TOPOLOGICAL INDICES OF CAFFEINE

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Abstract: Graph theory has provided chemists with a variety of useful tools, such as topological indices. A topological index Top(G) of a graph G is a number with the property that for every graph H isomorphic to G, Top(H) = Top(G). In this paper, we compute ABC index, ABC_4 index, Randic index, Sum connectivity index, GA index, GA_5 index, First Zagreb index, Second Zagreb index, First Multiple Zagreb index, Second Multiple Zagreb index, Augmented Zagreb index, Harmonic index and Hyper Zagreb index, First Zagreb polynomials, Second Zagreb polynomials, Third Zagreb polynomials, Forgotten topological index, Forgotten polynomials and Symmetric division index of Caffeine.

Keywords: ABC index, ABC_4 index, Randic connectivity index, Sum connectivity index, GA index , GA_5 index, First Zagreb index, Second Zagreb index, First Multiple Zagreb index, Second Multiple Zagreb index, Augmented Zagreb index, Harmonic index, Hyper Zagreb index, First Zagreb polynomials, Second Zagreb polynomials, Third Zagreb polynomials, Forgotten topological index, Forgotten polynomials, Symmetric division index and Caffeine.

I. INTRODUCTION

Caffeine is a chemical found in coffee, tea, cola, guarana, mate and other products. Caffeine is most commonly used to improve mental alertness, but it has many other uses. It is a central nervous system stimulant of the metylxanthine class. It is the world's most widely consumed psychoactive drug. its molecular formula is $C_8H_{10}N_4O_2$. Its structure is shown in following figure -1.

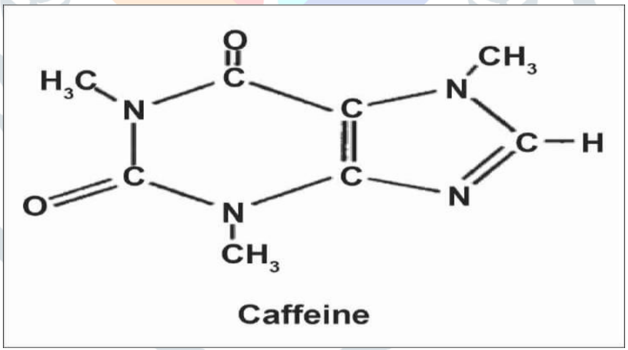

Figure1

Topological indices are the molecular descriptors that describe the structures of chemical compounds and they help us to predict certain physic-chemical properties like boiling point, enthalpy of vaporization, stability, etc. Molecules and molecular compounds are often modeled by molecular graph. A molecular graph is a representation of the structural formula of a chemical compound in terms of graph theory, whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. Note that hydrogen atoms are often omitted. All molecular graphs considered in this paper are finite, connected, loop less and without multiple edges. Let G = (V, E) be a graph with vertex set V and edge set E. The degree of a vertex u∊E(G) is denoted by d_u and is the number of vertices that are adjacent to u. The edge connecting the vertices u and v is denoted by uv.

The Atom-bond connectivity index, ABC index is one of the degree based molecular descriptor, which was introduced by Estrada et al. [7] in late 1990's and it can be used for modeling thermodynamic properties of organic chemical compounds, it is also used as a tool for explaining the stability of branched alkanes [8].
Some upper bounds for the atom-bond connectivity index of graphs can be found in [3]. The atom-bond connectivity index of chemical bicyclic graphs, connected graphs can be seen in [4, 30]. For further results on ABC index of trees see the papers [11, 21, 29, 31] and the references cited there in.

Definition.1.1. Let G = (V, E) be a molecular graph and d_u is the degree of the vertex u, then ABC index of G is defined as,

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

The fourth atom bond connectivity index, ABC_4 (G) index was introduced by M.Ghorbani et al. [15] in 2010. Further studies on ABC_4(G) index can be found in [9, 10].

Definition.1.2. Let G be a graph, then its fourth ABC index is defined as,

$$ABC_4(G) = \sum_{uv\in E(G)} \sqrt{\frac{s_u + s_v - 2}{s_u s_v}}.$$

Where S_u is sum of degrees of all neighbors of vertex u in G. In other words $s_u = \sum_{uv\in E(G)} d_v$, similarly S_V.

The first and oldest degree based topological index is Randic index [23] denoted by χ(G) and was introduced by Milan Randic in 1975. It provides a quantitative assessment of branching of molecules.

Definition.1.3. For the graph G Randic index is defined as,

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

Sum connectivity index belongs to a family of Randic like indices and it was introduced by Zhou and N. Trinajstic [33]. Further studies on Sum connectivity index can be found in [34, 35].

Definition.1.4. For a simple connected graph G, its sum connectivity index S(G) is defined as,

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

The Geometric-arithmetic index, GA(G) index of a graph G was introduced by D. Vukicevi'c et.al [27]. Further studies on GA index can be found in [2, 5, 32].

Definition.1.5. Let G be a graph and e = uv be an edge of G then.

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

The fifth Geometric-arithmetic index, GA_5(G) was introduced by A.Graovac et al [16] in 2011.

Definition.1.6. For a Graph G, the fifth Geometric-arithmetic index is defined as,

$$GA_5(G) = \sum_{uv\in E(G)} \frac{2\sqrt{s_u s_v}}{s_u + s_v}.$$

Where S_u is the sum of the degrees of all neighbors of the vertex u in G, similarly S_v.

A pair of molecular descriptors (or topological index), known as the First Zagreb index Z_1(G) and Second Zagreb index Z_2(G), first appeared in the topological formula for the total π-energy of conjugated molecules that has been derived in 1972 by I. Gutman and N.Trinajsti'c [17]. Soon after these indices have been used as branching indices. Later the Zagreb indices found applications in QSPR and QSAR studies. Zagreb indices are included in a number of programs used for the routine computation of topological indices POLLY, DRAGON, CERIUS, TAM, DISSI. Z_1(G) and Z_2(G) were recognize as measures of the branching of the carbon atom molecular skeleton [20], and since then these are frequently used for structure property modeling. Details on the chemical applications of the two Zagreb indices can be found in the books [25, 26]. Further studies on Zagreb indices can be found in [1, 18, 33, 34, 35].

Definition.1.7. For a simple connected graph G, the first and second Zagreb indices were defined as follows,

$$Z_1(G) = \sum_{e=uv\in E(G)} (d_u + d_v).$$

$$Z_2(G) = \sum_{e=uv\in E(G)} (d_u d_v).$$

Where d_v denotes the degree (number of first neighbors) of vertex v in G.

In 2012, M. Ghorbani and N. Azimi [14] defined the Multiple Zagreb topological indices of a graph G, based on degree of vertices of G.

Definition.1.8. For a simple connected graph G, the first and second multiple Zagreb indices were defined as follows

$$PM_1(G) = \prod_{e=uv\in E(G)} (d_u + d_v).$$

$$PM_2(G) = \prod_{e=uv\in E(G)} (d_u d_v).$$

Properties of the first and second Multiple Zagreb indices may be found in [6, 19].

The Augmented Zagreb index was introduced by Furtula et al [12]. This graph invariant has proven to be a valuable predictive index in the study of the heat of formation in octanes and heptanes, is a novel topological index in chemical graph theory, whose prediction power is better than atom-bond connectivity index. Some basic investigation implied that AZI index has better correlation properties and structural sensitivity among the very well established degree based topological indices.

Definition.1.9. Let G = (V, E) be a graph and du be the degree of a vertex u, then augmented Zagreb index is denoted by AZI(G) and is defined as,

$$AZI(G) = \sum_{uv\in E} \left[\frac{d_u d_v}{d_u + d_v - 2}\right]^3.$$

Further studies can be found in [22] and the references cited there in.

The Harmonic index was introduced by Zhong [36]. It has been found that the harmonic index correlates well with the Randic index and with the π-electron energy of benzenoid hydrocarbons.

Definition.1.10. Let G = (V, E) be a graph and du be the degree of a vertex u then Harmonic index is defined as,

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

Further studies on H (G) can be found in [28, 34].
G.H. Shirdel et.al [24] introduced a new distance-based of Zagreb indices of a graph G named Hyper-Zagreb Index.

Definition.1.11. The hyper Zagreb index is defined as,

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

Fath-Tabar [37] introduced the Third Zagreb index in 2011. Which is defined by.

Definition.1.12. For a simple connected graph G, the third Zagreb index is defined as,

$$ZG_3(G) = \sum_{e=uv\in E(G)} |d_u - d_v|.$$

Again in 2011Fath-Tabar [37] introduced the First, Second and Third Zagreb Polynomials which is defined by,

Definition.1.13. The First, Second and Third Zagreb Polynomials for a simple connected graph G is defined as,

$$ZG_1(G,x) = \sum_{e=uv\in E(G)} x^{d_u+d_v}.$$

$$ZG_2(G,x) = \sum_{e=uv\in E(G)} x^{d_u d_v}.$$

$$ZG_3(G,x) = \sum_{e=uv\in E(G)} x^{|d_u-d_v|}.$$

Definition.1.14. The forgotten topological index is also a degree based topological index, denoted by F(G) for simple graph G .It was encountered in [13], defined as,

$$F(G) = \sum_{e=uv\in E(G)} [(d_u)^2 + (d_v)^2]$$

Definition.1.15.The forgotten topological polynomials for a graph G defined as,

$$F(G,x) = \sum_{e=uv\in E(G)} x^{[(d_u)^2+(d_v)^2]}$$

Definition.1.16. There are some new degrees based graph invariants, which plays an important role in chemical graph theory. These topological indices are quite useful for determining total surface area and heat formation of some chemical compounds. These graphs invariants are as follow Symmetric division index,

$$SDD(G) = \sum_{e=uv} \left\{\frac{min(d_u,d_v)}{max(d_u,d_v)} + \frac{max(d_u,d_v)}{min(d_u,d_v)}\right\}.$$

II. Main results

Theorem.2.1. The Atom bond connectivity index of Caffeine is 10.87047.

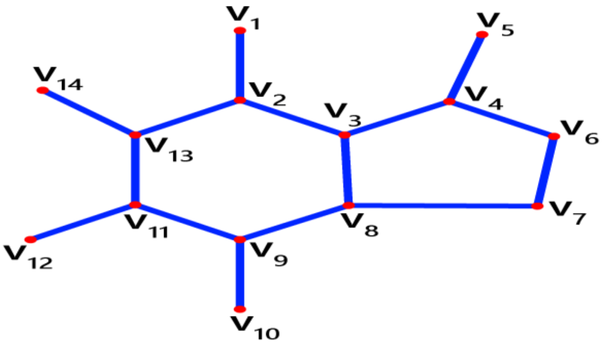

Figure-2

Proof: Consider Caffeine ($C_8H_{10}N_4O_2$). Let m_{ij} denotes edges connecting the vertices of degrees d_i and d_j. Two-dimensional structure of Caffeine (as shown in the Figure-2) contains edges of the type $m_{1,3}$, $m_{2,2}$, $m_{2;3}$ and $m_{3;3}$. From the figure-2, the number edges of these types are $|m_{1;3}|=5$, $|m_{2;2}|=1$, $|m_{2;3}|=2$ and $|m_{3;3}|=7$.

∴ The atom-bond connectivity index of Caffeine = ABC($C_8H_{10}N_4O_2$)

$$= \sum_{uv\in E} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}.$$

$$= |m_{1,3}|\sqrt{\frac{1+3-2}{1.3}} + |m_{2,2}|\sqrt{\frac{2+2-2}{2.2}} + |m_{2,3}|\sqrt{\frac{2+3-2}{2.3}} + |m_{3,3}|\sqrt{\frac{3+3-2}{3.3}}.$$

$$= 5 \times \sqrt{\frac{2}{3}} + 1 \times \frac{\sqrt{2}}{2} + 2 \times \frac{1}{\sqrt{2}} + 7 \times \frac{2}{3}.$$

∴ ABC($C_8H_{10}N_4O_2$) = 10.87047.

Theorem.2.2.The fourth atom bond connectivity index of Caffeine is 8.1516.

Proof: Let $e_{i,j}$ denotes the edges of Caffeine with i = S_u and j = S_v. It is easy to see that the summation of degrees of edge endpoints of Caffeine have six edge types $e_{3,7}$, $e_{3,6,}$ $e_{5,5}$, $e_{5,6,}$ $e_{5,8,}e_{6,9,}$ $e_{7,7}$, $e_{7,8}$, $e_{7,9}$ and $e_{8,9,}$ as shown in the following figure-2. clearly from the figure -2, $|e_{3,7}| = 4$, $|e_{3,6}| = 1$, $|e_{5,5}| = 1$, $|e_{5,6}| = 1$,$|e_{5,8}|= 1$, $|e_{6,9}| = 1$, $|e_{7,7}| = 3$, $|e_{7,8}| = 1$, $|e_{7,9}| = 1$,and $|e_{8,9}| = 1$.

The fourth atom-bond connectivity index of Caffeine = ABC_4($C_8H_{10}N_4O_2$).

$$= \sum_{uv\in E(G)} \sqrt{\frac{s_u + s_v - 2}{s_u s_v}}.$$

$$= |m_{3,7}|\left(\sqrt{\frac{3+7-2}{3.7}}\right) + |m_{3,6}|\left(\sqrt{\frac{3+6-2}{3.6}}\right) + |m_{5,5}|\left(\sqrt{\frac{5+5-2}{5.5}}\right) + |m_{5,6}|\left(\sqrt{\frac{5+6-2}{5.6}}\right) + |m_{5,8}|\left(\sqrt{\frac{5+8-2}{5.8}}\right) + |m_{6,9}|\left(\sqrt{\frac{6+9-2}{6.9}}\right) +$$
$$|m_{7,7}|\left(\sqrt{\frac{7+7-2}{7.7}}\right) + |m_{7,8}|\left(\sqrt{\frac{7+8-2}{7.8}}\right) + |m_{7,9}|\left(\sqrt{\frac{7+9-2}{7.9}}\right) + |m_{8,9}|\left(\sqrt{\frac{8+9-2}{8.9}}\right).$$

$$= 4 \times \sqrt{\frac{8}{21}} + 1 \times \sqrt{\frac{7}{18}} + 1 \times \sqrt{\frac{8}{25}} + 1 \times \sqrt{\frac{9}{30}} + 1 \times \sqrt{\frac{11}{40}} + 1 \times \sqrt{\frac{15}{54}} + 3 \times \sqrt{\frac{12}{49}} + 1 \times \sqrt{\frac{13}{56}} + 1 \times \sqrt{\frac{2}{9}} + 1 \times \sqrt{\frac{5}{24}}.$$

∴ ABC_4($C_8H_{10}N_4O_2$) = 8.1516.

Theorem.2.3.The Randic connectivity index of Caffeine is 6.5366.

Proof: Consider Randic connectivity index of Caffeine = χ($C_8H_{10}N_4O_2$)

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

$$= |m_{1,3}|\left(\frac{1}{\sqrt{1.3}}\right) + |m_{2,2}|\left(\frac{1}{\sqrt{2.2}}\right) + |m_{2,3}|\left(\frac{1}{\sqrt{2.3}}\right) + |m_{3,3}|\left(\frac{1}{\sqrt{3.3}}\right).$$

$$= 5 \times \left(\frac{1}{\sqrt{3}}\right) + 1 \times \left(\frac{1}{2}\right) + 2 \times \left(\frac{1}{\sqrt{6}}\right) + 7 \times \left(\frac{1}{3}\right).$$

∴ χ($C_8H_{10}N_4O_2$) = 6.5366.

Theorem.2.4. The sum connectivity index of Caffeine is 6.7522.

Proof: Consider the sum connectivity index of Caffeine = $S(C_8H_{10}N_4O_2)$

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

$$= |m_{1,3}|\left(\frac{1}{\sqrt{1+3}}\right) + |m_{2,2}|\left(\frac{1}{\sqrt{2+2}}\right) + |m_{2,3}|\left(\frac{1}{\sqrt{2+3}}\right) + |m_{3,3}|\left(\frac{1}{\sqrt{3+3}}\right).$$

$$= 5 \times \left(\frac{1}{2}\right) + 1 \times \left(\frac{1}{2}\right) + 2 \times \left(\frac{1}{\sqrt{5}}\right) + 7 \times \left(\frac{1}{\sqrt{6}}\right).$$

$\therefore S(C_8H_{10}N_4O_2) = 6.7522.$

Theorem.2.5.The Geometric-Arithmetic index of Caffeine is 14.2897.

Proof: Consider the Geometric-Arithmetic index of Caffeine = $GA(C_8H_{10}N_4O_2)$

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

$$= |m_{1,3}|\left(\frac{2\sqrt{1.3}}{1+3}\right) + |m_{2,2}|\left(\frac{2\sqrt{2.2}}{2+2}\right) + |m_{2,3}|\left(\frac{2\sqrt{2.3}}{2+3}\right) + |m_{3,3}|\left(\frac{2\sqrt{3.3}}{3+3}\right).$$

$$= 5 \times \left(\frac{2\sqrt{3}}{4}\right) + 1 \times \left(\frac{2\sqrt{4}}{4}\right) + 2 \times \left(\frac{2\sqrt{6}}{5}\right) + 7 \times \left(\frac{2\sqrt{9}}{6}\right).$$

$\therefore GA(C_8H_{10}N_4O_2) = 14.2897.$

Theorem.2.6. The fifth Geometric-Arithmetic index of Caffeine is 14.5457.

Proof: Consider the fifth Geometric-Arithmetic index of Caffeine = $GA_5(C_8H_{10}N_4O_2)$

$$= \sum_{uv\in E(G)} \frac{2\sqrt{s_u s_v}}{s_u + s_v}.$$

$$= |e_{3,7}|\left(\frac{2\sqrt{3.7}}{3+7}\right) + |e_{3,6}|\left(\frac{2\sqrt{3.6}}{3+6}\right) + |e_{5,5}|\left(\frac{2\sqrt{5.5}}{5+5}\right) + |e_{5,6}|\left(\frac{2\sqrt{5.6}}{5+6}\right) + |e_{5,8}|\left(\frac{2\sqrt{5.8}}{5+8}\right) + |e_{6,9}|\left(\frac{2\sqrt{6.9}}{6+9}\right) + |e_{7,7}|\left(\frac{2\sqrt{7.7}}{7+7}\right) + |e_{7,8}|\left(\frac{2\sqrt{7.8}}{7+8}\right) + |e_{7,9}|\left(\frac{2\sqrt{7.9}}{7+9}\right) + |e_{8,9}|\left(\frac{2\sqrt{8.9}}{8+9}\right).$$

$$= 4 \times \left(\frac{2\sqrt{21}}{10}\right) + 1 \times \left(\frac{2\sqrt{18}}{6}\right) + 1 \times \left(\frac{2\sqrt{25}}{10}\right) + 1 \times \left(\frac{2\sqrt{30}}{11}\right) + 1 \times \left(\frac{2\sqrt{40}}{13}\right) + 1 \times \left(\frac{2\sqrt{54}}{15}\right) + 3 \times \left(\frac{2\sqrt{49}}{14}\right) + 1 \times \left(\frac{2\sqrt{56}}{15}\right) + 1 \times \left(\frac{2\sqrt{63}}{16}\right) + 1 \times \left(\frac{2\sqrt{72}}{17}\right).$$

$\therefore GA_5(C_8H_{10}N_4O_2) = 14.5457.$

Theorem.2.7.The First Zagreb index of Caffeine is 76.

Proof: Consider First Zagreb index of Caffeine = $Z_1(C_8H_{10}N_4O_2)$

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

$$= |m_{1,3}|(1+3) + |m_{2,2}|(2+2) + |m_{2,3}|(2+3) + |m_{3,3}|(3+3).$$

$$= 5 \times (1+3) + 1 \times (2+2) + 2 \times (2+3) + 7 \times (3+3).$$

$$= 5 \times 4 + 6 \times 4 + 4 \times 5 + 2 \times 6.$$

$\therefore Z_1(C_8H_{10}N_4O_2) = 76.$

Theorem.2.8. The Second Zagreb index of Caffeine is 94.

Proof: The Second Zagreb index of Caffeine = $Z_2(C_8H_{10}N_4O_2)$

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

$$= |m_{1,3}|(1.3) + |m_{2,2}|(2.2) + |m_{2,3}|(2.3) + |m_{3,3}|(3.3).$$

$$= 5(3) + 1(4) + 2(6) + 7(9).$$

$\therefore Z_2(C_8H_{10}N_4O_2) = 94.$

Theorem.2.9. The First multiple Zagreb index of Caffeine is 2.8665×10^{10}.

Proof: The First multiple Zagreb index of Caffeine = $PM_1(C_8H_{10}N_4O_2)$

$$= \prod_{e=uv\in E(G)} (d_u + d_v)$$

$$= \prod_{e=uv\in 1,3} (d_u + d_v) \prod_{e=uv\in 2,2} (d_u + d_v) \prod_{e=uv\in 2,3} (d_u + d_v) \prod_{e=uv\in 3,3} (d_u + d_v)$$

$$= 4^5 \times 4^1 \times 5^2 \times 6^7.$$

$\therefore PM_1(C_8H_{10}N_4O_2) = 2.8665 \times 10^{10}.$

Theorem.2.10. The second multiple Zagreb index of Caffeine is 1.6737×10^{11}.

Proof: The second multiple Zagreb index of Caffeine = $PM_2(C_8H_{10}N_4O_2)$

$$= \prod_{e=uv\in E(G)} (d_u.d_v)$$

$$= \prod_{e=uv\in 1,3} (d_u.d_v) \prod_{e=uv\in 2,2} (d_u.d_v) \prod_{e=uv\in 2,3} (d_u.d_v) \prod_{e=uv\in 3,3} (d_u.d_v).$$

$$= 3^5 \times 4^1 \times 6^2 \times 9^7.$$

$\therefore PM_2(C_8H_{10}N_4O_2) = 1.6737 \times 10^{11}.$

Theorem.2.11.The Augmented Zagreb index of Caffeine is 120.6094.
Proof: The augmented Zagreb index of Caffeine = AZI(G) $(C_8H_{10}N_4O_2)$

$$= \sum_{uv\in E} \left[\frac{d_u d_v}{d_u + d_v - 2}\right]^3.$$

$$= |m_{1,3}| \left[\frac{1.3}{1+3-2}\right]^3 + |m_{2,2}| \left[\frac{2.2}{2+2-2}\right]^3 + |m_{2,3}| \left[\frac{2.3}{2+3-2}\right]^3 + |m_{3,3}| \left[\frac{3.3}{3+3-2}\right]^3.$$

$$= 5 \times \left(\frac{3}{2}\right)^3 + 1 \times \left(\frac{4}{2}\right)^3 + 2 \times \left(\frac{6}{3}\right)^3 + 7 \times \left(\frac{9}{4}\right)^3.$$

$\therefore AZI(G)(C_8H_{10}N_4O_2) = 120.6094.$

Theorem.2.12. The harmonic index of Caffeine is 6.1333.
Proof: The harmonic index of Caffeine = $H(C_8H_{10}N_4O_2)$

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

$$= |m_{1,3}| \left(\frac{2}{1+3}\right) + |m_{2,2}| \left(\frac{2}{2+2}\right) + |m_{2,3}| \left(\frac{2}{2+3}\right) + |m_{3,3}| \left(\frac{2}{3+3}\right).$$

$$= 5 \times \left(\frac{2}{4}\right) + 1 \times \left(\frac{2}{4}\right) + 2 \times \left(\frac{2}{5}\right) + 7 \times \left(\frac{2}{6}\right).$$

$H(C_8H_{10}N_4O_2) = 6.1333.$

Theorem.2.13.The hyper Zagreb index of Caffeine is 398.
Proof: The hyper Zagreb index of Caffeine = $HM(C_8H_{10}N_4O_2)$

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

$$= |m_{1,3}|(1+3)^2 + |m_{2,2}|(2+2)^2 + |m_{2,3}|(2+3)^2 + |m_{3,3}|(3+3)^2.$$

$$= 5 \times 4^2 + 1 \times 4^2 + 2 \times 5^2 + 7 \times 6^2.$$

$\therefore HM(C_8H_{10}N_4O_2) = 398.$

Theorem.2.14. The First Zagreb polynomials of Caffeine is $7x^6 + 2x^5 + 6x^4$.
Proof: Consider First Zagreb polynomials of Caffeine = $ZG_1(C_8H_{10}N_4O_2, x)$

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

$$= |m_{1,3}|x^{(1+3)} + |m_{2,2}|x^{(2+2)} + |m_{2,3}|x^{(2+3)} + |m_{3,3}|x^{(3+3)}.$$

$$= 5 \times x^4 + 1 \times x^4 + 2 \times x^5 + 7 \times x^6.$$

$\therefore ZG_1(C_8H_{10}N_4O_2, x) = 7x^6 + 2x^5 + 6x^4.$

Theorem.2.15. The Second Zagreb polynomials of Caffeine is $7x^9 + 2x^6 + x^4 + x^3$.
Proof: Consider Second Zagreb polynomials of Caffeine = $ZG_2(C_8H_{10}N_4O_2, x)$

$$= \sum_{e=uv\in E(G)} x^{d_u d_v}.$$

$$= |m_{1,3}|x^{(1.3)} + |m_{2,2}|x^{(2.2)} + |m_{2,3}|x^{(2.3)} + |m_{3,3}|x^{(3.3)}.$$

$$= 5 \times x^3 + 1 \times x^4 + 2 \times x^6 + 7 \times x^9.$$

$\therefore ZG_2(C_8H_{10}N_4O_2, x) = 7x^9 + 2x^6 + x^4 + x^3.$

Theorem.2.16. The Third Zagreb polynomials of Caffeine is $5x^2 + x + 8$.
Proof: Consider Third Zagreb polynomials of Caffeine = $ZG_3(C_8H_{10}N_4O_2, x)$

$$= \sum_{e=uv\in E(G)} x^{|d_u - d_v|}.$$

$$= |m_{1,3}|x^{|1-3|} + |m_{2,2}|x^{|2-2|} + |m_{2,3}|x^{|2-3|} + |m_{3,3}|x^{|3-3|}.$$
$$= 5 \times x^2 + 1 \times x^0 + 2 \times x^1 + 7 \times x^0.$$

∴ $ZG_3(C_8H_{10}N_4O_2, x) = 5x^2 + x + 8.$

Theorem.2.17.The Forgotten topological index of Caffeine is 210.

Proof: Consider Forgotten topological index of Caffeine = $F(C_8H_{10}N_4O_2)$

$$= \sum_{e=uv\in E(G)} [(d_u)^2 + (d_v)^2]$$
$$= |m_{1,3}|(1^2 + 3^2) + |m_{2,2}|(2^2 + 2^2) + |m_{2,3}|(2^2 + 3^2) + |m_{3,3}|(3^2 + 3^2).$$
$$= 5 \times 10 + 1 \times 8 + 2 \times 13 + 7 \times 18.$$

∴ $F(C_8H_{10}N_4O_2) = 210.$

Theorem.2.18. The Forgotten polynomials of Caffeine is $7x^{18} + 2x^{13} + 5x^{10} + x^8$.

Proof: Consider Forgotten polynomials of Caffeine = $F(C_8H_{10}N_4O_2, x)$

$$= \sum_{e=uv\in E(G)} x^{[(d_u)^2+(d_v)^2]}.$$
$$= |m_{1,3}|x^{(1^2+3^2)} + |m_{2,2}|x^{(2^2+2^2)} + |m_{2,3}|x^{(2^2+3^2)} + |m_{3,3}|x^{(3^2+3^2)}.$$
$$= 5 \times x^{10} + 1 \times x^8 + 2 \times x^{13} + 7 \times x^{18}.$$

∴ $F(C_8H_{10}N_4O_2, x) = 7x^{18} + 2x^{13} + 5x^{10} + x^8.$

Theorem.2.19.The Symmetric division index of Caffeine is 29.

Proof: Consider Symmetric division index of Caffeine = $SDD(C_8H_{10}N_4O_2)$

$$= \sum_{e=uv\in E(G)} \left\{\frac{min(d_u, d_v)}{max(d_u, d_v)} + \frac{max(d_u, d_v)}{min(d_u, d_v)}\right\}.$$
$$= |m_{1,3}|\left\{\frac{min(1.3)}{max(1.3)} + \frac{max(1.3)}{min(1.3)}\right\} + |m_{2,2}|\left\{\frac{min(2.2)}{max(2.2)} + \frac{max(2.2)}{min(2.2)}\right\} + |m_{2,3}|\left\{\frac{min(2.3)}{max(2.3)} + \frac{max(2.3)}{min(2.3)}\right\} + |m_{3,3}|\left\{\frac{min(3.3)}{max(3.3)} + \frac{max(3.3)}{min(3.3)}\right\}.$$
$$= 5 \times \frac{10}{3} + 1 \times 1 + 2 \times \frac{13}{6} + 7 \times 1.$$

∴ $SDD(C_8H_{10}N_4O_2) = 29.$

III. Conclusion

ABC index, ABC_4 index, Randic connectivity index, Sum connectivity index, GA index , GA_5 index, First Zagreb index, Second Zagreb index, First Multiple Zagreb index, Second Multiple Zagreb index, Augmented Zagreb index, Harmonic index and Hyper Zagreb index, First Zagreb polynomials, Second Zagreb polynomials, Third Zagreb polynomials, Forgotten polynomials, Forgotten topological index and Symmetric division index of Caffeine was computed.

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