^2 + 240x^2y^3+96x^2 y^4 + 108 x^3 y^3 + 24x^1y^3$.

$M_5(G) =D_y(D_x+D_y)(f(x,y)) |_{x = y = 1} = 580$.

Theorem 3.6. Let G be the graph of complex of Zinc (II) then its SK index is

SK(G) = 102.

Proof. The number of edges are $E_{\{2,2\}} = 14, E_{\{2,3\}} = 16, E_{\{2,4\}}= 4, E_{\{3,3\}}= 6$, and $E_{\{1,3\}} = 2$.

The SK index of complex $\sum_{uv\in E(G)}(\frac{d_u+d_v}{2})$

$= 14\frac{2+2}{2}+ 16\frac{2+3}{2} + 4\frac{2+4}{2} + 6\frac{3+3}{2} + 2 \frac{1+3}{2}$.

= 102.

The M-polynomial of complex of Zinc (II)

Let $f(x,y) = M(G;x,y) = 14 x^2 y^2 + 16 x^2y^3+ 4 x^2 y^4 + 6x^3y^3+2x^1 y^3$.

$D_x(f(x,y)) = 28 x^2 y^2 + 32x^2y^3+8 x^2 y^4 + 18 x^3 y^3 + 2x^1y^3$.

$D_y(f(x,y)) = 28 x^2 y^2 + 48x^2y^3+16 x^2 y^4 + 18 x^3 y^3 + 6x^1y^3$.

$(D_x+D_y)(f(x,y)) = 56 x^2 y^2 + 80x^2y^3+24x^2 y^4 + 36 x^3 y^3 + 8x^1y^3$.

$\frac{1}{2}(D_x+D(f(x,y)) = 28 x^2 y^2 + 40x^2y^3+12x^2 y^4 + 18 x^3 y^3 + 4 x^1y^3$.

$\frac{1}{2}(D_x+D_y)(f(x,y))|_{x = y =1} = 102$.

Theorem 3.7. Let G be the graph of complex of Zinc (II) then its SK_1 index is

$SK_1(G) = 122$.

Proof. The SK_1 index of complex of Zn (II)

$\sum_{uv\in E(G)}(\frac{d_u*d_v}{2})$.

$= 14\frac{2*2}{2}+ 16\frac{2*3}{2} + 4\frac{2*4}{2} + 6\frac{3*3}{2} + 2 \frac{1*3}{2}$.

= 122.

The M-polynomial of complex of Zinc (II)

Let $f(x,y) = M(G;x,y) = 14 x^2 y^2 + 16 x^2y^3+ 4 x^2 y^4 + 6x^3y^3+2x^1 y^3$.

$D_x(f(x,y)) = 28 x^2 y^2 + 32x^2y^3+8 x^2 y^4 + 18 x^3 y^3 + 2x^1y^3$.

$D_y(f(x,y)) = 28 x^2 y^2 + 48x^2y^3+16 x^2 y^4 + 18 x^3 y^3 + 6x^1y^3$.

$(D_xD_y) (f(x,y)) = 56 x^2 y^2 + 96x^2y^3+32x^2 y^4 + 54x^3 y^3 + 6x^1y^3$.

$\frac{1}{2}(D_xD_y) (f(x,y)) = 28 x^2 y^2 + 48x^2y^3+16x^2 y^4 + 27x^3 y^3 + 3x^1y^3$.

$SK_1(G) = \frac{1}{2}(D_x*D_y)(f(x,y))|_{x=y=1} = 122.$

Theorem 3.8. Let G be the graph of complex of Zinc (II) then its SK_2 index is

$SK_2(G) = 254.$

Proof. The SK_2 index of complex $\sum_{uv\in E(G)}(\frac{d_u+d_v}{2})^2$

$= 14(\frac{2+2}{2})^2 + 16(\frac{2+3}{2})^2+4(\frac{2+4}{2})^2+6(\frac{3+3}{2})^2+2(\frac{1+3}{2})^2.$

$= 254.$

The M-polynomial for complex of Zinc (II)

Let $f(x,y) = M(G;x,y) = 14x^2y^2 + 16x^2y^3 + 4x^2y^4 + 6x^3y^3 + 2x^1y^3.$

$J(f(x,y)) = 14x^4 + 16x^5 + 4x^6 + 6x^6 + 2x^4.$

$D_x^2J(f(x,y)) = 14*16x^4 + 16*25x^5 + 4*36x^6 + 6*36x^6 + 2*16x^4.$

$\frac{1}{4}D_x^2J(f(x,y)) = 14*4x^4 + 4*25x^5 + 1*36x^6 + 6*9x^6 + 2*4x^4.$

$SK_2(G) = \frac{1}{4}D_x^2J(f(x,y))|_{x=y=1} = 14*4 + 4*25 + 1*36 + 6*9 + 2*4.$

$SK_2(G) = \frac{1}{4}D_x^2J(f(x,y))|_{x=y=1} = 254.$

Topological index	Derivation from M(G;x,y)
Atom bond connectivity index	$S_x^{-1/2}Q_{-2}J\,D_x^{-1/2}D_y^{-1/2}(M(G;x,y))|_{x=y=1}$
Fourth atom bond connectivity index	$S_x^{-1/2}Q_{-2}J\,D_x^{-1/2}D_y^{-1/2}(M(G;x,y))|_{x=y=1}$
Forgotten index	$(D_x^2+D_y^2)(M(G;x,y))|_{x=y=1}$ and $Dx(F(G,x))|_{x=1}$
Redefined third Zagreb index	$D_xD_y(D_x+D_y)(M(G;x,y))|_{x=y=1}$
Fifth Zagreb index	$D_y(D_x+D_y)(M(G;x,y))|_{x=y=1}$
SK index	$\frac{1}{2}(D_x+D_y)(M(G;x,y))|_{x=y=1}$
SK_1 index	$\frac{1}{2}D_x*D_y)(M(G;x,y))|_{x=1}$
SK_2 index	$\frac{1}{4}D_x^2J(M(G;x,y))|_{x=1}$

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

(d_u,d_v)	(2,2)	(2,3)	(2,4)	(3,3)	(1,3)
No. of edges	14	16	4	6	2

Table 2: Edge partition of Zinc (II).

(S_u,S_v)	(4,4)	(4,5)	(5,6)	(5,5)	(5,7)	(7,9)	(6,9)	(7,7)	(3,6)	(7,28)	(4,6)
No. of edges	5	7	7	2	4	4	2	4	2	4	1

Table 3: Edge partition of Zinc (II) based on degree sum of neighbors of end vertices of each edge.

(d_u,d_v)	(2,2)	(2,3)	(2,4)	(3,3)	(1,3)
No. of edges	8	20	4	6	4

Table 4: Edge partition of Manganese (II).

(S_u,S_v)	(3,5)	(5,5)	(5,6)	(5,7)	(3,6)	(6,9)	(7,9)	(7,7)	(7,28)	(5,9)	(4,5)	(6,6)
No.of edges	2	8	8	4	2	2	3	3	4	1	4	1

Table 5: Edge partition of Manganese (II)based on degree sum of neighbors of end vertices of each edge.

(d_u,d_v)	(2,3)	(2,2)	(2,4)	(3,3)	(1,3)
No. of edges	20	8	4	6	4

Table 6: Edge partition of Cobalt (II).

(S_u,S_v)	(3,5)	(5,5)	(5,6)	(6,6)	(7,28)	(7,7)	(5,7)	(4,5)	(7,9)	(6,9)	(3,6)
No. of edges	2	6	8	2	4	4	4	4	4	2	2

Table 7: Edge partition of Cobalt (II) based on degree sum of neighbors of end vertices of each edge.

(d_u,d_v)	(2,3)	(2,2)	(2,4)	(3,3)	(1,3)
No. of edges	20	8	4	6	4

Table 8: Edge partition of Copper (II).

(S_u,S_v)	(3,5)	(5,5)	(5,6)	(6,6)	(5,7)	(7,9)	(6,9)	(3,6)	(4,5)	(7,7)	(7,28)	(6,7)
No. of edges	2	6	10	2	2	2	4	2	4	2	4	2

Table 9: Edge partition of Copper (II) based on degree sum of neighbors of end vertices of each edge.

Metal complex	ABC index	ABC_4index	F	$ReZG_3$ index	M_5index	SK index	SK_1 index	SK_2 index
Zn(II)	29.65	22.61	528	1244	580	102	122	254
Mn(II)	29,88	22	552	1292	616	104	125	263
Co(II)	29.88	22.25	552	1292	616	104	125	263
Cu(II)	29.88	22.88	552	1292	616	104	125	263

Table 10: Topological indices of metal complexes of Zinc (II), Manganese (II), Cobalt (II) and Copper (II) by using degree.

Metal complex	ABC index	ABC_4index	F (M-poly.)	F (Fogotten poly.)	$ReZG_3$ index	M_5index	SK index	SK_1 index	SK_2 index
Zn(II)	29.68	22.60	528	528	1244	580	102	122	254
Mn(II)	29.88	21.95	552	552	1292	616	104	125	263
Co(II)	29.88	22.33	552	552	1292	616	104	125	263
Cu(II)	29.88	22.46	552	552	1292	616	104	125	263

Table 11: Topological indices of metal complexes of Zinc (II), Manganese (II), Cobalt (II) and Copper (II) by using M-polynomials.

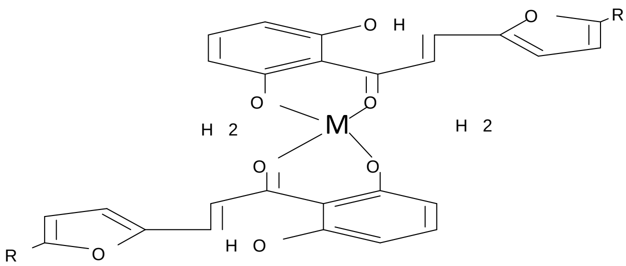

Figure 2. Metal complex of Manganese (II)with (E)-3-(furan-2-yl)-1-(2,6-dihydroxyphenyl)prop-2-en-1-one
R= H, M= Mn(II).

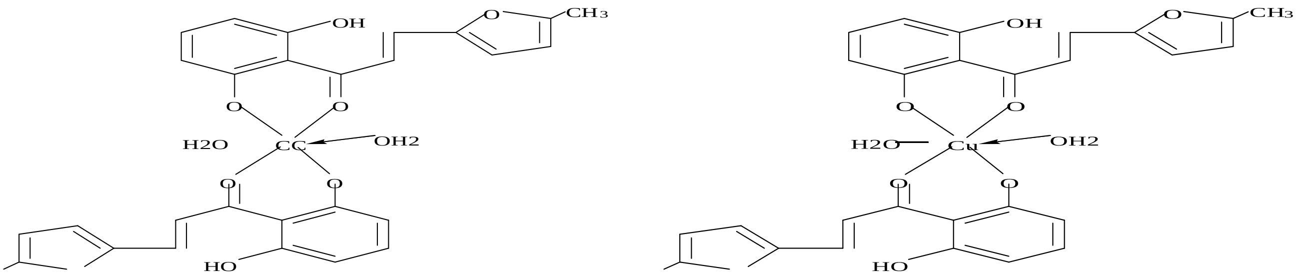

Figure 3. Metal complexes of cobalt (II) and copper (II) with chalcone of 5-methyl furaldehyde.

4. Conclusion

In this paper we have studied the atom bond connectivity index,fourth atom bond connectivity index,forgotten index,fifth Zagreb index,redefined third Zagreb index,SK index,SK_1indexand SK_2 index for complexes of Zinc(II),Manganese(II),Cobalt(II) and Copper(II) from M-polynomials.The forgotten index computed from M-polynomial and forgotten polynomial gives same results.The formula from M-polynomial in terms of differential operators for ABC index can be used for ABC_4 index with suitable changes.The ABC index and ABC_4 index for metal complexes of Zn(II),Mn(II),Co(II) and Cu(II) has close values.

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