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A NOTE ON SYMMETRIC DIVISION DEG ENERGY OF GRAPH AND IT'S APPLICATIONS

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Abstract. Symmetric division deg matrix is one of the degree based matrix of graph. Motivated by this, in this paper, we discuss the applications of symmetric division deg energy with respect to lower alkanes. We get a very good correlation with physical properties such as molar volumes(MV), molar refractions(MR) of alkanes. We further discuss the results on symmetric division deg energy with the consideration of minimum dominating set.

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1. Introduction

The energy of graph is an attractive and emerging subject for both researchers of mathematics and mathematical chemistry due to the remarkable applications of it. A conjugated hydrocarbon can be easily represented by a molecular graph. In molecular graph, vertices and edges are considered as follows. Carbon atoms will be considered as the vertices and bond between the carbon-carbon atoms will be considered as edges of the graph. Here Hydrogen atoms will be ignored. In 1978, Ivan Gutman [4] invented the concept of energy of graph, which is defined as the sum of the absolute values of the eigenvalues of the adjacency matrix of the graph. Many new matrix representations of different sort are introduced. Few matrices are based on degree of the vertices, (viz., Randic matrix, Sum connectivity matrix, Harmonic matrix etc.,) few are based on distance, eccentricity, coloring, partitioning, and some researchers linked the concepts of domination, covering, hub set, geodeic set concept with spectral graph theory. Symmetric division deg matrix was introduced by K. N Prakasha et. al., [10] and defined it as

$$SDD_{ij} = \begin{cases} \frac{min\{d_i,d_j\}}{max\{d_i,d_j\}} + \frac{max\{d_i,d_j\}}{min\{d_i,d_j\}} & \text{if } v_i \sim v_j, \\ 0 & otherwise. \end{cases}$$

Here d_i and d_j represents degree of the vertices v_i and v_j respectively.
We discuss the energy of two different sort of complements. They are as follows

Definition 1.1. [12] *The complement of a graph G is a graph $\overline{G}$ on the same vertices such that two distinct vertices of $\overline{G}$ are adjacent if and only if they are not adjacent in G.*

Definition 1.2. [12] *Let G be a graph and $P_k = \{V_1, V_2, ..., V_k\}$ be a partition of its vertex set V. Then the k-complement of G is obtained as follows: For all V_i and V_j in P_k, $i \neq j$ remove the edges between V_i and V_j and add the edges between the vertices of V_i and V_j which are not in G and is denoted by $\overline{(G)_k}$.*

Definition 1.3. [12] *Let G be a graph and $P_k = \{V_1,\ V_2,\ \cdots,\ V_k\}$ be a partition of its vertex set V. Then the $k(i)$-complement of G, is another sort of the complement of a graph, is obtained as follows: For each partition set V_r in P_k, remove the edges of G joining the vertices in V_r and add the edges of $\overline{G}$ (complement of G) joining the vertices of V_r, and is denoted by $\overline{G_{k(i)}}$.*

2. Applications of symmetric division deg energy by considering QSPR Analysis using Linear Regression Model

We consider the symmetric division deg energy $SDDE$ for modelling five physical properties such as surface tension(ST), boiling point(BP), molar volumes(MV), molar refractions(MR) and heats of vaporization(HV) of lower alkanes. We have tested the following linear regression model

$$P = a + b(SDDE) \tag{1}$$

where, P =physical property and $SDDE$ =symmetric division deg energy.
The below table gives the SDDE energy and five physical properties. The values of five physical properties are taken from [7], [8] and [13].

Table 1: Symmetric division deg energy, surface tension(st), boiling point(BP), molar volumes(MV), molar refractions(MR) and heats of vaporization(HV) of lower alkanes.

Alkane	SDD-Energy	ST	BP	MV	MR	HV
Butane	10.7703	12.46	152.01	100.4	24.3	22.44
Pentane	12.5498	16	36.1	115.2	25.27	26.4
2-Methylbutane	15.0643	15	27.9	116.4	25.29	24.6
Hexane	15.7506	18.42	68.7	130.7	29.91	31.6
2-Methylpentane	16.6411	17.38	60.3	131.9	29.95	29.9
3-Methylpentane	18.1773	18.12	63.3	129.7	29.8	30.3
2,2-Dimethylbutane	20.3464	16.3	49.7	132.7	29.93	27.7
2,3-Dimethylbutane	19.2756	17.37	58	130.2	29.81	29.1
Heptane	17.7859	20.26	98.4	146.5	34.55	36.6
2-Methylhexane	20.1909	19.29	90.1	147.7	34.59	34.8
3-Methylhexane	19.8584	19.79	91.9	145.8	34.46	35.1
3-Ethylhexane	22.0913	20.44	93.5	143.5	34.28	35.2
2,2-Dimethylpentane	21.8588	18.02	79.2	148.7	34.62	32.4
2,3-Dimethylpentane	22.3384	19.96	89.8	144.2	34.32	34.2

2,4-Dimethylpentane	20.6726	18.15	80.5	148.9	34.62	32.9
3,3-Dimethylpentane	23.4312	19.59	86.1	144.5	34.33	33
2,3,3-Trimethylbutane	24.5072	18.76	80.9	145.2	34.37	32
Octane	20.7924	21.76	125.7	162.6	39.19	41.5
2-Methylheptane	21.9368	20.6	117.6	163.7	39.23	39.7
3-Methylheptane	23.1285	21.17	118.9	161.8	39.1	39.8
4-Methylheptane	21.5057	21	117.7	162.1	39.12	39.7
3-Ethylhexane	22.0913	21.51	118.5	160.1	38.94	39.4
2,2-Dimethylhexane	25.2438	19.6	106.8	164.3	39.25	37.3
2,3-Dimethylhexane	24.0281	20.99	115.6	160.4	38.98	38.8
2,4-Dimethylhexane	23.9215	20.05	109.4	163.1	39.13	37.8
2,5-Dimethylhexane	24.2330	19.73	109.1	164.7	39.26	37.9
3,3-Dimethylhexane	24.9824	20.63	112	160.9	39.01	37.9
3,4-Dimethylhexane	25.4148	21.62	117.7	158.8	38.85	39
3-Ethyl-2-methylpentane	22.94	21.52	115.7	158.8	38.84	38.5
3-Ethyl-3-methylpentane	26.0390	21.99	118.3	157	38.72	38
2,2,3-Trimethylpentane	27.5529	20.67	109.8	159.5	38.92	36.9
2,2,4-Trimethylpentane	25.8675	18.77	99.2	165.1	39.26	36.1
2,3,3-Trimethylpentane	26.2640	21.56	114.8	157.3	38.76	37.2
2,3,4-Trimethylpentane	26.4878	21.14	113.5	158.9	38.87	37.6
Nonane	22.9543	22.92	150.8	178.7	43.84	46.4
Decane	25.8560	23.83	344.45	196	42.5	51.42
2-Methyloctane	25.0094	21.88	143.3	179.8	43.88	44.7
3-Methyloctane	25.1229	22.34	144.2	178	43.73	44.8
4-Methyloctane	24.8011	22.34	142.5	178.2	43.77	44.8
3-Ethylheptane	24.2058	22.81	143	176.4	43.64	44.8
4-Ethylheptane	24.0964	22.81	141.2	175.7	43.49	44.8
2,2-Dimethylheptane	27.1732	20.8	132.7	180.5	43.91	42.3
2,3-Dimethylheptane	27.2939	22.34	140.5	176.7	43.63	43.8
2,4-Dimethylheptane	25.559	21.3	133.5	179.1	43.74	42.9
2,5-Dimethylheptane	27.3698	21.3	136	179.4	43.85	42.9
2,6-Dimethylheptane	26.0710	20.83	135.2	180.9	43.93	42.8

3,3-Dimethylheptane	28.3425	22.01	137.3	176.9	43.69	42.7
3,4-Dimethylheptane	27.1018	22.8	140.6	175.3	43.55	43.8
3,5-Dimethylheptane	27.1533	21.77	136	177.4	43.64	43
4,4-Dimethylheptane	26.5254	22.01	135.2	176.9	43.6	42.7
3-Ethyl-2-methylhexane	26.1443	22.8	138	175.4	43.66	43.8
4-Ethyl-2-methylhexane	25.4970	21.77	133.8	177.4	43.65	43
3-Ethyl-3-methylhexane	27.6812	23.22	140.6	173.1	43.27	43
3-Ethyl-4-methylhexane	26.09	23.27	140.46	172.8	43.37	44
2,2,3-Trimethylhexane	29.2456	21.86	133.6	175.9	43.62	41.9
2,2,4-Trimethylhexane	29.1285	20.51	126.5	179.2	43.76	40.6
2,2,5-Trimethylhexane	29.4971	20.04	124.1	181.3	43.94	40.2
2,3,3-Trimethylhexane	29.1098	22.41	137.7	173.8	43.43	42.2
2,3,4-Trimethylhexane	29.5671	22.8	139	173.5	43.39	42.9
2,3,5-Trimethylpentane	28.0942	21.27	131.3	177.7	43.65	41.4
2,4,4-Trimethylhexane	29.0046	21.17	130.6	177.2	43.66	40.8
3,3,4-Trimethylhexane	30.6074	23.27	140.5	172.1	43.34	42.3
3,3-Diethylpentane	26.1803	23.75	146.2	170.2	43.11	43.4
2,2-Dimethyl-3-ethylpentane	28.0921	22.38	133.8	174.5	43.46	42
2,3-Dimethyl-3-ethylpentane	29.5053	23.87	142	170.1	42.95	42.6
2,4-Dimethyl-3-ethylpentane	26.7960	22.8	136.7	173.8	43.4	42.9
2,2,3,3-Tetramethylpentane	32.7512	23.38	140.3	169.5	43.21	41
2,2,3,4-Tetramethylpentane	31.1081	21.98	133	173.6	43.44	41
2,2,4,4-Tetramethylpentane	31.0549	20.37	122.3	178.3	43.87	38.1
2,3,3,4-Tetramethylpentane	31.6715	23.31	141.6	169.9	43.2	41.8

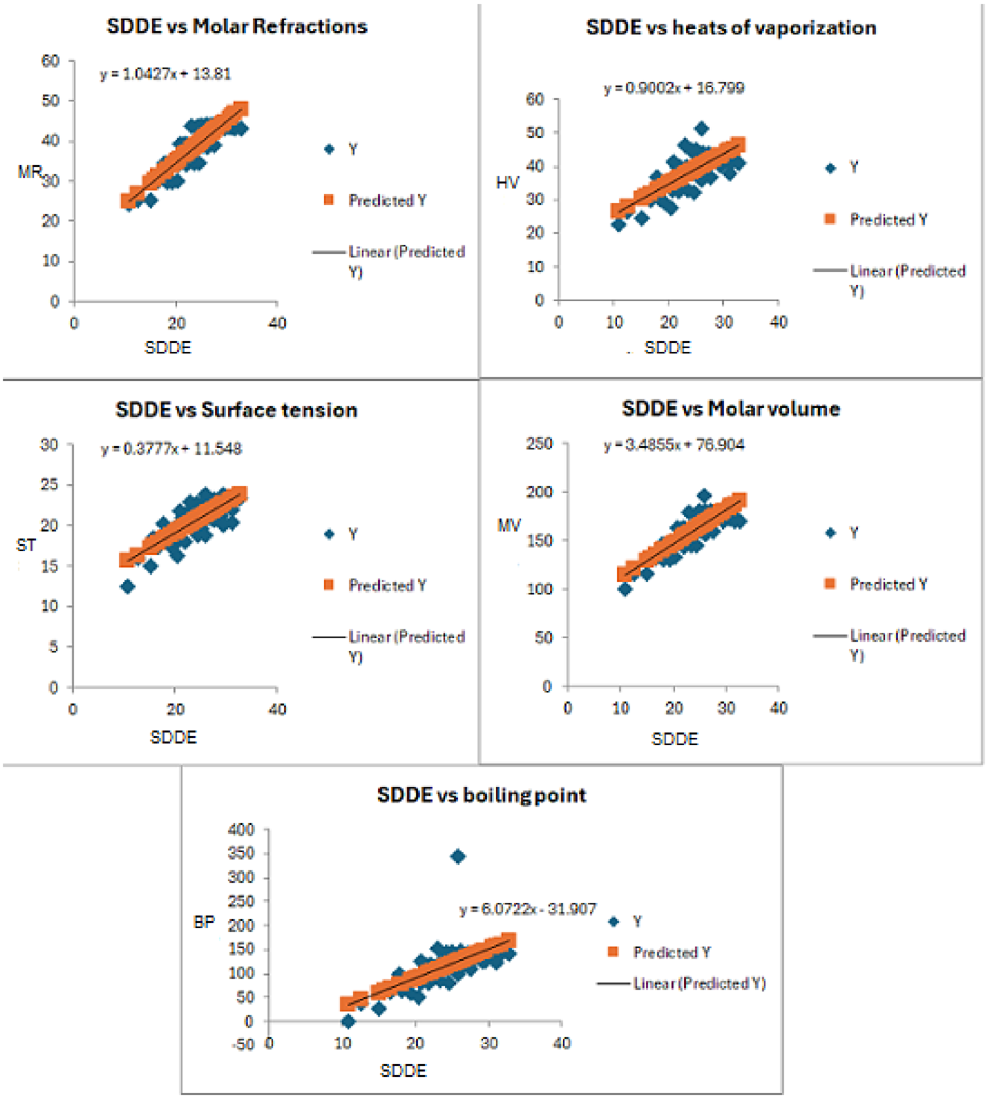

FIGURE 1. Linear fitting of the $SDDE$ with physical properties.

(In Figure 1, X stands for SDDE and Y stands for respective physical property.) We obtained the above linear models of the $SDDE$ with physical properties. Using equation 1, we can get the different linear equations for symmetric division deg energy and physical properties.

$$
\begin{aligned}
BP &= 6.0722[SDDE] - 31.907 \\
MV &= 3.4855[SDDE] + 76.904 \\
MR &= 1.0427[SDDE] + 13.81 \\
HV &= 0.9022[SDDE] + 16.799 \\
ST &= 0.3777[SDDE] + 15.647
\end{aligned}
$$

The correlation coefficient of the symmetric division deg energy with surface tension(ST), boiling point(BP), molar volumes(MV), molar refractions(MR) and heats of vaporization(HV) of lower alkanes are given in Table 2. The numbers highlighted in bold font indicates a high correlation between the symmetric division deg energy and the physico-chemical properties of lower alkanes.

Table 2: Correlation coefficient value of symmetric division deg energy with surface tension(ST), boiling point(BP), molar volumes(MV), molar refractions(MR) and heats of vaporization(HV) of lower alkanes.

ST	BP	MV	MR	HV
0.7628	0.6398	**0.8313**	**0.8706**	**0.7217**

The QSPR study of $SDDE$ reveals that can be useful in predicting the molar refractions and molar volumes of lower alkanes. Also from Table 2, one can easily verify that $SDDE(G)$ shows good correlation with surface tension(ST), molar volumes(MV), molar refractions(MR) and heats of vaporization(HV) of lower alkanes.

3. Extension of symmetric division deg energy by considering minimum dominating set

For a graph G, with vertex set $V = \{v_1, v_2, v_3, ..., v_n\}$, a subset D of V is called a dominating set of G if every vertex of $V - D$ is adjacent to some vertex in D [9].

Any dominating set with minimum cardinality is called a minimum dominating set[9]. Here we consider D as minimum dominating set. For more details on few energies related to domination sets refer [9], [11] and [14]. Motivated by the symmetric division deg matrix, in this paper we associate minimum dominating symmetric division deg matrix as follows.

$$SDD^D_{ij} = \begin{cases} \frac{min\{d_i,d_j\}}{max\{d_i,d_j\}} + \frac{max\{d_i,d_j\}}{min\{d_i,d_j\}} & \text{if } v_i \sim v_j, \\ 1 & \text{if } i = j \text{ and } v_i \in D, \\ 0 & otherwise. \end{cases}$$

Let χ_i represents minimum dominating symmetric division deg eigenvalues, then the minimum dominating symmetric division deg energy is given by

$$SDDE^D(G) = \sum_{i=1}^{n} |\chi_i| \tag{2}$$

Consider a dominating set υ, which represents any dominating set. As there are plethora of domination sets, we considered domination set which is in general represents any sort of domination such as minimum dominating set, global dominating set, double dominating set, total dominating set, restrained dominating set etc.,

Proposition 3.1. *The first three coefficients of* $\Phi^{\upsilon}(G,\chi)$ *are given as follows:*
(*i*) $a_0 = 1$,
(*ii*) $a_1 = -|\upsilon|$,
(*iii*) $a_2 = |\upsilon|C_2 - \sum_{i<j}\left(\frac{d_i}{d_j}+\frac{d_j}{d_i}\right)^2$.

Proof. (*i*) From the definition of characteristic polynomial $\Phi^{\upsilon}(G,\chi) = det[\chi I - SDD^{\upsilon}(G)]$, we get $a_0 = 1$.

(*ii*) Consider the sum of determinants of all 1×1 principal submatrices of $SDD^{\upsilon}(G)$ which is equal to the trace of $SDD^{\upsilon}(G)$.
$\Rightarrow a_1 = (-1)^1$ trace of $[SDD^{\upsilon}(G)] = -|\upsilon|$.

(*iii*)

$$\begin{aligned}(-1)^2 a_2 &= \sum_{1\leq i<j\leq n}\begin{vmatrix} a_{ii} & a_{ij}\\ a_{ji} & a_{jj}\end{vmatrix}\\ &= \sum_{1\leq i<j\leq n} a_{ii}a_{jj} - a_{ji}a_{ij}\end{aligned}$$

At $i = j$, the entry of the matrix will take the values 0 or 1 depends on the vertex belongs to dominating set or not.

$$= |\upsilon|C_2 - \sum_{i<j}\left(\frac{d_i}{d_j}+\frac{d_j}{d_i}\right)^2$$

□

Proposition 3.2. *If* $\chi_1, \chi_2, \ldots, \chi_n$ *are symmetric division deg eigenvalues of* $SDD^{\upsilon}(G)$*, then*

$$\sum_{i=1}^{n} {\chi_i}^2 = |\upsilon| + 2\sum_{i<j}\left(\frac{d_i}{d_j}+\frac{d_j}{d_i}\right)^2.$$

Proof. We know that

$$\begin{aligned}\sum_{i=1}^{n}\chi_i^2 &= 2\sum_{i<j}(a_{ij})^2 + |\upsilon|\\ &= |\upsilon| + 2\sum_{i<j}\left(\frac{d_i}{d_j}+\frac{d_j}{d_i}\right)^2.\end{aligned}$$

□

Theorem 3.3. *Let G be a graph with n vertices, then*

$$SDDE^{\upsilon}(G) \leq \sqrt{n\left(|\upsilon| + 2\sum_{i<j}\left(\frac{d_i}{d_j}+\frac{d_j}{d_i}\right)^2\right)}.$$

Proof. Let $\chi_1, \chi_2, \ldots, \chi_n$ be the eigenvalues of $P_k(G)$.
Now by Cauchy - Schwartz inequality we have

$$\left(\sum_{i=1}^{n} a_i b_i\right)^2 \leq \left(\sum_{i=1}^{n} {a_i}^2\right)\left(\sum_{i=1}^{n} {b_i}^2\right).$$

Let $a_i = 1$, $b_i =\mid \chi_i \mid$. Then
then

$$\left(\sum_{i=1}^{n} |\chi_i|\right)^2 \leq \left(\sum_{i=1}^{n} 1\right)\left(\sum_{i=1}^{n} |\chi_i|^2\right)$$

$$[SDDE^{v}]^2 \leq n\left(|v| + 2\sum_{i<j}\left(\frac{d_i}{d_j} + \frac{d_j}{d_i}\right)^2\right)$$

$$[SDDE^{v}] \leq \sqrt{n\left(|v| + 2\sum_{i<j}\left(\frac{d_i}{d_j} + \frac{d_j}{d_i}\right)^2\right)}.$$

This is an upper bound for $SDDE^{v}(G)$. □

Theorem 3.4. *Let G be a graph with n vertices. If $det(SDD^{v}(G))$ represents determinant of the matrix $SDD^{v}(G)$, then*

$$SDDE^{v}(G) \geq \sqrt{\left(|v| + 2\sum_{i<j}\left(\frac{d_i}{d_j} + \frac{d_j}{d_i}\right)^2\right) + n(n-1)(det(SDD^{v}(G)))^{\frac{2}{n}}}.$$

Theorem 3.5. *Let χ_1 be the largest minimum dominating symmetric division deg eigenvalue, then*

$$\chi_1(G) \geq \frac{2\sum_{i<j}\left(\frac{d_i}{d_j} + \frac{d_j}{d_i}\right) + k}{n}$$

where k is the domination number.

Proof. Here we consider X as any nonzero vector, then by using Lemma 3.17 of [2], we have,

$$\chi_1(G) = \max_{X \neq 0} \frac{X' A X}{X' X}$$

$$\chi_1(G) \geq \max_{X \neq 0} \frac{J' P^{v} J}{J' J} = \frac{2\sum_{i<j}\left(\frac{d_i}{d_j} + \frac{d_j}{d_i}\right) + k}{n}.$$

Here J represents a unit matrix. □

4. Symmetric division deg energy of some standard graphs

The important result in the spectral theory of trees is [5]

$$\phi(T,\lambda) = \lambda^n + \sum_{k\geq n}(-1)^k m(T,k)\lambda^{n-2k}$$

Here $m(T,k)$ stands for the number of $k-$matchings (= selections of k mutually independent edges) in the tree T. By definition, $m(T,1) = n-1$. The coefficient $m_{TI}(T,k)$ is equal to the sum of weights coming from all k-matchings of T.

Theorem 4.1. *Let T be a tree with $n \geq 4$ vertices*

$$SDDE(T) \geq E(T).$$

Proof. Here d_i and d_j be the degrees of the vertices. For $n \geq 4$,

$$\frac{min\{d_i,d_j\}}{max\{d_i,d_j\}} + \frac{max\{d_i,d_j\}}{min\{d_i,d_j\}} > 1.$$

Since the topological index $SDD(T) > 1$, then the corresponding energy will be

$$SDDE(T) \geq E(T)$$

□

For next two results $E(G)$ represents energy of graph with respect to adjacency matrix.

Theorem 4.2. *Let G be a regular graph of n vertices with regularity r, then*

$$SDDE(G) = 2E(G)$$

Theorem 4.3. *Let G be a semi-regular graph of of degrees $r \geq 1$ and $s \geq 1$, then*

$$SDDE(G) = \left(\frac{r^2+s^2}{rs}\right)E(G)$$

In next results $SDDE^D(G)$ represents minimum dominating symmetric division deg energy and $SDD^D(G)$ represents minimum dominating symmetric division deg matrix.

Theorem 4.4. *The minimum dominating symmetric division deg energy of a complete graph K_n is $SDDE^D(K_n) = 2(n-2) + \sqrt{4n^2-4n+9}$.*

Proof. The minimum dominating set $= D = \{v_1\}$. The minimum dominating symmetric division deg matrix is

$$SDD^D(K_n) = \begin{bmatrix} 1 & 2 & 2 & \dots & 2 & 2 \\ 2 & 0 & 2 & \dots & 2 & 2 \\ 2 & 2 & 0 & \dots & 2 & 2 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 2 & 2 & 2 & \dots & 0 & 2 \\ 2 & 2 & 2 & \dots & 2 & 0 \end{bmatrix}.$$

$$SDD^{v}(K_n) = \begin{vmatrix} \chi-1 & -2 & -2 & \dots & -2 & -2 \\ -2 & \chi & -2 & \dots & -2 & -2 \\ -2 & -2 & \chi & \dots & -2 & -2 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -2 & -2 & -2 & \dots & \chi & -2 \\ -2 & -2 & -2 & \dots & -2 & \chi \end{vmatrix}.$$

Characteristic equation is

$$(\chi+2)^{n-2}(\chi^2-(2n-3)\chi-2n)=0$$

and the spectrum is $Spec^{D}_{SDD}(K_n) = \begin{pmatrix} -2 & \frac{(2n-3)+\sqrt{4n^2-4n+9}}{2} & \frac{(2n-3)-\sqrt{4n^2-4n+9}}{2} \\ n-2 & 1 & 1 \end{pmatrix}$.

Therefore, $SDDE^{D}(K_n) = 2(n-2)+\sqrt{4n^2-4n+9}$. □

Theorem 4.5. *The minimum dominating symmetric division deg energy of star graph $K_{1,n-1}$ is*

$$SDDE^{D}(K_{1,n-1}) = \sqrt{1+\frac{4(n^2-2n+2)^2}{n-1}}.$$

Proof. The minimum dominating set $= D = \{v_0\}$. The minimum dominating symmetric division deg matrix is

$$SDD^{D}(K_{1,n-1}) = \begin{bmatrix} 1 & \frac{n^2-2n+2}{n-1} & \frac{n^2-2n+2}{n-1} & \dots & \frac{n^2-2n+2}{n-1} & \frac{n^2-2n+2}{n-1} \\ \frac{n^2-2n+2}{n-1} & 0 & 0 & \dots & 0 & 0 \\ \frac{n^2-2n+2}{n-1} & 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{n^2-2n+2}{n-1} & 0 & 0 & \dots & 0 & 0 \\ \frac{n^2-2n+2}{n-1} & 0 & 0 & \dots & 0 & 0 \end{bmatrix}.$$

$$\begin{vmatrix} \chi-1 & -\frac{n^2-2n+2}{n-1} & -\frac{n^2-2n+2}{n-1} & \dots & -\frac{n^2-2n+2}{n-1} & -\frac{n^2-2n+2}{n-1} \\ -\frac{n^2-2n+2}{n-1} & \chi & 0 & \dots & 0 & 0 \\ -\frac{n^2-2n+2}{n-1} & 0 & \chi & \dots & 0 & 0 \\ -\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -\frac{n^2-2n+2}{n-1} & 0 & 0 & \dots & \chi & 0 \\ -\frac{n^2-2n+2}{n-1} & 0 & 0 & \dots & 0 & \chi \end{vmatrix}.$$

Characteristic equation is

$$\chi^{n-2}\left[\chi^2-\chi-\frac{(n^2-2n+2)^2}{n-1}\right]=0$$

spectrum is $Spec^{D}_{SDD}(K_{1,n-1}) =$

$$\begin{pmatrix} 0 & \frac{1}{2}+\frac{1}{2}\sqrt{1+\frac{4(n^2-2n+2)^2}{n-1}} & \frac{1}{2}-\frac{1}{2}\sqrt{1+\frac{4(n^2-2n+2)^2}{n-1}} \\ n-2 & 1 & 1 \end{pmatrix}.$$

Therefore, $SDDE^{D}(K_{1,n-1}) = \sqrt{1+\frac{4(n^2-2n+2)^2}{n-1}}$. □

Definition 4.6. [6] *The double star graph $S_{n,m}$ is the graph constructed upon joining the centers v_0 and u_0 of two star graphs $K_{1,n-1}$ and $K_{1,m-1}$. The double star graph $S_{n,m}$ is basically a bipartite graph which will be having the vertex set $V(S_{n,m}) = V(K_{1,n-1}) \cup V(K_{1,m-1})$ and the edge set $E(S_{n,m}) = \{v_0u_0; v_0v_i; u_0u_j : 1 \leq i \leq n-1, 1 \leq i \leq n-1\}$*

Theorem 4.7. *The minimum dominating symmetric division deg energy of Double star graph $S_{n,n}$ is*

$$SDDE^D(S_{n,n}) = \sqrt{9 + \frac{4(n-1)(n^2+1)^2}{n^2}} + \sqrt{1 + \frac{4(n-1)(n^2+1)^2}{n^2}}.$$

Proof. The minimum dominating set $= D = \{u_0, v_0\}$. The minimum dominating symmetric division deg matrix is

$$\begin{bmatrix} 1 & n+\frac{1}{n} & n+\frac{1}{n} & \dots & n+\frac{1}{n} & 2 & 0 & 0 & \dots & 0 \\ n+\frac{1}{n} & 0 & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\ n+\frac{1}{n} & 0 & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ n+\frac{1}{n} & 0 & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\ 2 & 0 & 0 & \dots & 0 & 1 & n+\frac{1}{n} & n+\frac{1}{n} & \dots & n+\frac{1}{n} \\ 0 & 0 & 0 & \dots & 0 & n+\frac{1}{n} & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & n+\frac{1}{n} & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & \dots & 0 & n+\frac{1}{n} & 0 & 0 & \dots & 0 \end{bmatrix}.$$

The characteristic polynomial is

$$\begin{vmatrix} \chi-1 & -n-\frac{1}{n} & -n-\frac{1}{n} & \dots & -n-\frac{1}{n} & -2 & 0 & 0 & \dots & 0 \\ -n-\frac{1}{n} & \chi & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\ -n-\frac{1}{n} & 0 & \chi & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -n-\frac{1}{n} & 0 & 0 & \dots & \chi & 0 & 0 & 0 & \dots & 0 \\ -2 & 0 & 0 & \dots & 0 & \chi-1 & -n-\frac{1}{n} & -n-\frac{1}{n} & \dots & -n-\frac{1}{n} \\ 0 & 0 & 0 & \dots & 0 & -n-\frac{1}{n} & \chi & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & -n-\frac{1}{n} & 0 & \chi & \dots & 0 \\ 0 & 0 & 0 & \dots & 0 & -n-\frac{1}{n} & 0 & 0 & \dots & \chi \end{vmatrix}.$$

Characteristic equation is

$$(\chi)^{2n-4}[\chi^2 + \chi - \frac{(n-1)(n^2+1)^2}{n^2}][\chi^2 - 3\chi - \frac{(n-1)(n^2+1)^2}{n^2}] = 0$$

Hence, spectrum is

$$\begin{pmatrix} 0 & \frac{-1+B}{2} & \frac{-1-B}{2} & \frac{3+\sqrt{9+\frac{4(n-1)(n^2+1)^2}{n^2}}}{2} & \frac{3-\sqrt{9+\frac{4(n-1)(n^2+1)^2}{n^2}}}{2} \\ 2n-4 & 1 & 1 & 1 & 1 \end{pmatrix}$$

where $B = \sqrt{1 + \frac{4(n-1)(n^2+1)^2}{n^2}}$.

$$SDDE^D(S_{n,n}) = \sqrt{9 + \frac{4(n-1)(n^2+1)^2}{n^2}} + \sqrt{1 + \frac{4(n-1)(n^2+1)^2}{n^2}}.$$

□

Theorem 4.8. *The minimum dominating symmetric division deg energy of complete bipartite graph $K_{n,n}$ is*

$$SDDE^{\upsilon}(K_{n,n}) = (2n+1) + \sqrt{4n^2+4n-7}.$$

Proof. The minimum dominating set $= D = \{u_1, v_1\}$. The minimum dominating symmetric division deg matrix is

$$SDD^D(K_{n,n}) = \begin{bmatrix} 1 & 0 & 0 & 0 & \dots & 2 & 2 & 2 & 2 \\ 0 & 0 & 0 & 0 & \dots & 2 & 2 & 2 & 2 \\ 0 & 0 & 0 & 0 & \dots & 2 & 2 & 2 & 2 \\ 0 & 0 & 0 & 0 & \dots & 2 & 2 & 2 & 2 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 2 & 2 & 2 & 2 & \dots & 1 & 0 & 0 & 0 \\ 2 & 2 & 2 & 2 & \dots & 0 & 0 & 0 & 0 \\ 2 & 2 & 2 & 2 & \dots & 0 & 0 & 0 & 0 \\ 2 & 2 & 2 & 2 & \dots & 0 & 0 & 0 & 0 \end{bmatrix}.$$

The characteristic polynomial is

$$\begin{vmatrix} \chi-1 & 0 & 0 & 0 & \dots & -2 & -2 & -2 & -2 \\ 0 & \chi & 0 & 0 & \dots & -2 & -2 & -2 & -2 \\ 0 & 0 & \chi & 0 & \dots & -2 & -2 & -2 & -2 \\ 0 & 0 & 0 & \chi & \dots & -2 & -2 & -2 & -2 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ -2 & -2 & -2 & -2 & \dots & \chi-1 & 0 & 0 & 0 \\ -2 & -2 & -2 & -2 & \dots & 0 & \chi & 0 & 0 \\ -2 & -2 & -2 & -2 & \dots & 0 & 0 & \chi & 0 \\ -2 & -2 & -2 & -2 & \dots & 0 & 0 & 0 & \chi \end{vmatrix}.$$

Characteristic equation is

$$(\chi)^{2n-4}[\chi^2-(2n+1)\chi-(2n-2)][\chi^2+(2n-1)\chi-(2n-2)] = 0$$

Hence, spectrum is $Spec^D_{SDD}(K_{n,n})$
$=\begin{pmatrix} 0 & \frac{-(2n-1)+C}{2} & \frac{-(2n-1)-C}{2} & \frac{(2n+1)+D}{2} & \frac{(2n+1)-D}{2} \\ (2n-4) & 1 & 1 & 1 & 1 \end{pmatrix}.$
$C = \sqrt{4n^2+4n-7}$ and $D = \sqrt{4n^2-4n+9}$
Therefore, $SDDE^D(K_{n,n}) = (2n+1) + \sqrt{4n^2+4n-7}$. □

Theorem 4.9. *The minimum dominating symmetric division deg energy of a crown graph S_n^0 is*

$$SDDE^D(S_n^0) = (4n-8) + \sqrt{4n^2-4n+9} + \sqrt{4n^2+4n-7}$$

Proof. Let S_n^0 be the crown graph of order $2n$ and let the vertex set of this graph be $\{u_1, u_2, \cdots, u_n, v_1, v_2, \cdots, v_n\}$. The minimum dominating symmetric division deg matrix of S_n^0 is

$$SDD^D(S_n^0) = \begin{bmatrix} 1 & 0 & 0 & \ldots & 0 & 0 & 2 & \ldots & 2 & 2 \\ 0 & 0 & 0 & \ldots & 0 & 2 & 0 & \ldots & 2 & 2 \\ 0 & 0 & 0 & \ldots & 0 & 2 & 2 & \ldots & 0 & 2 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & 0 & 2 & 2 & \ldots & 2 & 0 \\ 0 & 2 & 2 & \ldots & 2 & 1 & 0 & \ldots & 0 & 0 \\ 2 & 0 & 2 & \ldots & 2 & 0 & 0 & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 2 & 2 & 0 & \ldots & 2 & 0 & 0 & \ldots & 0 & 0 \\ 2 & 2 & 2 & \ldots & 0 & 0 & 0 & \ldots & 0 & 0 \end{bmatrix}$$

$$SDD^D(S_n^0) = \begin{vmatrix} \chi-1 & 0 & 0 & \ldots & 0 & 0 & 2 & \ldots & 2 & -2 \\ 0 & \chi & 0 & \ldots & 0 & -2 & 0 & \ldots & -2 & -2 \\ 0 & 0 & \chi & \ldots & 0 & -2 & -2 & \ldots & 0 & -2 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & \chi & -2 & -2 & \ldots & -2 & 0 \\ 0 & -2 & -2 & \ldots & -2 & \chi-1 & 0 & \ldots & 0 & 0 \\ -2 & 0 & -2 & \ldots & -2 & 0 & \chi & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -2 & -2 & 0 & \ldots & -2 & 0 & 0 & \ldots & \chi & 0 \\ -2 & -2 & -2 & \ldots & 0 & 0 & 0 & \ldots & 0 & \chi \end{vmatrix}$$

The characteristic polynomial is

$$(\chi-2)^{n-2}(\chi+2)^{n-2}(\chi^2+(2n-5)\chi-(6n-8))(\chi^2+(2n-3)\chi-2n)=0$$

implying that the spectrum is
$Spec_{SDD^D}(S_n^0) =$

$$\begin{pmatrix} 2 & -2 & \frac{(2n-3)+A}{2} & \frac{(2n-3)-A}{2} & \frac{-(2n-5)+\sqrt{4n^2+4n-7}}{2} & \frac{-(2n-5)-\sqrt{4n^2+4n-7}}{2} \\ n-2 & n-2 & 1 & 1 & n-1 & n-1 \end{pmatrix}.$$

Here $A = \sqrt{4n^2-4n+9}$. Therefore, we obtain

$$SDDE^D(S_n^0) = (4n-8) + \sqrt{4n^2-4n+9} + \sqrt{4n^2+4n-7}.$$

□

Theorem 4.10. *The minimum dominating symmetric division deg energy of the cocktail party graph $K_{n\times 2}$ is*

$$SDDE^D(K_{n\times 2}) = (4n-7) + \sqrt{16n^2-8n+17}.$$

Proof. Let $K_{n\times 2}$ be the cocktail party graph of order $2n$ having vertex set $\{u_1, u_2, \cdots, u_n, v_1, v_2, \cdots, v_n\}$. The minimum dominating symmetric division deg matrix is

$$SDD^D(K_{n\times 2}) = \begin{bmatrix} 1 & 0 & 2 & 2 & \ldots & 2 & 2 & 2 & 2 \\ 0 & 1 & 2 & 2 & \ldots & 2 & 2 & 2 & 2 \\ 2 & 2 & 0 & 0 & \ldots & 2 & 2 & 2 & 2 \\ 2 & 2 & 0 & 0 & \ldots & 2 & 2 & 2 & 2 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 2 & 2 & 2 & 2 & \ldots & 0 & 0 & 2 & 2 \\ 2 & 2 & 2 & 2 & \ldots & 0 & 0 & 2 & 2 \\ 2 & 2 & 2 & 2 & \ldots & 2 & 2 & 0 & 0 \\ 2 & 2 & 2 & 2 & \ldots & 2 & 2 & 0 & 0 \end{bmatrix}$$

The characteristic polynomial is

$$\begin{vmatrix} \chi-1 & 0 & -2 & -2 & \ldots & -2 & -2 & -2 & -2 \\ 0 & \chi-1 & -2 & -2 & \ldots & -2 & -2 & -2 & -2 \\ -2 & -2 & 0 & 0 & \ldots & -2 & -2 & -2 & -2 \\ -2 & -2 & 0 & 0 & \ldots & -2 & -2 & -2 & -2 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ -2 & -2 & -2 & -2 & \ldots & 0 & 0 & -2 & -2 \\ -2 & -2 & -2 & -2 & \ldots & 0 & 0 & -2 & -2 \\ -2 & -2 & -2 & -2 & \ldots & -2 & -2 & 0 & 0 \\ -2 & -2 & -2 & -2 & \ldots & -2 & -2 & 0 & 0 \end{vmatrix}$$

In that case, the characteristic equation is

$$\chi^{n-2}(\chi^2 - (4n-7)\chi - (12n-8)(\chi+4)^{n-2} = 0$$

and hence the spectrum becomes

$$Spec_{SDD^D}(K_{n\times 2}) = \begin{pmatrix} -4 & 0 & \frac{(4n-7)+\sqrt{16n^2-8n+17}}{2} & \frac{(4n-7)-\sqrt{16n^2-8n+17}}{2} \\ n-2 & n-2 & 1 & 1 \end{pmatrix}.$$

The energy is

$$(4n-7) + \sqrt{16n^2 - 8n + 17}$$

Therefore we arrive at the required result. □

Theorem 4.11. *The minimum dominating symmetric division deg energy of the friendship graph F_n^3 is*

$$SDDE^D(F_n^3) = (4n-2) + \sqrt{9 + \frac{8}{n}(n^4 + 2n^2 - n + 1)}$$

Proof. Let F_n^3 be the friendship graph with $2n+1$ vertices and let v_0 be the common vertex which is the only member present in the minimum dominating set. The minimum dominating symmetric division deg matrix is

$$\begin{bmatrix} 1 & n+\frac{1}{n} & n+\frac{1}{n} & n+\frac{1}{n} & n+\frac{1}{n} & \dots & n+\frac{1}{n} & n+\frac{1}{n} \\ n+\frac{1}{n} & 0 & 2 & 0 & 0 & \dots & 0 & 0 \\ n+\frac{1}{n} & 2 & 0 & 0 & 0 & \dots & 0 & 0 \\ n+\frac{1}{n} & 0 & 0 & 0 & 2 & \dots & 0 & 0 \\ n+\frac{1}{n} & 0 & 0 & 2 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ n+\frac{1}{n} & 0 & 0 & 0 & 0 & \dots & 0 & 2 \\ n+\frac{1}{n} & 0 & 0 & 0 & 0 & \dots & 2 & 0 \end{bmatrix}$$

The characteristic polynomial is

$$\begin{vmatrix} \chi-1 & -(n+\frac{1}{n}) & -(n+\frac{1}{n}) & -(n+\frac{1}{n}) & -(n+\frac{1}{n}) & \dots & -(n+\frac{1}{n}) & -(n+\frac{1}{n}) \\ -(n+\frac{1}{n}) & \chi & -2 & 0 & 0 & \dots & 0 & 0 \\ -(n+\frac{1}{n}) & -2 & \chi & 0 & 0 & \dots & 0 & 0 \\ -(n+\frac{1}{n}) & 0 & 0 & \chi & -2 & \dots & 0 & 0 \\ -(n+\frac{1}{n}) & 0 & 0 & -2 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -(n+\frac{1}{n}) & 0 & 0 & 0 & 0 & \dots & \chi & -2 \\ -(n+\frac{1}{n}) & 0 & 0 & 0 & 0 & \dots & -2 & \chi \end{vmatrix}$$

The characteristic equation becomes

$$(\chi-2)^{n-1}(\chi+2)^n(\chi^2-3\chi-(\frac{2}{n})(n^4+2n^2-n+1))=0$$

implying that the spectrum is

$$Spec_{SDD^D}(F_n^3)=\begin{pmatrix} -2 & 2 & \frac{3+\sqrt{9+\frac{8}{n}((n^4+2n^2-n+1))}}{2} & \frac{3-\sqrt{9+\frac{8}{n}((n^4+2n^2-n+1))}}{2} \\ n & n-1 & 1 & 1 \end{pmatrix}.$$

Therefore, we get

$$SDDE^D(F_n^3)=(4n-2)+\sqrt{9+\frac{8}{n}(n^4+2n^2-n+1)}$$

□

Theorem 4.12. *The minimum dominating symmetric division deg energy of the complement $\overline{K_{n\times 2}}$ of the cocktail party graph of order $2n$ is*

$$SDDE^D\overline{(K_{n\times 2})}=n\sqrt{17}.$$

Proof. Let $\overline{K_{n\times 2}}$ be the complement of the cocktail party graph of order $2n$ with vertex set $\{u_1,\ u_2,\ \cdots,\ u_n,\ v_1,\ v_2,\ \cdots,\ v_n\}$. Here $\{u_1,\ u_2,\ \cdots,\ u_n\}$ is the minimum dominating set. Then the minimum dominating symmetric division deg matrix of $\overline{K_{n\times 2}}$ is

$$SDD^D(\overline{K_{n\times 2}}) = \begin{bmatrix} 1 & 0 & 0 & 0 & \dots & 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & \dots & 0 & 2 & 0 & 0 \\ 0 & 0 & 1 & 0 & \dots & 0 & 0 & 2 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 2 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & \dots & 0 & 0 & 0 & 0 \end{bmatrix}.$$

The characteristic polynomial is

$$\begin{vmatrix} \chi-1 & 0 & 0 & 0 & \dots & -2 & 0 & 0 & 0 \\ 0 & \chi-1 & 0 & 0 & \dots & 0 & -2 & 0 & 0 \\ 0 & 0 & \chi-1 & 0 & \dots & 0 & 0 & -2 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ -2 & 0 & 0 & 0 & \dots & \chi & 0 & 0 & 0 \\ 0 & -2 & 0 & 0 & \dots & 0 & \chi & 0 & 0 \\ 0 & 0 & -2 & 0 & \dots & 0 & 0 & \chi & 0 \\ 0 & 0 & 0 & -2 & \dots & 0 & 0 & 0 & \chi \end{vmatrix}.$$

Hence the characteristic equation becomes

$$(\chi^2 - \chi - 4)^{n-1})^n = 0$$

and therefore the spectrum is

$$Spec_{SDD^D}(\overline{K_{n\times 2}}) = \begin{pmatrix} \frac{1+\sqrt{17}}{2} & \frac{1-\sqrt{17}}{2} \\ n & n \end{pmatrix}.$$

Finally we get $SDDE^D(\overline{K_{n\times 2}}) = n\sqrt{17}$.

Theorem 4.13. *The symmetric division deg energy of the* $2(i)$*-complement of the double star graph* $S_{n,n}$ *is*

$$SDDE^D(\overline{(S_{n,n})_{2(i)}}) = \sqrt{25n+9} + \sqrt{16n^2+n+9} + 4(n-1).$$

Proof. The symmetric division deg matrix for the 2(i)-complement of the double star graph is

$$SDD^D(\overline{(S_{n,n})_{2(i)}}) = \begin{bmatrix} 1 & 2.5 & 2.5 & \dots & 2.5 & 0 & 0 & 0 & \dots & 0 \\ 2.5 & 0 & 2 & \dots & 2 & 0 & 2 & 2 & \dots & 2 \\ 2.5 & 2 & 0 & \dots & 2 & 0 & 2 & 2 & \dots & 2 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 2 & 2 & 2 & \dots & 0 & 0 & 2 & 2 & \dots & 2 \\ 0 & 0 & 0 & \dots & 0 & 1 & 2.5 & 2.5 & \dots & 2.5 \\ 0 & 2 & 2 & \dots & 2 & 2.5 & 0 & 2 & \dots & 2 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 2 & 2 & \dots & 2 & 2.5 & 2 & 2 & \dots & 2 \\ 0 & 2 & 2 & \dots & 2 & 2.5 & 2 & 2 & \dots & 0 \end{bmatrix}.$$

The characteristic polynomial is

$$\begin{vmatrix} \chi-1 & -2.5 & -2.5 & \dots & -2.5 & 0 & 0 & 0 & \dots & 0 \\ -2.5 & \chi & -2 & \dots & -2 & 0 & -2 & -2 & \dots & 2 \\ -2.5 & -2 & \chi & \dots & -2 & 0 & -2 & -2 & \dots & 2 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -2 & -2 & -2 & \dots & \chi & 0 & -2 & -2 & \dots & 2 \\ 0 & 0 & 0 & \dots & 0 & \chi-1 & -2.5 & -2.5 & \dots & -2.5 \\ 0 & -2 & -2 & \dots & -2 & -2.5 & \chi & -2 & \dots & 2 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & -2 & -2 & \dots & -2 & -2.5 & -2 & -2 & \dots & 2 \\ 0 & -2 & -2 & \dots & -2 & -2.5 & -2 & -2 & \dots & \chi \end{vmatrix}.$$

Then the characteristic equation becomes

$$(\chi+2)^{2n-2}\left(\chi^2+(4n-1)\chi-(\frac{9n}{4}+2)\right)\left(\chi^2+\chi-(6.25n+2)\right)=0$$

and hence, the spectrum is
$Spec_{SDD^D}(\overline{(S_{n,n})_{2(i)}}) =$

$$\begin{pmatrix} \frac{(4n-1)+\sqrt{16n^2+n+9}}{2} & \frac{(4n-1)-\sqrt{16n^2+n+9}}{2} & \frac{-1+\sqrt{25n+9}}{2} & \frac{-1+\sqrt{25n+9}}{2} & -2 \\ 1 & 1 & 1 & 1 & 2n-2 \end{pmatrix}.$$

Therefore,

$$SDDE^D(\overline{(S_{n,n})_{2(i)}}) = \sqrt{25n+9}+\sqrt{16n^2+n+9}+4(n-1)$$

□

5. Conclusion

In this paper, we discussed about application of symmetric division deg $SDDE(G)$ of a graph G. QSPR analysis using linear regression model showed that there is a good correlation between symmetric division deg energy $SDDE(G)$, molar volumes and molar refractions of lower alkanes. Further we discuss symmetric division deg energy $SDDE(G)$ of graphs by considering the minimum domination parameter.

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