Degree Based Topological Indices of Polysiloxanes

Muge TOGAN, Aysun YURTTAS GUNES, Musa DEMIRCI
Ismail Naci CANGUL*,
Bursa Uludag University, Faculty of Arts & Science,
Mathematics Department, Gorukle-Bursa 16059 Turkey

Abstract

Molecules can be modelled by graphs to obtain their required properties by means of only mathematical methods and formulae. In this paper, we consider several degree based topological graph indices of a chemical molecule called polysiloxanes.

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1 Introduction

The term polysiloxane refers to a class of compounds whose molecules consist of a silicon-oxygen backbone $(-Si-O-Si-O-Si-O-Si-)n$ arranged either in a linear or cyclic (ring) pattern. Each silicon in the chain has two additional oxygen atoms attached to it. In many cases, the polysiloxanes also have one or more alkyl groups attached to the main chain replacing one or more of the oxygens. An alkyl group is an alkane, a saturated hydrocarbon, lacking one hydrogen atom. Examples of alkyl groups are the methyl $(-CH3-)$ and ethyl $(-CH2CH3-)$ groups. Its chemical formula is $(R2SiO)n$, where R is usually methylsiloxanes $(-CH3-)$, although it can be H or an alkyl or aryl group. In a common type of siloxane, all the oxygens that are not a part of the backbone of the chain are replaced by methyl groups.

Polysiloxane has shown greater resistance to the effects of UV radiation than organic polymers containing a carbon-carbon backbone. Polysiloxanes can be oils, greases, rubbers or plastics depending on molecular weight. Polysiloxanes exhibit superb abrasion and corrosion resistance, anti-graffiti properties, strong chemical resistance and resilience to dirt pickup. Some useful properties of polysiloxanes include flexibility, resistance to water and oxidation, chemical inertness, permeability to gases, low glass transition temperature and low surface energy. These properties make polysiloxanes suitable for a wide range

*Corresponding Author

of commercial applications, such as electrical insulation, electronical coatings, household sealants for cooking apparatus, automobile gaskets, airplane seals, textiles or paper coatings and lubricating greases, [12].

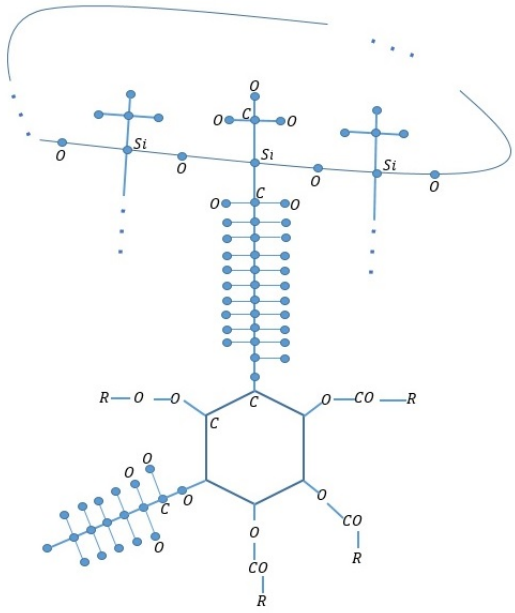

Figure 1: Polysiloxanes

Graph indices are used in different ways to study several properties of chemical substances. They are defined as topological graph invariants measuring several properties of graphs that are modeling real life cases. They can be classified to three groups according to the way they are defined: by vertex degrees, by matrices or by distances, see e.g. [1, 2]. The first and second Zagreb indices $M_1(G)$ and $M_2(G)$ are defined by Gutman and Trinajstic, [9], by $M_1(G) = \sum_{u \in V(G)} d_G^2(u)$ and $M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v)$, respectively, and become popular due to their uses in QSAR and QSPR studies. In [4], some results on the first Zagreb index together with some other indices are given and these indices are calculated for some graph operations in [5].

The forgotten index of a graph G denoted by $F(G)$ or $M_3(G)$ was defined by $F(G) = \sum_{u \in V(G)} d_G^3(u)$, see [7, 8]. The hyper-Zagreb index is defined as a variant of the Zagreb indices as $HM(G) = \sum\limits_{uv \in E} (d_u + d_v)^2$, see e.g. [7].

Inspired by the study of heat of formation for some alkanes, Furtula et al. proposed an index called Augmented Zagreb index, which gives a better prediction power in [6]. It is defined by $AZI(G) = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v - 2}$. The Harmonic index was introduced by Zhong [16], who found that it correlates

well with Π-electron energy of benzenoid hydrocarbons and it was defined by $H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}$. Ranjini et al., [13], defined the redefined first, second and third Zagreb indices for a graph G as $ReZG_1(G) = \sum_{uv \in E(G)} \frac{d_u + d_v}{d_u \cdot d_v}$, $ReZG_2(G) = \sum_{uv \in E(G)} \frac{d_u \cdot d_v}{d_u + d_v}$ and $ReZG_3(G) = \sum_{uv \in E(G)} (d_u \cdot d_v)(d_u + d_v)$. Milicevic et al., [11], reformulated the Zagreb indices in terms of the edge degrees instead of the vertex-degrees as $RM_1(G) = \sum_{uv \in E(G)} d(e)^2$, $RM_2(G) = \sum_{e,e' \in E(G)} d(e)d(e')$ where e, e' are pairs of incident edges of the graph G. Aram and Dehgardi, [3], introduced the concept of reformulated F-index as $RF(G) = \sum_{uv \in E(G)} d(uv)^3$. Kulli, [10], introduced the first and second K Banhatti indices, intending to take into account the contributions of pairs of incident elements. They are defined as $B_1(G) = \sum_{u,e} [d_G(u) + d(e)]$, $B_2(G) = \sum_{u,e} d_G(u)d(e)$.

2 Main Results

Now we will determine some well-known topological indices of polysiloxanes.

Lemma 1 *The first and second Zagreb indices of G^* are $M_1(G^*) = 812n$ and $M_2(G^*) = 1040n$.*

Proof. We partition the edges of G^* into edges of type $E_{(d_u, d_v)}$ where uv is an edge. In G^*, we get the edges of type $E_{(1,3)}, E_{(1,4)}, E_{(2,3)}, E_{(2,4)}, E_{(3,3)}, E_{(3,4)}$ and $E_{(4,4)}$. The number of edges of these types for one unit are 6, 78, 12, 2, 6, 6 and 31, respectively. First, we calculate $M_1(G)$ for one unit:

$$\begin{aligned} M_1(G^*) &= \mid E_{(1,3)} \mid (1+3) + \mid E_{(1,4)} \mid (1+4) + \mid E_{(2,3)} \mid (2+3) \\ &+ \mid E_{(2,4)} \mid (2+4) + \mid E_{(3,3)} \mid (3+3) \\ &+ \mid E_{(3,4)} \mid (3+4) + \mid E_{(4,4)} \mid (4+4) = 812. \end{aligned}$$

For n units, we get the result as $M_1(G^*) = 812n$. As $M_2(G) = \sum_{uv \in E(G)} d_u d_v$, we get the result by similar calculations. ■

Lemma 2 *The third Zagreb index (forgotten index) of G^* is $F(G^*) = 2832n$.*

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

$$F(G^*) = \sum_{u \in V} {d_u}^3 = 1^3 \cdot 84 + 2^3 \cdot 7 + 3^3 \cdot 12 + 4^3 \cdot 37 = 2832.$$

For n units, we have $F(G^*) = 2832n$. ■

Using the same counting method, we can prove the following results:

Lemma 3 *The hyper Zagreb index of G^* is $HM(G^*) = 4912n$.*

Lemma 4 *The Augmented Zagreb index of G^* is $AZI(G^*) = 1056,27 \cdot n$.*

Lemma 5 *The harmonic index of G^* is $H(G^*) = 51,13 \cdot n$.*

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

$$\begin{aligned} H(G^*) &= \mid E_{(1,3)} \mid \frac{2}{1+3} + \mid E_{(1,4)} \mid \frac{2}{1+4} + \mid E_{(2,3)} \mid \frac{2}{2+3} \\ &+ \mid E_{(2,4)} \mid \frac{2}{2+4} + \mid E_{(3,3)} \mid \frac{2}{3+3} + \mid E_{(3,4)} \mid \frac{2}{3+4} + \mid E_{(4,4)} \mid \frac{2}{4+4} \\ &= 6 \cdot \frac{1}{2} + 78 \cdot \frac{2}{5} + 12 \cdot \frac{2}{5} + 2 \cdot \frac{1}{3} + 6 \cdot \frac{1}{3} + 6 \cdot \frac{2}{7} + 31 \cdot \frac{1}{4} = 51,13. \end{aligned}$$

■ The following can be deduced similarly:

Lemma 6 *The re-defined versions of the Zagreb indices of G^* are $ReZG_1(G) = 140n$, $ReZG_2(G) = 165,25 \cdot n$, $ReZG_3(G) = 6884n$.*

Lemma 7 *The reformulated Zagreb indices of G^* are $RM_1(G^*) = 2228n$ and $RM_2(G^*) = 3022n$.*

Lemma 8 *The reformulated F-index of G^* is $RF(G^*) = 9836n$.*

Proof. As $RF(G) = \sum_{uv \in E(G)} d(uv)^3$, the calculations are similar to $RM_1(G^*)$. ■

Lemma 9 *The Banhatti indices of G^* are $B_1(G^*) = 1872n$ and $B_2(G^*) = 3288n$.*

Proof. We know that $B_1(G) = \sum_{u,e} d_G(u) + d(e)$, i.e.,

$$\begin{aligned} B_1(G^*) &= 6[(1+2)+(2+3)] + 78[(4+3)+(1+3)] + 12[(2+3)+(3+3)] \\ &+ 6[(3+4)+(3+4)] + 2[(4+4)+(2+4)] + 6[(4+5)+(3+5)] \\ &+ 31[(6+4)+(6+4)] = 1872. \end{aligned}$$

For n units, we obtain $B_1(G^*) = 1872n$. For B_2, a similar proof applies. ■

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Muge TOGAN, Aysun YURTTAS GUNES, Musa DEMIRCI, Ismail Naci CANGUL
capkinm@uludag.edu.tr, ayurttas@uludag.edu.tr, mdemirci@uludag.edu.tr, cangul@uludag.edu.tr