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M-polynomial and entropy of para-line graph of naphthalene

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ABSTRACT

The objective of this paper is to explore the stability of naphthalene (m, n). For a single unit of naphthalene, its stability is less relative to selfdimerization. For two units of naphthalene, there is a slight increase in stability and self-dimerization decreases as well. However, for (m, n) unit of Naphthalene, its stability increases rapidly and self-dimerization decreases proportionately. The M-Polynomial is extracted from praline graph of naphthalene which further yielded several degree-based topological indices. The analytical information function of a graph is entropy which uses probability density on the set of vertices. This paper computes the entropy of para-line graph of naphthalene (m, n) and its relationship with Randic index.

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1. Introduction

Mathematical models which are constructed from polynomials interpretations of chemical compounds, applied to forecast its estates. Rich instrument is mathematical chemistry like polynomials and functions which prognosticate premises of compounds. The indices which indicated the topology of the chemical compounds are also numerical limitations of graph and generally graph immutable. The structures of molecules are narrated numerically by topological indices.

A graph having vertex set V(L) = E(G) is line graph L(G) = L in which two vertices correspond to the edges of graph G adjoining if and only if the parallel edges having a vertex in common two. A subdivision graph is obtained by putting a vertex in the mid of every edge. The line graph of subdivision with 2a vertices called para-line graph PL = PL(G). $C_{10}H_8$ is the chemical formula of Naphthalene. In 1820, white solid with a pungent odor are expressed in two different reports and a pungent odor is obtained from coal tar. In 1821, these two reports are mentioned by John Kidd then he explained many estates of this substance. Many techniques of production are introduced by him. Also he introduced Naphthalene. The word Naphthalene is obtained from a kind of Naphtha. In 1826, Michael

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2313-626X/© 2019 The Authors. Published by IASE. This is an open access article under the CC BY-NC-ND license (http://creativecommons.org/licenses/by-nc-nd/4.0/) Faraday proposed the chemical formula of Naphthalene. Erlenmeyer (1866) introduced the formation of two fused benzene rings. After three years, Call Grabe established this formula. Black Walnut and many essential oils are the sources to find Naphthalene. In the production of phthalic anhydride, it seems very helpful. Körner (1973) introduced entropy function to read the smallest number of edges which are compulsory for characterizing the knowledge source (Dehmer and Mowshowitz, 2011). Para-line graph of Naphthalene has shown in Fig. 1.

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2. M-polynomial

M-Polynomial was introduced by Deutsch and Klavžar (2015). In the factors of distance based topological indices, M polynomial played important role. It is the most general progressive polynomial. And also closed formula along with ten distance based topological indices (Furtula et al., 2010; Kulli, 2016; Vukičević and Furtula, 2009) are given by Mpolynomial. It is explained as:

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

where,

 $\delta = Min\{d_v : v \in V(G)\}$, $\Delta = Max\{d_v : v \in V(G)\}$

The number of corners are represented by m_{ij} . There are many helpful applications of algebraic polynomials in chemistry like Hosoya polynomials. Key polynomial is Hosoya polynomial in the field of topological indices of distance based. Hosoya polynomial is also known as wiener polynomial

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(Kirby and Pollak, 1998). We can calculate wiener index by taking the first derivative of Hosoya polynomial. Wiener (1947) introduced Wiener index in chemical graph theory. It is oldest topological index affiliated to molecular branching. In regulating distance based topological indices, this polynomial played critical role. For estimating the alkanes boiling point, wiener suggested wiener index firstly in 1947. M polynomial also played the identical occupation in driving the secure structure of numberless degree based topological indices (Ajmal et al., 2016; Kulli, 2016; Klavžar and Gutman, 1996). Consequently, in Table 1, explicit expressions for some continuous degree based Topological indices are listed in Table 1.

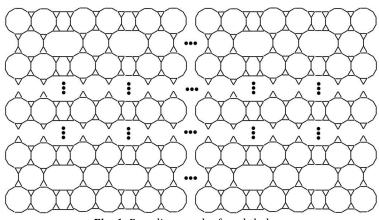


Fig. 1: Para-line graph of naphthalene

Table 1: M-polynomial topological indices

Sr. No.	Topological Indices	f(t, s)	Derivation from M(G, t, s)
1	First Zagreb Index	t + s	$M_1(G) = (D_t + D_s)f(t, s) _{t=s=1}$
2	Second Zagreb Index	ts	$M_1(G) = (D_t D_s) f(t, s) _{t=s=1}$
3	Second Modified Zagreb Index	$\frac{1}{ts}$	${}^{m}M_1(G)=(\delta_t\delta_s)f(t,s) _{t=s=1}$
4	General Randic Index, $\alpha \neq 0$	$(ts)^{\alpha}$	$R_{\alpha}(G) = (D_{\alpha}^{t}D_{\alpha}^{s})f(t,s) _{t=s=1}$
5	Inverse General Randic Index, $\alpha \neq 0$	$\frac{1}{(ts)^{\alpha}}$	$RR_{\alpha}(G) = (\delta_{\alpha}^{t}\delta_{\alpha}^{s})f(t,s) _{t=s=1}$
6	Symmetric Division Index	$\frac{t^2 + s^2}{ts}$	$SDD(G) = (D_t \delta_s + \delta_t D_s) f(t,s) _{t=s=1}$
7	Harmonic Index	$\frac{1}{t+s}$	$H(G) = 2\delta_t f(t,s) _{t=1}$
8	Inverse Sum Index	$\frac{ts}{t+s}$	$I(G) = \delta_t J D_t D_s f(t,s) _{t=1}$
9	Augmented Zagreb	$\left[\frac{\mathrm{ts}}{\mathrm{t+s-2}}\right]^3$	$A(G) = \delta_t^3 Q - 2J D_t^3 D_s^3 f(t,s) _{t=1}$

where in Table 1,

$$\begin{split} D_{s} &= s \frac{\partial}{\partial s} M(G;t,s) | t = s = 1 \\ D_{t} &= t \frac{\partial}{\partial t} M(G;t,s) | t = s = 1 \\ \delta_{t} &= \int_{0}^{t} \frac{M(G;y,s)}{y} dt \\ \delta_{s} &= \int_{0}^{t} \frac{M(G;t,y)}{y} ds \\ J &= M(G;t,t) \\ Q_{\alpha} &= x^{\alpha} M(G;t,s), \\ \alpha &\neq 0 \end{split}$$

3. Entropy

Körner (1973) introduced entropy function to read the smallest number of edges which are compulsory for characterizing the knowledge source (Dehmer and Mowshowitz, 2011). The analytical information function of a graph is entropy which explained with a probability density on the set of vertices. Körner (1973) measured the main estates of entropy graph in various papers from 1973 till 1992. The idea of entropy was expanded through evolution of statistical mechanics. Shannon (1948) firstly proposed this idea into information theory. Entropy of G is stated as:

$$I(G, \alpha) = \log(R_{\alpha}(G)) - \frac{\alpha}{R_{\alpha}(G)} \sum_{u,v \in E} (d_{l}d_{m})^{\alpha}$$

where, $R_{\alpha}(G) = \sum_{u,v \in E} (d_{l}d_{m})^{\alpha}$

4. Results of m-polynomial and entropy

4.1. M-polynomial of para-line graph of naphthalene

The edge partition of degree based topological indices of Para-line Graph of (m, n) Naphthalene is given below in the Table 2.

Table 2: Edge partition of degree based topological indices

_	of para-line graph of (m, n) naphthalene				
	$(d_l, d_m), l, m \in E(G)$	E _{l,m}	Number of Edges		
	(2,2)	E _{2,2}	4m + 6n + 4		
	(2,3)	E _{2,3}	8m + 4n - 8		
	(3,3)	E _{3,3}	45mn - 22m - 20n + 4		
	(2,3)	E _{2,3}	8m + 4n - 8		

Theorem 4.1.1: Let G be a Para-line graph of Naphthalene. Its M-polynomial is:

$$\begin{array}{ll} \mathsf{M}(\mathsf{G};\mathsf{t},\mathsf{s}) &=& (4m+6n+4)\mathsf{t}^2\mathsf{s}^2 + (8m+4n-8)\mathsf{t}^2\mathsf{s}^3 \\ + (45mn-22m-20n+4)\mathsf{t}^3\mathsf{s}^3 \end{array}$$

Proof: Suppose that G be a Para-line graph of Naphthalene. The 'edge set' is divided into three parts:

 $\begin{array}{lll} E_1(G) &=& \{e=lm \in E(G) \colon d_l=2, d_m=2\}, \\ E_2(G) &=& \{e=lm \in E(G) \colon d_l=2, d_m=3\}, \\ E_3(G) &=& \{e=lm \in E(G) \colon d_l=3, d_m=3\} \end{array}$

such that

$$\begin{split} |E_1(G)| &= 4m + 6n + 4, \\ |E_2(G)| &= 8m + 4n - 8, \\ |E_3(G)| &= 45mn - 22m - 20n + 4. \end{split}$$

Now from the definition of M-Polynomial, it is deduced that:

$$\begin{split} \mathsf{M}(\mathsf{G};\mathsf{t},\mathsf{s}) &= \sum_{i\leq j} \mathsf{m}_{ij} \, (\mathsf{G}) \mathsf{t}^i \mathsf{s}^j \\ \mathsf{M}(\mathsf{G};\mathsf{t},\mathsf{s}) &= \sum_{1\leq 6} \mathsf{m}_{16} \, (\mathsf{G}) \mathsf{t}^2 \mathsf{s}^2 + \sum_{2\leq 6} \mathsf{m}_{26} \, (\mathsf{G}) \mathsf{t}^2 \mathsf{s}^3 + \sum_{3\leq 6} \\ \mathsf{m}_{36} \, (\mathsf{G}) \mathsf{t}^3 \mathsf{s}^3 \\ \mathsf{M}(\mathsf{G};\mathsf{t},\mathsf{s}) &= |\mathsf{E}_1(\mathsf{G})| \mathsf{t}^2 \mathsf{s}^2 + |\mathsf{E}_2(\mathsf{G})| \mathsf{t}^2 \mathsf{s}^3 + |\mathsf{E}_3(\mathsf{G})| \mathsf{t}^3 \mathsf{s}^3 \\ \mathsf{M}(\mathsf{G};\mathsf{t},\mathsf{s}) &= (4\mathsf{m} + 6\mathsf{n} + 4) \mathsf{t}^2 \mathsf{s}^2 + (8\mathsf{m} + 4\mathsf{n} - 8) \mathsf{t}^2 \mathsf{s}^3 + \\ (45\mathsf{mn} - 22\mathsf{m} - 20\mathsf{n} + 4) \mathsf{t}^3 \mathsf{s}^3. \end{split}$$

Next some degree-based topological indices of para-line graph of Naphthalene are computed from this M-polynomial and proof is completed.

Proposition 4.1.2: Let G be a Para-line graph of Naphthalene graph, then calculated nine indices of M-polynomial,

$$\begin{split} M_1(G) &= -76m - 76n + 270mn \\ M_2(G) &= -134m - 132n + 405mn + 4 \\ {}^{m}M_2(G) &= -\frac{1}{9}m - \frac{1}{18}n + 5mn + \frac{1}{9} \\ R_{\alpha}(G) &= (2)^{\alpha} \times (2)^{\alpha} \times 4(m + 3n + 2) + (2)^{\alpha} \times (3)^{\alpha} \\ &\times 12(2m + n - 2) + (3)^{\alpha} \times (3)^{\alpha} \\ &\times 3(45mn - 22m - 20m + 4) \\ RR_{\alpha}(G) &= \frac{2}{2 \times 2^{\alpha} \times 2^{\alpha}}(m + 3n - 2) \\ &+ \frac{4}{2 \times 2^{\alpha} \times 3^{\alpha}}(2m + 2n - 2) \\ &+ \frac{1}{3 \times 3^{\alpha} \times 3^{\alpha}}(45mn - 22m - 20n \\ &+ 4) \\ SSD(G) &= -\frac{44}{3}m - \frac{40}{3}n + 90mn + \frac{8}{3} \\ H(G) &= -\frac{32}{15}m - \frac{31}{15}n + 15mn + \frac{2}{15} \\ I(G) &= -\frac{97}{5}m - \frac{96}{5}n + \frac{135}{2}mn + \frac{2}{5} \\ A(G) &= -\frac{15865}{32}m - \frac{7863}{16}n + \frac{98415}{64}mn + \frac{139}{16} \end{split}$$

Proof: Applying the formula of 1st Zagreb index

$$\begin{split} &M_1(G;t,s) = (D_t + D_s)M(G;t,s)|_{t=s=1} \\ &D_tM(G;t,s) = t\frac{\partial}{\partial t}M(G;t,s) \\ &D_tM(G;t,s)|_{t=s=1} = -42m - 40n + 135mn + 4 \end{split}$$

$$\begin{split} &D_s M(G;t,s) = t \frac{\partial}{\partial t} M(G;t,s) \\ &D_s M(G;t,s)|_{t=s=1} = -34m - 36n + 135mn - 4 \,, \end{split}$$

after putting the value, we have obtained the result and also 3D plot of 1st Zagreb index has been show in Fig. 2.

$$M_1(G) = -76m - 76n + 270mn.$$

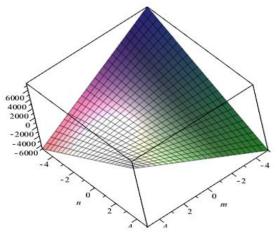


Fig. 2: 3D plot of 1st Zagreb index

By applying formula of 2nd Zagreb index

$$M_2(G; t, s) = (D_t D_s) M(G; t, s)|_{t=s=1},$$

we have already find

$$\begin{split} &D_s M(G;t,s)|_{t=s=1} = -34m - 36n + 135mn - 4 \\ &(D_t D_s) M(G;t,s) = t \frac{\partial}{\partial t} D_s M(G;t,s) \\ &(D_t D_s) M(G;t,s)|_{t=s=1} = -134m - 132n + 405mn + 4 \end{split}$$

So,

 $M_2(G) = -134m - 132n + 405mn + 4.$

By utilizing the formula of 2nd modified Zagreb index, we have obtained the result and the 3D plot of 2nd Zagreb index is shown by utilizing the formula of 2nd modified Zagreb index, we have obtained the result and the 3D plot of 2nd Zagreb index is shown in Fig. 3.

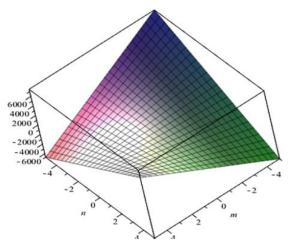


Fig. 3: 3D plot of 2nd Zagreb index

$$\label{eq:mM2} \begin{split} {}^{m}M_{2} &= \delta_{t}\delta_{s}|_{t=s=1}\\ \delta_{s}|_{t=s=1} &= {}^{s}\int_{0}\frac{M(t,y)}{y}dy\\ \delta_{s}|_{t=s=1} &= {}^{-8}m - {}^{7}_{3}n + 15mn + {}^{2}_{3}\\ \delta_{t}\delta_{s}|_{t=s=1} &= {}^{t}\int_{0}\frac{M(y,s)}{y}dy\\ \delta_{t}\delta_{s}|_{t=s=1} &= {}^{-1}_{9}m - {}^{1}_{18}n + 5mn + {}^{1}_{9} \end{split}$$

hence,

$${}^{m}M_{2}(G) = -\frac{1}{9}m - \frac{1}{18}n + 5mn + \frac{1}{9}$$

The 3D plot of 2nd modified Zagreb index is given in Fig. 4.

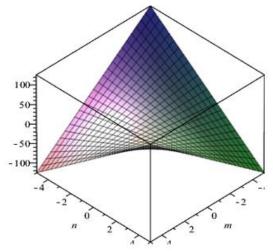


Fig. 4: 3D plot of 2nd modified Zagreb index

Using the definition of symmetric division Zagreb index

$$SSD(G) = D_t \delta_s + \delta_t D_s|_{t=s=1}$$

$$D_t \delta_s|_{t=s=1} = \frac{-38}{3}m - \frac{34}{3} + 45mn + \frac{8}{3}m + \frac{34}{3}m + \frac$$

adding both, we have

$$\delta_t D_s|_{t=s=1} = -2m - 2n + 45mn.$$

Hence, we obtained the result and has shown 3D plot of symmetric division index given in Fig. 5.

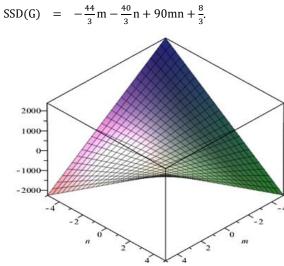


Fig. 5: 3D plot of symmetric division index

Using the formula of Inverse sum index along with its 3D graph is given in Fig. 6.

$$\begin{split} I(G) &= \delta_s J D_t D_s |_{t=1} \\ J D_t D_s |_{t=1} &= (16m+24n+16)t^4 + 6(8m+4n-8)t^5 + \\ 9(45mn-22m-20n+4)t^6 \\ \delta_s J D_t D_s |_{t=1} &= -\frac{97}{5}m - \frac{96}{5}n + \frac{135}{2}mn + \frac{2}{5} \end{split}$$

hence,

I(G) =
$$-\frac{97}{5}m - \frac{96}{5}n + \frac{135}{2}mn + \frac{2}{5}$$

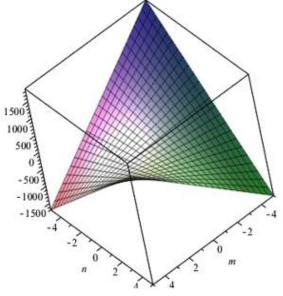


Fig. 6: 3D plot of inverse sum index

Applying the definition of harmonic index, we got the result and has shown the graph of Harmonic index in Fig. 7.

 $\begin{array}{ll} H(G) &=& 2\delta_t J|_{t=1} \\ J|_{t=1} &= (4m+6n+4)t^4 + (8m+4n-8)t^5 + (45mn-22m-20n+4)t^6 \\ 2\delta_t J|_{t=1} &= -\frac{32}{15}m - \frac{31}{15}n + 15mn + \frac{2}{15} \end{array}$

S0,

H(G) =
$$-\frac{32}{15}m - \frac{31}{15}n + 15mn + \frac{2}{15}$$

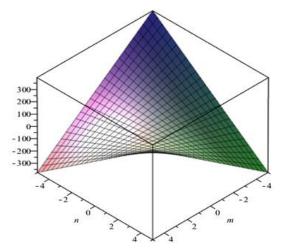


Fig. 7: 3D plot of harmonic index

By using Randic' index;

$$R_{\alpha}(G) = D_t^{\alpha} D_s^{\alpha}|_{t=s=1}$$

we have already find

$$\begin{split} & D_s^{\alpha} = 2 \times 2^{\alpha} (4m+6n+4) t^{\alpha} s^{\alpha} + 3 \times 3^{\alpha} (8m+4n-8) t^2 s^3 + 3 \times 3^{\alpha} \\ & + 3 \times 3^{\alpha} (45mn-22m-20n+4) t^{\alpha} s^{\alpha} \\ & D_t^{\alpha} D_s^{\alpha} = 2 \times 2^{\alpha} \times (2)^{\alpha} (4m+6n+4) t^{\alpha} s^{\alpha} + 3 \times (3)^{\alpha} \times \\ & (2)^{\alpha} (8m+4n-8) t^2 s^{\alpha} + 3 \times (3)^{\alpha} \times (3)^{\alpha} (45mn-22m-20n+4) t^{\alpha} s^{\alpha} \\ & D_t^{\alpha} D_s^{\alpha} = 2 \times 2^{\alpha} \times (2)^{\alpha} (4m+6n+4) t^{\alpha} s^{\alpha} + 3 \times (3)^{\alpha} \times \\ & (2)^{\alpha} (8m+4n-8) t^{\alpha} s^{\alpha} + 3 \times (3)^{\alpha} \times (3)^{\alpha} (45mn-22m-20n+4) t^{\alpha} s^{\alpha} \\ & D_t^{\alpha} D_s^{\alpha} |_{t=s=1} = 2 \times (2)^{\alpha} \times 2^{\alpha} (4m+6n+4) + 3 \times (3)^{\alpha} \times \\ & (2)^{\alpha} (8m+4n-8) + 3 \times 3^{\alpha} \times 3^{\alpha} (45mn-22m-20n+4) \end{split}$$

S0,

$$\begin{split} R_{\alpha}(G) &= (2)^{\alpha} \times (2)^{\alpha} \times 4(m+3n+2) + (2)^{\alpha} \times (3)^{\alpha} \times \\ 12(2m+n-2) + (3)^{\alpha} \times (3)^{\alpha} \times 3(45mn-22m-20m+4). \end{split}$$

The 3D plot of Randic index is given in Fig. 8.

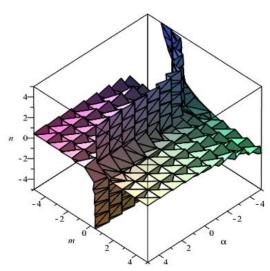


Fig. 8: 3D plot of Randic index

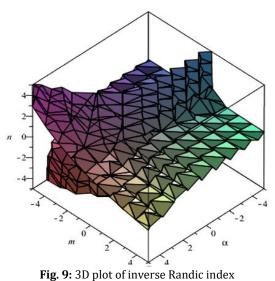
Putting the formula of inverse Randic' index

$$\begin{split} & RR_{\alpha}(G) = \delta_{t}^{\alpha} \delta_{s}^{\alpha}|_{t=s=1} \\ & \delta_{s}^{\alpha} = \frac{1}{2 \times 2^{\alpha}} (4m + 6n + 4) t^{2} s^{2} + \frac{1}{2 \times 3^{\alpha}} (8m + 4n - 8) t^{2} s^{3} + \frac{1}{3 \times 3^{\alpha}} (45mn - 22m - 20n + 4) t^{3} s^{3} \end{split}$$

now we find $\delta^{\alpha}_{t} \delta^{\alpha}_{s}$

$$\begin{split} &\delta_t^\alpha \delta_s^\alpha = \frac{1}{2 \times 2^\alpha \times 2^\alpha} (4m + 6n + 4) t^2 s^2 + \frac{1}{2 \times 3^\alpha 2^\alpha} (8m + 4n - 8) t^2 s^3 + \frac{1}{3 \times 3^\alpha \times 2^\alpha} (45mn - 22m - 20n + 4) t^3 s^3 \\ &\delta_t^\alpha \delta_s^\alpha |_{t=s=1} = \frac{1}{2 \times 2^\alpha \times 2^\alpha} (4m + 6n + 4) t^2 s^2 + \frac{1}{2 \times 3^\alpha \times 2^\alpha} (8m + 4n - 8) + \frac{1}{3 \times 3^\alpha \times 2^\alpha} (45mn - 22m - 20n + 4) \\ &\delta_t^\alpha \delta_s^\alpha |_{t=s=1} = \frac{2}{2 \times 2^\alpha \times 2^\alpha} (m + 3n - 2) + \frac{4}{2 \times 2^\alpha \times 3^\alpha} (2m + 2n - 2) + \frac{1}{3 \times 3^\alpha \times 3^\alpha} (45mn - 22m - 20n + 4) \\ &\text{RR}_\alpha(G) = \frac{2}{2 \times 2^\alpha \times 2^\alpha} (m + 3n - 2) + \frac{4}{2 \times 2^\alpha \times 3^\alpha} (2m + 2n - 2) + \frac{1}{3 \times 3^\alpha \times 3^\alpha} (45mn - 22m - 20n + 4). \end{split}$$

The 3D plot of Inverse Randic index has shown in Fig. 9.



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Utilizing the formula of augmented Zagreb index;

$$\begin{split} & A(G) = \delta_t^3 Q_{-2} J D_t^3 D_s^3 |_{t=s=1} \\ & D_t^3 D_s^3 = 2 \times 2^3 \times 2^3 (4m + 6n + 4) t^2 s^2 + 3 \times 3^3 \times 2^3 (8m + 4n - 8) t^2 s^3 + 3 \times 3^3 \times 3^3 (45mn - 22m - 20n + 4) t^3 s^3 \\ & J D_t^3 D_s^3 = 2 \times 2^3 \times 2^3 (4m + 6n + 4) t^4 + 3 \times 3^3 \times 2^3 (8m + 4n - 8) t^5 + 3 \times 3^3 \times 3^3 (45mn - 22m - 20n + 4) t^6 \\ & Q_{-2} J D_t^3 D_s^3 = t^{-2} \{2 \times 2^3 \times 2^3 (4m + 6n + 4) t^4 + 3 \times 3^3 \times 2^3 (8m + 4n - 8) t^5 + 3 \times 3^3 \times 3^3 \times 3^3 \times 3^3 (45mn - 22m - 20n + 4) t^6 \} \\ & Q_{-2} J D_t^3 D_s^3 = \{2 \times 2^3 \times 2^3 (4m + 6n + 4) t^2 + 3 \times 3^3 \times 2^3 (8m + 4n - 8) t^3 + 3 \times 3^3 \times 3^3 \times 3^3 (45mn - 22m - 20n + 4) t^6 \} \\ & Q_{-2} J D_t^3 D_s^3 = \{2 \times 2^3 \times 2^3 (4m + 6n + 4) t^2 + 3 \times 3^3 \times 2^3 (8m + 4n - 8) t^3 + 3 \times 3^3 \times 3^3 \times 3^3 (45mn - 22m - 20n + 4) t^4 \} \\ & \delta_t^3 Q_{-2} J D_t^3 D_s^3 = 2 \times 2^3 \times 2^3 \times 2^3 \times 2^3 (4m + 6n + 4) t^2 + 3 \times 2^3 \times 2^3 \times 3^3 (8m + 4n - 8) t^3 + 3 \times 3^3 \times 3^3 \times 3^3 \times 3^3 (45mn - 22m - 20n + 4) t^4 . \end{split}$$

So, after obtaining the results, we have also shown in Fig. 10.

 $\delta_{t}^{3}Q_{-2}JD_{t}^{3}D_{s}^{3}|_{t=s=1} = 2 \times 2^{3} \times 2^{3} \times \frac{1}{2^{3}}(4m + 6n + 4) + 3 \times 2^{3} \times \frac{1}{3^{3}}(8m + 4n - 8) + 3 \times 3^{3} \times 3^{3} \times 3^{3} \times \frac{1}{4^{3}}(45mn - 22m - 20n + 4)$ $\delta_{t}^{3}Q_{-2}JD_{t}^{3}D_{s}^{3}|_{t=s=1} = -\frac{15865}{32}m - \frac{7863}{16}n + \frac{98415}{64}mn + \frac{139}{16}$ $A(G) = -\frac{15865}{32}m - \frac{7863}{16}n + \frac{98415}{64}mn + \frac{139}{16}$

Fig. 10: 3D plot of augmented Zagreb index

5. Entropy of para-line graph of naphthalene

Now we find entropy of para-line graph of (m, n) Naphthalene.

Theorem 5.1: Let G be a para-line graph of Naphthalene. Then its entropy is:

 $I(G; \alpha) = \log(2 \times (4)^{\alpha}(2m + 3n + 2) + 4 \times 6^{\alpha}(2m + n - 2) + 9^{\alpha}(45mn - 22m - 20n + 4)) - \alpha(\frac{\beta}{2})$

where

$$\begin{split} \beta &= 2 \times 4^{\alpha} log(4)(2m+3n+2) + 4 \times 6^{\alpha} log(6)(4m+n-2) + 9^{\alpha} log(9)(45mn-22m-20n+4) \\ \gamma &= 2 \times 4^{\alpha}(2m+3n+2) + 4 \times 6^{\alpha}(2m+n-2) + \\ 9^{\alpha}(45mn-22m-20n+4) \end{split}$$

Proof: Let G be a Para-line graph of Naphthalene and $E_{\{l,m\}}$ denotes number of edges connecting the vertices d_l and d_m . The general Randic index formula is

 $R_{\alpha}(G) = \sum_{l,m \in E(G)} (d_l d_m)^{\alpha},$

this implies that

$$\begin{split} & R_{\alpha}(G) = \sum_{l,m \in E_{1}(G)} (d_{l}d_{m})^{\alpha} + \sum_{l,m \in E_{2}(G)} (d_{l}d_{m})^{\alpha} + \\ & \sum_{l,m \in E_{3}(G)} (d_{l}d_{m})^{\alpha} \\ & = (4)^{\alpha} |E_{1}(G)| + (6)^{\alpha} |E_{2}(G)| + (9)^{\alpha} |E_{3}(G)| \\ & = (4)^{\alpha} (4m + 6n + 4) + (6)^{\alpha} (8m + 4n - 8) + \\ & (9)^{\alpha} (45mn - 22m - 20n + 4) \\ & = 2 \times (4)^{\alpha} (2m + 3n + 2) + 4 \times (6)^{\alpha} (2m + n - 2) + \\ & (9)^{\alpha} (45mn - 22m - 20n + 4), \end{split}$$

now the formula for entropy is:

$$\begin{split} I(G;\alpha) &= \log R_{\alpha}(G) - \frac{\alpha}{R_{\alpha}(G)} \sum_{l,m \in E(G)} \left(\left(d_{l}d_{m} \right)^{\alpha} \log(d_{l}d_{m}) \right) \\ I(G;\alpha) &= \log(2 \times (4)^{\alpha}(2m + 3n + 2) + 4 \times (6)^{\alpha}(2m + n - 2) + (9)^{\alpha}(45mn - 22m - 20n + 4)) - \\ \alpha(\frac{1}{2 \times 4^{\alpha}(2m + 3n + 2) + 4.6^{\alpha}(2m + n - 2) + 9^{\alpha}(45mn - 22m - 20n + 4))} \times \\ (4^{\alpha}\log(4)(4m + 6n + 4) + 6^{\alpha}\log(6)(8m + 4n - 8) + \\ 9^{\alpha}\log(9)(45mn - 22m - 20n + 4)) \\ I(G;\alpha) &= \log(2 \times (4)^{\alpha}(2m + 3n + 2) + 4 \times (6)^{\alpha}(2m + n - 2) + (9)^{\alpha}(45mn - 22m - 20n + 4)) - \alpha(\frac{1}{\gamma}) \times \beta \\ I(G;\alpha) &= \log(2 \times (4)^{\alpha}(2m + 3n + 2) + 4 \times (6)^{\alpha}(2m + n - 2) + 9^{\alpha}(45mn - 22m - 20n + 4)) - \alpha\left(\frac{\beta}{\nu}\right), \end{split}$$

where,

$$\begin{split} \beta &= 2 \times 4^{\alpha} log(4)(2m+3n+2) + 4 \times 6^{\alpha} log(6)(4m+n-2) + 9^{\alpha} log(9)(45mn-22m-20n+4) \\ \gamma &= 2 \times 4^{\alpha}(2m+3n+2) + 4 \times 6^{\alpha}(2m+n-2) + 9^{\alpha}(45mn-22m-20n+4), \end{split}$$

hence completed the proof.

6. Conclusion

We have studied scene family but our main target is the study of Naphthalene. It is helpful for making plastic, crystals, toilet deodorant blocks and moth balls. We have computed nine topological indices from M-polynomial and also discussed the entropy of naphthalene. These indices also played an important role to explain various chemical structures and physical properties of atoms, molecules and correlate the structure of molecules to their biological activity and also increased the stability and solubility of (m, n) Naphthalene. We have obtained relationship between Entropy and Randic index of this graph. These results will be helpful for the mankind and provides a support to recognize deep topology of the Para-line graph of (m, n) Naphthalene.

Compliance with ethical standards

Conflict of interest

The authors declare that they have no conflict of interest.

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