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Study of Two-dimensional Generalized Canonical Sine-Cosine Transform

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ABSTRACT

This paper is concerned with the definition of two-dimensional (2-D) generalized canonical SC- transform it is extended to the distribution of compact support by using kernel method. We have discussed inversion theorem for that transform. Lastly we have proved Uniqueness theorem for that transform.

Keywords: 2-D canonical transform, 2-D sine-cosine transform, 2-D sine-sine transform, 2-D cosine-cosine transform, 2-D fractional Fourier transform, generalized function.

I. INTRODUCTION

Now a days fractional Fourier transforms plays important role in information processing [5]. The fractional Fourier transform as an extension of the Fourier transform. It has been used many applications such as optical system analysis, filter design, solving differential equations. Phase retrieval and pattern recognition etc. [8] [3],In fact the fractional Fourier transform is special case of the canonical transform. The canonical transform is defined as

$$\left\{CT f(t)\right\}(s)=\frac{1}{\sqrt{2\pi ib}}\int_{-\infty}^{\infty} e^{-i\left(\frac{s}{b}\right)t} e^{\frac{i}{2}\left(\frac{a}{b}\right)t} f(t)\,dt \quad b\neq 0 \qquad \text{..........(1)}$$

$$=\sqrt{d}\,e^{\frac{i}{2}\left(cds^2\right)f(d.s)} \quad b=0$$

And the constraint that ad-bc=1 must be satisfied. The canonical transform defined above in (1) are all one-dimensional [1-D], in [1] [2], [10],[11],[12],[13],[14],[15], they have generalized them from one–dimensional into the (2-D) cases, [4] ,[06],[07].The two-dimensional canonical sine-cosine transform it is extended to the distribution of compact support by using kernel method [09] .

The two-dimensional canonical sine-cosine transform is defined as.

$$\left\{2DCSCT\ f(t,x)\right\}(s,w)=-i\frac{1}{\sqrt{2\pi ib}}\frac{1}{\sqrt{2\pi ib}}e^{\frac{i}{2}\left(\frac{d}{b}\right)s^2} e^{\frac{i}{2}\left(\frac{d}{b}\right)w^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\sin\left(\frac{s}{b}t\right)\cos\left(\frac{w}{b}x\right)e^{\frac{i}{2}\left(\frac{a}{b}\right)t^2}.e^{\frac{i}{2}\left(\frac{a}{b}\right)x^2} f(t,x)\,dxdt$$

When $b \neq 0$

Notation and terminology of this paper is as per [17], [18]. The paper is organized as follows. Section. 2 gives the definition of 2-D canonical sine-cosine transform on the space of generalized function in section. 3 inversion theorem is proved in section. 4 Uniqueness theorems proved lastly the conclusion is stated.

II. DEFINITION TWO DIMENSIONAL (2D) GENERALIZED CANONICAL SINE-COSINE TRANSFORM $[2DCSCT]$

Let $E'(R\times R)$ denote the dual of $E(R\times R)$ therefore the generalized canonical sine-cosine transform of $f(t,x)\in E'(R\times R)$ is defined as

$$\{2DCSCT\, f(t,x)\}(s,w)=\langle f(t,x),K_s(t,s)K_c(x,w)\rangle$$

$$\{2DCSCT\, f(t,x)\}(s,w)$$
$$=(-i)\frac{1}{\sqrt{2\pi ib}}\frac{1}{\sqrt{2\pi ib}}e^{\frac{i}{2}\left(\frac{d}{b}\right)s^2}e^{\frac{i}{2}\left(\frac{d}{b}\right)w^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\sin\left(\frac{s}{b}t\right)\cos\left(\frac{w}{b}x\right)e^{\frac{i}{2}\left(\frac{a}{b}\right)t^2}e^{\frac{i}{2}\left(\frac{a}{b}\right)x^2}f(t,x)\,dxdt$$

Where $K_s(t,s)=(-i)\frac{1}{\sqrt{2\pi ib}}e^{\frac{i}{2}\left(\frac{d}{b}\right)s^2}e^{\frac{i}{2}\left(\frac{a}{b}\right)t^2}\sin\left(\frac{s}{b}t\right)$ when $b\neq 0$

$$=\sqrt{d}\,e^{\frac{i}{2}\left(cds^2\right)}\delta(t-ds) \qquad \text{when } b=0$$

and $K_c(x,w)=\frac{1}{\sqrt{2\pi ib}}e^{\frac{i}{2}\left(\frac{d}{b}\right)w^2}e^{\frac{i}{2}\left(\frac{a}{b}\right)x^2}\cos\left(\frac{w}{b}x\right)$ when $b\neq 0$

$$=\sqrt{d}\,e^{\frac{i}{2}\left(cdw^2\right)}\delta(x-dw) \qquad \text{when } b=0$$

where $\gamma_{E,k}\{K_s(t,s)K_c(x,w)\}=\sup_{\substack{-\infty<t<\infty\\ -\infty<x<\infty}}\left|D_t^k\, D_x^l\, K_s(t,s)K_c(x,w)\right|<\infty$

III. THEOREM :(INVERSION)

If $\{2DCSCT\, f(t,x)\}(s,w)$ is canonical sine- cosine transform of $f(t,x)$ then

$$f(t,x)=-ie^{\frac{-i}{2}\left(\frac{a}{b}\right)t^2}e^{\frac{-i}{2}\left(\frac{a}{b}\right)x^2}\sqrt{\frac{2\pi i}{b}}\sqrt{\frac{2\pi i}{b}}.$$
$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{\frac{-i}{2}\left(\frac{d}{b}\right)s^2}e^{\frac{-i}{2}\left(\frac{d}{b}\right)w^2}\sin\left(\frac{s}{b}t\right)\cos\left(\frac{w}{b}x\right)\{2DCSCT\ f(t,x)\}(s,w)\,dsdw,$$

Proof: The two dimensional canonical sine- cosine transform if $f(t,x)$ is given by

$$\{2DCSCT\, f(t,x)\}(s,w)$$
$$= -i\frac{1}{\sqrt{2\pi ib}}\frac{1}{\sqrt{2\pi ib}}e^{\frac{i}{2}\left(\frac{d}{b}\right)s^2}e^{\frac{i}{2}\left(\frac{d}{b}\right)w^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\sin\left(\frac{s}{b}t\right)\cos\left(\frac{w}{b}x\right)e^{\frac{i}{2}\left(\frac{a}{b}\right)t^2}e^{\frac{i}{2}\left(\frac{a}{b}\right)x^2}f(t,x)dxdt$$

$$f(s,w) = \{2DCSCT\, f(t,x)\}(s,w)$$
$$\therefore f(s,w)$$
$$= -i\frac{1}{\sqrt{2\pi ib}}\frac{1}{\sqrt{2\pi ib}}e^{\frac{i}{2}\left(\frac{d}{b}\right)s^2}.e^{\frac{i}{2}\left(\frac{d}{b}\right)w^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\sin\left(\frac{s}{b}t\right)\cos\left(\frac{w}{b}t\right)e^{\frac{i}{2}\left(\frac{a}{b}\right)t^2}e^{\frac{i}{2}\left(\frac{a}{b}\right)x^2}f(t,x)dxdt$$

$$f(s,w).\sqrt{2\pi ib}\sqrt{2\pi ib}\; e^{-\frac{i}{2}\left(\frac{d}{b}\right)s^2}.e^{-\frac{i}{2}\left(\frac{d}{b}\right)w^2}$$
$$= -i\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\sin\left(\frac{s}{b}t\right)\cos\left(\frac{w}{b}x\right)e^{\frac{i}{2}\left(\frac{a}{b}\right)t^2}e^{\frac{i}{2}\left(\frac{a}{b}\right)x^2}f(t,x)dxdt$$

$$\therefore C_1(s,w) = f(s,w)\sqrt{2\pi ib}\sqrt{2\pi ib}\; e^{-\frac{i}{2}\left(\frac{d}{b}\right)s^2}e^{-\frac{i}{2}\left(\frac{d}{b}\right)w^2}$$

And $g(t,x) = e^{\frac{i}{2}\left(\frac{a}{b}\right)t^2}e^{\frac{i}{2}\left(\frac{a}{b}\right)x^2}f(t,x)$

$$C_1(s,w) = -i\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}g(t,x).\sin\left(\frac{s}{b}t\right).\cos\left(\frac{w}{b}x\right)dxdt$$

$$C_1(s,w) = \{2DCSCTg(t,x)\}\left(\frac{s}{b},\frac{w}{b}\right)$$

Where $\{2DCSCTg(t,x)\}\left(\frac{s}{b},\frac{w}{b}\right)$ is 2D Canonical sine-cosine transform of g(t,x).2D canonical sine -cosine transform g(t,x) with argument

$\therefore \frac{s}{b} = \eta$ and $\frac{w}{b} = \xi$ Therefore, $\frac{ds}{b} = d\eta$ and $\frac{dw}{b} = d\xi$

$$\therefore C_1(s,w) = \{2DCSCTg(t,x)\}(\eta,\xi)$$

By using inversion formula we get $\therefore g(t,x) = -i\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}C_1(s,w)\sin(\eta t)\cos(\xi x)d\eta d\xi$

$$g(t,x) = -i\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}F(s,w)\sqrt{2\pi ib}\sqrt{2\pi ib}\; e^{-\frac{i}{2}\left(\frac{d}{b}\right)s^2}e^{-\frac{i}{2}\left(\frac{d}{b}\right)w^2}\sin(\eta t)\cos(\xi x)d\eta d\xi$$

$$e^{\frac{i}{2}\left(\frac{a}{b}\right)t^2} e^{\frac{i}{2}\left(\frac{a}{b}\right)x^2} f(t,x) = -i\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} F(s,w)\sqrt{2\pi ib}\,\sqrt{2\pi ib}\; e^{-\frac{i}{2}\left(\frac{d}{b}\right)s^2} e^{-\frac{i}{2}\left(\frac{d}{b}\right)w^2} \sin\left(\frac{s}{b}t\right)\cos\left(\frac{w}{b}x\right)\frac{ds}{b}\frac{dw}{b}$$

$$e^{\frac{i}{2}\left(\frac{a}{b}\right)t^2} e^{\frac{i}{2}\left(\frac{a}{b}\right)x^2} f(t,x)$$
$$= -i\sqrt{2\pi ib}\,\sqrt{2\pi ib}\,\frac{1}{b}\frac{1}{b}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{\frac{-i}{2}\left(\frac{d}{b}\right)s^2} e^{\frac{-i}{2}\left(\frac{d}{b}\right)w^2} \sin\left(\frac{s}{b}t\right)\cos\left(\frac{w}{b}x\right) f(s,w)\,ds\,dw$$

$$f(t,x)$$
$$= -i\, e^{-\frac{i}{2}\left(\frac{a}{b}\right)t^2} e^{-\frac{i}{2}\left(\frac{a}{b}\right)x^2}\sqrt{\frac{2\pi i}{b}}\sqrt{\frac{2\pi i}{b}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{\frac{i}{2}\left(\frac{d}{b}\right)s^2} e^{\frac{i}{2}\left(\frac{d}{b}\right)w^2} \sin\left(\frac{s}{b}t\right)\cos\left(\frac{w}{b}x\right)\{2DCSCT\, f(t,x)\}(s,w)\,ds\,dw$$

IV. THEOREM:(UNIQUENESS)

If $\{2DCSCT\ f(t,x)\}\,(s,w)$ and $\{2DCSCT\ g(t,x)\}\,(s,w)$ are 2D canonical sine-cosine transform and

$\sup pf \subset s_a$, and s_b and, $\sup p\, g \subset s_a, and \quad s_b$

Where $s_a = \{t : t \in R^n,\ \ |t| \le a, a > 0\}$ and $s_b = \{x : x \in R^n,\ \ |x| \le b, b > 0\}$

If $\{2DCSCT\ f(t,x)\}\,(s,w) = \{2DCSCT\ g(t,x)\}\,(s,w)$

then, f = g in the sense of equality in $D'(I)$

Proof: By inversion theorem $f - g$

$$= \left(-ie^{\frac{-i}{2}\left(\frac{a}{b}\right)t^2} e^{\frac{-i}{2}\left(\frac{a}{b}\right)x^2}\sqrt{\frac{2\pi i}{b}}\sqrt{\frac{2\pi i}{b}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{\frac{-i}{2}\left(\frac{d}{b}\right)s^2} e^{\frac{-i}{2}\left(\frac{d}{b}\right)w^2}\sin\left(\frac{s}{b}t\right)\cos\left(\frac{w}{b}x\right)\right.$$
$$\left.\{2DCSCT\ f(t,x)\}(s,w)\,ds\,dw\right)$$

$$-\left(-ie^{\frac{-i}{2}\left(\frac{a}{b}\right)t^2} e^{\frac{-i}{2}\left(\frac{a}{b}\right)x^2}\sqrt{\frac{2\pi i}{b}}\sqrt{\frac{2\pi i}{b}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{\frac{-i}{2}\left(\frac{d}{b}\right)s^2} e^{\frac{-i}{2}\left(\frac{d}{b}\right)w^2}\sin\left(\frac{s}{b}t\right)\cos\left(\frac{w}{b}x\right)\right.$$
$$\left.\{2DCSCT\ g(t,x)\}(s,w)\,ds\,dw\right)$$

$$\therefore f - g = -i\sqrt{\frac{2\pi i}{b}}\sqrt{\frac{2\pi i}{b}}\, e^{-\frac{i}{2}\left(\frac{a}{b}\right)t^2} e^{-\frac{i}{2}\left(\frac{a}{b}\right)x^2}\int_{-\infty}^{\infty} e^{-\frac{i}{2}\left(\frac{d}{b}\right)s^2} e^{-\frac{i}{2}\left(\frac{d}{b}\right)s^2}\sin\left(\frac{s}{b}x\right)\cos\left(\frac{w}{b}x\right)$$
$$\left[\{2DCSCT f(t,x)\} - \{2DCSCT g(t,x)\}\right] ds\,dw$$

Thus f = g in $D'(I)$

V. CONCLUSION

In this paper two-dimensional canonical sine-cosine is Generalized in the form the distributional sense, we have inversion theorem for this transform is proved. Lastly uniqueness theorem is also proved.

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Different Versions of Vertex Degrees of the Molecular Graph and Topological Indices

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ABSTRACT

Research work in chemical graph theory is mainly focused on degree based and types of topological indices of molecular graphs. In the chemical graph theory, many degrees based topological indices have been introduced and studied which are given by the [1] general formula TI(G) $=\sum_{u\,v\in E(G)} F\left(\deg(u_i), \deg(v_j)\right)$.In this paper different versions of vertex degree and corresponding first Zagreb index, second Zagreb index and forgotten index are investigated for2-methylbutane.

Keywords: Degree,forgotten index, modified version of topological index, molecular graph, multiplication-degree,sum-degree, Zagreb index.

I. INTRODUCTION

Molecules and molecular compounds are often modelled by molecular graphs. A molecular graph is presentation of the structural formula of a chemical compound in terms of graph theory whose vertices correspond to the atoms of compound and edges correspond to chemical bonds. Degree based Zagreb indices and forgotten index are the basic degree basedtopological indices. There are different ways to define vertex degree and compute the topological indices by using the classical formulas or graph polynomials[2-14]. Let G(V,E) be a graph with n vertices and m edges.The degree of a vertex u∈V(G) is denoted by d_u and is the number of vertices adjacent to u. The edge connecting the vertices u and v is denoted by uv.The maximum and minimum degree of a vertex among vertices of G are denoted by $\Delta = \max\{d_v|v \in V(G)\}$, $\delta = \min\{d_v|v \in V(G)\}$respectively.The general formula for topological index is TI(G) $=\sum_{u\,v\in E(G)} F\left(deg(u_i), deg(v_j)\right)$,where F(x,y) is some function with property F(x,y) = F(y,x).

The R-degree first Zagreb index, R-degree second Zagreb index and R-degree forgotten index are defined as [15] $M_{R^1}(G)=\sum_{uv\in E(G)} [r(u)+r(v)]$,$M_{R^2}(G)=\sum_{uv\in E(G)} r(u)r(v)$ and

$F_R(G) = \sum_{uv\in E(G)}[r(u)^2 + r(v)^2]$,where R-degree of a vertex visr(v =M_v+ S_v,S_v is sumdegree and M_v is multiplication-degree of v.

The revan-degree first Zagreb index, revan-degree second Zagreb index and revan-degree forgotten index are defined as[16]

$rM_1(G) = \sum_{uv\in E(G)}[r_G(u) + r_G(v)]$,$rM_2(G) = \sum_{uv\in E(G)} r_G(u)r_G(v)$ and

$rF(G) = \sum_{uv\in E(G)}[r_G(u)^2 + r_G(v)^2]$,where revan-degree of a vertex u is

$r_G(u) = \Delta(G)+\delta(G)-d_G(u)$.

The reverse-degree first Zagreb index, reverse-degree second Zagreb index and reverse-degree forgotten index are defined as

$cM_1(G) = \sum_{uv\in E(G)}(c_u + c_v)$,$cM_2(G) = \sum_{uv\in E(G)}(c_u c_v)$ and $cF(G) = \sum_{uv\in E(G)}(c_u^2 + c_v^2)$,wherethe reverse-degreeof a vertex v is $c_v = \Delta(G) - d_G(v) + 1$.

The S-degree first Zagreb index, S-degree second Zagreb index and S-degree forgotten index are defined as [17-18]

$M_{S^1}(G) = \sum_{uv\in E(G)} [S(u) + S(v)]$, $M_{S^2}(G) = \sum_{uv\in E(G)} S(u)S(v)$and

$F_S(G) = \sum_{uv\in E(G)} [S(u)^2 + S(v)^2]$, where S-degree of a vertex $S(v) = |M_v - S_v|$.

The modifiedleap degreefirst Zagreb index, leap degree second Zagreb index and leap degree forgotten index are defined as [19]

$LM_1^*(G) = \sum_{uv\in E(G)} [d_2(u) + d_2(v)]$,$LM_2(G) = \sum_{uv\in V(G)} d_2(u)d_2(v)$ and

$LF(G) = \sum_{uv\in V(G)}[(d_2^2(u) + d_2^2(v)]$.

The modifiedHDRfirst Zagreb index,HDR second Zagreb index and modified HDR forgotten index are defined as[20]

$HDRM_1^*(G) = \sum_{uv\in E(G)}[d_{hr}(u) + d_{hr}(v)]$,$HDRM_2(G) = \sum_{uv\in E(G)}[d_{hr}(u)d_{hr}(v)]$ and

$HDRF^*(G) = \sum_{uv\in E(G)}[d_{hr}^2(u) + d_{hr}^2(v)]$,where $d_{hr}(u) = |\{u,v\in V(G)/d(u,v) = \frac{R}{2}\}|$,

d(u,v)is the distance between the vertices u and vin V(G) and R is radius of G.

The first Zagreb coindex and second Zagreb coindexand forgotten coindexare defined as [21-23]

$\overline{M_1}(G) = \sum_{uv\notin E(G)} (d_u + d_v)$, $\overline{M_2}(G) = \sum_{uv\notin E(G)} (d_u d_v)$ and $\overline{F}(G) = \sum_{uv\notin E(G)} (d_u^2 + d_v^2)$.

The non-neighbor first Zagreb index and non-neighbor second Zagreb index and non-neighbor forgotten index are defined as [24]

$\overline{M_1(G)} = \sum_{uv\in E(G)} (\overline{d_G(u)} + \overline{d_G(v)})$,$\overline{M_2(G)} = \sum_{uv\in E(G)} \overline{d_G(u)d_G(v)}$ and

$\overline{F(G)} = \sum_{uv\in E(G)} [\overline{d_G(u)}^2 + \overline{d_G(v)}^2]$.

The downhillfirst Zagreb index,downhill second Zagreb index and downhill forgotten index are defined as[25-26]

$DWM_1(G) = \sum_{v\in V(G)}(d_{dn}(v))^2$,$DWM_2(G) = \sum_{vu\in E(G)} d_{dn}(v)d_{dn}(u)$ and $DWF(G) = \sum_{v\in V(G)}(d_{dn}(v))^3$.

An uphillfirst Zagreb index, uphill second Zagreb index and uphill forgotten index are defined as [27]

$UPM_1(G) = \sum_{v\in V(G)}(d_{up}(v))^2$,$UPM_2(G) = \sum_{v\in V(G)} d_{up}(u)\, d_{up}(v)$ and $UPF(G) = \sum_{v\in V(G)}(d_{up}(v))^3$.

The neighborhoodfirst Zagreb index,modified version of neighborhoodsecond Zagreb index and neighborhood forgotten index are defined as [28-29]

$M_{N1}(G) = \sum_{v\in V(G)} [\delta_G(v)]^2$,$M_{N2}^*(G) = \sum_{uv\in E(G)} [\delta_G(u)\delta_G(v)]$ and $F_N(G) = \sum_{v\in V(G)}[\delta_G(v)]^3$.

The ev-degree Randic index of the graph G is defined as [30-31]$R^\beta(G) = \sum_{e\in E(G)} c_e^{-\frac{1}{2}}$.

The ve-degree first Zagreb index, ev-degree modified second Zagreb index and ve-degree forgotten index are defined as

$M_1^{ve}(G) = \sum_{v\in V(G)} d_{ve}(v)^2$, $M_2^{*ev}(G) = \sum_{e\in E(G)} \frac{1}{d_{ev}(e)}$ and $F^{ve}(G) = \sum_{v\in V(G)} d_{ve}(v)^3$.

In this paper R, revan, reverse,S, leap, HDR, coindex, non-neighbor, downhill, uphill,neighborhood degreesum and vedegrees based first Zagreb index, second Zagreb index and forgotten index of 2-methylbutane are investigated. All the symbols and notations used in this paper are standard and mainly taken from books of graph theory [32-34].

II. MATERIALS AND METHODS

A molecular graph G(V, E) is constructed by representing each atom of molecule by vertex and bonds between them by edges. Let V(G) be vertex set and E(G) be edge set.The chemical structure and molecular graph of 2-methylbutane are shown in figure 1. Let molecular graph of 2-methylbutane is denoted by G.The vertices 1,4 and 5 are pendent vertices with degree 1. The degree of vertex 2 is 3 and that of 3 is 2. The maximum,minimum degree among vertices of Gand different versions of vertex degree are observed for molecular graph G. In this paper R, revan, reverse, S, leap, HDR, coindex, non-neighbor, downhill, uphill, neighborhood degreesum and ve degrees based first Zagreb index, second Zagreb index and forgotten index of 2-methylbutane are computed by using definitions of these topological indices.

III. RESULTS AND DISCUSSION

The maximum degree among vertices of G is 3 and minimum degree is 1. Let molecular graph of 2-methylbutane is denoted by G.The basic definitions of first Zagreb index, second Zagreb index and forgotten index are used to compute topological indices (table 1).The edge partition of 2-methylbutane is the underlying point in the determination of different versions of vertex degree of a graph (table 2).

Theorem 1. R-degree firstZagreb index, R-degree second Zagreb index and R-degree forgotten index of 2-methylbutane are(i)M_{R^1} (G)= 49,(ii)M_{R^2} (G)= 149and (iii)F_R(G)= 307.

Proof. Byusingdefinitions and edge degree partition of molecular graph G, we get

(i)$M_{R^1}(G) = \sum_{uv\in E(G)}[r(u)+r(v)]$

$=\sum_{13\in E(G)}(6+6)+\sum_{12\in E(G)}(4+7)+\sum_{23\in E(G)}(7+7)$=2(6+6)+(4+7)+(7+7)= 49.

(ii)$RM_2(G) = \sum_{uv\in E(G)} [r(u)r(v)]$

$= \sum_{13\in E(G)}(6*6)+\sum_{12\in E(G)}(4*7)+\sum_{23\in E(G)}(7*7)$=2(6*6)+(4*7)+(7*7)= 149.

(iii) $F_R(G)= \sum_{uv\in E(G)}[r(u)^2+r(v)^2]$

$= \sum_{13\in E(G)}(6^2+6^2)+\sum_{12\in E(G)}(4^2+7^2)+\sum_{23\in E(G)}(7^2+7^2)$

$= 2(6^2+6^2)+(4^2+7^2)+(7^2+7^2)$= 307.

Theorem 2. Revan-degree firstZagreb index, revan-degree second Zagreb index and revan-degree forgotten index of 2-methylbutaneare(i)rM_1(G) = 16,(ii)rM_2(G) = 14and(iii)rF(G) = 38.

Proof. Byusingdefinitions and edge degree partition of molecular graph G, we get

(i)$rM_1(G)=\sum_{uv\in E(G)} [r_G(u)+r_G(v)]$

$= \sum_{13\in E(G)} (3+1)+\sum_{12\in E(G)} (3+2)+\sum_{23\in E(G)} (2+1)$= 2(3+1)+(3+2)+(2+1)= 16.

(ii)$rM_2(G)=\sum_{uv\in E(G)} [r_G(u)r_G(v)]$

$= \sum_{13\in E(G)} (3*1)+\sum_{12\in E(G)} (3*2)+\sum_{23\in E(G)} (2*1)$= 2(3)+6+2= 14.

(iii)$rF(G)=\sum_{uv\in E(G)}[r_G(u)^2+r_G(v)^2]$

$= \sum_{□□\in □(□)} (3^2+1^2)+\sum_{□□\in □(□)} (3^2+2^2)+\sum_{□□\in □(□)} (2^2+1^2)$= 2(10)+13+5= 38.

Theorem 3. Reverse-degreefirstZagreb index, reverse-degree second Zagreb index and reverse-degree forgotten index of 2-methylbutane are

(i)$cM_1(G)$= 16,(ii)$cM_2(G)$= 14and (iii)cF(G)= 38.

Proof. Byusingdefinitions and edge degree partition of molecular graph G,we get

(i)$cM_1(G)=\sum_{uv\in E(G)}(c_u+c_v)$

$= \sum_{13\in □(□)}(3+1)+\sum_{12\in □(□)}(3+2)+\sum_{23\in □(□)}(2+1)$= 2(4)+5+3= 16.

(ii)$cM_2(G)=\sum_{uv\in E(G)}(c_u c_v)$

$= \sum_{13\in □(□)}(3*1)+\sum_{12\in □(□)}(3*2)+\sum_{23\in □(□)}(2*1)$= 2(3)+6+2= 14.

(iii)$cF(G)=\sum_{uv\in E(G)}(c_u^2+c_v^2)$

$= \sum_{13\in □(□)}(3^2+1^2)+\sum_{12\in □(□)}(3^2+2^2)+\sum_{23\in □(□)}(2^2+1^2)$

$= 2(3^2+1^2)+(3^2+2^2)+(2^2+1^2)$= 38.

Theorem 4.S-degree first Zagreb index, S-degree second Zagreb index and S-degree forgotten index of 2-methylbutane are(i)$M_{S^1}(G)$= 8,(ii)$M_{S^2}(G)$ = 2and (iii)$F_S(G)$ = 18.

Proof. Byusingdefinitions and edge degree partition of molecular graph G, we get

(i)$M_{S^1}(G)=\sum_{uv\in E(G)} [S(u)+S(v)]$

$= \sum_{13\in □(□)} (0+2)+\sum_{12\in □(□)} (0+1)+\sum_{23\in □(□)} (1+2)$= 2(2)+1+3= 8.

(ii)$M_{S^2}(G)=\sum_{uv\in E(G)} S(u)S(v)$

$= \sum_{13\in □(□)} (0*2)+\sum_{12\in □(□)} (0*1)+\sum_{23\in □(□)} (1*2)$= 1*2= 2.

(iii)$F_S(G)=\sum_{uv\in E(G)} [S(u)^2+S(v)^2]$

$= \sum_{13\in □(□)} (0+2^2)+\sum_{12\in □(□)} (0+1)^2+\sum_{23\in □(□)} (1^2+2^2)$= $2(2)^2+1^2+3^2$= 18.

Theorem 5. Leapmodified first Zagreb index, leap second Zagreb index and leap forgotten index of2-methylbutane are(i)$LM_1^*(G)$ = 12,(ii)$LM_2(G)$ = 8and (iii)LF(G) = 20.

Proof. Byusingdefinitions and edge degree partition of molecular graph G, we get

(i)$LM_1^*(G)=\sum_{uv\in \boldsymbol{E(G)}} [d_2(u)+d_2(v)]$

$= \sum_{□□\in □(□)} (1+2)+\sum_{□□\in □(□)} (2+1)$= 2(1+2)+2(2+1)= 12.

(ii)$LM_2(G)=\sum_{uv\in \boldsymbol{V(G)}} d_2(u)d_2(v)$

$= \sum_{□□\in □(□)} (1*2)+\sum_{□□\in □(□)} (2*1)$= 2(1*2)+2(2*1)= 8.

(iii)$LF(G)=\sum_{uv\in V(G)}[d_2^2(u)+d_2^2(v)]$

$= \sum_{12\in □(G)}(1^2+2^2)+\sum_{21\in □(G)}(2^2+1^2)$= $2(1^2+2^2)+2(2^2+1^2)$= 20.

Theorem 6.HDRmodifiedfirst Zagreb index, HDR second Zagreb index andHDR modified forgotten index of2-methylbutaneare

(i)$HDRM_1^*(G)$ = 16,(ii)$HDRM_2(G)$ = 14and (iii)HDRF*(G) = 38.

Proof. Byusingdefinitions and edge degree partition of molecular graph G, we get

(i)$HDRM_1^*(G)=\sum_{uv\in E(G)}[d_{hr}(u)+d_{hr}(v)]$

$= \sum_{□□\in □(□)}(1+3)+\sum_{□□\in □(□)}(3+2)+\sum_{34\in □(□)}(1+2)$= 2(1+3) +1(3+2) +1(1+2)= 16.

(ii)$HDRM_2(G)=\sum_{uv\in E(G)}[d_{hr}(u)d_{hr}(v)]$

$= \sum_{□□\in □(□)}(1*3)+\sum_{□□\in □(□)}(3*2)+\sum_{34\in □(□)}(1*2)$= 2(1*3) +1(3*2) +1(1*2)= 14.

(iii)$HDRF^*(G)=\sum_{uv\in E(G)}[d_{hr}^2(u)+d_{hr}^2(v)]$

$=\sum_{12\in E(G)}(1^2+3^2)+\sum_{23\in E(G)}(3^2+2^2)+\sum_{34\in E(G)}(1^2+2^2)$

$= 2(1^2+3^2)+1(3^2+2^2)+1(1^2+2^2)$= 38.

Theorem 7. FirstZagreb coindex, second Zagreb coindex and forgotten coindex of 2-methylbutaneare(i)$\overline{M_1}$(G) = 11,(ii)$\overline{M_2}$(G) = 7and (iii)$\overline{F}$(G) = 19.

Proof. Byusingdefinitions and edge degree partition of molecular graph G, we get

(i) $\overline{M_1}(G)=\sum_{uv\notin E(G)} (d_u + d_v)$

$= \sum_{51\notin E(G)} (1 + 1)+\sum_{53\notin E(G)} (1 + 2)+\sum_{24\notin E(G)} (3 + 1)$= 2(1+1) +1(1+2) +1(3+1)= 11.

(ii)$\overline{M_2}(G) =\sum_{uv\notin E(G)} (d_u d_v)$

$= \sum_{51\notin E(G)} (1 * 1)+\sum_{53\notin E(G)} (1 * 2)+\sum_{24\notin E(G)} (3 * 1)$= 2(1*1) +1(1*2) +1(3*1)= 7.

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

$= \sum_{51\notin E(G)} (1^2 + 1^2)+\sum_{53\notin E(G)} (1^2 + 2^2)+\sum_{24\notin E(G)} (3^2 + 1^2)$

= $2(1^2+1^2) +1(1^2+2^2) +1(3^2+1^2)$= 19.

Theorem 8. Non-neighborfirst Zagreb index, non-neighbor second Zagreb index and non-neighborforgotten index of 2-methylbutane are (i)$\overline{M_1(G)}$= 16,(ii) $\overline{M_2(G)}$= 14and (iii)$\overline{F(G)}$ = 38.

Proof. Byusingdefinitions and edge degree partition of molecular graph G,we get

(i)$\overline{M_1(G)} =\sum_{uv\in E(G)} (\overline{d_G(u)} + \overline{d_G(v)})$

$= \sum_{12\in E(G)}(3 + 1)+\sum_{23\in E(G)}(2 + 1)+\sum_{34\in E(G)}(3 + 2)$= 2(3+1) +1(2+1) +1(3+2)= 16.

(ii)$\overline{M_2(G)} =\sum_{uv\in E(G)} \overline{d_G(u) d_G(v)}$

$= \sum_{12\in E(G)}(3 * 1)+\sum_{23\in E(G)}(2 * 1)+\sum_{34\in E(G)}(3 * 2)$= 2(3*1) +1(2*1) +1(3*2)= 14.

(iii)$\overline{F(G)}= \sum_{uv\in E(G)}[\overline{d_G(u)}^2 + \overline{d_G(v)}^2]$

$= \sum_{12\in E(G)}(3^2 + 1^2)+\sum_{23\in E(G)}(2^2 + 1^2)+\sum_{34\in E(G)}(3^2 + 2^2)$

= $2(3^2+1^2) +1(2^2+1^2) +1(3^2+2^2)$= 38.

Theorem 9. Downhillfirst Zagreb index, downhill second Zagreb index and downhillforgotten index of 2-methylbutane are(i)DWM_1(G) = 48,(ii) DWM_2(G) =32and (iii) DWF(G) = 128.

Proof. Byusingdefinitions and edge degree partition of molecular graph G, we get

(i)$DWM_1(G)=\sum_{v\in V(G)}(d_{dn}(v))^2$

$= \sum_{v\in V(G)}(d_{dn}(n-1))^2$= $(n-2)(n-1)^2$= 48.

(ii) $DWM_2(G)=\sum_{vu\in E(G)} d_{dn}(v)d_{dn}(u)$

$= \sum_{vu\in V(G)} d_{dn}(n-1)d_{dn}(n-1)+\sum_{vu\in V(G)} d_{dn}(n-1)d_{dn}(0)$= (n-3)(n-1)(n-1)= 32.

(iii)$DWF(G) =\sum_{v\in V(G)}(d_{dn}(v))^3$

$= \sum_{v\in V(G)}(d_{dn}(n-1))^3$= $(n-3)(n-1)^3$= 128.

Theorem 10. Uphillfirst Zagreb index, uphill second Zagreb index and uphill forgotten index of 2-methylbutane are(i)UPM_1(G) =39, (ii)UPM_2(G) = 26and (iii)UPF(G) = 105.

Proof. Byusingdefinitions and edge degree partition of molecular graph G, we get

(i)$UPM_1(G) =\sum_{v\in V(G)}(d_{up}(v))^2$

$= \sum_{v\in V(G)}(d_{up}(n-2))^2+\sum_{v\in V(G)}(d_{up}(n-3))^2$= $3(n-2)^2+(n-2)(n-3)^2$= 39.

(ii)$UPM_2(G) =\sum_{v\in V(G)} d_{up}(v)\, d_{up}(u)$

$\sum_{v\in V(G)}(n-2)(n-3)+\sum_{v\in V(G)}(d_{up}(n-3)\ (n-3)$= 3[(n-2)(n-3)]+(n-3)[(n-3)(n-3)]= 26.

(iii)$UPF(G) =\sum_{v\in V(G)}(d_{up}(v))^3$

$= \sum_{v\in V(G)}(d_{up}(n-2))^3+\sum_{v\in V(G)}(d_{up}(n-3))^3$= $3(n-2)^3+(n-2)(n-3)^3$= 105.

Theorem 11. NeighborhoodfirstZagreb index, neighborhoodsecond Zagreb index and neighborhoodforgotten index of 2-methylbutane are

(i)M_{N1}(G)= 58,(ii) M_{N2}(G) = 53and (iii)F_N(G) = 213.

Proof. Byusingdefinitions and edge degree partition of molecular graph G, we get

(i) $M_{N1}(G) = \sum_{v\in V(G)} [\delta_G(v)]^2$

$= \sum_{1\in V(G)} 2^2 + \sum_{2\in V(G)} 5^2 + \sum_{5\in V(G)} 3^2 + \sum_{3\in V(G)} 4^2 = 2*2^2+5^2+3^2+4^2 = 58.$

(ii) $M_{N2}(G) = \sum_{uv\in E(G)} [\delta_G(u)\delta_G(v)]$

$= \sum_{12\in E(G)} (2*5) + \sum_{25\in E(G)} (5*3) + \sum_{23\in E(G)} (5*4) + \sum_{34\in E(G)} (4*2)$

= 2*5+5*3+5*4+4*2= 53.

(iii) $F_N(G) = \sum_{v\in V(G)} [\delta_G(v)]^3$

$= \sum_{1\in V(G)} 2^3 + \sum_{2\in V(G)} 5^3 + \sum_{5\in V(G)} 2^3 + \sum_{3\in V(G)} 4^3 = 2*2^3+5^3+2^3+4^3 = 213.$

Theorem 12. The ve-degree firstZagreb index, ev-degree modified second Zagreb index and ve-degree forgotten index of 2-methylbutane are

(i) $M_1^{ve}(G) = 54$,(ii) $M_2^{*ev}(G) = 1.033$and(iii) $F^{ve}(G) = 190$.

Proof. Byusingdefinitions and edge degree partition of molecular graph G,we get

(i) $M_1^{ve}(G) = \sum_{v\in V(G)} d_{ve}(v)^2$

$= \sum_{1\in V(G)} d_{ve}(3)^2 + \sum_{2\in V(G)} d_{ve}(4)^2 + \sum_{4\in V(G)} d_{ve}(2)^2 = 2*9+2*16+4 = 54.$

(ii) $M_2^{*ev}(G) = \sum_{e\in E(G)} \frac{1}{d_{ev}(e)}$

$= \sum_{12\in E(G)} \frac{1}{2} + \sum_{23\in E(G)} \frac{1}{5} + \sum_{34\in E(G)} \frac{1}{3} = 2*\frac{1}{4} + \frac{1}{5} + \frac{1}{3} = 1.033.$

(iii) $F^{ve}(G) = \sum_{v\in V(G)} d_{ve}(v)^3$

$= \sum_{1\in V(G)} d_{ve}(3)^3 + \sum_{2\in V(G)} d_{ve}(4)^3 + \sum_{4\in V(G)} d_{ve}(2)^3 = 2*27+2*64+8 = 190.$

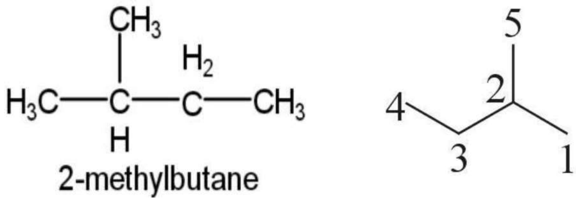

Figure 1. The chemical structure and molecular graph of 2-methylbutane.

Table 1. Basic formulas of topological indices.

Topological index	First Zagreb index	Second Zagreb index	Forgotten index
f(x,y)	x+y	xy	x^2+y^2

Table 2. Edge degree partition of 2-methylbutane.

(d_u, d_v)	(1,3)	(1,2)	(2,3)
Number of edges	2	1	1

IV. CONCLUSION

The revan, reverse, HDR and non-neighbor degrees-basedstudied topological indices have similar values for respective topological indices. From degree of vertices of a molecular graph: R, revan, reverse, S, leap, HDR, coindex, non-neighbor, downhill, uphill, neighborhood and ve degrees are observed for 2-methylbutane and then corresponding first Zagreb index, second Zagreb index and forgotten index are computed. This concept can be applied to any molecular graph to investigate corresponding degree based topological indices.

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Equations Dealing with Topological Indices : Zagreb Indices

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ABSTRACT

The main aim of study of chemical graph theory is to compute the distance and degree based topological indices and bounds in topological indices of molecular graphs. Topological equations comprise degree based topological indices, degree of a graph, degree of a complement graph and coindices. Some topological equations based on first, second, third, hyper Zagreb indices, forgotten index, Banhatti indicesand Sombor index are investigated for polycyclic aromatic hydrocarbons (PAHs).

KEYWORDS: Complement of graph, degree, line graph, molecular graph, polycyclic aromatic compound, topological equation, topological index.

I. INTRODUCTION

Let G be a simple,finite, connected graph with vertex set V(G) and edge set E(G). Family of descriptors that all have the general form D(G) = $\sum_{u=v} F(d_u, d_v)$,where summation goes all over all pairs of vertices u,v of the molecular graph G and d_u denotes the degree of vertex u was studied by I.Gutman[1].Topological indices of a simple graph are numerical descriptors that are derived from graph of chemical compounds. Conventional way of computing the topological indices of molecular graph is by using classical formulas, graph exponentials, M-polynomials and degree-distance polynomials[2-12].For a simple connected graph G, the first and second Zagreb indices are defined as [13]

$M_1(G) = \sum_{uv\in E(G)}(d_u + d_v)$ and $M_2(G) = \sum_{uv\in E(G)} d_u\, d_v$.

The hyper Zagreb index is defined as [14]

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

The topological analysis of polycyclic aromatic hydrocarbonsusing irregularity indices was done by J.Konsalraj et al.in [15].The first and second Zagreb coindices and forgotten coindex are defined as [16-19]

$\overline{M_1}(G) = \sum_{uv\notin E(G)}(d_u + d_v)$, $\overline{M_2}(G) = \sum_{uv\notin E(G)} d_u\, d_v$ and $\overline{F}(G) = \sum_{uv\notin E(G)}(d_u^2 + d_v^2)$.

The hyper Zagreb index is related to F(G) and M_2(G)[20] by,

$HZ(G) = F(G) + 2M_2(G)$. (1)

Let G is graph of order n and size m then the following equations relate first and second Zagreb indices as[21-22]

$\overline{M_2}(G) = 2m^2-\frac{1}{2}M_1(G)-M_2(G)$, (2)

$\overline{M_2}(\overline{G}) = m(n-1)^2-(n-1)M_1(G)+M_2(G)$, (3)

$M_1(\overline{G}) = M_1(G)+n(n-1)^2-4m(n-1)$, (4)

$M_1(L(G)) = 4m-2M_1(G)+2M_2(G)+F(G)$, (5)

$\overline{M_1}(\overline{G}) = 2m(n-1)-M_1(G)$, (6)

and $RM_2(G) = M_2(G) - M_1(G)+m$. (7)

The Banhatti indices are related to first Zagreb index and hyper Zagreb index by

$B_1(G) = 3M_1(G)-4m$ and $B_2(G) = HM_1(G) - 2M_1(G)$, (8)

where $B_1(G)$ and $B_2(G)$ are first and second Banhatti indices [23-24] and $HM_1(G)$ is hyper first Zagreb index.

The complement of a graph G, denoted by $\overline{G}$, is a simple graph on the same set of vertices u and v are connected by an edge uv, if and only if they are not adjacent in G. The degree of a vertex v in $\overline{G}$ is given by $d_{\overline{G}}(v) = |V(G)|-1-d_G(v)$, where $|V(G)| = n$. Let L(G) be the line graph of G then $d_G(e)= d_u+d_v-2$[25].The irregularity measure index is defined as

$IRM(G) = F(G)-2M_2(G)$, where $IRM(G) = \sum_{xy\in E(G)}[d(x)-d(y)]^2$ (9)

and the F-coindex is defined as $\overline{F}(G) = (n-1)M_1(G)-F(G)$. (10)

In complement form forgotten index is expressed as

$F(\overline{G})= n(n-1)^3-6m(n-1)^2+3(n-1)M_1(G)-F(G)$,

$\overline{F}(\overline{G})= 2m(n-1)^2 -2(n-1)M_1(G)+F(G)$

and $\overline{M_1}(\overline{G}) = \overline{M_1}(G)$ and $\overline{F}(\overline{G}) \neq \overline{F}(G)$. (11)

If G is any graph, then the Sombor index (with $p = \frac{1}{2}$) is [26]

$SO_{\frac{1}{2}}(G) = M_1(G)+2RR(G)$ (12)

where $SO_p(G) = \sum_{uv\in E(G)}(d_u{}^p + d_v{}^p)^{\frac{1}{p}}$, we call $SO_p(G)$ as the p-Sombor index, where $p \neq 0$ clearly, SO_1 is the first Zagreb index and SO_2 original Sombor index and RR(G) is reciprocal Randic index given by $RR(G) = \sum_{uv\in E(G)}(d_u d_v)^{\frac{1}{2}}$.

The third Zagreb index is defined as

$M_3(G) = F(G)+2M_2(G)$. (13)

Polycyclic aromatic hydrocarbons (PAHs) are a class of chemicals that occur naturally in coal, crude oil, and gasoline. By calculation we obtain $|V(G)| = 6n^2+6n$ and $|E(G)| = 9n^2+3n$ for PAHs.From figure 1,it is observed that $PAH_1= C_6H_6$ and $PAH_2 = C_{24}H_{12}$. In PAHs there are two types of edges based on the degree of end vertices of each edge as [27-35] E_{13}, E_{33}, which are expressed by $E_{13}= \{uv\in E(G)|d_u=1, d_v=3\}$, $|E_{13}|= 6n$, $E_{33}= \{uv\in E(G)|d_u=3, d_v=3\}$, $|E_{33}|= 9n^2-3n$.Topological equations comprises degree based topological indices, degree of a graph, degree of a complement graph and coindices.Let G bethemoleculargraphofPolycyclicaromatichydrocarbons (PAHs) and G'be the line graph of the moleculargraph of first member of Polycyclic aromatic hydrocarbons (PAHs) n > 2. There are $9n^2+ 3n$ nodes and $18n^2$ linksinG'.Outof $9n^2+3n$ nodesinG', $9n^2-3n$ nodesareof degree 2 and 6n nodes of degree 4. Let us consider the edge partition of G'basedondegree,thefirstedgepartitionhas12nlinkswith $d_{L(G)}(u)= 2$, $d_{L(G)}(v)= 4$ andthesecondedgepartitionhas $18n^2-12n$ linkswith $d_{L(G)}(u)= d_{L(G)}(v) = 4$.Let $d_G(e)$ denote the degree of an edge e in G, which is defined as $d_G(e) = d_u+d_v-2$,with e = uv.By calculation we get the first and second Zagreb indices as $M_1(G) = 54n^2+6n$ and $M_2(G) = 81n^2-9n$. The notations used in this paper are standard and mainly taken from standard books of chemical graph theory [36-38].In this paper topological equations based on first, second, third, hyper Zagreb indices, forgotten indices, Banhatti indices, irregularitymeasure indexand Sombor index are investigated for polycyclic aromatic hydrocarbons (PAHs).

II. MATERIALS AND METHODS

A molecular graph G(V, E) is constructed by representing each atom of molecule by vertex and bonds between them by edges. Let V(G) be vertex set and E(G) be edge set. The molecular graph of first three members of polycyclic aromatic hydrocarbons and line graph of benzeneare shown in figure 1 and 2 respectively.Let the molecular graph of polycyclic aromatic hydrocarbons is denoted by G and line graph of PAHs by G'.The degree and edge degree of vertices of these molecular graphs are observed and used in the computation of $M_1(G)$, $M_2(G)$ and RR(G).In this paper Zagreb indices, forgotten indices, Banhatti indices, Sombor index and irregularity measure index of polycyclic aromatic hydrocarbons(PAHs) are computed by using topological equations (1-13).

III. RESULTS AND DISCUSSION

Let molecular graphs of PAHs is denoted by G and line graph of first member of PAHs by G'. The definitions of first Zagreb index, second Zagreb index and forgotten index are used to compute these topological indices by using edge partition. The edge partition for degree and edge of molecular graph PAHs graph is represented in table 1. In this section we compute the topological indices by using equations (1-13).By using formulas and edge partition from table 1,the first and second Zagreb indices are obtained as $M_1(G) = \sum_{uv\in E(G)} (d_u + d_v) = 6n(4)+(9n^2-3n)6=54n^2+6n$, $M_2(G) = \sum_{uv\in E(G)} (d_u d_v) = 6n(3)+(9n^2-3n)9=81n^2-9n$.

Theorem 1. The first Zagreb indices of polycyclic aromatic hydrocarbons are

(i)$M_1(\overline{G})=-n(35n^2-76n-19)$,(ii)$M_1(L(G)) = 12n(21n-1)$and (iii)$\overline{M_1}(\overline{G}) =6n(3n^2-11n-2)$.

Proof. Byusingtopological equations (4-6),figure (1-2) and edge degree partition of PAHs, we get

(i)$M_1(\overline{G}) = M_1(G)+n(n-1)^2-4m(n-1)$

$=54n^2+6n+n(n-1)^2-4(9n^2+3n)(n-1)= -n(35n^2-76n-19)$.

(ii)$M_1(L(G)) = 4m-2M_1(G)+2M_2(G)+F(G)$

$= 4(9n^2+3n)-2(54n^2+6n)+2(81n^2-9n)+162n^2+6n= 12n(21n-1)$.

(iii)$\overline{M_1}(\overline{G}) = 2m(n-1)-M_1(G)$

$= 2(9n^2+3n)(n-1)-(54n^2+6n)= 6n(3n^2-11n-2)$.

Theorem 2. $\overline{M_2}(G)$,$\overline{M_2}(\overline{G})$ and $RM_2(G)$ of polycyclic aromatic hydrocarbons are

(i)$\overline{M_2}(G)=-6n(15n-2)$,(ii)$\overline{M_2}(\overline{G}) = 3n^2(n-4)(3n-11)$ and (iii)$RM_2(G) = 12n(3n-1)$.

Proof. Byusing equations (2, 3 and 7) and edge degree partition of PAHs, we get

(i)$\overline{M_2}(G) = 2m^2-\frac{1}{2}M_1(G)-M_2(G)$

$= 2(9n^2+3n)^2-\frac{1}{2}(54n^2 + 6n) - (81n^2-9n)= -6n(15n-2)$.

(ii)$\overline{M_2}(\overline{G}) = m(n-1)^2-(n-1)M_1(G)+M_2(G)$

$= (9n^2+3n)(n-1)^2-(n-1)(54n^2+6n)+81n^2-9n= 3n^2(n-4)(3n-11)$.

(iii)$RM_2(G) = M_2(G) - M_1(G) + m$

$= 81n^2 - 9n - 54n^2 - 6n + 9n^2+3n= 12n(3n-1)$.

Theorem 3.$\overline{F}(G)$,$\overline{F}(\overline{G})$ and$F(\overline{G})$of polycyclic aromatic hydrocarbons are

(i)$\overline{F}(G) = 6n(9n^2-35n-2)$,(ii)$\overline{F}(\overline{G}) = 2n(9n^3-69n^2+59n+12)$and

(iii) $F(\overline{G})$= -n(53n^3-249n^2+321n+43).

Proof. By using equations (10-11) and edge degree partition of PAHs, we get

(i) $\overline{F}(G)$= (n-1)M$_1$(G)-F(G)

F(G) = $\sum_{uv\in E(G)}(d_u - d_v)^2$+2M$_2$(G)=6n(1-3)^2 + 2(81n^2-9n) = 162n^2 + 6n.

$\overline{F}(G)$ = (n-1)(54n^2+6n) – (162n^2+6n) = 6n(9n^2-35n-2).

(ii) $\overline{F}(\overline{G})$= 2m(n-1)^2-2(n-1)M$_1$(G)+F(G)

= 2(9n^2+3n)(n-1)^2-2(n-1)(54n^2+6n)+162n^2+6n= 2n(9n^3-69n^2+59n+12).

(iii) $F(\overline{G})$=n(n-1)^3-6m(n-1)^2+3(n-1)M$_1$(G)-F(G)

= n(n-1)^3-6(9n^2+3n)(n-1)^2+3(n-1)(54n^2+6n)-(162n^2+6n)= -n(53n^3-249n^2+321n+43).

Theorem 4. The hyper Zagreb index, Sombor index (with p = $\frac{1}{2}$), second and first Banhatti indicesof polycyclic aromatic hydrocarbons are(i)HZ(G) = 324n^2-12n,(ii)$SO_{\frac{1}{2}}$(G) = 108n^2+8.78n,(iii)B$_2$(G) = 216n^2-24n and (iv)B$_1$(G) = 6n(21n+1).

Proof. Byusingequations (1,12 and 8) and edge degree partition of PAHs, we get

(i)HZ(G) = F(G)+2M$_2$(G)

= 162n^2+6n+2(81n^2-9n)= 324n^2-12n.

(ii)$SO_{\frac{1}{2}}$(G) = M_1(G)+2RR(G)

RR(G) = $\sum_{uv\in E(G)}(d_u d_v)^{\frac{1}{2}}$= (6n)$3^{\frac{1}{2}}$+(9n^2-3n)3 = 27n^2+1.39n.

$SO_{\frac{1}{2}}$(G) = 54n^2+6n+54n^2+2.78n= 108n^2+8.78n.

(iii) B$_2$(G) = HM$_1$(G)-2M$_1$(G).

HM$_1$(G) = $\sum_{uv\in E(G)}(d_u + d_v)^2$= 6n$(1+3)^2$+(9n^2-3n)$(3+3)^2$= 324n^2-12n.

B$_2$(G) = 324n^2-12n-2(54n^2+6n)= 216n^2-24n.

(iv) B$_1$(G) = 3M$_1$(G)-4m.

= 3(54n^2+6n)-4(9n^2+3n)= 6n(21n+1).

Theorem 5. The third Zagreb index and irregularity measure index of PAHsare

(i)M$_3$(G) = 324n^{2}and (ii)IRM(G) = 24n.

Proof. Byusing equations (13, 9) and edge degree partition of PAHs, we get

(i)M$_3$(G) = F(G)+2M$_2$(G)

=(162n^2+6n)+2(81n^2-3n)= 324n^2.

(ii)IRM(G) = F(G)-2M$_2$(G).

F(G) = 162n^2+6n and M$_2$(G) = 81n^2-9n.

IRM(G) = 162n^2+6n-2 (81n^2-9n)= 24n.

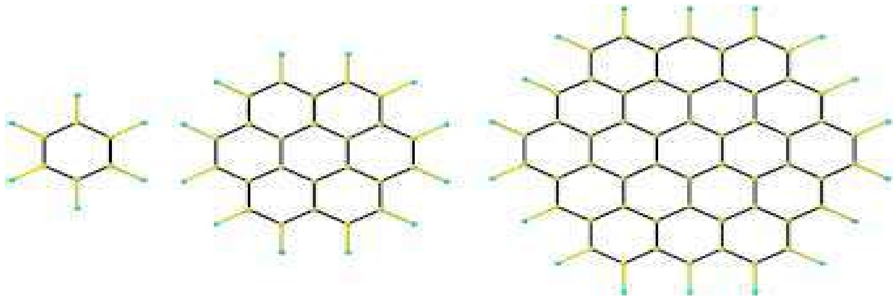

Figure 1:Molecular graphs of PAH$_1$, PAH$_2$ and PAH$_3$.

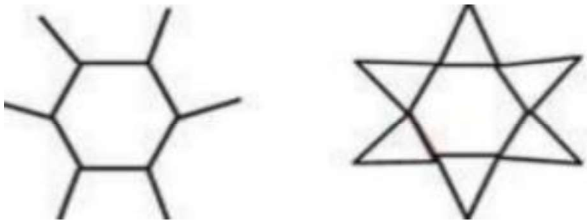

Figure 2:The molecular graphs ofPAH1and L(PAH1).

Table 1. Edge degree partition of polycyclic aromatic compounds.

(d_u, d_v)	(1,3)	(3,3)
$d_G(e)$	2	4
Number of edges	6n	$9n^2$-3n

IV. CONCLUSION

The first, second,third Zagreb indices, forgotten indices, Sombor index, first,second Banhatti indices and irregularity measure index are computed by using topological equations for polycyclic aromatic hydrocarbons. The relations $\overline{M_1}(\overline{G}) = \overline{M_1}(G)$ and $\overline{F}(\overline{G}) \neq \overline{F}(G)$arevalid for PAHs.This is novel idea to compute the degree based topological indices by using topological equations of the molecular compounds.

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Energy Storage Applications of Conducting Polymers and Its Nanocomposite : A Special Emphasis on Supercapacitor

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ABSTRACT

The implication of the conducting polymers (CPs) for various technological applications rapidly increased. Owing to the electrical conductivity approaching those of metallic conductors and other extra ordinary properties makes it distinguishable from the other synthesized materials. Herein, we discussed a broad overview of recent advances in the applications of CPs for the supercapacitor. We first focus the fundamentals of CPs, synthesis techniques and properties. We then highlight the potential supercapacitor applications of CPs, specifically polyaniline, polypyrrole and its nanocomposites with various other materials. Finally, we conclude present study by offering our perspectives on the current challenges and future opportunities for the CPs in supercapacitor applications.

Keywords: Energy Storage Devices, Supercapacitor, Polyaniline, Polypyrrole

I. INTRODUCTION

Recently, improved and advanced technologies have been changes the human life and make it lavish and comfortable. Worldwide, various scientific, academic and industrial groups are devoted their research work to develop new technologies.However, no advanced technology can work without the use of energies such as mechanical, chemical, electrical and thermal etc. As a result, more research into energy harvesting and storage is required for advancement in a variety of fields.Recently, the developed world has faced a number of serious global issues, including insufficient energy production, the availability of portable water, global warming, and so on. [1, 2]. The main cause of these serious issues is the rapidly increasing population and human standard of living. Electrical energy has become a part of everyday life. The production of electrical energy and its long-term reserves is a major and serious impediment to research. Solar energy, wind energy, tidal energy and biomass energy production are considered worrisome options. However, it has many flaws, including a large workforce, a large land business, accuracy, inefficiency, and high costs. As a result, scientists are looking for alternatives to traditional global energy sources such as super capacitors, batteries, fuel cells, and so on. [3, 4].

Recently, energy production from renewable energy sources has been increased rapidly. However, its contribution to global energy production is only low or less than 1%. The energy generated from the power plant is used for various applications such as direct lighting, cooling and communication devices [5]. Saving energy through storage devices in the absence of renewable sources requires a variety of applications. But nowadays there are insufficient efficient storage devices that can store a large number of charges and distribute them as needed. Thus, storage systems such as batteries and electrochemical capacitors (ECs) have taken more interest in saving the energy produced and have played an important role in storing maximum energy [6].

The improvement in the available storage devices with new designs and techniques are not helping to store the energy to the desired level. Therefore, utilizing new advanced technology and with new materials the properties of energy storage devices can be enhanced in desired performance. The selection of the novel materials and techniques can give us the user friendly, light weight, less hazardous, economically cheap and highly efficient energy storage devices. Concerned to the storage of energy in electrochemical form have many superior advantages such as direct energy conversion, portability, absence of moving parts and convenient for mass production. However still it has some critical issues in the developments of electrochemical energy storage devices such as environmental security, light weight, portability, efficiency and low cost etc. [7].

From the last decades the huge efforts are devoted by the many scientists and researchers to develop and enhanced the physical and chemical properties of electrochemical storage system. Electrochemical energy storage systems are broadly classified in three major types based on their properties i.e. (I) batteries, (II) fuel cells and (III) supercapacitors.

Super capacitor is an emerging and become the most promising energy storage device in recent years. Basically, the same principles are used in supercapacitors as conventional capacitors. Supercapacitors are distinguished with high surface area electrodes and thin dielectrics by conventional capacitors to obtain more capacitances. Super capacitors fall between the battery and the capacitor i.e., energy density greater than conventional capacitors and higher energy density than batteries [8].

Supercapacitors have better option for energy storage devices than batteries and fuel cells. However, it faces the challenges such as low energy density, high cost, high self-discharging rate and practical use. Thus, the researchers have scope to enhance the performance, modified electrode structure, achieved the desired thickness of the electrode layer, and porosity. Recently, carbon species (activated carbon, graphene, carbon nanotubes, etc.), metal compounds and conducting polymers are the three main types used as electrode materials for energy storage devices. As well as transition metal oxide (RuO_2, NiO, MnO_2, Co_3O_4, IrO_2 Mn_3O_4,) nanomaterials, carbon nanomaterials, binary, ternary nanocomposites, conducting polymers and conducting polymers nanocomposites and so on. Carbon species-based electrodes with high conductivity and stability usually have excellent cycling stability and high-power density as supercapacitor electrodes. However, carbon-based electrodes for supercapacitors are usually exhibits low energy density because of the limitation in energy storage mechanism. Metal compounds owing to high activity and good intrinsic electrochemical properties in supercapacitors still they have problems like low conductivity, high cost and limited natural abundance [9].

Conducting polymers (CPs), like Poly (3,4- ethylenedioxythiophene) (PEDOT), polypyrrole (Ppy) and polyaniline (PANi), have gained more attention as promising candidates for energy storage devices. CPs has the excellent and unique electronic, optoelectronic, and electrochemical features. As well as CPshave pseudocapacitive features, facile synthesis protocol, good environmental and chemical stability, tunable conductivity, low production cost, etc.Their simple components (C, H, N or S) also indicate the high affordability. CPs based devices show high specific capacitance compared with electrochemical double-layer supercapacitors, and has faster kinetics than most inorganic batteries, which can narrow the gap between inorganic batteries and carbon-based capacitors. The combination of conducting polymers and carbon materials, metal compounds is quite popular with excellent performance taking advantage of each component, shown superior performance in asymmetric supercapacitor [10, 11].

The superiority of supercapacitors decides by cyclic life which depends upon the stability of the electrode materials during charge/discharge cycles. Conducting polymers incorporated with nanomaterials attain higher stability of the electrode material in terms of cyclic life. Also, the decoration of polymer nanocomposites with nanomaterials enhances the electrochemical conductivity, thermal stability and optical and mechanical properties and large surface area to stored charges [12].

The recent development concern to the supercapacitors have been discussed in the following headings using the polyaniline and its nanocomposites as well as polypyrrole and its nanocomposites.

II. SUPERCAPACITOR APPLICATIONS OF CONDUCTING POLYMERS AND ITS NANOCOMPOSITE

Payami, E., et. al; developed ternary nanocomposite consisting of modified GO (GO-Fc), Mn_3O_4 nanoparticles, and polyaniline (PANI) via a simple physically mixing procedure. As synthesized ternary nanocomposite further used as a battery-type supercapacitor and obtained results reveals the promising ability via supercapacitor parameters high power density and cyclic stability [13].Röse, P. et.al; synthesized polyaniline (PANI) nanofibers via chemical oxidative synthesis route using sodium phytate as a plant derived dopant. Electrochemical properties of the synthesized PANI as electrode material for supercapacitors shows the high specific capacitance analyzed by galvanostatic charge/discharge (GCD) curves. The PANI electrode shows the capacitance retention of 67.6% of its initial value, low solution resistance (Rs) value of 281×10^{-1} Ohm and charge transfer resistance value (Rct) of 7.44 Ohm. As well as after 1000 charge discharge cycles retained 95.3% in coulombic efficiency without showing any significant degradation of the material [14].Deshmukh, P. R. et. al; prepared the polyaniline-ruthenium oxide (PANI-RuO_2) nanocomposite thin films by a chemical bath deposition (CBD) method. The PANI–RuO_2 exhibits specific capacitance of 830 Fg^{-1} with 216 $Whkg^{-1}$ and 4.16 $kWkg^{-1}$ specific energy and power respectively [15].Gui, D., et.al; synthesized three polyaniline (PANI)/grapheneoxide (GO) nanocomposite electrode materials by chemical polymerization with the mass ratio (mANI:mGO) 1000:1, 100:1, and 10:1 in ice water, respectively. The electrochemical behavior of the PANI/GO with the mass ratio (mANI:mGO)1000:1 possessed excellent capacitive behavior with a specific capacitance as high as 355.2 F g^{-1}at 0.5 A g^{-1} in 1 mol $L^{-1}H_2SO_4$electrolyte and after 1000 cycles, the specific capacitance of the composite still has 285.8 F g^{-1} [16].Mishra, A. K. et.al; synthesized graphene via hydrogen-induced exfoliation and functionalized to decorate with metal oxide (RuO_2, TiO_2, and Fe_3O_4) nanoparticles and polyaniline using the chemical route. Electrochemical performance of as-prepared nanocomposites is examined using cyclic voltammetry and galvanostatic charge discharge techniques for supercapacitor applications. A maximum specific capacitance of 80, 125, 265, 60, 180, and 375 F/g for HEG, f-HEG, RuO_2-f-HEG, TiO_2-f- HEG, Fe_3O_4-f-HEG, and PANI-f-HEG nanocomposites, respectively, is obtained with 1 M H2SO4 as the electrolyte at the voltage sweep rate of 10 mV/s. The specific capacitance for each nanocomposite sustains up to 85% even at higher voltage sweep rate of 100 mV/s [17].Khalid, M., et.al; using electrodeposition process synthesized composite thin films of polyaniline (PANI) nanofibers and graphene oxide (GO) nanoplatelets for electrochemical capacitors. An electrochemical property of thin films shows capacitance of 662 F g^{-1} at a low current density of 0.025 mA cm^2 with simultaneous high energy density (64.5 Wh kg^{-1}) and high-power density (1159 Wh kg^{-1}) [18].Viswanathan, A., et.al; synthesized reduced graphene oxide, copper oxide and polyaniline (GCP) nanocomposites by facile in-situ single step chemical method by varying the weight percentage of each of the constituent materials. The weight percentage of composites G12%: Cu_2O/CuO 40%: P48% (G12CP) exhibits the maximum specific capacitance of 684.93 Fg^{-1}, specific capacity of 821.91 Cg^{-1}, energy density of 136.98Wh kg^{-1}, and power density of 1315.76Wkg^{-1} at the current density of 0.25 Ag^{-1}. The composite shows the retention of 84% of its initial capacitance up to 5000 cycles at a scan rate of 700mVs^{-1} [19].Devadas, B., et al; Synthesized the polymer@Cdots composites by in situ chemical oxidative polymerization method and studied the specific capacitances. The specific capacitances of composites were 676 and 529 F/g for PPy@ Cdots and PANI@Cdots, respectively, at current density of 1 A/g [20].Ashokkumar, S. P., et al; reported the electrochemical performance of polyaniline (PANI)/copper oxide (CuO) nanocomposites (PCN) for energy storage device applications. The Cyclic Voltametry (CV) result shows the specific capacitance PANI is 294 F/g and 424 F/g for highest concentration PCN2 nanocomposites and GCD reveals the cyclic stability up to 4000 cycles [21].

III. CONCLUSION

In this review paper, we have discussed recent progress in the development of conducting polymers-based supercapacitor.Owing to the excellent properties of the conducting polymers it is employed for the supercapacitor applications. Worldwide various research groups devoted their research to improve the super capacitive performance of the conducting polymers. The mainly polyaniline and polypyrrole were highly studied due to some exceptional qualities compared to the other conducting polymers. We have thoroughly summaries the recent development in the fields of supercapacitor using polyaniline and polypyrrole. Finally, we conclude that the present work may be highly useful for the upcoming researcher.

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