

Degree-Based Topological Indices of Square of Alkanes

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Abstract : Graph operations are crucial in many applications of graph theory, as they allow large graphs to be constructed from smaller ones. This study focuses on one specific graph-theoretical operation: the square graph. Alkanes, which are the simplest hydrocarbons composed solely of hydrogen (H) and carbon (C) atoms without any functional groups, are the subject of our investigation. In this paper, we compute several topological indices for the square 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), Symmetric Division Deg Index (SDD). Additionally, we provide a graphical and numerical comparison of these topological indices.

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

1. Introduction

Consider an undirected chemical graph *G* with no loops or multiple edges. In such graphs, atoms are represented by vertices V , and the bonds between atoms are represented by edges *E*. The order of a graph is defined as the number of vertices in *G*, while the size of a graph is the number of edges. The degree of a vertex d_g is the number of edges connected to it. For further details on notations and terminologies, R. J. Wilson's book is recommended [1].The Handshaking Lemma, discovered by Leonard Euler in 1736, is particularly useful for calculating the total number of edges in a graph *G*. Often referred to as the first theorem of graph theory [2]. Chemical graph theory should be regarded not only as equivalent to other fields of Theoretical chemistry is not only equivalent to other fields but also complementary and crucial for a deeper understanding of the nature of chemical structures and modelling molecular structures. One of the most significant areas of graph theory includes quantitative structural properties (QSPR) and structural activity relationships (QSAR). Topological indices provide valuable information about the shape of a molecule. By converting a chemical structure into a numerical value, topological indices are particularly useful in QSPR/QSAR investigations. These indices play a vital role in helping chemists model the molecular structure of chemical compounds and study their chemical and physical characteristics. Various types of topological indices have been developed, such as degree-based [3][4][5], distance-based [6], and counting-related topological indices [7][8]. These indices are calculated for numerous graphs and many newly constructed graphs using different graph operations [9]. The concept of topological indices originated from 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:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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.

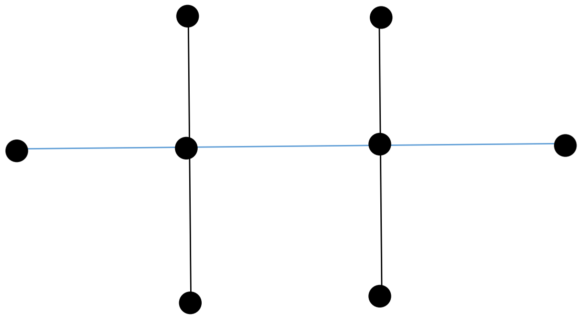

Figure 1 : C_2H_6

Definition 2.2 The square of a graph *G* is obtained from *G* by adding new edges between every two vertices having distance two in *G* and is denoted by G^2 .

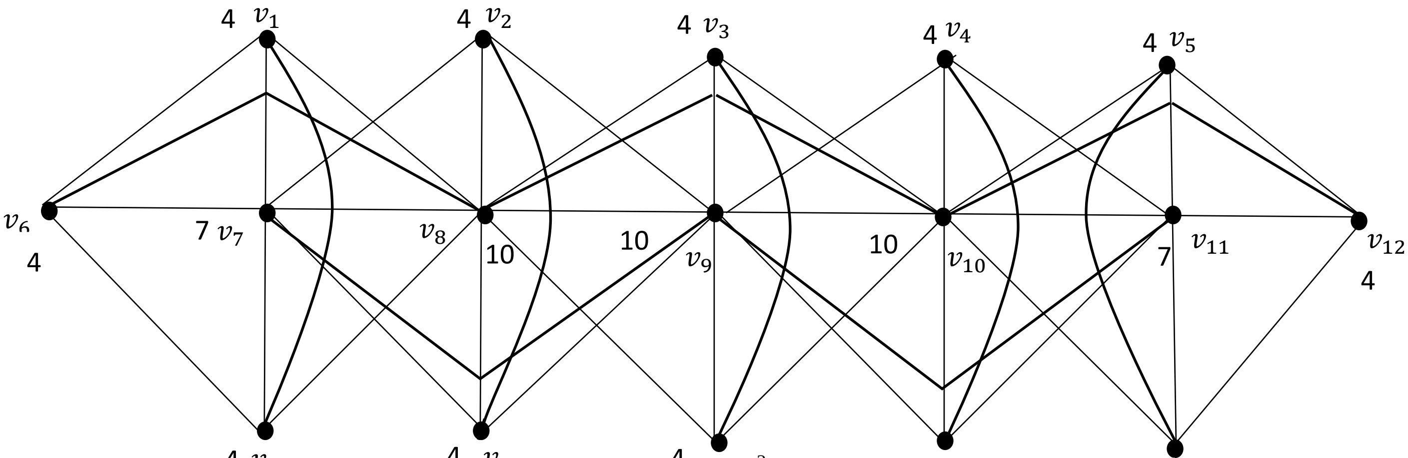

Figure 2 : $)^2$:

3. Topological Indices of Square of Alkanes

The vertex set of the square of alkane C_kH_{2k+2} is $3k+2$ and the edge set of the square of alkane C_kH_{2k+2} is $9k+1$. The edge set of the square of alkane is partitioned into five sets based on degree of the end vertices.

$E_{4,4}$	$E_{4,7}$	$E_{4,10}$	$E_{7,10}$	$E_{10,10}$
k + 4	10	6k - 10	4	2k - 7

Table 3. Edge set partition of Square of alkane

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

$$ABC\left[\left(C_kH_{2k+2}\right)^2\right]=1.523522981+k\left[\frac{12\sqrt{30}+5\sqrt{6}+12\sqrt{2}}{20}\right].$$

$$GA\left[\left(C_kH_{2k+2}\right)^2\right]=1.523058484+k\left[\frac{21+12\sqrt{10}}{7}\right]. \qquad k\geq 4$$

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

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

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

$$=(k+4)\sqrt{\frac{4+4-2}{4(4)}}+10\sqrt{\frac{4+7-2}{4(7)}}+(6k-10)\sqrt{\frac{4+10-2}{4(10)}}+4\sqrt{\frac{7+10-2}{7(10)}}+(2k-7)\sqrt{\frac{10+10-2}{10(10)}}$$

$$ABC\left[\left(C_kH_{2k+2}\right)^2\right]=1.523522981+k\left[\frac{12\sqrt{30}+5\sqrt{6}+12\sqrt{2}}{20}\right].$$

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

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

$$GA\left[\left(C_kH_{2k+2}\right)^2\right]=\sum_{E_{4,4}}\frac{2\sqrt{d_ud_v}}{d_u+d_v}+\sum_{E_{4,7}}\frac{2\sqrt{d_ud_v}}{d_u+d_v}+\sum_{E_{4,10}}\frac{2\sqrt{d_ud_v}}{d_u+d_v}+\sum_{E_{7,10}}\frac{2\sqrt{d_ud_v}}{d_u+d_v}+\sum_{E_{10,10}}\frac{2\sqrt{d_ud_v}}{d_u+d_v}$$

$$=(k+4)\left[\frac{2\sqrt{4(4)}}{4+4}\right]+10\left[\frac{2\sqrt{4(7)}}{4+7}\right]+(6k-10)\left[\frac{2\sqrt{4(10)}}{4+10}\right]+4\left[\frac{2\sqrt{7(10)}}{7+10}\right]+(2k-7)\left[\frac{2\sqrt{10(10)}}{10+10}\right]$$

$$GA\left[\left(C_kH_{2k+2}\right)^2\right]=1.523058484+k\left[\frac{21+12\sqrt{10}}{7}\right].$$

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

$$F\left[\left(C_kH_{2k+2}\right)^2\right]=1128k-1186.$$

$$ISI\left[\left(C_kH_{2k+2}\right)^2\right]=\left[\frac{204}{7}\right]k-13.64629488. \qquad k\geq 4$$

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

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

$$F\left[\left(C_kH_{2k+2}\right)^2\right]=\sum_{E_{4,4}}(d_u^2+d_v^2)+\sum_{E_{4,7}}(d_u^2+d_v^2)+\sum_{E_{4,10}}(d_u^2+d_v^2)+\sum_{E_{7,10}}(d_u^2+d_v^2)+\sum_{E_{10,10}}(d_u^2+d_v^2)$$

$$=(k+4)\left(4^2+4^2\right)+10\left(4^2+7^2\right)+\left(6k-10\right)\left(4^2+10^2\right)+4\left(7^2+10^2\right)+\left(2k-7\right)\left(10^2+10^2\right)$$

$$F\left[\left(C_kH_{2k+2}\right)^2\right]=1128k-1186.$$

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

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

$$ISI\left[\left(C_kH_{2k+2}\right)^2\right]=\sum_{E_{4,4}}\left[\frac{1}{\frac{1}{d_u}+\frac{1}{d_v}}\right]+\sum_{E_{4,7}}\left[\frac{1}{\frac{1}{d_u}+\frac{1}{d_v}}\right]+\sum_{E_{4,10}}\left[\frac{1}{\frac{1}{d_u}+\frac{1}{d_v}}\right]+\sum_{E_{7,10}}\left[\frac{1}{\frac{1}{d_u}+\frac{1}{d_v}}\right]+\sum_{E_{10,10}}\left[\frac{1}{\frac{1}{d_u}+\frac{1}{d_v}}\right]$$

$$=(k+4)\left[\frac{1}{\frac{1}{4}+\frac{1}{4}}\right]+10\left[\frac{1}{\frac{1}{4}+\frac{1}{7}}\right]+\left(6k-10\right)\left[\frac{1}{\frac{1}{4}+\frac{1}{10}}\right]+4\left[\frac{1}{\frac{1}{7}+\frac{1}{10}}\right]+\left(2k-7\right)\left[\frac{1}{\frac{1}{10}+\frac{1}{10}}\right]$$

$$ISI\left[\left(C_kH_{2k+2}\right)^2\right]=\left[\frac{204}{7}\right]k-13.64629488.$$

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

$\chi\left[\left(C_kH_{2k+2}\right)^2\right]$ is $\left[\frac{9+6\sqrt{10}}{20}\right]k+1.086774979$.

$RR\left[\left(C_kH_{2k+2}\right)^2\right]$ is $\left(24+12\sqrt{10}\right)k-30.86412592$. $\quad k\geq 4$

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

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

$$\chi\left[\left(C_kH_{2k+2}\right)^2\right]=\sum_{E_{4,4}}\left[\frac{1}{\sqrt{d_ud_v}}\right]+\sum_{E_{4,7}}\left[\frac{1}{\sqrt{d_ud_v}}\right]+\sum_{E_{4,10}}\left[\frac{1}{\sqrt{d_ud_v}}\right]+\sum_{E_{7,10}}\left[\frac{1}{\sqrt{d_ud_v}}\right]+\sum_{E_{10,10}}\left[\frac{1}{\sqrt{d_ud_v}}\right]$$

$$=(k+4)\left[\frac{1}{\sqrt{4(4)}}\right]+10\left[\frac{1}{\sqrt{4(7)}}\right]+\left(6k-10\right)\left[\frac{1}{\sqrt{4(10)}}\right]+4\left[\frac{1}{\sqrt{7(10)}}\right]+\left(2k-7\right)\left[\frac{1}{\sqrt{10(10)}}\right]$$

$$\chi\left[\left(C_kH_{2k+2}\right)^2\right]=\left[\frac{9+6\sqrt{10}}{20}\right]k+1.086774979.$$

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

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

$$RR\left[\left(C_kH_{2k+2}\right)^2\right]=\sum_{E_{4,4}}\sqrt{d_u d_v}+\sum_{E_{4,7}}\sqrt{d_u d_v}+\sum_{E_{4,10}}\sqrt{d_u d_v}+\sum_{E_{7,10}}\sqrt{d_u d_v}+\sum_{E_{10,10}}\sqrt{d_u d_v}$$

$$=(k+4)\sqrt{4(4)}+10\sqrt{4(7)}+(6k-10)\sqrt{4(10)}+4\sqrt{7(10)}+(2k-7)\sqrt{10(10)}$$

$$RR\left[\left(C_kH_{2k+2}\right)^2\right]=\left(24+12\sqrt{10}\right)k-30.86412592.$$

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

$$AG_1\left[\left(C_kH_{2k+2}\right)^2\right]=\left[\frac{30+21\sqrt{10}}{10}\right]k+0.3898284692$$

$$M_1\left[\left(C_kH_{2k+2}\right)^2\right]=132k-70 \qquad k\geq 4$$

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

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

$$AG_1\left[\left(C_kH_{2k+2}\right)^2\right]=\sum_{E_{4,4}}\left[\frac{d_u+d_v}{2\sqrt{d_u d_v}}\right]+\sum_{E_{4,7}}\left[\frac{d_u+d_v}{2\sqrt{d_u d_v}}\right]+\sum_{E_{4,10}}\left[\frac{d_u+d_v}{2\sqrt{d_u d_v}}\right]+\sum_{E_{7,10}}\left[\frac{d_u+d_v}{2\sqrt{d_u d_v}}\right]+\sum_{E_{10,10}}\left[\frac{d_u+d_v}{2\sqrt{d_u d_v}}\right]$$

$$=(k+4)\left[\frac{4+4}{2\sqrt{4(4)}}\right]+10\left[\frac{4+7}{2\sqrt{4(7)}}\right]+(6k-10)\left[\frac{4+10}{2\sqrt{4(10)}}\right]+4\left[\frac{7+10}{2\sqrt{7(10)}}\right]+(2k-7)\left[\frac{10+10}{2\sqrt{10(10)}}\right]$$

$$AG_1\left[\left(C_kH_{2k+2}\right)^2\right]=\left[\frac{30+21\sqrt{10}}{10}\right]k+0.3898284692.$$

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

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

$$M_1\left[\left(C_kH_{2k+2}\right)^2\right]=\sum_{E_{4,4}}\left(d_u+d_v\right)+\sum_{E_{4,7}}\left(d_u+d_v\right)+\sum_{E_{4,10}}\left(d_u+d_v\right)+\sum_{E_{7,10}}\left(d_u+d_v\right)+\sum_{E_{10,10}}\left(d_u+d_v\right)$$

$$=(k+4)(4+4)+10(4+7)+(6k-10)(4+10)+4(7+10)+(2k-7)(10+10)$$

$$M_1\left[\left(C_kH_{2k+2}\right)^2\right]=132k-70.$$

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

$$M_2\left[\left(C_kH_{2k+2}\right)^2\right]=456k-476$$

$$M_2^*(G)\left[\left(C_kH_{2k+2}\right)^2\right]=\left[\frac{93}{400}\right]k+\left[\frac{241}{700}\right]$$

$$HM\left[\left(C_kH_{2k+2}\right)^2\right]=2040k-2138 \qquad k\geq 4$$

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

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

.

$$M_2\left[\left(C_kH_{2k+2}\right)^2\right]=\sum_{E_{4,4}}\left(d_u\times d_v\right)+\sum_{E_{4,7}}\left(d_u\times d_v\right)+\sum_{E_{4,10}}\left(d_u\times d_v\right)+\sum_{E_{7,10}}\left(d_u\times d_v\right)+\sum_{E_{10,10}}\left(d_u\times d_v\right)$$

$$=(k+4)(4\times4)+10(4\times7)+(6k-10)(4\times10)+4(7\times10)+(2k-7)(10\times10)$$

$$M_2\left[\left(C_kH_{2k+2}\right)^2\right]=456k-476\,.$$

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

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

$$M_2^*(G)\left[\left(C_kH_{2k+2}\right)^2\right]=\sum_{E_{4,4}}\left[\frac{1}{d_ud_v}\right]+\sum_{E_{4,7}}\left[\frac{1}{d_ud_v}\right]+\sum_{E_{4,10}}\left[\frac{1}{d_ud_v}\right]+\sum_{E_{7,10}}\left[\frac{1}{d_ud_v}\right]+\sum_{E_{10,10}}\left[\frac{1}{d_ud_v}\right]$$

$$=(k+4)\left[\frac{1}{4(4)}\right]+10\left[\frac{1}{4(7)}\right]+(6k-10)\left[\frac{1}{4(10)}\right]+4\left[\frac{1}{7(10)}\right]+(2k-7)\left[\frac{1}{10(10)}\right]$$

$$M_2^*(G)\left[\left(C_kH_{2k+2}\right)^2\right]=\left[\frac{93}{400}\right]k+\left[\frac{241}{700}\right].$$

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

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

$$HM\left[\left(C_kH_{2k+2}\right)^2\right]=\sum_{E_{4,4}}\left(d_u+d_v\right)^2+\sum_{E_{4,7}}\left(d_u+d_v\right)^2+\sum_{E_{4,10}}\left(d_u+d_v\right)^2+\sum_{E_{7,10}}\left(d_u+d_v\right)^2+\sum_{E_{10,10}}\left(d_u+d_v\right)^2$$

$$=(k+4)(4+4)^2+10(4+7)^2+(6k-10)(4+10)^2+4(7+10)^2+(2k-7)(10+10)^2$$

$$HM\left[\left(C_kH_{2k+2}\right)^2\right]=2040k-2138\,.$$

Theorem 3.6. The Symmetric Division Deg index of Square of a alkane are given by

$$SDD\left[\left(C_kH_{2k+2}\right)^2\right]=\left[\frac{117}{5}\right]k-\left[\frac{229}{70}\right]. \qquad k\geq 4$$

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

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

$$SDD\left[\left(C_kH_{2k+2}\right)^2\right]=\sum_{E_{4,4}}\left[\frac{d_u^{\,2}+d_v^{\,2}}{d_ud_v}\right]+\sum_{E_{4,7}}\left[\frac{d_u^{\,2}+d_v^{\,2}}{d_ud_v}\right]+\sum_{E_{4,10}}\left[\frac{d_u^{\,2}+d_v^{\,2}}{d_ud_v}\right]+\sum_{E_{7,10}}\left[\frac{d_u^{\,2}+d_v^{\,2}}{d_ud_v}\right]+\sum_{E_{10,10}}\left[\frac{d_u^{\,2}+d_v^{\,2}}{d_ud_v}\right]$$

$$=(k+4)\left[\frac{4^2+4^2}{4(4)}\right]+10\left[\frac{4^2+7^2}{4(7)}\right]+(6k-10)\left[\frac{4^2+10^2}{4(10)}\right]+4\left[\frac{7^2+10^2}{7(10)}\right]+(2k-7)\left[\frac{10^2+10^2}{10(10)}\right]$$

$$SDD\left[\left(C_kH_{2k+2}\right)^2\right]=\left[\frac{117}{5}\right]k-\left[\frac{229}{70}\right].$$

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