Topological Indices of Triphenylene Based Discotic Liquid Crystals

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Abstract

Most of the topological graph indices are the degree based ones. Probably the largest degree based class of graph indices is known as the Zagreb indices. There are several variants of Zagreb indices and they are considered here. In this work, some of those indices for a molecular structure called as the spherulitic crystalline compound are calculated. We also determine those indices for the subdivision graph, which is one of the most important derived graphs, of the spherulitic crystalline compound.

Keywords: Graph, Triphenylene, discotic liquid crystal, Zagreb indices, topological indices

Mathematics Subject Classification: 05C07, 05C30, 05C50

1 Introduction

Graph theory is one of the fastest growing subjects of Mathematics due to its applications in many areas of Mathematics and also in all other sciences. When there are relations beetwen things, we can model this by a graph. The vertices are modelling e.g. atoms, persons, countries, companies, parts of body, neurons in the brain, people in a social network, etc. and edges are modelling the interactions between the things represented by the vertices. Since 1947 when the first application of graphs in Chemistry were given, graphs are intensively used in Chemistry and its related areas such as Pharmacology. One class of such molecular structures is the discotic liquid crystals (DLCs) which are unique nanostructures having remarkable electronic and optoelectronic properties. The history of these fascinating materials goes back to 1977 when Chandrasekhar and

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his colleagues reported that not only rod-like molecules, but also compounds with disc-like molecular shapes are able to form mesophases.

The symmetrically fused aromatic hydrocarbon triphenylene has been known in chemical literature for a long time. This compound was isolated from the pyrolytic products of benzene [5], see Figure 1.

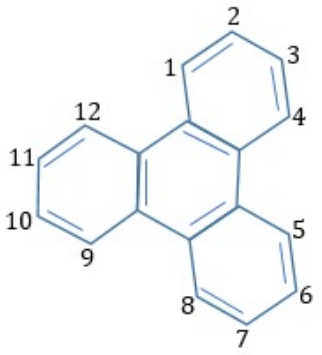

Figure 1: Triphenylene

The potential of triphenylene as a novel core for DLCs was mentioned in [3] and right a few months after the discovery of mesomorphism in disc-shaped molecules. Ever since, triphenylene has attained considerable attention of liquid crystal scientists due to following reasons: its derivatives are thermally and chemically stable, its chemical properties are easily obtainable, they have a variety of mesophases and their one-dimensional charge and energy transfer properties offer an important number of potential applications. For this reason, many scientists tried to obtain varieties of triphenylene-based DLCs [4, 6]. These kind of materials have been extensively studied for their physico-chemical properties such as ferroelectric switching [13], one-dimensional charge migration [2], electroluminescence [23], one-dimensional energy migration [18], alignment and self-assembling behaviour on surfaces [25] and many other properties. Nowadays, we have over 500 discotic liquid crystals based on triphenylene in the literature.

An oligomer is a molecular structure of chemicals that consists of a usually small number of repeating units. When the number of monomers is infinite, the structure is called polymer. A dimer is an oligomer consisting of two monomers joined by bonds that can be either strong or weak, covalent or intermolecular. A liquid crystal dimer (LCD) consists of molecules having two mesogenic groups usually linked by a flexible spacer or sometimes by a rigid structure. The easiest

way to prepare a dimer is by joining both monomers by means of a flexible spacer, the chemistry of triphenylene dimers actually began with a rather complicated molecule where both triphenylene units are connected by a calamitic molecule. The chemical compound in Figure 2 is a spherulitic crystalline compound melting at 167^oC.

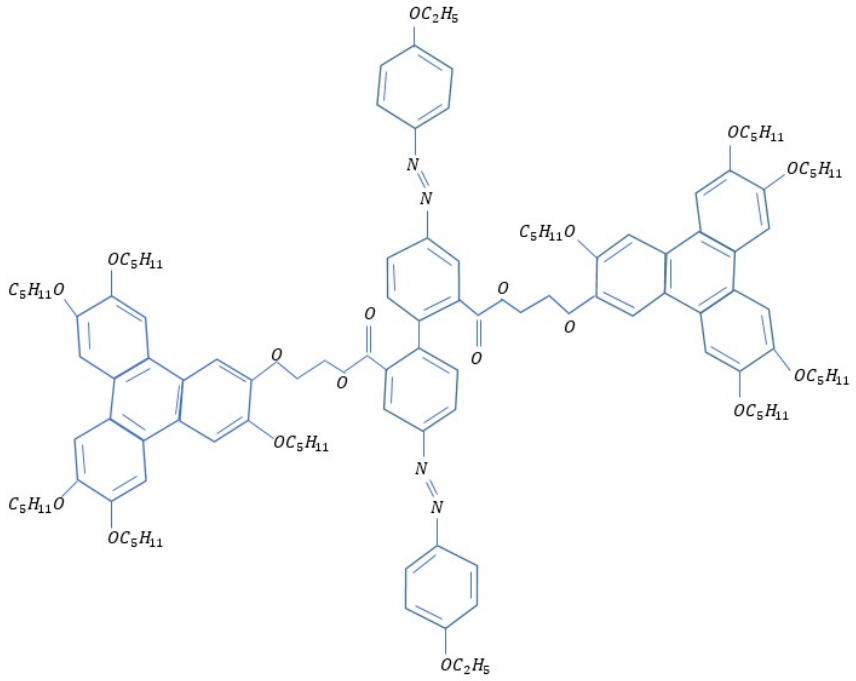

Figure 2: Cr167I

Topological graph indices are defined and used in many areas to study several properties of different objects, mostly atoms and molecules. A large number of topological graph indices have been defined and studied by many chemists and mathematicians as most graphs are generated from molecules by replacing atoms with vertices and chemical bonds with edges. They are defined as topological graph invariants measuring several physical, chemical, biological, pharmacological, pharmaceutical etc. properties of graphs which are modelling real life cases. They can mainly be grouped into three classes according to the way they are defined: by vertex degrees, by matrices or by distances.

Let $G = (V(G), E(G))$ be a simple graph with $\mid V(G) \mid = n$ vertices and $\mid E(G) \mid = m$ edges. That is, there are no loops nor multiple edges. For a vertex $v \in V(G)$, we denote the degree of v by $d_G(v)$ or d_v.

Two of the most important topological graph indices are called the first and second Zagreb indices denoted by $M_1(G)$ and $M_2(G)$, respectively:

$$M_1(G) = \sum_{u \in V(G)} d_G^2(u) \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v). \tag{1.1}$$

They were first defined in 1972 by Gutman and Trinajstic, [12], and are referred to due to their uses in QSAR and QSPR studies. In [8], some results on the first Zagreb index together with some other indices are given. For some graph operations, these indices are calculated in [9].

The total π-electron energy depends on the degree based sums $M_1(G)$ and $F(G) = \sum_{u \in V(G)} d_G^3(u)$. They were first appeared in the study of structure-dependency of total π-electron energy in [12]. The first index was later named as the first Zagreb index and the second sum has never been further studied. The sum $F(G)$ was recently named as the forgotten index or the F-index by Furtula and Gutman, [11]. Sometimes, it is alternatively denoted by $M_3(G)$ and it was shown to have an exceptional applicative potential.

The hyper-Zagreb index was defined as a variety of the classical Zagreb indices as

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

see e.g. [11].

Inspired by the study of heat of formation for heptanes and octanes in [10], Furtula et al. proposed another index called augmented Zagreb index which gives a better prediction power. It is defined by

$$AZI(G) = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v - 2}.$$

The harmonic index defined as below was introduced by Zhong [26] and correlates well with Π-electron energy of benzenoid hydrocarbons

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

Ranjini et al., [20], re-defined the Zagreb indices, i.e. the redefined first, second and third Zagreb indices for a graph G and these are

$$ReZG_1(G) = \sum_{uv \in E(G)} \frac{d_u + d_v}{d_u \cdot d_v},$$

$$ReZG_2(G) = \sum_{uv \in E(G)} \frac{d_u \cdot d_v}{d_u + d_v},$$

$$ReZG_3(G) = \sum_{uv \in E(G)} (d_u \cdot d_v)(d_u + d_v).$$

Milicevic et al., [19], reformulated the Zagreb indices in terms of the edge degrees instead of the vertex-degrees as

$$RM_1(G) = \sum_{uv \in E(G)} d(uv)^2,$$

$$RM_2(G) = \sum_{e,e' \in E(G)} d(e)d(e').$$

Aram and Dehgardi, [1], introduced the concept of reformulated F-index as

$$RF(G) = \sum_{uv \in E(G)} d(uv)^3.$$

Kulli, [16], introduced the first and second K Banhatti indices, intending to take into account the contributions of pairs of incident elements. They are defined as

$$B_1(G) = \sum_{u,e} [d_G(u) + d(e)],$$

$$B_2(G) = \sum_{u,e} d_G(u)d(e).$$

In this paper, we calculate the topological indices of the spherulitic crystalline compound seen in Figure 2 and denote this compound by G^* throughout the paper.

2 Topological indices of the spherulitic crystalline compound

Now we will determine some well-known topological indices of G^*. There is a large number of papers on Zagreb indices, see, e.g. [1, 11, 14, 15, 17, 19, 26].

Theorem 2.1. *The first and second Zagreb indices of G^* are $M_1(G^*) = 1.510$ and $M_2(G^*) = 1.877$.*

Proof. We partition the edges of G^* into edges of the types $E_{(d_u,d_v)}$ where uv is an edge. In G^*, we get the edges of types $E_{(1,3)}, E_{(1,4)}, E_{(2,2)}, E_{(2,3)}, E_{(2,4)}, E_{(3,3)}$,

and $E_{(4,4)}$. The number of edges of these types are 8, 120, 14, 60, 12, 23 and 42, respectively. Recall that $M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)$, therefore we get

$$\begin{aligned} M_1(G^*) &= \mid E_{(1,3)} \mid (1+3) + \mid E_{(1,4)} \mid (1+4) + \mid E_{(2,2)} \mid (2+2) \\ &+ \mid E_{(2,3)} \mid (2+3) + \mid E_{(2,4)} \mid (2+4) + \mid E_{(3,3)} \mid (3+3) + \mid E_{(4,4)} \mid (4+4) \\ &= 2 \cdot 4 + 120 \cdot 5 + 14 \cdot 4 + 60 \cdot 5 + 12 \cdot 6 + 23 \cdot 6 \\ &+ 42 \cdot 8 = 1.510. \end{aligned}$$

As $M_2(G) = \sum_{uv \in E(G)} d_u d_v$, we get the result by similar calculations. □

The two indices studied in the next two theorems have been calculated in [17] for Carbon nanocones.

Theorem 2.2. *The third Zagreb index (forgotten index) of G^* is $F(G^*) = 4.950$.*

Proof. We know that $F(G) = \sum_{u \in V(G)} {d_u}^3$, i.e.,

$$\begin{aligned} F(G^*) &= \sum_{u \in V(C_8H_{11}NO_2)} {d_u}^3 = 1^3 \cdot 2 + 2^3 \cdot 38 + 3^3 \cdot 36 + 10[4^3 \cdot 5 + 2^3 + 1^3 \cdot 11] \\ &+ 2[4^3 \cdot 2 + 2^3 + 1^3 \cdot 5] = 4.950 \end{aligned}$$

as required. □

Theorem 2.3. *The hyper-Zagreb index of G^* is $HM(G^*) = 8.704$.*

Proof. We know that $HM(G) = \sum_{uv \in E(G)} (d_u + d_v)^2$, *i.e.*,

$$\begin{aligned} HM(G^*) &= \mid E_{(1,3)} \mid (1+3)^2 + \mid E_{(1,4)} \mid (1+4)^2 + \mid E_{(2,2)} \mid (2+2)^2 \\ &+ \mid E_{(2,3)} \mid (2+3)^2 + \mid E_{(2,4)} \mid (2+4)^2 + \mid E_{(3,3)} \mid (3+3)^2 \\ &+ \mid E_{(4,4)} \mid (4+4)^2 \\ &= 2(1+3)^2 + 120(1+4)^2 + 14(2+2)^2 + 60(2+3)^2 \\ &+ 12(2+4)^2 + 23(3+3)^2 + 42(4+4)^2 \\ &= 8.704 \end{aligned}$$

giving us the result. □

Theorem 2.4. *The augmented Zagreb index of G^* is $AZI(G^*) = 2037,623$.*

Proof. We know that $AZI(G) = \sum_{uv \in E(G)} (\frac{d_u \cdot d_v}{d_u + d_v - 2})^3$, i.e.,

$$\begin{aligned} AZI(G) &= \mid E_{(1,3)} \mid (\frac{1 \cdot 3}{1+3-2})^3 + \mid E_{(1,4)} \mid (\frac{1 \cdot 4}{1+4-2})^3 + \mid E_{(2,2)} \mid (\frac{2 \cdot 2}{2+2-2})^3 \\ &+ \mid E_{(2,3)} \mid (\frac{2 \cdot 3}{2+3-2})^3 + \mid E_{(2,4)} \mid (\frac{2 \cdot 4}{2+4-2})^3 \\ &+ \mid E_{(3,3)} \mid (\frac{3 \cdot 3}{3+3-2})^3 + \mid E_{(4,4)} \mid (\frac{4 \cdot 4}{4+4-2})^3 \\ &= 2(\frac{3}{2})^3 + 120(\frac{4}{3})^3 + 14 \cdot 2^3 + 60 \cdot 2^3 + 12 \cdot 2^3 + 23(\frac{9}{4})^3 + 42(\frac{8}{3})^3 \\ &= 2.037,623. \end{aligned}$$

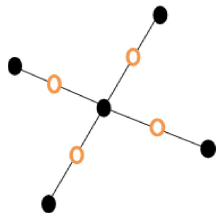

Figure 3: The subdivision graph $S(S_4)$

□

The following indices can be proved in a similar enumerative methods:

Theorem 2.5. *The harmonic index of* G^* *is* $H(G^*) = 102.163$.

Theorem 2.6. *The re-defined versions of Zagreb indices of* G^* *are* $ReZG_1(G^*) = 262$, $ReZG_2(G^*) = 318$ *and* $ReZG_3(G^*) = 11.186$.

Theorem 2.7. *The reformulated Zagreb indices of* G^* *are* $RM_1(G^*) = 3.780$ *and* $RM_2(G^*) = 7.074$.

Theorem 2.8. *The reformulated F-index of* G^* *are* $RF(G^*) = 16.300$.

Theorem 2.9. *The Banhatti indices of* G^* *are* $B_1(G^*) = 2.838$ *and* $B_2(G^*) = 4.244$.

3 Topological indices of the subdivision graph of the spherulitic crystalline compound

The subdivision graph (or sometimes called as subgraph) $S(G)$ of a simple graph G is defined as the new graph obtained by adding an extra vertex into each edge of G. Equivalently, $S(G)$ is obtained by replacing each edge of the graph by a path of length 2. See e.g. Figure 3. The subdivision graphs have been studied in literature, see e.g. [14], [21], [22] and [24].

The main reason to study the subdivision graphs is that, by means of topological indices, it makes combinatorically possible to calculate several properties of large graphs having some symmetry as most subdivision graphs have symmetrical shapes, in terms of a smaller graph G. Another reason is that we can obtain classified information about a series of graphs from a parent graph and calculate several properties which are usually in terms of topological indices.

In Molecular Chemistry, several chemical operations result in molecular graphs which are subdivision graphs of some other molecular graphs of some chemical

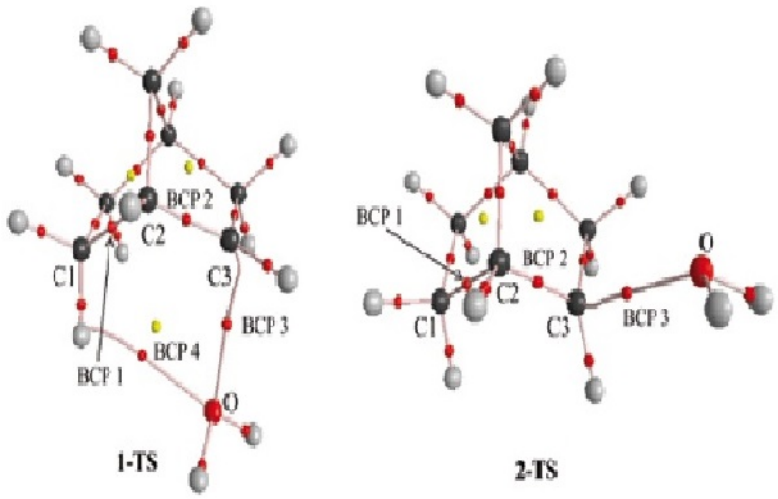

Figure 4: Molecular graphs of the transition state of solvolysis of 2-endo- and 2-exo-norbornanols

compounds. In Figure 4, an example to this situation is given, [7]. It shows the molecular graph of the transition state of the first step of the nucleophilically unassisted solvolysis of protonated 2-endo- and 2-exo-norbornanol. There are three critical points: nuclear attractor critical point, bond critical point and ring critical point.

The next result gives the topological indices of spherulitic crystalline compound:

Theorem 3.1. *Let $S(G^*)$ be the subdivision graph of G^*. Then several topological graph indices of it are as below:*

(i) $M_1(S(G^*)) = 2.626$ *and* $M_2(S(G^*)) = 3.068$
(ii) $F(S(G^*)) = 7.182$
(iii) $HM(S(G^*)) = 13.378$
(iv) $AZI(S(G^*)) = 4.464$
(v) $H(S(G^*)) = 252,9333\cdots$
(vi) $ReZG_1(S(G^*)) = 549$, $ReZG_2(S(G^*)) = 610,133\cdots$ *and* $ReZG_3(S(G^*)) = 33.436$
(vii) $RM_1(S(G^*)) = 3780$
(viii) $RF(S(G^*)) = 16.348$.

Proof. Note that all edges of the subdivision graph are of type $(2, k)$ for some positive integer k. The edge partition of $S(G^*)$ is given in the following table:

(r,s)-edges	their number
$(2,1)$-edges	128
$(2,2)$-edges	100
$(2,3)$-edges	114
$(2,4)$-edges	216

Hence the above indices can be obtained as in Section 2. □

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