Mean Degree Based Topological Indices for Rhomtrees and Line Graph of Rhomtrees

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Abstract:

Rhotrix theory deals with array of numbers in rhomboid mathematical form. The graphical representation of rhotrix of dimension n is known as rhomtree. Since the degree of all the vertices in rhomtree is less than or equal to four the graphical structure of rhomtree is isomorphic to some molecular graph.A topological index is a numeric quantity which is derived from a molecular graph does not depend on labeling or pictorial representation of a graph. It is found that there exist strong connection between the chemical characteristics of chemical compounds and their topological indices. Among different topological indices, degree-based topological indices have some important applications in chemical graph theory. In this paper mean degree based topological indices of rhomtrees and line graph of rhomtrees are computed.

Keywords: Rhotrix, Geometric Arithmetic Mean index, Atom Bond Connectivity index, Root Mean Square index and Contra Harmonic Mean index

1.Introduction

In a molecular graph the vertices correspond to atoms and edges correspond the bonds between them. A topological index is a numeric quantity which is derived from a molecular graph does not depend on labeling or pictorial representation of a graph. It is found that there exist a strong connection between the characteristics of chemical compounds and their topological indices[3]. Topological indices are used for studying quantitative structure-activity relationship (QSAR)and quantitative structure-property relationship (QSPR) for predicting different properties of chemical compounds and biological activities in chemistry, biochemistry and nanotechnology [4, 10].Among different topological indices, degree-based topological indices are most studied and have some important applications in chemical graph theory[7].

Baig et.al [2] computed the Geometric Arithmetic index GA(G) = $\sum_{uv\in E(G)} \frac{\sqrt{d_G(u)d_G(v)}}{\frac{1}{2}\left(d_G(u)+d_G(v)\right)}$ and the Atom Bond Connectivity index (ABC)[6] ABC(G) = $\sum_{uv\in E(G)} \sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}}$ for regular triangulene Oxide network. In this paper similar to the above indices, Root Mean Square index(RMS) and Contra harmonic Mean index(CHM)of a graph G are defined and are respectively given by RMS(G)= $\sum_{uv\in E(G)} \sqrt{\frac{d_G^2(u)+d_G^2(v)}{2}}$ and CHM(G)= $\sum_{uv\in E(G)} \frac{d_G^2(u)+d_G^2(v)}{d_G(u)+d_G(v)}$.The above four mean degree based topological indices are calculated for rhomtree and line graph of rhomtree in sections 2 and 3.

Construction of Rhomtree

The structure of n-dimensional rhotrix is as follows:

$$R_n = \left\langle \begin{array}{ccccccccc} & & & & a_{11} & & & & \\ & & & a_{21} & c_{11} & a_{12} & & & \\ & & a_{31} & c_{21} & a_{22} & c_{12} & a_{13} & & \\ & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \\ a_{t1} & c_{t-11} & & & h(R) & & & c_{1t-1} & a_{1t} \\ & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \\ & & a_{tt-2} & c_{t-1t-2} & a_{t-1t-1} & c_{t-2t-1} & a_{t-2t} & & \\ & & & a_{tt-1} & c_{t-1t-1} & a_{t-1t} & & & \\ & & & & a_{tt} & & & & \end{array} \right\rangle$$

Where a_{11}, a_{12}, … a_{tt} denote the major entries and c_{11}, c_{12}, … $c_{t-1}c_{t-1}$ in R_n denote the minor entries of the rhotrix by sani[8,9]. A Rhotrix would always have an odd dimension. Any n-dimensional Rhotrix R_n, will have $|R_n| = \frac{1}{2}(n^2+1)$ entries by Ajibade [1] and $n \in 2Z^+ + 1$. A heart of a Rhotrix denoted by h(R) is defined as the element at the perpendicular intersection of the two diagonals of a Rhotrix. Let $\hat{R}(n)$ be a set consisting all real rhotrices of dimension$n \in 2Z^+ + 1$ and let R(n) be ay rhotrix in $\hat{R}(n)$. Then the graphical representation of rhotrix R(n) is a rhomtree T(m), with m=$\frac{1}{2}(n^2+1)$ number of vertices and $\frac{1}{2}(n^2-1)$ number of edges, having four components of binary branches and each component is bridged to the root vertex by one incident edge.

If n=7, then $\hat{R}(7)$ is a set consisting of all real rhotrices of dimension three and let R(7) be any element in $\hat{R}(7)$ given by

$$R_7 = \left\langle \begin{array}{ccccccc} & & & a_{11} & & & \\ & & a_{21} & c_{11} & a_{12} & & \\ & a_{31} & c_{21} & a_{22} & c_{12} & a_{13} & \\ a_{14} & c_{31} & a_{32} & c_{22} & a_{23} & c_{13} & a_{14} \\ & a_{42} & c_{32} & a_{33} & c_{23} & a_{24} & \\ & & a_{43} & c_{33} & a_{34} & & \\ & & & a_{44} & & & \end{array} \right\rangle$$

with r_{13} = h(R) is the heart of the rhotrix. If we take each entry in R(7) as a node point and connecting all of the entries as network of twenty five vertices using a particular pattern or style for the construction, in such a way that the heart vertex will serve as the root of the tree while the non heart vertices will serve as branches, then a rhomtree T(25) corresponding to the rhotrix R(7) ids obtained and shown in fig.1.

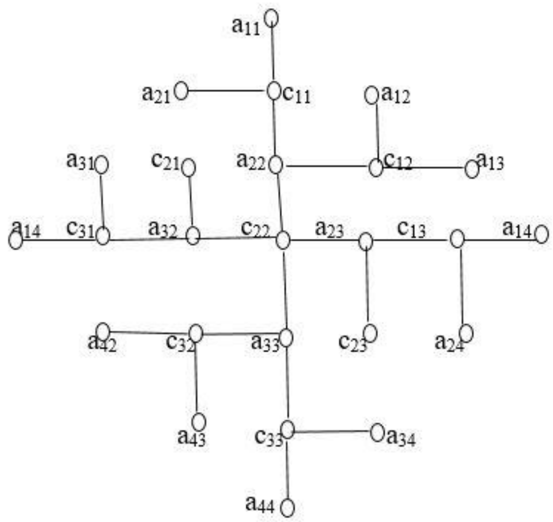

fig.1 Rhomtree T(25)

The line graph of L[T(25)] is given in Fig.2

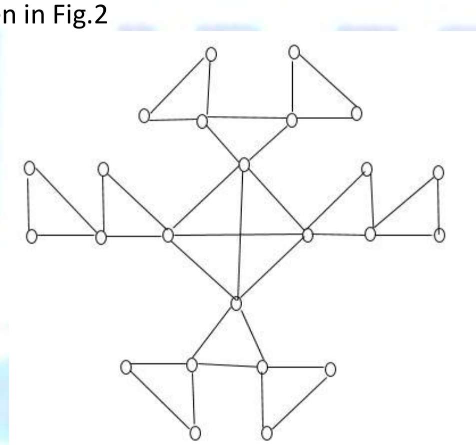

fig.2 L(T(25))

Let G=T(m) be the rhomtree of order m=$\frac{1}{2}(n^2+1)$. The partitions of the vertex set V(G) are denoted by $V_i(G)$, where v∈V_i(G) if d(v)=i. Thus the following partitions of the vertex set are obtained.

V_1= {v∈V(G): d(v)=1},V_3= {v∈V(G):d(v)=3} and V_4= {v∈V(G):d(v)=4}

From the structure of rhomtree, the cardinality of V_1,V_3 and V_4 are given below:
$|V_1| = \frac{1}{4}(n^2+7)$, $|V_3| = \frac{1}{4}(n^2-9)$ and $|V_4| = 1$

The edge set of G can also be divided into three partitions based on the sum of degrees of the end vertices and it is denoted by E_j so that if $e = uv \in E_j$ then d(u) + d(v) = j for $\delta(G) \leq j \leq \Delta(G)$. Thus the edge set of G is the union of E_4, E_6 and E_7. The edge sets E_4, E_6 and E_7, which are subsets of E(G) are as follows:
E_4={e=uv∈E(G): d(u)=1, d(v)=3}, E_6={e=uv∈E(G) :d(u)=3, d(v)=3} and
E_7= {e=uv∈E(G): d(u)=3, d(v)=4}.

In this case from direct calculations, the cardinality of E_4, E_6 and E_7 are respectively $\frac{1}{4}(n^2+7)$, $\frac{1}{4}(n^2-25)$ and 4. The partitions of the vertex set V(G) and edge set E(G) are given in Table 1 and Table 2 respectively.

Vertex partition	V_1	V_3	V_4
Cardinality	$\frac{1}{4}(n^2+7)$	$\frac{1}{4}(n^2-9)$	1

Table1: The vertex partition of Rhomtree T(m)

Edge partition	E_4	E_6	E_7
Cardinality	$\frac{1}{4}(n^2+7)$	$\frac{1}{4}(n^2-25)$	4

Table 2: The edge partition of Rhomtree T(m)

Similarly the vertex set and edge set of line graph of rhomtree can be partitioned. The partitions of the vertex set of L(G) are given by
$V_2^*=\{v\in V(L(G)): d(v)=2\}$,$V_4^*=\{v\in V(L(G)):d(v)=4\}$ and $V_5^*=\{v\in V(L(G)):d(v)=5\}$.
The partitions of the edge set of L(G) are given by
$E_4^*=\{e=uv\in E(L(G)): d(u)=2 , d(v)=2\}$, $E_6^*=\{e=uv\in E(L(G)) :d(u)=2, d(v)=4\}$ and
$E_7^*=\{e=uv\in E(G): d(u)=2, d(v)=5\}$, $E_8^*=\{e=uv\in E(G): d(u)=4, d(v)=4\}$,
$E_9^*=\{e=uv\in E(G): d(u)=4, d(v)=5\}$, $E_{10}^*=\{e=uv\in E(G): d(u)=5, d(v)=5\}$.
The cardinality of partitions of V(L(G)) and E(L(G)) are respectively given in table 3 and 4

Vertex Partition of L(G)	V_2^*	V_4^*	V_5^*
Cardinality	$\frac{1}{4}(n^2+7)$	$\frac{1}{4}(n^2-25)$	4

Table 3: The Vertex partition of L(T(m))

Edge partition of L(G)	E_4^*	E_6^*	E_7^*	E_8^*	E_9^*	E_{10}^*
Cardinality	n-1	$\frac{1}{2}(n^2-4n+7)$	2	$\frac{1}{4}(n^2+4n-69)$	6	6

Table 4: The Edge partition of L(T(m))

2. GA-index, AMS index of T(m) and L(T(m))

Theorem 2.1 The GA- index of RhomtreeT(m) is given byGA(G)= $\frac{1}{56}\left(n^2\left(7\sqrt{3}+14\right)+\sqrt{3}(177)-350\right)$

Proof The GA-index of T(m) is

$$GA((G)) = \sum_{uv\in E(G)} \frac{2\sqrt{d(u)d(v)}}{(d(u)+d(v))}$$

$$= \sum_{uv\in E_4^*} \frac{2\sqrt{d(u)d(v)}}{(d(u)+d(v))} + \sum_{uv\in E_6^*} \frac{2\sqrt{d(u)d(v)}}{(d(u)+d(v))} + \sum_{uv\in E_7^*} \frac{2\sqrt{d(u)d(v)}}{(d(u)+d(v))}$$

$$= |E_4^*|\left(\frac{\sqrt{3}}{2}\right) + |E_6^*|(1) + |E_7^*|\left(\frac{4\sqrt{3}}{7}\right)$$

$$= \frac{1}{4}(n^2+7)\left(\frac{\sqrt{3}}{2}\right) + \frac{1}{4}(n^2-25)(1) + 4\left(\frac{4\sqrt{3}}{7}\right) = \frac{1}{56}\left(n^2(7\sqrt{3}+14) + \sqrt{3}(177) - 350\right)$$

Theorem 2.2 The GA index of Line graph of Rhomtree L(T(m)) is given by

GA(L(T(m))= $n+5+\frac{1}{2}(n^2-4n+7)\left(\frac{2\sqrt{2}}{3}\right)+2\left(\frac{2\sqrt{10}}{7}\right)+\frac{1}{4}(n^2+4n-69)(1)+8\frac{\sqrt{5}}{3}$

Proof The GA-index of Line graph of T(m) is

$$GA(L(G)) = \sum_{uv\in E(G)} \frac{2\sqrt{d(u)d(v)}}{(d(u)+d(v))}$$

$$= \sum_{uv\in E_4^*} \frac{2\sqrt{d(u)d(v)}}{(d(u)+d(v))} + \sum_{uv\in E_6^*} \frac{2\sqrt{d(u)d(v)}}{(d(u)+d(v))} + \sum_{uv\in E_7^*} \frac{2\sqrt{d(u)d(v)}}{(d(u)+d(v))} + \sum_{uv\in E_8^*} \frac{2\sqrt{d(u)d(v)}}{(d(u)+d(v))} +$$

$$\sum_{uv\in E_9^*} \frac{2\sqrt{d(u)d(v)}}{(d(u)+d(v))} + \sum_{uv\in E_{10}^*} \frac{2\sqrt{d(u)d(v)}}{(d(u)+d(v))}$$

$$= |E_4^*|(1) + |E_6^*|\left(\frac{2\sqrt{2}}{3}\right) + |E_7^*|\left(\frac{2\sqrt{10}}{7}\right) + + |E_8^*|(1) + |E_9^*|\left(\frac{4\sqrt{5}}{9}\right) + |E_{10}^*|(1)$$

$$= (n-1)(1) + \frac{1}{2}(n^2-4n+7)\left(\frac{2\sqrt{2}}{3}\right) + 2\left(\frac{2\sqrt{10}}{7}\right) + \frac{1}{4}(n^2+4n-69)(1) + 6\left(\frac{4\sqrt{5}}{9}\right) + 6(1)$$

$$= n+5+\frac{1}{2}(n^2-4n+7)\left(\frac{2\sqrt{2}}{3}\right)+2\left(\frac{2\sqrt{10}}{7}\right)+\frac{1}{4}(n^2+4n-69)(1)+8\frac{\sqrt{5}}{3}$$

Theorem 2.3 The Atom Bond Connectivity index of Rhomtree T(m) is given by

ABC(T(m))= $\frac{1}{24}\left[4n^2+\sqrt{\frac{2}{3}}(6n^2+42)+48\sqrt{\frac{5}{3}}-100\right]$

Proof The ABC-index of T(m) is

$$ABC(L(G)) = \sum_{uv\in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}$$

$$= \sum_{uv\in E_4^*} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}} + \sum_{uv\in E_6^*} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}} + \sum_{uv\in E_7^*} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}$$

$$= |E_4^*|\left(\sqrt{\frac{2}{3}}\right) + |E_6^*|\left(\frac{2}{3}\right) + |E_7^*|\left(\frac{1}{2}\sqrt{\frac{5}{3}}\right)$$

$$= \frac{1}{4}(n^2+7)\left(\sqrt{\frac{2}{3}}\right) + \frac{1}{4}(n^2-25)\left(\frac{2}{3}\right) + 4\left(\frac{1}{2}\sqrt{\frac{5}{3}}\right) = \frac{1}{24}\left[4n^2 + \sqrt{\frac{2}{3}}(6n^2+42) + 48\sqrt{\frac{5}{3}} - 100\right]$$

Theorem 2.4 The Atom Bond Connectivity index of Line graph of Rhomtree L(T(m)) is given by

ABC(L(T(m)))= $(n-1)\frac{1}{\sqrt{2}} + \frac{1}{2\sqrt{2}}(n^2-2n+7) + \frac{1}{4}(n^2+4n-69)\left(\frac{1}{2}\sqrt{\frac{3}{2}}\right) + 6\left(\frac{1}{2}\sqrt{\frac{7}{5}}\right) + 6\left(\frac{2\sqrt{2}}{5}\right) + 2\left(\frac{1}{\sqrt{2}}\right)$

Proof The ABC-index of Line graph of T(m) is

$$ABC(L(G)) = \sum_{uv\in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}$$

$$= \sum_{uv\in E_4^*} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}} + \sum_{uv\in E_6^*} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}} + \sum_{uv\in E_7^*} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}$$

$$+ \sum_{uv\in E_8^*} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}} + \sum_{uv\in E_9^*} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}} + \sum_{uv\in E_{10}^*} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}$$

$$= |E_4^*|\left(\sqrt{\frac{2}{4}}\right) + |E_6^*|\left(\sqrt{\frac{4}{8}}\right) + |E_7^*|\left(\sqrt{\frac{5}{10}}\right) + |E_8^*|\left(\sqrt{\frac{6}{16}}\right) + |E_9^*|\left(\sqrt{\frac{7}{20}}\right) + |E_{10}^*|\left(\sqrt{\frac{8}{25}}\right)$$

$$= (n-1)\left(\sqrt{\frac{1}{2}}\right) + \frac{1}{2}(n^2-4n+7)\left(\sqrt{\frac{1}{2}}\right) + 2\left(\sqrt{\frac{1}{2}}\right) + \frac{1}{4}(n^2+4n-69)\left(\frac{1}{2}\sqrt{\frac{3}{2}}\right) + 6\left(\frac{1}{2}\sqrt{\frac{7}{5}}\right) + 6\left(\frac{2\sqrt{2}}{5}\right)$$

$$= (n-1)\frac{1}{\sqrt{2}} + \frac{1}{2\sqrt{2}}(n^2-2n+7) + \frac{1}{4}(n^2+4n-69)\left(\frac{1}{2}\sqrt{\frac{3}{2}}\right) + 6\left(\frac{1}{2}\sqrt{\frac{7}{5}}\right) + 6\left(\frac{2\sqrt{2}}{5}\right) + 2\left(\frac{1}{\sqrt{2}}\right)$$

3. RMS index , CHM index of Rhomtree and Line Graph of Rhomtree:

Theorem 3.1 The Root Mean Square index of Rhomtree T(m) is given by

RMS(T(m))= $\frac{1}{4}(n^2+7)\sqrt{5} + \frac{3}{4}(n^2-25) + \frac{20}{\sqrt{2}}$

Proof The RMS index of T(m) is

$$RMS(G)=\sum_{uv\in E(G)}\sqrt{\frac{d(u)^2+d(v)^2}{2}}$$

$$=\sum_{uv\in E_4^*}\sqrt{\frac{d(u)^2+d(v)^2}{2}}+\sum_{uv\in E_6^*}\sqrt{\frac{d(u)^2+d(v)^2}{2}}+\sum_{uv\in E_7^*}\sqrt{\frac{d(u)^2+d(v)^2}{2}}$$

$$=|E_4|\times\sqrt{\frac{10}{2}}+|E_6|\sqrt{\frac{18}{2}}+|E_7|\times\sqrt{\frac{25}{2}}$$

$$=\frac{1}{4}\left(n^2+7\right)\sqrt{5}+\frac{3}{4}\left(n^2-25\right)+\frac{20}{\sqrt{2}}$$

Theorem 3.2 The Root Mean square index of Line graph of Rhomtree L(T(m)) is given by

RMS (L(T(m)))= $(n^2+6n-41)+\left(\frac{n^2-4n+7}{2}\right)\left(\sqrt{10}\right)+2\left(\sqrt{\frac{29}{2}}\right)+6\left(\sqrt{\frac{41}{2}}\right)$

Proof RMS index of Line graph of T(m) is

$$RMS(L(G))=\sum_{uv\in E(G)}\sqrt{\frac{d(u)^2+d(v)^2}{2}}$$

$$=\sum_{uv\in E_4^*}\sqrt{\frac{d(u)^2+d(v)^2}{2}}+\sum_{uv\in E_6^*}\sqrt{\frac{d(u)^2+d(v)^2}{2}}+\sum_{uv\in E_7^*}\sqrt{\frac{d(u)^2+d(v)^2}{2}}$$

$$+\sum_{uv\in E_8^*}\sqrt{\frac{d(u)^2+d(v)^2}{2}}+\sum_{uv\in E_9^*}\sqrt{\frac{d(u)^2+d(v)^2}{2}}+\sum_{uv\in E_{10}^*}\sqrt{\frac{d(u)^2+d(v)^2}{2}}$$

$$=|E_4^*|\left(\sqrt{\frac{2^2+2^2}{2}}\right)+|E_6^*|\left(\sqrt{\frac{2^2+4^2}{2}}\right)+|E_7^*|\left(\sqrt{\frac{3^2+4^2}{2}}\right)+|E_8^*|\left(\sqrt{\frac{4^2+4^2}{2}}\right)+|E_9^*|\left(\sqrt{\frac{4^2+5^2}{2}}\right)+|E_{10}^*|\left(\sqrt{\frac{5^2+5^2}{2}}\right)$$

$$=(n-1)(2)+\left(\frac{n^2-4n+7}{2}\right)\left(\sqrt{10}\right)+2\left(\sqrt{\frac{29}{2}}\right)+\frac{1}{4}\left(n^2+4n-69\right)(4)+6\left(\sqrt{\frac{41}{2}}\right)+6(5)$$

$$=(n^2+6n-41)+\left(\frac{n^2-4n+7}{2}\right)\left(\sqrt{10}\right)+2\left(\sqrt{\frac{29}{2}}\right)+6\left(\sqrt{\frac{41}{2}}\right)$$

Theorem 3.3 The Contra harmonic Mean index of Rhomtree T(m) is given by

CHM(T(m)= $\frac{1}{56}\left(77n^2-5\right)$

Proof

$$CHM(T(m)) = \sum_{uv\in E(G)} \frac{d(u)^2 + d(v)^2}{d(u)+d(v)}$$

$$= \sum_{uv\in E_4^*} \frac{d(u)^2 + d(v)^2}{d(u)+d(v)} + \sum_{uv\in E_6^*} \frac{d(u)^2 + d(v)^2}{d(u)+d(v)} + \sum_{uv\in E_7^*} \frac{d(u)^2 + d(v)^2}{d(u)+d(v)}$$

$$= |E_4^*|\left(\frac{5}{2}\right) + |E_6^*|(3) + |E_7^*|\left(\frac{25}{7}\right)$$

$$= \frac{1}{4}(n^2+7)\left(\frac{5}{2}\right) + \frac{1}{4}(n^2-25)(3) + 4\left(\frac{25}{7}\right)$$

$$= \frac{1}{56}(77n^2 - 5)$$

Theorem 3.4 The Contra harmonic Mean index of Line graph of Rhomtree L(T(m)) is given by

CHM (L(T(m)))= $\frac{1}{21}(56n^2 - 14n + 132)$

Proof The CHM-index of line graph of T(m) is

$$CHM(L(G)) = \sum_{uv\in E(G)} \frac{d(u)^2 + d(v)^2}{d(u)+d(v)}$$

$$= \sum_{uv\in E_4^*} \frac{d(u)^2 + d(v)^2}{d(u)+d(v)} + \sum_{uv\in E_6^*} \frac{d(u)^2 + d(v)^2}{d(u)+d(v)} + \sum_{uv\in E_7^*} \frac{d(u)^2 + d(v)^2}{d(u)+d(v)} + \sum_{uv\in E_8^*} \frac{d(u)^2 + d(v)^2}{d(u)+d(v)} + \sum_{uv\in E_9^*} \frac{d(u)^2 + d(v)^2}{d(u)+d(v)} + \sum_{uv\in E_{10}^*} \frac{d(u)^2 + d(v)^2}{d(u)+d(v)}$$

$$= |E_4^*|\left(\frac{2^2+2^2}{4}\right) + |E_6^*|\left(\frac{2^2+4^2}{6}\right) + |E_7^*|\left(\frac{2^2+5^2}{7}\right) + |E_8^*|\left(\frac{4^2+4^2}{8}\right) + |E_9^*|\left(\frac{4^2+5^2}{9}\right) + |E_{10}^*|\left(\frac{5^2+5^2}{10}\right)$$

$$= (n-1)(2) + \left(\frac{n^2-4n+7}{2}\right)\left(\frac{10}{3}\right) + 2\left(\frac{29}{7}\right) + \frac{1}{4}(n^2+4n-69)(4) + 6\left(\frac{41}{9}\right) + 6(5)$$

$$= \frac{1}{21}(56n^2 - 14n + 132)$$

Conclusion

The molecular name for T(25) is 4,4- Bis-(1-isopropyl-2-methyl-propyl)-2,3,5,6-tetramethyl-heptane and that of T(41) is 4-(1-Isopropyl-2-methyl-propyl)-5-[1-(1-isopropyl-2-methyl-propyl)-2,3-dimethyl-butyl]-2,3,6,7,8-pentamethyl-5-(1,2,3-trimethyl-butyl)-nonane. Since the rhomtrees are isomorphic to molecular graphs the mean degree based indices which are computed in this paper may be applicable to study the characteristics of chemical compounds and drugs.

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