INDIAN JOURNAL OF SCIENCE AND TECHNOLOGY

RESEARCH ARTICLE

# On Entropy Measures of Thiophene Dendrimers Using Degree Based Structural Descriptors

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OPEN ACCESS

**Received:** 12-11-2022

**Accepted:** 25-01-2023

**Published:** 09-03-2023

**Citation:** Xavier DA, Theertha Nair A , Varghese ES, Baby A (2023) On Entropy Measures of Thiophene Dendrimers Using Degree Based Structural Descriptors. Indian Journal of Science and Technology 16(10): 707-716. https://doi.org/10.17485/IJST/v16i10.2179

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**Funding:** None

**Competing Interests:** None



Published By Indian Society for Education and Environment (iSee)

**ISSN**
Print: 0974-6846
Electronic: 0974-5645

## Abstract

**Objectives**: This study evaluates various degree-based topological indices and corresponding entropy measures of thiophene dendrimers. **Methods**:We begin by implementing the traditional edge partition method for estimating the structural correlation of two variations of thiophene dendrimers before focusing about graph entropy measurements, using Shannon's entropy model. **Findings:** Various degree based molecular descriptors of two variations of thiophene dendrimers and their corresponding entropies have been obtained. In addition, a comparative analysis of these descriptors have also been carried out. **Novelty:** The concept of investigating a structure as the result of arbitrary communication is the key innovative notion. This insight allowed Shannon's entropy estimates to be utilized for calculating the structural information content of a chemical compound. Due to the wide range of applications, thiophene dendrimers stand out in the field of organic electronics. As a result, these evaluations can be used for exploring the data required for conducting experiments using this dendrimer family.

**Keywords:** Dendrimers; Thiophene dendrimers; Degree based Topological Indices; Entropy measures

## 1 Introduction

Topological indices are numbers calculated from conventional formulas obtained after applying mathematical operations on the graphs using various methods. The need for using tools like topological indices arised from the fact that physical and chemical attributes are given as numbers which have further given them a measure that allowed for comparisons and correlations. These descriptors are crucial tools in QSAR/QSPR research because they serve as molecular descriptors. The Shannon's entropy concept-inspired graph entropies with topological indices to act as the units of information for calculating the structural information of chemical graphs and complicated networks. Discrete mathematics, biology, and chemistry are just a few of the fields where the graph entropy measures are crucial[1–3].

Dendrimer is a member of a group of macromolecules that combine the benefits of oligomers and polymers. The most popular organic semiconductors for use in organic electronics are one-dimensional linear oligothiophenes and polythiophenes because of their exceptional optical, redox, self-organizing and transport capabilities. Among them, the most prominent examples of dendrimers for organic electrical applications are all-thiophene dendrimers (DOT), which are recently developed. These thiophene dendrimers are structurally stiff and shape-persistent, in contrast to ordinary dendrimers that have flexible backbones. As a result, these materials exhibit significant isotropic characteristics. Additionally, to adjust optical and electrical characteristics, these structurally specified molecules may be further functionalized with different functional groups at various places. They can be used as top-notch building blocks to create brand-new thiophene-based compounds for use in organic electronics. Each of the thiophene dendrons and dendrimers up to a fourth generation (a 90-mer) have been successfully synthesized utilizing trimethylsilyl (R=TMS) as protecting groups. Tetrabutylammonium fluoride (TBAF) can detach the TMS protecting groups from these unique all-thiophene dendrimers, resulting in "pure" all-thiophene dendrimers (R=H). The chemical structures of these structures are shown in Figure 1 [4,5]. Chemical graph theory has a significant impact in the present world. Many different branches of chemistry have found use for topological indices including Quantitative Structure-Property Relationships (QSPR), Quantitative Biology, and Quantitative Structure -Activity Relationships (QSAR), etc [1,6–10]. Different approaches are used to find the various topological indices including distance based, degree based, eccentricity based and so on. We focus on the degree based topological indices which are useful in carrying out various chemical experiments. Even though, this group of dendrimers play a major role in organic electronics, no significant amount of work has been carried out yet to examine the topological aspects of this dendrimer family and hence this work is so relevant to fill the research gap. Our contribution consists of computing graph entropies based on the unique functional information, which relates the number of vertices with various degrees and the number of edges connecting vertices with different degrees. From this index, it is possible to analyse mathematical values and further investigate some physico-chemical properties of the molecule. Therefore, it is an efficient method in avoiding expensive and time-consuming laboratory experiments. For further information regarding the concept refer [11–15].

In this study, various degree based molecular descriptors of two variations of thiophene dendrimers and their corresponding entropies have been calculated.

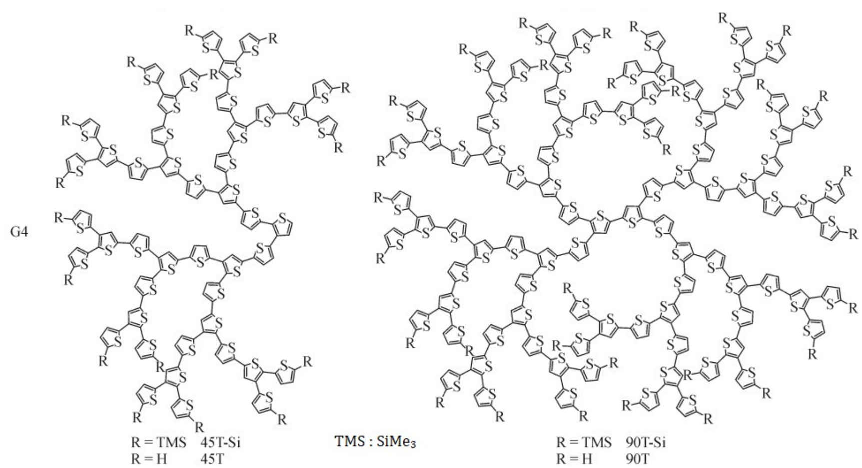


**Fig 1.** Chemical structure of thiophene dendrimers

## 2 Methodology

We examine a simple, finite, connected graph G with a set of vertex values of V and a set of edge values of E. The total number of edges that are incident on a vertex $x$, denoted by the symbol $d_x$, is that vertex's degree. Using Shannon's model, the entropy measurements have been determined [14]. The mathematical equations of various indices based on degree have been given in Table 1. Let $DT(G)$ denote the degree based topological index of a graph $G$, then we get,

$$DT(G) = \sum_{g \in E(G)} t(g)$$

where $t$ is the functional characterizing the degree based topological index.

The entropy measure is denoted by $ENT_{DT}(G)$ and is defined as,

$$ENT_{DT}(G) = log(DT(G)) - \frac{1}{DT(G)} log\left[\prod_{g\in E(G)} [t(g)]^{[t(g)]}\right] \quad (1)$$

**Table 1.** Degree based indices of graph$G$

| Degree Based Index | Mathematical Formula |
|---|---|
| First Zagreb | $M_1(G) = \sum_{g=xy\in E(G)}(d_x + d_y)$ |
| Second Zagreb | $M_2(G) = \sum_{g=xy\in E(G)}(d_x \times d_y)$ |
| Harmonic | $H(G) = \sum_{g=xy\in E(G)} \frac{2}{d_x+d_y}$ |
| Hyper Zagreb | $HM(G) = \sum_{g=xy\in E(G)}[d_x + d_y]^2$ |
| Forgotten | $F(G) = \sum_{g=xy\in E(G)}[d_x]^2 + [d_y]^2$ |
| Randic | $R(G) = \sum_{g=xy\in E(G)} \frac{1}{\sqrt{d_x\times d_y}}$ |
| Reciprocal Randic | $RR(G) = \sum_{g=xy\in E(G)} \sqrt{d_x \times d_y}$ |
| Sum-connectivity index | $SC(G) = \sum_{g=xy\in E(G)} \frac{1}{\sqrt{d_x+d_y}}$ |
| Geometric arithmetic | $GA(G) = \sum_{g=xy\in E(G)} \frac{2\sqrt{d_x\times d_y}}{d_x+d_y}$ |
| Atom bond connectivity | $ABC(G) = \sum_{g=xy\in E(G)} \frac{\sqrt{d_x+d_y-2}}{\sqrt{d_x\times d_y}}$ |
| Irregularity measure | $irr(G) = \sum_{g=xy\in E(G)}\lvert d_x - d_y\rvert$ |
| Sigma | $\sigma(G) = \sum_{g=xy\in E(G)}(d_x - d_y)^2$ |

## 3 Degree Based Indices and Entropies

In this section, we compute the degree based indices in Table 1 for the oligothiophene dendrimers with two different protecting groups; TMS and H. Further, we have extended this work by computing the degree based entropies for these dendrimers.

**Theorem 1** For $n \geq 1$,

$M_1(DOT_{TMS}(n)) = 228 \times 2^n - 190$

$M_2(DOT_{TMS}(n)) = 280 \times 2^n - 241$

$H(DOT_{TMS}(n)) = (\frac{362}{21} \times 2^n) - \frac{73}{5}$

$HM(DOT_{TMS}(n)) = 1200 \times 2^n - 988$

$F(DOT_{TMS}(n)) = 640 \times 2^n - 506$

$R(DOT_{TMS}(n)) = (\frac{1}{\sqrt{3}} \times 2^n) - 4\sqrt{6} + 4\sqrt{6} \times 2^n + (\frac{23}{3} \times 2^n) - 5$

$RR(DOT_{TMS}(n)) = 4\sqrt{3} \times 2^n - 24\sqrt{6} + 24\sqrt{6} \times 2^n + 44 \times 2^n - 35$

$SC(DOT_{TMS}(n)) = 6\sqrt{5} \times 2^n - \frac{3\sqrt{6}}{2} - \frac{24\sqrt{5}}{5} + \frac{4\sqrt{6}\times 2^n}{3} + \frac{2^{n+1}\sqrt{7}}{7} + 2^{n+1} - 2$

$GA(DOT_{TMS}(n)) = \frac{8\sqrt{3}\times 2^n}{7} - \frac{48\sqrt{6}}{5} + \frac{48\sqrt{6}\times 2^n}{5} + \frac{84\times 2^n}{5} - 13$

$ABC(DOT_{TMS}(n)) = 14\sqrt{2} \times 2^n - 14\sqrt{2} + 3\sqrt{3} \times 2^n + \frac{\sqrt{15}\times 2^n}{3} + (\frac{16}{3} \times 2^n) - 6$

$irr(DOT_{TMS}(n)) = 44 \times 2^n - 24$

$\sigma(DOT_{TMS}(n)) = 80 \times 2^n - 24$

Proof. The graph $DOT_{TMS}(n)$ $: n \geq 1$ has $44 \times 2^n - 37$ edges. The degree of vertices of $DOT_{TMS}(n)$ can be $1, 2, 3$ or 4. We observed and inferred 5 partitions for the edge set based on the vertex degree, which are $(2,2)$, $(2,3)$, $(3,3)$, $(3,4)$ and $(4,1)$. The edge partitions $(d_x, d_y)$, $xy \in E(DOT_{TMS}(n))$ and the corresponding number of edges in each partition is given in Table 2. The molecular graph of fourth generation thiophene(R=TMS) dendrimer is given in Figure 2.

**Table 2.** Edge partition of oligothiophene-TMS dendrimer

| Edge partition$(d_x, d_y)$ | Number of edges |
|---|---|
| $(2,2)$ | $4\times 2^n-4$ |
| $(2,3)$ | $24\times 2^n-24$ |
| $(3,3)$ | $8\times 2^n-9$ |
| $(3,4)$ | $2^{n+1}$ |
| $(4,1)$ | $3\times 2^{n+1}$ |

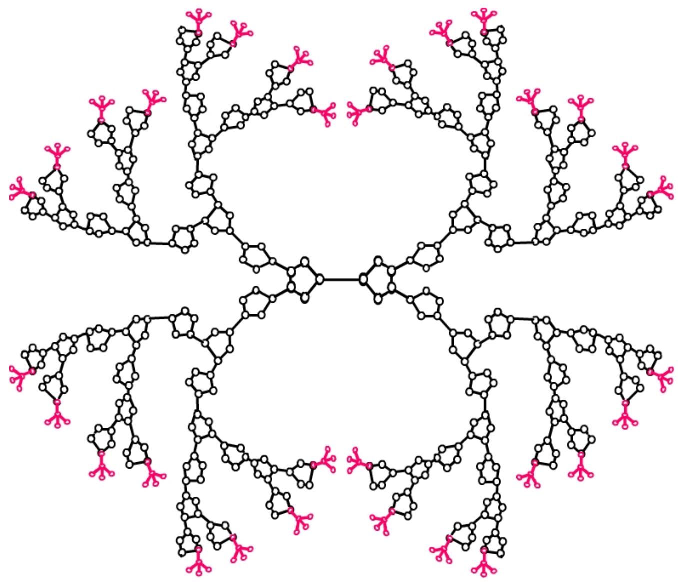

**Fig 2.** Thiophene dendrimer with varying group as TMS; $DOT_{TMS}(4)$

Using Table 3 and by applying formulas in Tables 1 and 2, we derive the following.

Let ;

$a_{22}$=$4\times 2^n-4$

$a_{23}$=$24\times 2^n-24$

$a_{33}$=$8\times 2^n-9$

$a_{34}$=$2^{n+1}$

$a_{41}$=$3\times 2^{n+1}$

$M_1(DOT_{TMS}(n)) = 4\times(a_{22})+5\times(a_{23})+6\times(a_{33})+7\times(a_{34})+5\times(a_{41}) = 228\times 2^n-190$

$M_2(DOT_{TMS}(n)) = 4\times(a_{22})+6\times(a_{23})+9\times(a_{33})+12\times(a_{34})+4\times(a_{41}) = 280\times 2^n-241$

$H(DOT_{TMS}(n)) = (\frac{1}{2})\times(a_{22})+(\frac{2}{5})\times(a_{23})+(\frac{1}{3})\times(a_{33})+(\frac{2}{7})\times(a_{34}) \quad +(\frac{2}{5})(a_{41}) = \left(\frac{362}{21}\times 2^n\right)-\frac{73}{5}$

$HM(DOT_{TMS}(n)) = 16\times(a_{22})+25\times(a_{23})+36\times(a_{33})+49\times(a_{34})+25\times(a_{41}) = 1200\times 2^n-988$

$F(DOT_{TMS}(n)) = 8\times(a_{22})+13\times(a_{23})+18\times(a_{33})+25\times(a_{34})+17\times(a_{41}) = 640\times 2^n-506$

$R(DOT_{TMS}(n)) = \frac{1}{2}\times(a_{22})+(\frac{1}{\sqrt{6}})\times(a_{23})+(\frac{1}{3})\times(a_{33})+(\frac{\sqrt{3}}{6})\times(a_{34})+\frac{1}{2}\times(a_{41})$

$$=(\frac{1}{\sqrt{3}}\times 2^n)-4\sqrt{6}+4\sqrt{6}\times 2^n+(\frac{23}{3}\times 2^n)-5$$

$RR(DOT_{TMS}(n)) = 2\times(a_{22})+\sqrt{6}\times(a_{23})+3\times(a_{33})+2\sqrt{3}\times(a_{34})+2\times(a_{41})$

$=4\sqrt{3}\times 2^n-24\sqrt{6}+24\times 2^n\times\sqrt{6}+44\times 2^n-35$

$SC(DOT_{TMS}(n)) = (\frac{1}{2})\times(a_{22})+(\frac{1}{\sqrt{5}})\times(a_{23})+(\frac{1}{\sqrt{6}})\times(a_{33})+(\frac{1}{\sqrt{7}})\times(a_{34}) \quad +(\frac{1}{\sqrt{5}})\times(a_{41})$

$=6\sqrt{5}\times 2^n-\frac{3\sqrt{6}}{2}-\frac{24\sqrt{5}}{5}+\frac{4\sqrt{6}\times 2^n}{3}+\frac{2^{n+1}\times\sqrt{7}}{7}+2^{n+1}-2$

$$GA(DOT_{TMS}(n)) = 1\times(a_{22}) + 2\times(\tfrac{\sqrt{6}}{5})\times(a_{23}) + 1\times(a_{33}) \quad +\tfrac{4}{7}\times\sqrt{3}\times(a_{34}) + (\tfrac{4}{5})\times(a_{41})$$
$$= \frac{8\sqrt{3}\times 2^n}{7} - \frac{48\sqrt{6}}{5} + \frac{48\sqrt{6}\times 2^n}{5} + \frac{84\times 2^n}{5} - 13$$

$$ABC(DOT_{TMS}(n)) = (\tfrac{1}{\sqrt{2}})\times(a_{22}) + (\tfrac{1}{\sqrt{2}})\times(a_{23}) + (\tfrac{2}{3})\times(a_{33}) \quad +(\tfrac{\sqrt{5}}{\sqrt{12}})\times(a_{34}) + (\tfrac{\sqrt{3}}{2})\times(a_{41})$$
$$= 14\sqrt{2}\times 2^n - 14\sqrt{2} + 3\sqrt{3}\times 2^n + \frac{\sqrt{15}\times 2^n}{3} + (\frac{16}{3}\times 2^n) - 6$$

$$irr(DOT_{TMS}(n)) = 1\times(a_{23}) + 1\times(a_{34}) + 3\times(a_{41}) == 44\times 2^n - 24$$
$$\sigma(DOT_{TMS}(n)) = 1\times(a_{23}) + 1\times(a_{34}) + 9\times(a_{41}) = 80\times 2^n - 24$$

**Theorem 2** For $n \geq 1$,

$$ENT_{M_1}(DOT_{TMS}(n)) = log(228\times 2^n - 190) - \frac{log(2^{(80\times 2^n - 86)}\times 3^{(48\times 2^n - 54)}\times 5^{(150\times 2^n - 120)}\times 7^{(7\times 2^{n+1})})}{(228\times 2^n - 190)}$$
$$ENT_{M_2}(DOT_{TMS}(n)) = log(280\times 2^n - 241) - \frac{log(2^{(272\times 2^n - 176)}\times 3^{(312\times 2^n - 306)})}{(280\times 2^n - 241)}$$
$$ENT_H\ (DOT_{TMS}(n)) \ = log\left((\tfrac{362}{21}\times 2^n) - \tfrac{73}{5}\right) - \frac{(105\times log(2^{(1694-2050\times 2^n)}\times 1560823428673649^{(30\times 2^n - 24)}\times 1574279231806271^{2^{n+1}}\times 3122621576798651^{(8\times 2^n - 9)}))}{(1810\times 2^n - 1533)}$$
$$ENT_{HM}(DOT_{TMS}(n)) = log(1200\times 2^n - 988) - \frac{log(2^{(3742\times 2^n - 3040)}\times 5^{(46\times 2^n - 42)}\times 48850679458489^{(8\times 2^n - 9)}\times 481482486096809^{(30\times 2^n - 24)}\times 2448436768113089^{(2^{n+1})}))}{(1200\times 2^n - 988)}$$
$$ENT_F(DOT_{TMS}(n)) = log(640\times 2^n - 506) - \frac{l\,og(2^{(524\times 2^n - 303)}\times 13^{(312\times 2^n - 312)}\times 1577835582516359^{(3\times 2^{n+1})}\times 2407412430484045^{(2^{n+1})}\times 4690457353031223^{(8\times 2^n - 9)}))}{(640\times 2^n - 506)}$$
$$ENT_R(DOT_{TMS}(n)) = log((\tfrac{1}{\sqrt{3}}\times 2^n) - 4\sqrt{6} + 4\sqrt{6}\times 2^n + (\tfrac{23}{3}\times 2^n) - 5) - \frac{(3log(2^{(1646-1701\times 2^n)}\times 3^{(26\times 2^n - 24)}\times 130169451236315^{(24\times 2^n - 24)}\times 1048750362812539^{(2^{n+1})}\times 3122621576798651^{(8\times 2^n - 9)}))}{(2^n\sqrt{3} - 12\sqrt{6} + 23\times 2^n + 12\sqrt{6}\times 2^n - 15)}$$
$$ENT_{RR}(DOT_{TMS}(n)) = log\left(4\times 2^n\times\sqrt{3} - 24\sqrt{6} + 24\times 2^n\times\sqrt{6} + 44\times 2^n - 35\right) - \frac{log(2^{(1120-1200\times 2^n)}\times 3^{(48\times 2^n - 51)}\times 421041878423467^{(24\times 2^n - 24)}\times 5206867775977999^{(2^{n+1})})}{4\times 2^n\times\sqrt{3} - 24\sqrt{6} + 24\times 2^n\times\sqrt{6} + 44\times 2^n - 35}$$
$$ENT_{SC}(DOT_{TMS}(n)) = log\left(6\sqrt{5}\times 2^n - \tfrac{3\sqrt{6}}{2} - \tfrac{24\sqrt{5}}{5} + \tfrac{4\sqrt{6}\times 2^n}{3} + \tfrac{2^{n+1}\times\sqrt{7}}{7} + 2^{n+1} - 2\right) - \left(\frac{1}{6\sqrt{5}\times 2^n - \frac{3\sqrt{6}}{2} - \frac{24\sqrt{5}}{5} + \frac{4\sqrt{6}\times 2^n}{3} + \frac{2^{n+1}\times\sqrt{7}}{7} + 2^{n+1} - 2}\right)\times log\left((\tfrac{1}{2})^{\frac{(4\times 2^n - 4)}{2}}\times(\tfrac{1}{\sqrt{5}})^{\frac{(24\times 2^n - 24)}{\sqrt{5}}}\times(\tfrac{1}{\sqrt{6}})^{\frac{(8\times 2^n - 9)}{\sqrt{6}}}\times(\tfrac{1}{\sqrt{7}})^{\frac{(2^{n+1})}{\sqrt{7}}}\times(\tfrac{1}{\sqrt{5}})^{\frac{(3\times 2^{n+1})}{\sqrt{5}}}\right)$$
$$ENT_{GA}(DOT_{TMS}(n)) = log\left(\tfrac{8\sqrt{3}\times 2^n}{7} - \tfrac{48\sqrt{6}}{5} + \tfrac{48\sqrt{6}\times 2^n}{5} + \tfrac{84\times 2^n}{5} - 13\right) - \left(\frac{1}{\left(\frac{8\sqrt{3}\times 2^n}{7} - \frac{48\sqrt{6}}{5} + \frac{48\sqrt{6}\times 2^n}{5} + \frac{84\times 2^n}{5} - 13\right)}\right)\times log\left(1^{(4\times 2^n - 4)}\times(\tfrac{2\sqrt{6}}{5})^{\left(\frac{2\sqrt{6}(24\times 2^n - 24)}{5}\right)}\times(1)^{(8\times 2^n - 9)}\times(\tfrac{4}{5})^{\left(\frac{4\left(3\times 2^{n+1}\right)}{5}\right)}\times(\tfrac{4\sqrt{3}}{7})^{(\frac{4\sqrt{3}(2^{n+1})}{7})}\right)$$
$$ENT_{ABC}(DOT_{TMS}(n)) = log\left(14\sqrt{2}\times 2^n - 14\sqrt{2} + 3\sqrt{3}\times 2^n + \tfrac{\sqrt{15}\times 2^n}{3} + (\tfrac{16}{3}\times 2^n) - 6\right) - \left(\frac{1}{14\sqrt{2}\times 2^n - 14\sqrt{2} + 3\sqrt{3}\times 2^n + \frac{\sqrt{15}\times 2^n}{3} + (\frac{16}{3}\times 2^n) - 6}\right)\times log\left((\tfrac{1}{\sqrt{2}})^{\frac{(4\times 2^n - 4)}{\sqrt{2}}}\times(\tfrac{1}{\sqrt{2}})^{\frac{(24\times 2^n - 24)}{\sqrt{2}}}\times(\tfrac{2}{3})^{\left(\frac{2(8\times 2^n - 9)}{3}\right)}\times(\tfrac{\sqrt{3}}{2})^{\frac{(\sqrt{3}(3\times 2^{n+1}))}{2}}\times(\tfrac{\sqrt{5}}{\sqrt{12}})^{(\frac{\sqrt{5}(2^{n+1})}{\sqrt{12}})}\right)$$
$$ENT_{irr}(DOT_{TMS}(n)) = log(44\times 2^n - 24) - \frac{log(3^{(18\times 2^n)})}{(44\times 2^n - 24)}$$
$$ENT_\sigma(DOT_{TMS}(n)) = log(80\times 2^n - 24) - \frac{log(3^{(108\times 2^n)})}{(80\times 2^n - 24)}$$

Proof.
Let ;
$a_{22} = 4 \times 2^n - 4$
$a_{23} = 24 \times 2^n - 24$
$a_{33} = 8 \times 2^n - 9$
$a_{34} = 2^{n+1}$
$a_{41} = 3 \times 2^{n+1}$
Using Theorem 1 and by applying equation 1, we obtain the following;
Let $m_1 = M_1(DOT_{TMS}(n)) = 228 \times 2^n - 190$

$$ENT_{M_1}(DOT_{TMS}(n)) = log(m_1) - (\frac{1}{m_1}) \times log((4^4)^{a_{22}} \times (5^5)^{a_{23}} \times (6^6)^{a_{33}} \times (7^7)^{a_{34}} \times (5^5)^{a_{41}})$$

Similarly, For $m_2 = M_2(DOT_{TMS}(n)) = 280 \times 2^n - 241$

$$ENT_{M_2}(DOT_{TMS}(n)) = log(m_2) - (\frac{1}{m_2}) \times log((4^4)^{a_{22}} \times (6^6)^{a_{23}} \times (9^9)^{a_{33}} \times (12^{12})^{a_{34}} \times (4^4)^{a_{41}})$$

For $m_3 = H(DOT_{TMS}(n)) = \frac{(362\times 2^n)}{21} - \frac{73}{5}$ ,

$$ENT_H(DOT_{TMS}(n)) = log(m_3) - (\frac{1}{m_3}) \times log(((\frac{1}{2})^{(\frac{1}{2})})^{a_{22}} \times ((\frac{2}{5})^{(\frac{2}{5})})^{a_{23}} \times ((\frac{1}{3})^{(\frac{1}{3})})^{a_{33}} \times ((\frac{2}{7})^{(\frac{2}{7})})^{a_{34}} \times ((\frac{2}{5})^{(\frac{2}{5})})^{a_{41}})$$

For $m_4 = HM(DOT_{TMS}(n)) = 1200 \times 2^n - 988$,

$$ENT_{HM}(DOT_{TMS}(n)) = log(m_4) - (\frac{1}{m_4}) \times log((16^{16})^{a_{22}} \times (25^{25})^{a_{23}} \times (36^{36})^{a_{33}} \times (49^{49})^{a_{34}} \times (25^{25})^{a_{41}})$$

For $m_5 = F(DOT_{TMS}(n)) = 640 \times 2^n - 506$,

$$ENT_F(DOT_{TMS}(n)) = log(m_5) - (\frac{1}{m_5}) \times log((8^8)^{a_{22}} \times (13^{13})^{a_{23}} \times (18^{18})^{a_{33}} \times (25^{25})^{a_{34}} \times (17^{17})^{a_{41}})$$

For $m_6 = R(DOT_{TMS}(n)) = (\frac{1}{\sqrt{3}} \times 2^n) - 4\sqrt{6} + 4\sqrt{6} \times 2^n + (\frac{23}{3} \times 2^n) - 5$

$$ENT_R(DOT_{TMS}(n)) = log(m_6) - (\frac{1}{m_6}) \times log(((\frac{1}{2})^{(\frac{1}{2})})^{a_{22}} \times ((\frac{1}{\sqrt{6}})^{(\frac{1}{\sqrt{6}})})^{a_{23}} \times ((\frac{1}{3})^{(\frac{1}{3})})^{a_{33}} \times ((\frac{\sqrt{3}}{6})^{(\frac{\sqrt{3}}{6})})^{a_{34}} \times (\frac{1}{2})^{\frac{1}{2}})^{a_{41}})$$

For $m_7 = RR(DOT_{TMS}(n)) = 4 \times 2^n \times \sqrt{3} - 24\sqrt{6} + 24 \times 2^n \times \sqrt{6} + 44 \times 2^n - 35$

$$ENT_{RR}(DOT_{TMS}(n)) = log(m_7) - (\frac{1}{m_7}) \times log((2^2)^{a_{22}} \times ((\sqrt{6})^{(\sqrt{6})})^{a_{23}} \times (3^3)^{a_{33}} \times ((2\sqrt{3})^{(2\sqrt{3})})^{a_{34}} \times (2^2)^{a_{41}})$$

For $m_8 = SC(DOT_{TMS}(n)) = 6\sqrt{5} \times 2^n - \frac{3\sqrt{6}}{2} - \frac{24\sqrt{5}}{5} + \frac{4\sqrt{6}\times 2^n}{3} + \frac{2^{n+1}\times\sqrt{7}}{7} + 2^{n+1} - 2$
$ENT_{SC}(DOT_{TMS}(n))$

$$= log(m_6) - (\frac{1}{m_8}) \times log(((\frac{1}{2})^{(\frac{1}{2})})^{a_{22}} \times ((\frac{1}{\sqrt{5}})^{(\frac{1}{\sqrt{5}})})^{a_{23}} \times ((\frac{1}{\sqrt{6}})^{(\frac{1}{\sqrt{6}})})^{a_{33}} \times ((\frac{1}{\sqrt{7}})^{(\frac{1}{\sqrt{7}})})^{a_{34}} \times ((\frac{1}{\sqrt{5}})^{(\frac{1}{\sqrt{5}})})^{a_{41}})$$

For $m_9 = GA(DOT_{TMS}(n)) = \frac{8\sqrt{3}\times 2^n}{7} - \frac{48\sqrt{6}}{5} + \frac{48\sqrt{6}\times 2^n}{5} + \frac{84\times 2^n}{5} - 13$
$ENT_{GA}(DOT_{TMS}(n))$

$$= log(m_9) - (\frac{1}{m_9}) \times log((1^1)^{a_{22}} \times ((\frac{2\sqrt{6}}{5})^{(\frac{2\sqrt{6}}{5})})^{a_{23}} \times (1^1)^{a_{33}} \times ((\frac{4\sqrt{3}}{7})^{(\frac{4\sqrt{3}}{7})})^{a_{34}} \times ((\frac{4}{5})^{(\frac{4}{5})})^{a_{41}})$$

For $m_{10} = ABC(DOT_{TMS}(n)) = 14\sqrt{2} \times 2^n - 14\sqrt{2} + 3\sqrt{3} \times 2^n + \frac{\sqrt{15}\times 2^n}{3} + (\frac{16}{3} \times 2^n) - 6$

$ENT_{ABC}\left(DOT_{TMS}\left(n\right)\right)$

$$= log(m_{10}) - (\frac{1}{m_{10}}) \times log(((\frac{1}{\sqrt{2}})^{(\frac{1}{\sqrt{2}})})^{a_{22}} \times ((\frac{1}{\sqrt{2}})^{(\frac{1}{\sqrt{2}})})^{a_{23}} \times ((\frac{2}{3})^{(\frac{2}{3})})^{a_{33}} \times ((\frac{\sqrt{5}}{\sqrt{12}})^{(\frac{\sqrt{5}}{\sqrt{12}})})^{a_{34}} \times ((\frac{\sqrt{3}}{2})^{(\frac{\sqrt{3}}{2})})^{a_{41}})$$

For $m_{11} = irr(DOT_{TMS}(n)) = 44 \times 2^n - 24$,

$$ENT_{irr}(DOT_{TMS}(n)) = log(m_{11}) - (\frac{1}{m_{11}}) \times log((1^1)^{a_{23}} \times (1^1)^{a_{34}} \times (3^3)^{a_{41}})$$

For $m_{12} = \sigma(DOT_{TMS}(n)) = 80 \times 2^n - 24$,

$$ENT_{\sigma}(DOT_{TMS}(n)) = log(m_{12}) - (\frac{1}{m_{12}}) \times log((1^1)^{a_{23}} \times (1^1)^{a_{34}} \times (9^9)^{a_{41}})$$

On substituting the values and simplifying the equations, we get the result.

**Theorem 3** For $n \geq 1$,
$M_1(DOT_H(n)) = 180 \times 2^n - 190$
$M_2(DOT_H(n)) = 224 \times 2^n - 241$
$H(DOT_H(n)) = (\frac{44}{3} \times 2^n) - \frac{73}{5}$
$HM(DOT_H(n)) = 916 \times 2^n - 988$
$F(DOT_H(n)) = 468 \times 2^n - 506$
$R(DOT_H(n)) = (\frac{10\sqrt{6}\times 2^n}{3}) - 4\sqrt{6} + (\frac{20}{3} \times 2^n) - 5$
$RR(DOT_H(n)) = 20\sqrt{6} \times 2^n - 24\sqrt{6} + 40 \times 2^n - 35$
$SC(DOT_H(n)) = 4\sqrt{5} \times 2^n - (\frac{3\sqrt{6}}{2}) - (\frac{24\sqrt{5}}{5}) + (\frac{4\sqrt{6}\times 2^n}{3}) + 4 \times 2^n - 2$
$GA(DOT_H(n)) = 8\sqrt{6} \times 2^n - (\frac{48\sqrt{6}}{5}) + 16 \times 2^n - 13$
$ABC(DOT_H(n)) = 14\sqrt{2} \times 2^n - 14\sqrt{2} + (\frac{16}{3} \times 2^n) - 6$
$irr(DOT_H(n)) = 20 \times 2^n - 24$
$\sigma(DOT_H(n)) = 20 \times 2^n - 24$

Proof. The graph $DOT_H(n) : n \geq 1$ has $36 \times 2^n - 37$ edges. The degree of vertices of $DOT_H(n)$ can be 2 or 3. We observed and inferred 3 partitions for the edge set based on the vertex degree, which are $(2,2)$, $(2,3)$ and $(3,3)$. The edge partitions $(d_x, d_y)$, $xy \in E(DOT_H(n))$ and the corresponding number of edges in each partition is given in Table 3. The molecular graph of fourth generation thiophene (R=H) dendrimer is given in Figure 3. Using datas from Table 1 and following the similar procedure as in Theorem 1, we obtain the results.

**Table 3.** Edge partition of dendrimer

| Edge partition $(d_x, d_y)$ | Number of edges |
|---|---|
| $(2,2)$ | $2^{n+3} - 4$ |
| $(2,3)$ | $20 \times 2^n - 24$ |
| $(3,3)$ | $8 \times 2^n - 9$ |

**Theorem 4** For $n \geq 1$,
$ENT_{M_1}(DOT_H(n)) = log(180 \times 2^n - 190) - \frac{log(256^{(2^{n+3}-4)} \times 3125^{(20\times 2^n - 24)} \times 46656^{(8\times 2^n - 9)})}{(180\times 2^n - 190)}$
$ENT_{M_2}(DOT_H(n)) = log(224 \times 2^n - 241) - \frac{log(256^{(2^{n+3}-4)} \times 46656^{(20\times 2^n - 24)} \times 387420489^{(8\times 2^n - 9)})}{(224\times 2^n - 241)}$
$ENT_H(DOT_H(n)) = log((\frac{44}{3} \times 2^n) - \frac{73}{5}) - \frac{(15log(2^{(1694-1440\times 2^n)} \times 1560823428673649^{(20\times 2^n - 24)} \times 3122621576798651^{(8\times 2^n - 9)}))}{(220\times 2^n - 219)}$
$ENT_{HM}\left(DOT_H\left(n\right)\right) = log\left(916 \times 2^n - 988\right)$
$-(\frac{1}{916\times 2^n - 988}) \times log((16^{16(2^{n+3}-4)}) \times (25^{25(20\times 2^n - 24)}) \times (36^{36(8\times 2^n - 9)}))$
$ENT_F\left(DOT_H\left(n\right)\right) = \ log(468 \times 2^n - 506) \ - \frac{log(2^{376\times 2^n - 303} \times 13^{260\times 2^n - 312} \times 4690457353031223^{8\times 2^n - 9})}{(468\times 2^n - 506)}$
$ENT_R(DOT_H(n)) = log((\frac{10\sqrt{6}\times 2^n}{3}) - 4\sqrt{6} + (\frac{20}{3} \times 2^n) - 5)$
$+ \frac{(3\times log(2^{1646-1400\times 2^n} \times 390508353708945^{20\times 2^n - 24} \times 3122621576798651^{8\times 2^n - 9}))}{(12\sqrt{6} - 20\times 2^n - 10\sqrt{6}\times 2^n + 15)}$

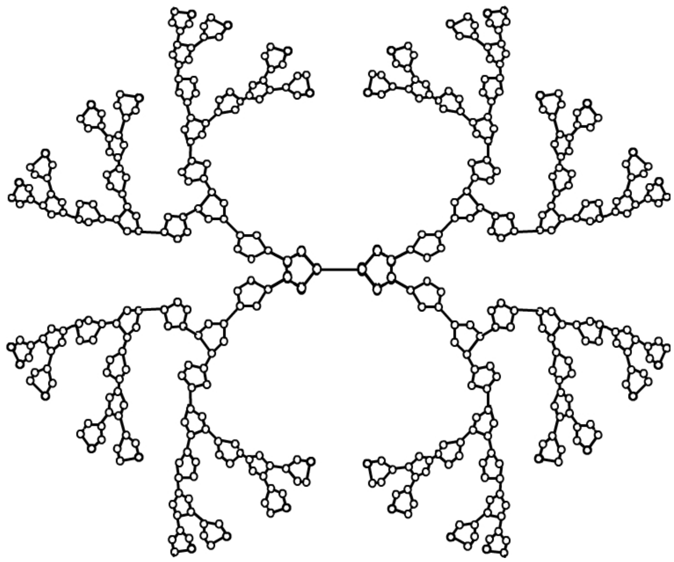

**Fig 3.** Thiophene dendrimer with varying group as H ; $DOT_H(4)$

$$ENT_{RR}(DOT_H(n)) = log(20\sqrt{6}\times 2^n - 24\sqrt{6} + 40\times 2^n - 35) + \frac{log(2^{1120-924\times 2^n}\times 3^{44\times 2^n-51}\times 421041878423467^{20\times 2^n-24})}{(24\sqrt{6}-40\times 2^n-20\sqrt{6}\times 2^n+35)}$$

$$ENT_{SC}(DOT_H(n)) = log\left(4\sqrt{5}\times 2^n - \left(\frac{3\sqrt{6}}{2}\right) - \left(\frac{24\sqrt{5}}{5}\right) + \left(\frac{4\sqrt{6}\times 2^n}{3}\right) + 4\times 2^n - 2\right) - \left(\frac{1}{4\sqrt{5}\times 2^n - \left(\frac{3\sqrt{6}}{2}\right) - \left(\frac{24\sqrt{5}}{5}\right) + \left(\frac{4\sqrt{6}\times 2^n}{3}\right) + 4\times 2^n - 2}\right)\times log\left(\left(\frac{1}{2}\right)^{\frac{\left(2^{n+3}-4\right)}{2}}\times\left(\frac{1}{\sqrt{5}}\right)^{\frac{(20\times 2^n-24)}{\sqrt{5}}}\times\left(\frac{1}{\sqrt{6}}\right)^{\frac{(8\times 2^n-9)}{\sqrt{6}}}\right)$$

$$ENT_{GA}(DOT_{TMS}(n)) = log\left(8\sqrt{6}\times 2^n - \left(\frac{48\sqrt{6}}{5}\right) + 16\times 2^n - 13\right) - \left(\frac{1}{(8\sqrt{6}\times 2^n - (\frac{48\sqrt{6}}{5}) + 16\times 2^n - 13}\right)\times log\left(1^{1(2^{n+3}-4)}\times\left(\frac{2\sqrt{6}}{5}\right)^{\left(\frac{2\sqrt{6}(20\times 2^n-24)}{5}\right)}\times(1)^{(8\times 2^n-9)}\right)$$

$$ENT_{ABC}(DOT_{TMS}(n)) = log\left(14\sqrt{2}\times 2^n - 14\sqrt{2} + \left(\frac{16}{3}\times 2^n\right) - 6\right) - \left(\frac{1}{14\sqrt{2}\times 2^n - 14\sqrt{2} + (\frac{16}{3}\times 2^n) - 6}\right)\times log\left(\left(\frac{1}{\sqrt{2}}\right)^{\frac{(2^{n+3}-4)}{\sqrt{2}}}\times\left(\frac{1}{\sqrt{2}}\right)^{\frac{(20\times 2^n-24)}{\sqrt{2}}}\times\left(\frac{2}{3}\right)^{\left(\frac{2(8\times 2^n-9)}{3}\right)}\right)$$

$$ENT_{irr}(DOT_H(n)) = log(20\times 2^n - 24)$$

$$ENT_{\sigma}(DOT_H(n)) = log(20\times 2^n - 24)$$

Proof. Using Equation 1, Theorem 3 and Table 3 and following the similar pattern used in Theorem 2, we obtain the required degree based entropy measures for oligothiophene-H dendrimer.

## 4 Comparison of Various Degree Measures

A graphical comparison of the degree based descriptors and entropy measures of thiophene dendrimers have been obtained in this section. Figure 4 depicts the comparison graph of oligothiophene-TMS dendrimer and Figure 5 depicts the comparison graph of oligothiophene-H dendrimer. These plots aid the reader in visually interpreting and comprehending the behavior of these descriptors and their corresponding entropies with respect to the parameters involved. This data analysis technique not only benefits in the collection of numerical values, but also relates different chemical attributes, allowing for a better understanding and correlation of the features involved in the study.

## 5 Discussion

Molecular descriptors, which are inextricably linked to the idea of molecular structure, play a critical role in scientific study, serving as the theoretical foundation of a complex network of information. The distinctive characteristics of a compound's physical, chemical and biological properties are determined by its structure. Topological indices are two-

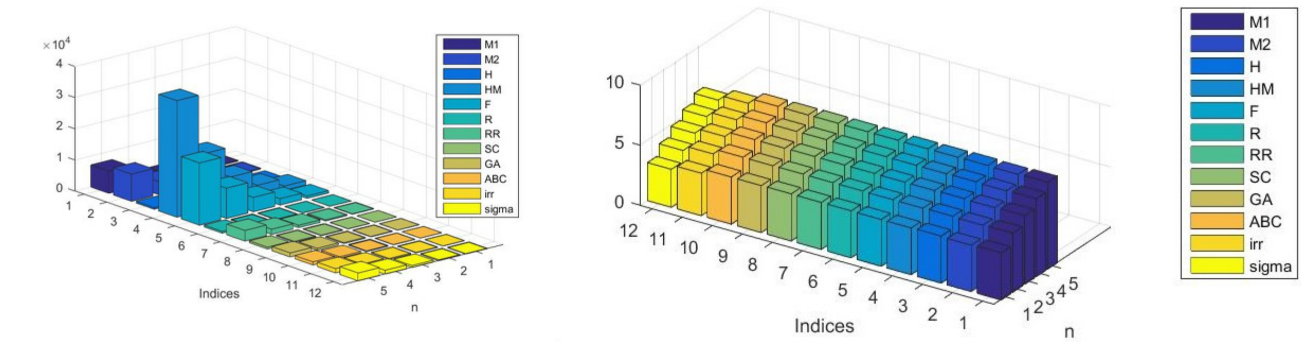


**Fig 4.** Comparison graph of Degree based Entropy measures of oligothiophene-TMS dendrimer

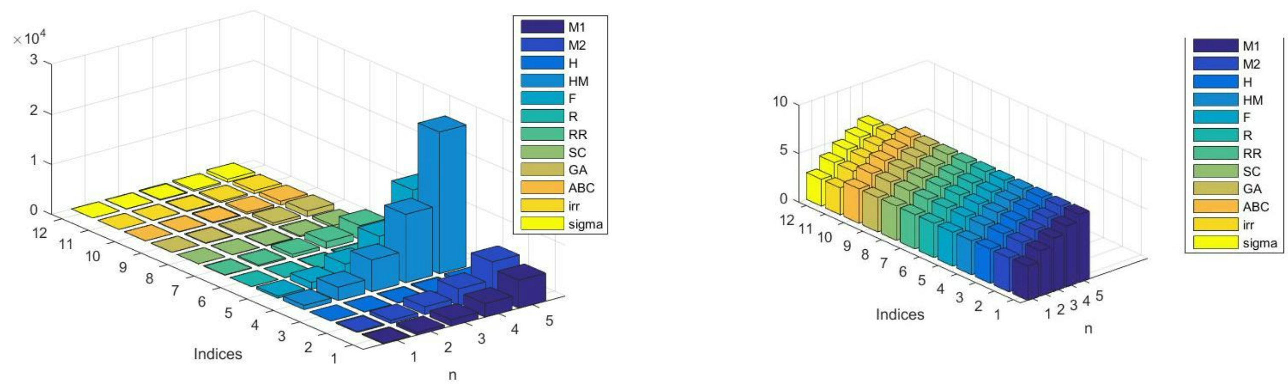


**Fig 5.** Comparison graph of Degree based molecular Indices of oligothiophene-H dendrimer

dimensional descriptors that are obtained from the structural representation of molecules. These descriptors are most usefully applied in QSAR and QSPR analysis. The molecular mechanism of a chemical may be inferred from its structure using a mathematical function called a QSAR model. The main phases in QSAR analysis are model generation, model validation, and its interpretation. Another crucial characteristic of descriptors is their Shannon entropy distribution, since those with larger entropies are predicted to provide more insightful prediction models. A method for evaluating the distribution and information content stored in descriptors is the Shannon entropy. The associated importance of this method is found in the determination of the physical implications of the graph-theoretical descriptors for Quantitative Structure-Property and Structure-Activity relationships in branching tree-like polymers. The Shannon's entropy is also frequently used to evaluate the variety of chemical resources and to analyze the information content of molecular descriptors within data sets of molecules. These descriptors and accompanied entropy measures serve as a gate way for further experimental research work. Future scope of research can be extended in formulating various other attributes including distance based indices, neighborhood degree indices, temperature indices, M-polynomial approach for certain indices, reverse degree based indices and a great variety of descriptors, for the family of thiophene dendrimers.

## 6 Conclusion

We have used Shannon's approach in finding the entropy measures of these thiophene dendrimers from their corresponding degree based molecular indices values. The graphical comparison between various entropy measures and also the indices values of these structures have also been portayed. Since the degree-based entropy has several possibilities in several fields of study, including computer science, chemistry, pharmaceuticals and biological therapies, a significant amount of research has to be carried out for enhancing the topological attributes of various chemical graphs. Accordingly, scientists can benefit from these numerical and graphical interpretation for various analysis of the structure. For a better understanding of the topic, several entropy measures and molecular indices have also been analyzed graphically. The neighborhood degree based indices using m polynomials and corresponding entropies can also be evaluated as a part of further research in this topic. Future study can extend this concept to different chemical structures.

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