Degree-Based Topological Indices of Cubic of Alkanes

Vidyashree K[1], Vishu Kumar M[2]

[1]Department of Mathematics, Nagarjuna College of Engineering and Technology, Devanahalli, Bangalore – 562 164, India

[2]Department of Mathematics, School of Applied Sciences, REVA University, Yelahanka, Bangalore – 560 064, India

Abstract : Graph operations are important in many graph theory applications because they allow the creation of large graphs from smaller ones. This work focuses on a specific graph theoretical process, the cube graph. Our research focuses on alkanes, the simplest hydrocarbons composed only of hydrogen (H) and carbon (C) atoms with no functional groups. In this paper, we compute several topological indices for the cube of alkanes, namely, Atom Bond Connectivity Index (ABC), Geometric Arithmetic (GA), Forgotten Index (F), Inverse Sum Indeg Index (ISI), Randic Index (χ), Reciprocal Randic Index (RR), Arithmetic Geometric Index (AG_1), First Zagreb Index (M_1), Second Zagreb Index (M_2), Modified Second Zagreb Index (M_2^*), Hyper Zagreb Index (HM), and Symmetric Division Deg Index (SDD). Additionally, we provide a graphical and numerical comparison of these topological indices.

Key Words : degree based topological indices, alkanes, cube of alkanes.

1. Introduction

Consider a chemical graph G that is undirected, without loops, and has few edges. In these graphs, edges (E) represent bonds between atoms, and vertices (V) represent the atoms. The size of a graph is determined by the number of edges, while its order is determined by the number of vertices in graph G. The degree of a vertex is the number of edges connected to it. For further information on notations and terminologies, the book by R.J. Wilson is recommended reading [1]. Leonard Euler's 1736 discovery, the Handshaking Lemma, which is often considered the first theorem of graph theory, is particularly useful for determining the number of edges in a graph G [2].

Chemical graph theory is intended to complement other fields of study, while theoretical chemistry can provide deeper insights into chemical structures and molecular structure modeling. Two important subfields of chemical graph theory are quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR). Topological indices, which convert a chemical structure into a numerical value, play a critical role in QSPR/QSAR studies, providing information about the morphology of molecules. These indices are fundamental in modeling the molecular structures of chemical substances and analyzing their physical and chemical properties. Several topological indices, such as distance-based [3], degree-based [4][5][6], and counting-related indices [7][8], are computed using various graph operations for numerous types of graphs, including newly constructed ones [9]. The concept of topological indices was inspired by the work of Wiener [10].

2. Prelimiaries

Assume the graph G, the Atom Bond Connectivity index [11] is defined as follows:

$$ABC(G)=\sum_{uv\in E(G)}\sqrt{\frac{d_u+d_v-2}{d_u d_v}} \qquad (1)$$

Furtula & Vukicevic [12] introduced the Geometric Arithmetic index as follows:

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

B. Furtula, I. Gutman [13] introduced the forgotten topological index as follows:

$$F(G)=\sum_{uv\in E(G)}\left(d_u^2+d_v^2\right) \quad (3)$$

Pattabiraman [14] introduced the Inverse Sum Indeg Index (ISI) as follows:

$$ISI(G)=\sum_{uv\in E(G)}\frac{1}{\frac{1}{d_u}+\frac{1}{d_v}} \quad (4)$$

Milan Randic [15] introduced the Randic Index as follows:

$$\chi(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_u d_v}} \quad (5)$$

I. Gutman, B. Furtula, C. Elphick [16] introduced the Reciprocal Randic Index as follows:

$$RR(G)=\sum_{uv\in E(G)}\sqrt{d_u d_v} \quad (6)$$

V S Shegehalli, R Kanabur [17], introduced the Arithmetic-Geometric Index as follows:

$$AG_1(G)=\sum_{uv\in E(G)}\frac{d_u+d_v}{2\sqrt{d_u d_v}} \quad (7)$$

Trinajstic N and Gutman I [18] , introduced First Zagreb Index as follows:

$$M_1(G)=\sum_{uv\in E(G)}\left(d_u+d_v\right) \quad (8)$$

Trinajstic N and Gutman I [18] , introduced Second Zagreb Index as follows:

$$M_2(G)=\sum_{uv\in E(G)}\left(d_u\times d_v\right) \quad (9)$$

Hao J, Theorems [19] introduced Modified Second Zagreb Index on 2011 as follows:

$$M_2^*(G)=\sum_{uv\in E(G)}\frac{1}{d_u\times d_v} \quad (10)$$

Shirdel G H, H. Rezapour, Sayadi A M [20], introduced Hyper Zagreb Index as follows:

$$HM(G)=\sum_{uv\in E(G)}\left(d_u+d_v\right)^2 \quad (11)$$

Vukicevic D, M. Gasperov [21] introduced Symmetric Division Deg Index as follows:

$$SDD(G)=\sum_{uv\in E(G)}\frac{\left(d_u^2+d_v^2\right)}{d_u d_v} \quad (12)$$

Definition 2.1 Alkanes consist entirely of single-bonded hydrogen and carbon atoms, with carbon and hydrogen arranged in tree-like structures, as illustrated in Figure 1. The general formula for alkanes is C_mH_{2m+2} where

$m \geq 1$.. They are commercially significant, serving as primary components in lubricants and gasoline. The first four alkanes are primarily used for cooking, heating, and power generation.
Graph operations are vital in various applications of chemical graph theory and other fields. By applying graph operations to alkanes, we can create new molecular structures.

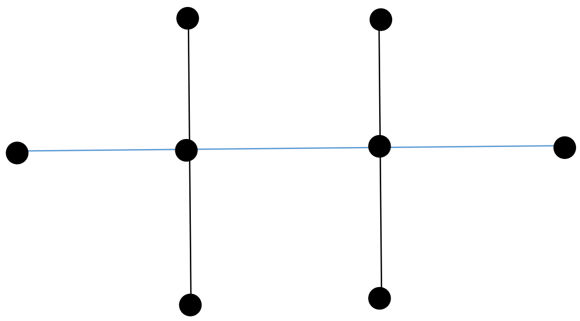

Figure 1 : C_2H_6

Definition 2.2 The cube of a graph *G* is obtained from *G* by adding new edges between every two vertices having distance three in *G* and is denoted by G^3.

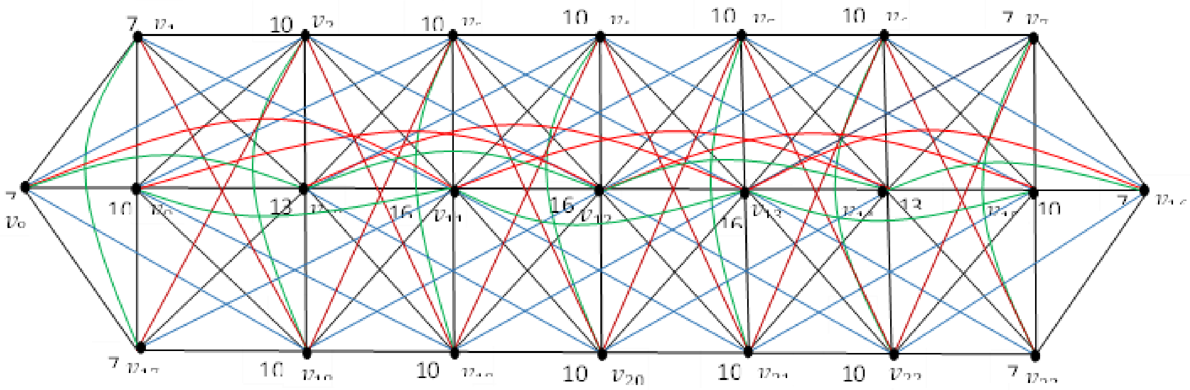

Figure 2 : $(C_7H_{16})^3$:

3. Topological Indices of Cube of Alkanes

The vertex set of the cube of alkane C_kH_{2k+2} is $3k+2$ and the edge set of the cube of alkane C_kH_{2k+2} is $18k-8$. The edge set of the cube of alkane is partitioned into nine sets based on degree of the end vertices.

Table 3. Edge set partition of Cube of alkane

$E_{7,7}$	$E_{7,10}$	$E_{7,13}$	$E_{7,16}$	$E_{10,10}$	$E_{10,13}$	$E_{10,16}$	$E_{13,16}$	$E_{16,16}$
6	18	6	6	5k - 6	14	10(k - 4)	6	3(k – 6)

Theorem 3.1. The Atom Bond Connectivity index and Geometric Arithmetic index of Cube of a alkane are given by

$$ABC\left[\left(C_kH_{2k+2}\right)^3\right]=7.0213k+0.1577$$
$$GA\left[\left(C_kH_{2k+2}\right)^3\right]=17.7301k-8.1094 \qquad k\geq 7$$

Proof. From equation 1, we compute the atom bond connectivity index as below,

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

$$ABC\left[\left(C_kH_{2k+2}\right)^3\right]=\sum_{E_{7,7}}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}+\sum_{E_{7,10}}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}+\sum_{E_{7,13}}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}+\sum_{E_{7,16}}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}+$$
$$\sum_{E_{10,10}}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}+\sum_{E_{10,13}}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}+\sum_{E_{10,16}}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}+\sum_{E_{13,16}}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}+\sum_{E_{16,16}}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}$$
$$=6\sqrt{\frac{7+7-2}{7(7)}}+18\sqrt{\frac{7+10-2}{7(10)}}+6\sqrt{\frac{7+13-2}{7(13)}}+6\sqrt{\frac{7+16-2}{7(16)}}+(5k-6)\sqrt{\frac{10+10-2}{10(10)}}+$$
$$14\sqrt{\frac{10+13-2}{10(13)}}+10(k-4)\sqrt{\frac{10+16-2}{10(16)}}+6\sqrt{\frac{13+16-2}{13(16)}}+3(k-6)\sqrt{\frac{16+16-2}{16(16)}}$$

$$ABC\left[\left(C_kH_{2k+2}\right)^3\right]=7.0213k+0.1577$$

From equation 2, we compute the geometric arithmetic index as follows,

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

$$GA\left[\left(C_kH_{2k+2}\right)^3\right]=\sum_{E_{7,7}}\frac{2\sqrt{d_ud_v}}{d_u+d_v}+\sum_{E_{7,10}}\frac{2\sqrt{d_ud_v}}{d_u+d_v}+\sum_{E_{7,13}}\frac{2\sqrt{d_ud_v}}{d_u+d_v}+\sum_{E_{7,16}}\frac{2\sqrt{d_ud_v}}{d_u+d_v}+\sum_{E_{10,10}}\frac{2\sqrt{d_ud_v}}{d_u+d_v}+\sum_{E_{10,13}}\frac{2\sqrt{d_ud_v}}{d_u+d_v}+\sum_{E_{10,16}}\frac{2\sqrt{d_ud_v}}{d_u+d_v}+\sum_{E_{13,16}}\frac{2\sqrt{d_ud_v}}{d_u+d_v}+\sum_{E_{16,16}}\frac{2\sqrt{d_ud_v}}{d_u+d_v}$$

$$=6\left[\frac{2\sqrt{7(7)}}{7+7}\right]+18\left[\frac{2\sqrt{7(10)}}{7+10}\right]+6\left[\frac{2\sqrt{7(13)}}{7+13}\right]+6\left[\frac{2\sqrt{7(16)}}{7+16}\right]+(5k-6)\left[\frac{2\sqrt{10(10)}}{10+10}\right]+$$
$$14\left[\frac{2\sqrt{10(13)}}{10+13}\right]+10(k-4)\left[\frac{2\sqrt{10(16)}}{10+16}\right]+6\left[\frac{2\sqrt{13(16)}}{13+16}\right]+3(k-6)\left[\frac{2\sqrt{16(16)}}{16+16}\right]$$
$$GA\left[\left(C_kH_{2k+2}\right)^3\right]=17.7301k-8.1094$$

Theorem 3.2. The Forgotten index and Inverse Sum Indeg index of Cube of a alkane are given by

$$F\left[\left(C_kH_{2k+2}\right)^3\right]=6096k-11932$$

$$ISI\left[\left(C_kH_{2k+2}\right)^3\right]=110.5385k-146.3539 \qquad k\geq 7$$

Proof. From equation 3, we compute the forgotten index as below,

$$F(G)=\sum_{uv\in E(G)}\left(d_u^2+d_v^2\right)$$

$$F\left[\left(C_kH_{2k+2}\right)^3\right]=\sum_{E_{7,7}}(d_u^2+d_v^2)+\sum_{E_{7,10}}(d_u^2+d_v^2)+\sum_{E_{7,13}}(d_u^2+d_v^2)+\sum_{E_{7,16}}(d_u^2+d_v^2)+$$

$$\sum_{E_{10,10}}(d_u^2+d_v^2)+\sum_{E_{10,13}}(d_u^2+d_v^2)+\sum_{E_{10,16}}(d_u^2+d_v^2)+\sum_{E_{13,16}}(d_u^2+d_v^2)+\sum_{E_{16,16}}(d_u^2+d_v^2)$$

$$=6\left(7^2+7^2\right)+18\left(7^2+10^2\right)+6\left(7^2+13^2\right)+6\left(7^2+16^2\right)+(5k-6)\left(10^2+10^2\right)+14\left(10^2+13^2\right)+10(k-4)\left(10^2+16^2\right)+6\left(13^2+16^2\right)+3(k-6)\left(16^2+16^2\right)$$

$$F\left[\left(C_kH_{2k+2}\right)^3\right]=6096k-11932$$

From equation 4, we compute the inverse sum indeg index as below,

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

$$ISI\left[\left(C_kH_{2k+2}\right)^3\right]=\sum_{E_{7,7}}\left[\frac{1}{\frac{1}{d_u}+\frac{1}{d_v}}\right]+\sum_{E_{7,10}}\left[\frac{1}{\frac{1}{d_u}+\frac{1}{d_v}}\right]+\sum_{E_{7,13}}\left[\frac{1}{\frac{1}{d_u}+\frac{1}{d_v}}\right]+\sum_{E_{7,16}}\left[\frac{1}{\frac{1}{d_u}+\frac{1}{d_v}}\right]+\sum_{E_{10,10}}\left[\frac{1}{\frac{1}{d_u}+\frac{1}{d_v}}\right]+\sum_{E_{10,13}}\left[\frac{1}{\frac{1}{d_u}+\frac{1}{d_v}}\right]+\sum_{E_{10,16}}\left[\frac{1}{\frac{1}{d_u}+\frac{1}{d_v}}\right]+\sum_{E_{13,16}}\left[\frac{1}{\frac{1}{d_u}+\frac{1}{d_v}}\right]+\sum_{E_{16,16}}\left[\frac{1}{\frac{1}{d_u}+\frac{1}{d_v}}\right]$$

$$=6\left[\frac{1}{\frac{1}{7}+\frac{1}{7}}\right]+18\left[\frac{1}{\frac{1}{7}+\frac{1}{10}}\right]+6\left[\frac{1}{\frac{1}{7}+\frac{1}{13}}\right]+6\left[\frac{1}{\frac{1}{7}+\frac{1}{16}}\right]+(5k-6)\left[\frac{1}{\frac{1}{10}+\frac{1}{10}}\right]+14\left[\frac{1}{\frac{1}{10}+\frac{1}{13}}\right]+10(k-4)\left[\frac{1}{\frac{1}{10}+\frac{1}{16}}\right]+6\left[\frac{1}{\frac{1}{13}+\frac{1}{16}}\right]+3(k-6)\left[\frac{1}{\frac{1}{16}+\frac{1}{16}}\right]$$

$$ISI\left[\left(C_kH_{2k+2}\right)^3\right]=110.5385k-146.3539$$

Theorem 3.3. The Randic index and Reciprocal Randic index of Cube of a alkane are given by

$\chi\left[\left(C_kH_{2k+2}\right)^3\right]$ is $1.4781k+0.9611$.

$RR\left[\left(C_kH_{2k+2}\right)^3\right]$ is $224.4911k-294.4735 \qquad k\geq 7$

Proof. From equation 5, we compute the Randic index as below,

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

$$\chi\left[\left(C_kH_{2k+2}\right)^3\right]=\sum_{E_{7,7}}\left[\frac{1}{\sqrt{d_ud_v}}\right]+\sum_{E_{7,10}}\left[\frac{1}{\sqrt{d_ud_v}}\right]+\sum_{E_{7,13}}\left[\frac{1}{\sqrt{d_ud_v}}\right]+\sum_{E_{7,16}}\left[\frac{1}{\sqrt{d_ud_v}}\right]+\sum_{E_{10,10}}\left[\frac{1}{\sqrt{d_ud_v}}\right]+\sum_{E_{10,13}}\left[\frac{1}{\sqrt{d_ud_v}}\right]+\sum_{E_{10,16}}\left[\frac{1}{\sqrt{d_ud_v}}\right]+\sum_{E_{13,16}}\left[\frac{1}{\sqrt{d_ud_v}}\right]+\sum_{E_{16,16}}\left[\frac{1}{\sqrt{d_ud_v}}\right]$$

$$=6\left[\frac{1}{\sqrt{7(7)}}\right]+18\left[\frac{1}{\sqrt{7(10)}}\right]+6\left[\frac{1}{\sqrt{7(13)}}\right]+6\left[\frac{1}{\sqrt{7(16)}}\right]+(5k-6)\left[\frac{1}{\sqrt{10(10)}}\right]+14\left[\frac{1}{\sqrt{10(13)}}\right]+10(k-4)\left[\frac{1}{\sqrt{10(16)}}\right]+6\left[\frac{1}{\sqrt{13(16)}}\right]+3(k-6)\left[\frac{1}{\sqrt{16(16)}}\right]$$

$$\chi\left[\left(C_kH_{2k+2}\right)^3\right]=1.4781k+0.9611$$

From equation 6, we compute the Reciprocal Randic index as below,

$$RR(G)=\sum_{uv\in E(G)}\sqrt{d_u d_v}$$

$$RR\left[\left(C_kH_{2k+2}\right)^3\right]=\sum_{E_{7,7}}\sqrt{d_ud_v}+\sum_{E_{7,10}}\sqrt{d_ud_v}+\sum_{E_{7,13}}\sqrt{d_ud_v}+\sum_{E_{7,16}}\sqrt{d_ud_v}+\sum_{E_{10,10}}\sqrt{d_ud_v}+\sum_{E_{10,13}}\sqrt{d_ud_v}+\sum_{E_{10,16}}\sqrt{d_ud_v}+\sum_{E_{13,16}}\sqrt{d_ud_v}+\sum_{E_{16,16}}\sqrt{d_ud_v}$$

$$=6\sqrt{7(7)}+18\sqrt{7(10)}+6\sqrt{7(13)}+6\sqrt{7(16)}+(5k-6)\sqrt{10(10)}+14\sqrt{10(13)}+10(k-4)\sqrt{10(16)}+6\sqrt{13(16)}+3(k-6)\sqrt{16(16)}$$

$$RR\left[\left(C_kH_{2k+2}\right)^3\right]=224.4911k-294.4735$$

Theorem 3.4. The Arithmetic Geometric index and First Zagreb index Cube of a alkane are given by

$$AG_1\left[\left(C_kH_{2k+2}\right)^3\right]=18.2774k-7.8600$$

$$M_1\left[\left(C_kH_{2k+2}\right)^3\right]=456k-592 \qquad k\geq 7$$

Proof. From equation 7, we compute the arithmetic geometric index as below,

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

$$AG_1\left[\left(C_kH_{2k+2}\right)^3\right]=\sum_{E_{7,7}}\left[\frac{d_u+d_v}{2\sqrt{d_ud_v}}\right]+\sum_{E_{7,10}}\left[\frac{d_u+d_v}{2\sqrt{d_ud_v}}\right]+\sum_{E_{7,13}}\left[\frac{d_u+d_v}{2\sqrt{d_ud_v}}\right]+\sum_{E_{7,16}}\left[\frac{d_u+d_v}{2\sqrt{d_ud_v}}\right]+\sum_{E_{10,10}}\left[\frac{d_u+d_v}{2\sqrt{d_ud_v}}\right]+\sum_{E_{10,13}}\left[\frac{d_u+d_v}{2\sqrt{d_ud_v}}\right]+\sum_{E_{10,16}}\left[\frac{d_u+d_v}{2\sqrt{d_ud_v}}\right]+\sum_{E_{13,16}}\left[\frac{d_u+d_v}{2\sqrt{d_ud_v}}\right]+\sum_{E_{16,16}}\left[\frac{d_u+d_v}{2\sqrt{d_ud_v}}\right]$$

$$=6\left[\frac{7+7}{2\sqrt{7(7)}}\right]+18\left[\frac{7+10}{2\sqrt{7(10)}}\right]+6\left[\frac{7+13}{2\sqrt{7(13)}}\right]+6\left[\frac{7+16}{2\sqrt{7(16)}}\right]+(5k-6)\left[\frac{10+10}{2\sqrt{10(10)}}\right]+14\left[\frac{10+13}{2\sqrt{10(13)}}\right]+10(k-4)\left[\frac{10+16}{2\sqrt{10(16)}}\right]+6\left[\frac{13+16}{2\sqrt{13(16)}}\right]+3(k-6)\left[\frac{16+16}{2\sqrt{16(16)}}\right]$$

$$AG_1\left[\left(C_kH_{2k+2}\right)^3\right]=18.2774k-7.8600\ .$$

From equation 8, we compute the first Zagreb index as below,

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

$$M_1\left[\left(C_kH_{2k+2}\right)^3\right]=\sum_{E_{7,7}}(d_u+d_v)+\sum_{E_{7,10}}(d_u+d_v)+\sum_{E_{7,13}}(d_u+d_v)+\sum_{E_{7,16}}(d_u+d_v)+\sum_{E_{10,10}}(d_u+d_v)+\sum_{E_{10,13}}(d_u+d_v)+\sum_{E_{10,16}}(d_u+d_v)+\sum_{E_{13,16}}(d_u+d_v)+\sum_{E_{16,16}}(d_u+d_v)$$

$$=6(7+7)+18(7+10)+6(7+13)+6(7+16)+(5k-6)(10+10)+14(10+13)+10(k-4)(10+16)+6(13+16)+3(k-6)(16+16)$$

$$M_1\left[\left(C_kH_{2k+2}\right)^3\right]=456k-592$$

Theorem 3.5. The Second Zagreb index, Modified Second Zagreb index and Hyper Zagreb index of Cube of a alkane are given by

$$M_2\left[\left(C_kH_{2k+2}\right)^3\right]=2868k-5768$$

$$M_2^*(G)\left[\left(C_kH_{2k+2}\right)^3\right]=0.1242k+0.2553$$

$$HM\left[\left(C_kH_{2k+2}\right)^3\right]=11832k-23468 \qquad k\geq 7$$

Proof. From equation 9, we compute the second zagreb index as below,

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

$$M_2\left[(C_kH_{2k+2})^3\right]=\sum_{E_{7,7}}(d_u\times d_v)+\sum_{E_{7,10}}(d_u\times d_v)+\sum_{E_{7,13}}(d_u\times d_v)+\sum_{E_{7,16}}(d_u\times d_v)+\sum_{E_{10,10}}(d_u\times d_v)+\sum_{E_{10,13}}(d_u\times d_v)+\sum_{E_{10,16}}(d_u\times d_v)+\sum_{E_{13,16}}(d_u\times d_v)+\sum_{E_{16,16}}(d_u\times d_v)$$

$$=6(7\times7)+18(7\times10)+6(7\times13)+6(7\times16)+(5k-6)(10\times10)+14(10\times13)+10(k-4)(10\times16)+6(13\times16)+3(k-6)(16\times16)$$

$$M_2\left[(C_kH_{2k+2})^3\right]=2868k-5768.$$

From equation 10, we compute the modified second zagreb index as below,

$$M_2^*(G)=\sum_{uv\in E(G)}\frac{1}{d_u\times d_v}$$

$$M_2^*(G)\left[(C_kH_{2k+2})^3\right]=\sum_{E_{7,7}}\left[\frac{1}{d_ud_v}\right]+\sum_{E_{7,10}}\left[\frac{1}{d_ud_v}\right]+\sum_{E_{7,13}}\left[\frac{1}{d_ud_v}\right]+\sum_{E_{7,16}}\left[\frac{1}{d_ud_v}\right]+\sum_{E_{10,10}}\left[\frac{1}{d_ud_v}\right]+\sum_{E_{10,13}}\left[\frac{1}{d_ud_v}\right]+\sum_{E_{10,16}}\left[\frac{1}{d_ud_v}\right]+\sum_{E_{13,16}}\left[\frac{1}{d_ud_v}\right]+\sum_{E_{16,16}}\left[\frac{1}{d_ud_v}\right]$$

$$=6\left[\frac{1}{7(7)}\right]+18\left[\frac{1}{7(10)}\right]+6\left[\frac{1}{7(13)}\right]+6\left[\frac{1}{7(16)}\right]+(5k-6)\left[\frac{1}{10(10)}\right]+14\left[\frac{1}{10(13)}\right]+10(k-4)\left[\frac{1}{10(16)}\right]+6\left[\frac{1}{13(16)}\right]+3(k-6)\left[\frac{1}{16(16)}\right]$$

$$M_2^*(G)\left[(C_kH_{2k+2})^3\right]=0.1242k+0.2553.$$

From equation 11, we compute the hyper zagreb index as below,

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

$$HM\left[(C_kH_{2k+2})^3\right]=\sum_{E_{7,7}}(d_u+d_v)^2+\sum_{E_{7,10}}(d_u+d_v)^2+\sum_{E_{7,13}}(d_u+d_v)^2+\sum_{E_{7,16}}(d_u+d_v)^2+\sum_{E_{10,10}}(d_u+d_v)^2+\sum_{E_{10,13}}(d_u+d_v)^2+\sum_{E_{10,16}}(d_u+d_v)^2+\sum_{E_{13,16}}(d_u+d_v)^2+\sum_{E_{16,16}}(d_u+d_v)^2$$

$$=6(7+7)^2+18(7+10)^2+6(7+13)^2+6(7+16)^2+(5k-6)(10+10)^2+14(10+13)^2+10(k-4)(10+16)^2+6(13+16)^2+3(k-6)(16+16)^2$$

$$HM\left[(C_kH_{2k+2})^3\right]=11832k-23468.$$

Theorem 3.6. The Symmetric Division Degree index of Cube of a alkane are given by

$$SDD\left[(C_kH_{2k+2})^3\right]=38.2500k-14.7440. \qquad k\geq 7$$

Proof. From equation 12, we compute the symmetric division degree index as below,

$$SDD(G)=\sum_{uv\in E(G)}\frac{(d_u^2+d_v^2)}{d_ud_v}$$

$$SDD\left[(C_kH_{2k+2})^3\right]=\sum_{E_{7,7}}\left[\frac{d_u^2+d_v^2}{d_ud_v}\right]+\sum_{E_{7,10}}\left[\frac{d_u^2+d_v^2}{d_ud_v}\right]+\sum_{E_{7,13}}\left[\frac{d_u^2+d_v^2}{d_ud_v}\right]+\sum_{E_{7,16}}\left[\frac{d_u^2+d_v^2}{d_ud_v}\right]+\sum_{E_{10,10}}\left[\frac{d_u^2+d_v^2}{d_ud_v}\right]+\sum_{E_{10,13}}\left[\frac{d_u^2+d_v^2}{d_ud_v}\right]+\sum_{E_{10,16}}\left[\frac{d_u^2+d_v^2}{d_ud_v}\right]+\sum_{E_{13,16}}\left[\frac{d_u^2+d_v^2}{d_ud_v}\right]+\sum_{E_{16,16}}\left[\frac{d_u^2+d_v^2}{d_ud_v}\right]$$

$$=6\left[\frac{7^2+7^2}{7(7)}\right]+18\left[\frac{7^2+10^2}{7(10)}\right]+6\left[\frac{7^2+13^2}{7(13)}\right]+6\left[\frac{7^2+16^2}{7(16)}\right]+(5k-6)\left[\frac{10^2+10^2}{10(10)}\right]+14\left[\frac{10^2+13^2}{10(13)}\right]+10(k-4)\left[\frac{10^2+16^2}{10(16)}\right]+6\left[\frac{13^2+16^2}{13(16)}\right]+3(k-6)\left[\frac{16^2+16^2}{16(16)}\right]$$

$$SDD\left[(C_kH_{2k+2})^3\right]=38.2500k-14.7440.$$

References:

[1] R.J. Wilson, Introduction to Graph Theory, New York: John Wiley and Sons, 1986.
[2] G. Chartrand, l. Lesniak and zhang, graphs & digraphs, 6th Edition ed., Boca Raton: Chapman and Hall/CRC, 2015, 640. DOI:https://doi.org/10.1201/b19731

[3] M. Hu, H. Ali, M. A. Binyamin, B. Ali, J.-B. Liu, On Distance-Based Topological Desceiptors of Chemical Interconnection Networks, Journal of Mathematics, 10, 2021. DOI: https://doi.org/10.1155/2021/5520619
[4] D.K. Ch., M. Marjan, M. Emina, M. Igor, Bonds for symmetric division deg index of graphs, Faculty of Sciences and Mathematics, 33(3), 638-698, 2019. DOI: 10.2298/FIL1903683D
[5] M. Alaeiyan, M. S. Sardar, S. Zafar, Z. Zahid, Computation of topological indices of line graph of Jahangir Graph, International Journal of Applied Mathematics, 91-107, 2018. DOI:10.18642/ijamml_7100121966
[6] G. Hong, Z. Gu, M. Javid, H.M. Awais, M.K. Siddiqui, Degree based topological invariants of metal-organic networks, IEEE access, 8, 68288-68300, 2020. DOI:10.1109/ACCESS.2020.2985729
[7] A. Yousaf, M. Nadeem, An Efficient Technique to Construct Certain Counting Polynomials and Related Topological Indices for 2D-Planar Graphs, Journal of the International Society for Polycyclic Aromatic Compounds, 14, 2021. DOI:10.1080/10406638.2021.1892780
[8] S. Hayat, M. Imran, Computation of topological indices of certain networks, Applied Mathematics and Computation, 213-228, 2014. DOI:10.1016/j.amc.2014.04.091
[9] M.S. Sardar, I. Siddique, D. Alrowaili, M.A. Ali, S. Akhtar, Computation of topological indices of double and strong double graphs of circumcoronene series of benzenoid Hm, Journal of Mathematics, 11, 2022.DOI:10.1155/2022/5956802
[10] H. Wiener, Structural determination of paraffin boiling point, Journal of the American Chemical Society, 17-20, January 1947.DOI:10.1021/ja01193a005
[11]D. S. Revankar, Priyanka S. Hande, and S. P. Hande, "On Atom-Bond Connectivity Status Index of Graphs", Advances in Mathematics: Scientific Journal 10 (2021), no.3, 1197–1213. DOI: https://doi.org/10.37418/amsj.10.3.9
[12] B. Furtula and D. Vukicevic, Topological index based on the ratios of geometrical and arithmetic means of end-vertex degrees of edges, J. Math. Chem., 46, 1369-1376, 2009.DOI:10.1007/s10910-009-9520-x
[13] B.Furtula and I. Gutman, A forgotten topological index, Journal of Mathematical Chemistry. 53, no. 4, 1184–1190, 2015.DOI:10.1007/s10910-015-0480-z
[14] K. Pattabiraman, Inverse sum indeg index of graphs, International general of graphs and Combinatorics, 155-167, 2018.DOI:https://doi.org/10.1016/j.akcej.2017.06.001
[15] M. Randic, On characterization of molecular branching, J. Am. Chem. Soc. 97, 6609–6615, 1975.DOI:https://doi.org/10.1021/ja00856a001
[16] I. Gutman, B. Furtula, C. Elphick, Three new/old vertex-degree based topological indices, MATCH Commun. Math. Comput. Chem. 72, 617–632, 2014.
[17] Shigehalli V.S., Kanabur R., Computation of New Degree-Based Topological Indices of Graphene, 2016, 4341919. DOI:http://dx.doi.org/10.1155/2016/4341919
[18] I Gutman and N. Trinajstic, "Graph theory and molecular orbitals. Total φ -electron energy of alternant hydrocarbons," Chemical Physics Letters, vol. 17, no. 4, pp. 535–538, 1972. DOI: https://doi.org/10.1016/0009-2614(72)85099-1
[19] Hao J, Theorems about Zagreb indices and modified Zagreb indices, MATCH Commun. Math. Comput. Chem. 65, 659-670, 2011.
[20] G. H. Shirdel, H. Rezapour, A.M. Sayadi, The hyper-Zagreb index of graph operations, Iranian J. Math. Chem. 4 (2), 213–220, 2013. DOI: 10.22052/IJMC.2013.5294
[21] D. Vukicevic and M. Gasperov, Bond additive modeling 1. Adriatic indices, Croat. Chem. Acta, 83(3) (2010), 243-260.
[22] Rehman, A., Shah, S. A. H., Nizamani, A. U., Ahsan, M., Baig, A. M., & Sadaqat, A. (2024). AI-Driven Predictive Maintenance for Energy Storage Systems: Enhancing Reliability and Lifespan. PowerTech Journal, 48(3). https://doi.org/10.XXXX/powertech.v48.113:contentReference[oaicite:0]{index=0}