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Some Topological Measures for Nicotine

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Abstract

A topological index is a quantity expressed as a number that help us to catch symmetry of chemical compounds. With the help of quantitative structure property relationship (QSPR), we can guess physical and chemical properties of several chemical compounds. Here, we will compute Shingali & Kanabour, Gourava and hype Gourava indices for the chemical compound Nicotine.

1 Introduction

Mathematical chemistry is a branch of mathematics in which tools of mathematics are use to solve the problems arising in chemistry [1]. In chemical graph theory, we discuss the chemical compounds in mathematical language. A graph having no loop or multiple edge in known as simple graph [2]. A molecular graph is a simple connected graph in which atoms and bounds are represented by vertex and edge set respectively [3]. The degree of vertex is the number of edges fall on that vertex. The first topological index was presented by Winer [4] in 1947, when was trying to find out the boiling point of alkane.

$$W(G) = \sum_{(u,v)\subseteq V(G)} d_G(u,v).$$

Gutman in 1975, [5] introduced the Zagreb indices. The first and second Zagreb indices are among the oldest molecular structure descriptors. A special number, in graph theoretical term, representing a molecular structure, is known as topological descriptor. A topological descriptor when correlates with a molecular property, it can be determine as graph-theoretic index or topological index. The First and

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second Zagreb indices are the oldest molecular descriptors invented in 1975 by Gutman [5] and their properties are extensively investigated. They are defined as:

$$M_1(G) = \sum_{uv\in E(G)} (d_u + d_v).$$

$$M_2(G) = \sum_{uv\in E(G)} (d_u \times d_v).$$

Shingali & Kanabour in [6] introduce the following topological indices,

$$\chi(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}}$$

$$R'(G) = \sum_{uv\in E(G)} \frac{1}{max\{d_u, d_v\}}$$

$$AG_1(G) = \sum_{uv\in E(G)} \frac{d_u + d_v}{2\sqrt{d_u \times d_v}}$$

$$SK(G) = \sum_{uv\in E(G)} \frac{d_2 + d_v}{2}$$

$$SK_1(G) = \sum_{uv\in E(G)} \frac{d_2 \times d_v}{2}$$

$$SK_2(G) = \sum_{uv\in E(G)} \left(\frac{d_2 + d_v}{2}\right)^2.$$

In 2017, Kulli [7] introduce the the idea of Gourava indices as,

$$GO_1(G) = \sum_{uv\epsilon E(G)} [(d_u + d_v) + (d_u \times d_v)]$$

$$GO_1(G) = \sum_{uv\epsilon E(G)} [(d_u + d_v) \times (d_u \times d_v)].$$

In [8] Kulli introduce the idea of hyper Gourava indices as,

$$HGO_1(G) = \sum_{uv\epsilon E(G)} [(d_u + d_v) + (d_u \times d_v)]^2$$

$$HGO_1(G) = \sum_{uv\epsilon E(G)} [(d_u + d_v) \times (d_u \times d_v)]^2.$$

For more about topological invariants one can find out detail [9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21].

2 Shingali & Kanabour, Gourava and Hyper Gourava Indices for Nicotine

Nicotine is a chemical compound, which is made by a few sorts of plants, including the tobacco plant. Nicotine has a many curative uses. There's developing proof that it might be valuable in treating Parkinson's disease [22, 23, 24]. The chemical structure of Nicotine is given in Figure 1, having chemical formula $C_{10}H_{14}N_2$. Figure 2 shows the molecular graph of Nicotine.

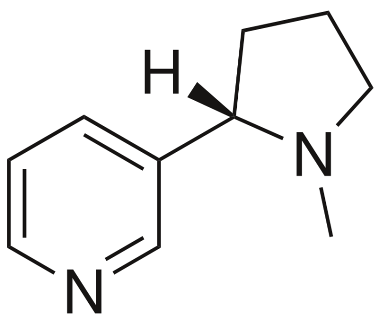

Figure 1: Graph of Nicotine.

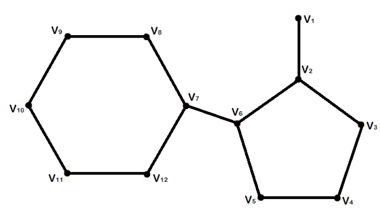

Figure 2: Molecular graph of Nicotine.

It can be observe from molecular graph of Nicotine that there are four type of edges are present in the molecular graph of Nicotine. The degree based edge partition and reverse edge partition is given in Table 1.

Table 1: Partition of $E(Nicotine)$.

(d_u, d_v)	Frequency
(1,3)	1
(2,2)	6
(2,3)	4
(3,3)	2

Theorem 2.1. *Let G be the graph of Nicotine. The Shingali & Kanabour indices for Nicotine are*

1. $\chi(G) = 6.1053.$
2. $R'(G) = 5.3333.$
3. $AG_1(G) = 31.0621.$
4. $SK(G) = 30.$
5. $SK_1(G) = 34.5.$
6. $SK_2(G) = 71.$

Proof.

$$
\begin{aligned}
1.\ \chi(G) &= \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}} \\
&= \left(\frac{1}{\sqrt{1+3}}\right)(1) + \left(\frac{1}{\sqrt{2+2}}\right)(6) \\
&\quad + \left(\frac{1}{\sqrt{2+3}}\right)(4) + \left(\frac{1}{\sqrt{3+3}}\right)(2) \\
&= 6.1053.
\end{aligned}
$$

2. $$\begin{aligned} R'(G) &= \sum_{uv\in E(G)} \frac{1}{max\{d_u, d_v\}} \\ &= \left(\frac{1}{3}\right)(1) + \left(\frac{1}{2}\right)(6) \\ &\quad + \left(\frac{1}{3}\right)(4) + \left(\frac{1}{3}\right)(2) \\ &= 5.3333. \end{aligned}$$

3. $$\begin{aligned} AG_1(G) &= \sum_{uv\in E(G)} \frac{d_u + d_v}{2\sqrt{d_u \times d_v}} \\ &= \left(\frac{1+3}{2\sqrt{1\times 3}}\right)(5) + \left(\frac{2+2}{2\sqrt{2\times 2}}\right)(9) \\ &\quad + \left(\frac{2+3}{2\sqrt{2\times 3}}\right)(14) + \left(\frac{3+3}{2\sqrt{3\times 3}}\right)(6) \\ &= 31.0621. \end{aligned}$$

4. $$\begin{aligned} SK(G) &= \sum_{uv\in E(G)} \frac{d_u + d_v}{2} \\ &= \left(\frac{1+3}{2}\right)(1) + \left(\frac{2+2}{2}\right)(6) \\ &\quad + \left(\frac{2+3}{2}\right)(4) + \left(\frac{3+3}{2}\right)(2) \\ &= 30. \end{aligned}$$

5. $$\begin{aligned} SK_1(G) &= \sum_{uv\in E(G} \frac{d_u \times d_v}{2} \\ &= \left(\frac{1\times 3}{2}\right)(1) + \left(\frac{2\times 2}{2}\right)(6) \\ &\quad + \left(\frac{2\times 3}{2}\right)(4) + \left(\frac{3\times 3}{2}\right)(2) \\ &= 34.5. \end{aligned}$$

$$6.\ SK_2(G) = \sum_{uv\in E(G)} \left(\frac{d_u+d_v}{2}\right)^2$$
$$= \left(\frac{1+3}{2}\right)^2(1) + \left(\frac{2+2}{2}\right)^2(6) + \left(\frac{2+3}{2}\right)^2(4) + \left(\frac{3+3}{2}\right)^2(2)$$
$$= 71.$$

□

Theorem 2.2. *Let G be the graph of Nicotine. Then the Gourava indices for Nicotine are*

1. $GO_1(G) = 129.$
2. $GO_2(G) = 336.$

Proof.

$$1.\ GO_1(G) = \sum_{uv\epsilon E(G)} [(d_u+d_v)+(d_u\times d_v)]$$
$$= [(1+3)+(1\times 3)](1) + [(2+2)+(2\times 2)](6) + [(2+3)+(2\times 3)](4) + [(3+3)+(3\times 3)](2)$$
$$= 129.$$

$$2.\ GO_2(G) = \sum_{uv\in E(G)} [(d_u+d_v)\times(d_u\times d_v)]$$
$$= [(1+3)\times(1\times 3)](1) + [(2+2)\times(2\times 2)](6) + [(2+3)\times(2\times 3)](4) + [(3+3)\times(3\times 3)](2)$$
$$= 336.$$

□

Theorem 2.3. *Let G be the graph of Nicotine. Then the hyper Gourava indices for Nicotine are*

1. $HGO_1(G) = 1367$.

2. $HGO_2(G) = 11112$.

Proof.

$$
\begin{aligned}
1.\ HGO_1(G) &= \sum_{uv\in E(G)} [(d_u + d_v) + (d_u \times d_v)]^2 \\
&= [(1+3) + (1\times 3)]^2(1) + [(2+2) + (2\times 2)]^2(6) \\
&\quad [(2+3) + (2\times 3)]^2(4) + [(3+3) + (3\times 3)]^2(2) \\
&= 1367.
\end{aligned}
$$

$$
\begin{aligned}
2.\ HGO_2(G) &= \sum_{uv\in E(G)} [(d_u + d_v) \times (d_u \times d_v)]^2 \\
&= [(1+3) \times (1\times 3)]^2(1) + [(2+2) \times (2\times 2)]^2(6) \\
&\quad [(2+3) \times (2\times 3)]^2(4) + [(3+3) \times (3\times 3)]^2(2) \\
&= 11112.
\end{aligned}
$$

□

Conclusion

In this article, we computed results for chemical compound Nicotine. We compute Shingali & Kanabour, Gourava and hyper Gourava indices for Nicotine. Our results can help to guess many physical and chemical properties of Nicotine. It is demonstrated certainty that topological indices help to anticipate numerous properties without setting off to the wet lab.

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