

Various Energies of Vitamin D₃

M. R. Rajesh Kanna¹, S. Roopa¹ and H.L. Parashivamurthy²

¹ Department of Mathematics, Sri D. Devaraja Urs Government First Grade College, Hunsur, Karnataka, India.

² Research Scholar, Research and Development Centre, Bharathiar University, Coimbatore - 641 046, India.

²Department of Mathematics, BGS Institute of Technology, B.G Nagar, Bellur- 571448, India.

Corresponding Author: M. R. Rajesh Kanna

(Email:mr.rajeshkanna@gmail.com, roopa.s.kumar@gmail.com and hlpmathsbgs@gmail.com)

Abstract: The concept of energy of a graph was introduced by I. Gutman in the year 1978. In this paper, we compute Energy, Seidel energy, Distance energy, Harary energy, Maximum degree energy, Randic energy and Laplacian energy of Vitamin D₃.

MSC: 05C12, 05C90.

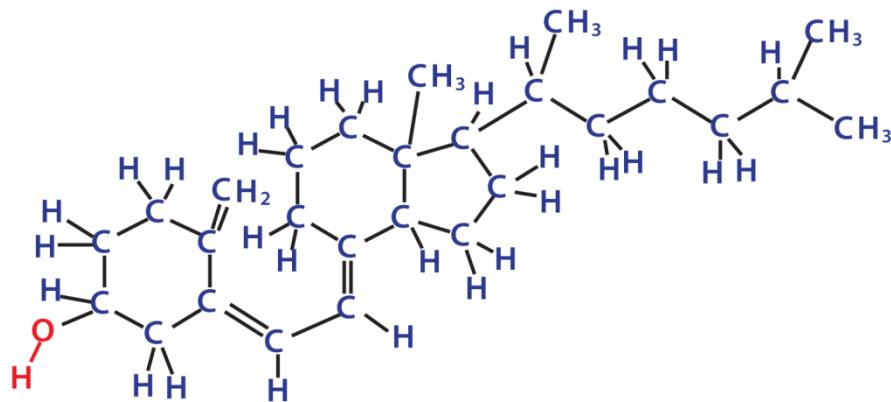
Keywords: Eigenvalues, Energy, Seidel energy, Distance energy, Harary energy, Maximum degree energy, Randic energy, Laplacian energy of Vitamin D₃.

Date of Submission: 15-02-2019

Date of acceptance: 04-03-2019

I. INTRODUCTION

Vitamin D₃ is the common name for cholecalciferol. Its molecular formula is C₂₇H₄₄O. Its structure is shown in the following figure. Vitamin D₃ is made by the body naturally when skin is exposed to the sun. It is more natural and easier for the body to absorb. Vitamin D₃ can be taken as a supplement to improve overall health. Vitamin D₃ also encourages the kidneys to recycle phosphate back into the blood, which helps the blood stay at the right ph.



Historically, vitamin D₃ loss has been associated with rickets, a disease caused by low levels of vitamin D₃ that commonly affects children. Oily fish like salmon, codfish, mackerel, and blue fish are great natural sources of vitamin D₃.

Energy of a Graph

Study on energy of graphs goes back to the year 1978, when I. Gutman [1] defined this while working with energies of conjugated hydrocarbon containing carbon atoms. All graphs considered in this article are assumed to be simple without loops and multiple edges. Let A = (a_{ij}) be the adjacency matrix of the graph G with its eigenvalues ρ₁, ρ₂, ..., ρ_n assumed in decreasing order. Since A is real symmetric, the eigenvalues of G are real numbers whose sum equal to zero. The sum of the absolute eigenvalues of G is called the energy E(G) of

$$\text{G. i.e., } E(G) = \sum_{i=1}^n |\rho_i|.$$

Theories on the mathematical concepts of graph energy can be seen in the reviews [2] and the references cited there in.

II. MAIN RESULTS

Theorem 2.1. The energy of vitamin D₃ is 35.047446.

Proof. Molecular graph of vitamin D₃ is as shown in the following figure - 1. Here vertices are numbered from V₁ to V₂₈.

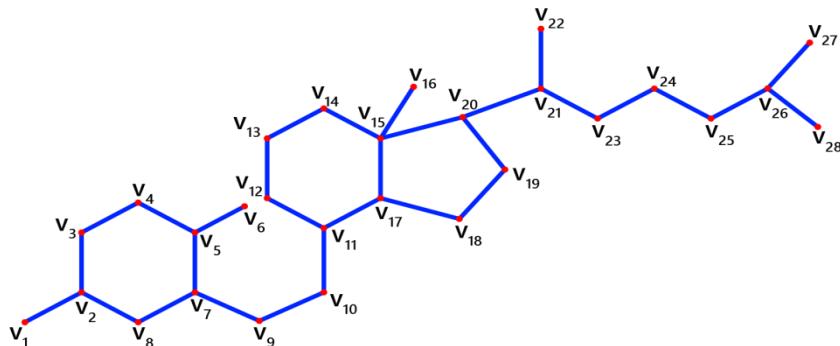


Figure 2.

Adjacency matrix of vitamin D₃ is

$$A(C_{27} H_{44} O) =$$

$$\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

Adjacency eigenvalues are

$$\begin{aligned} \rho_1 &\approx -2.4355614, \rho_2 \approx -2.2730185, \rho_3 \approx -2.0906754, \rho_4 \approx -1.8863824, \rho_5 \approx -1.6300101, \rho_6 \approx -1.4936866, \\ \rho_7 &\approx -1.439932, \rho_8 \approx -1.3004642, \rho_9 \approx -1.0995714, \rho_{10} \approx -0.8777241, \rho_{11} \approx -0.5891457, \rho_{12} \approx -0.2878489, \\ \rho_{13} &\approx -0.1197024, \rho_{14} \approx 2.439D-16, \rho_{15} \approx 3.243D-16, \rho_{16} \approx 0.2065951, \rho_{17} \approx 0.3405332, \rho_{18} \approx 0.6146199, \\ \rho_{19} &\approx 0.8994470, \rho_{20} \approx 1, \rho_{21} \approx 1.2396439, \rho_{22} \approx 1.4343512, \rho_{23} \approx 1.487193, \rho_{24} \approx 1.6186651, \\ \rho_{25} &\approx 1.84971, \rho_{26} \approx 2.0140548, \rho_{27} \approx 2.2760577, \rho_{28} \approx 2.5428521. \end{aligned}$$

The energy of vitamin D₃

$$E(C_{27}H_{44}O) = | -2.4355614 | + | -2.2730185 | + | -2.0906754 | + | -1.8863824 | + | -1.6300101 | \\ + | -1.4936866 | + | -1.439932 | + | -1.3004642 | + | -1.0995714 | + | -0.8777241 | \\ + | -0.5891457 | + | -0.2878489 | + | -0.1197024 | + | 2.439D - 16 | + | 3.243D - 16 | \\ + | 0.2065951 | + | 0.3405332 | + | 0.6146199 | + | 0.8994470 | + | 1. | + | 1.2396439 | \\ + | 1.4343512 | + | 1.487193 | + | 1.6186651 | + | 1.84971 | + | 2.0140548 | + | 2.2760577 | \\ + | 2.5428521 |$$

The energy of vitamin D₃ is 35.047446.

III. SEIDEL ENERGY

Let G be a simple graph of order n with vertex set $V = \{v_1, v_2, v_3, \dots, v_n\}$ and edge set E . The Seidel matrix of G is the $n \times n$ matrix defined by $S(G) := (s_{ij})$, where

$$s_{ij} = \begin{cases} -1, & \text{if } v_{ij} \in E \\ 1, & \text{if } v_{ij} \notin E \\ 0, & \text{if } v_i = v_j \end{cases}$$

The characteristic polynomial of $S(G)$ is denoted by $f_n(G, \rho) = \det(\rho I - S(G))$. The Seidel eigenvalues of the graph G are the eigenvalues of $S(G)$. Since $S(G)$ is real and symmetric, its eigenvalues are real numbers. The Seidel energy [3] of G defined as

$$SE(G) = \sum_{i=1}^n |\rho_i|.$$

Theorem 3.1. The Seidal energy of vitamin D₃ is 90.966062.

Proof. Seidel matrix of vitamin D₃ is

$$S(C_{27}H_{44}O) =$$

Seidel eigenvalues are

$$\begin{aligned} \rho_1 &\approx -5.7069245, \rho_2 \approx -5.4912402, \rho_3 \approx -4.7711865, \rho_4 \approx -4.3155957, \rho_5 \approx -4.0701165, \\ \rho_6 &\approx -3.9233158, \rho_7 \approx -3.4684857, \rho_8 \approx -3.2596336, \rho_9 \approx -2.6770556, \rho_{10} \approx -2.2768152, \\ \rho_{11} &\approx -1.7390131, \rho_{12} \approx -1.4377609, \rho_{13} \approx -1, \rho_{14} \approx -0.8372871, \rho_{15} \approx -0.4439705, \\ \rho_{16} &\approx -0.0646316, \rho_{17} \approx 0.2157664, \rho_{18} \approx 0.8495716, \rho_{19} \approx 1.4060756, \rho_{20} \approx 1.5836108 \\ \rho_{21} &\approx 1.7905088, \rho_{22} \approx 1.9088485, \rho_{23} \approx 2.2752917, \rho_{24} \approx 2.556669, \rho_{25} \approx 2.9231917, \\ \rho_{26} &\approx 3.4800546, \rho_{27} \approx 3.6940462, \rho_{28} \approx 22.799398. \end{aligned}$$

The Seidel energy of vitamin D₃ is

$$\begin{aligned} \text{SE}(\text{C}_{27}\text{H}_{44}\text{O}) = & | -5.7069245 | + | -5.4912402 | + | -4.7711865 | + | -4.3155957 | + | -4.0701165 | + \\ & | -3.9233158 | + | -3.4684857 | + | -3.2596336 | + | -2.6770556 | + | -2.2768152 | \\ & + | -1.73901 | + | -1.4377609 | + | -1.1 | + | -0.8372871 | + | -0.4439705 | \\ & + | -0.0646316 | + | 0.2157664 | + | 0.8495716 | + | 1.4060756 | + | 1.5836108 | \\ & + | 1.7905088 | + | 1.9088485 | + | 2.2752917 | + | 2.556669 | + | 2.9231917 | \\ & + | 3.4800546 | + | 3.6940462 | + | 22.799398 | \end{aligned}$$

The Seidal energy of vitamin D₃ is 90.966062

IV. DISTANCE ENERGY

On addressing problem for loop switching, R. L. Graham, H. O. Pollak [4] defined distance matrix of a graph. The concept of distance energy was defined by G. Indulal et al. [5] in the year 2008. Let G be a simple graph of order n with vertex set $V = \{v_1, v_2, \dots, v_n\}$ and edge set E. Let d_{ij} be the distance between the vertices v_i and v_j , then the $n \times n$ matrix $D(G) = (d_{ij})$ is called the distance matrix of G. The characteristic polynomial of $D(G)$ is denoted by $f(G; \rho) = |\rho I - D(G)|$, where I is the unit matrix of order n. The roots $\rho_1, \rho_2, \dots, \rho_n$ assumed in non increasing order are called the distance eigenvalues of G. The distance energy of a graph G is defined as

$$DE(G) = \sum_{i=1}^n |\rho_i|.$$

Since $D(G)$ is a real symmetric matrix with zero trace, these distance eigenvalues are real with sum equal to zero.

Theorem 4.1. The Distance energy of vitamin D₃ is 330.1068.

Proof. Distance matrix of vitamin D₃ is

$$D(\text{C}_{27}\text{H}_{44}\text{O}) =$$

0	1	2	3	4	5	3	2	4	5	6	7	8	9	8	9	7	8	9	9	10	11	11	12	13	14	15	15
1	0	1	2	3	4	2	1	3	4	5	6	7	8	7	8	6	7	8	8	9	10	10	11	12	13	14	14
2	1	0	1	2	3	3	2	4	5	6	7	8	9	8	9	7	8	9	9	10	11	11	12	13	14	15	15
3	2	1	0	1	2	2	3	3	4	5	6	7	8	7	8	6	7	8	8	9	10	11	11	12	13	14	14
4	3	2	1	0	1	1	2	2	3	4	5	6	7	6	7	5	6	7	7	8	9	10	10	11	12	13	13
5	4	3	2	1	0	2	3	3	4	5	6	7	8	7	8	6	7	8	8	9	10	9	11	12	13	14	14
3	2	3	2	1	2	0	1	1	2	3	4	5	6	5	6	4	5	6	6	7	8	8	9	10	11	12	12
2	1	2	3	2	3	1	0	2	3	4	5	6	7	6	7	5	6	7	7	8	9	9	10	11	12	13	13
4	3	4	3	2	3	1	2	0	1	2	3	4	5	4	5	3	4	5	5	6	7	8	9	10	11	11	11
5	4	5	4	3	4	2	3	1	0	1	2	3	4	3	4	2	3	4	4	5	6	6	7	8	9	10	10
6	5	6	5	4	5	3	4	2	1	0	1	2	3	2	3	1	2	3	3	4	5	5	6	7	8	9	9
7	6	7	6	5	6	4	5	3	2	1	0	1	2	3	4	2	3	4	4	5	6	6	7	8	9	10	10
8	7	8	7	6	7	5	6	4	3	2	1	0	1	2	3	3	4	4	3	4	5	5	6	7	8	9	9
9	8	9	8	7	8	6	7	5	4	3	2	1	0	1	2	2	3	3	2	3	4	4	5	6	7	8	8
8	7	8	7	6	7	5	6	4	3	2	3	2	1	0	1	1	2	2	1	2	3	3	4	5	6	7	7
9	8	9	8	7	8	6	7	5	4	3	4	3	2	1	0	2	3	3	2	3	4	4	5	6	7	8	8
7	6	7	6	5	6	4	5	3	2	1	2	3	2	1	2	0	1	2	2	3	4	4	5	6	7	8	8
8	7	8	7	6	7	5	6	4	3	2	3	4	3	2	3	1	0	1	2	3	4	4	5	6	7	8	8
9	8	9	8	7	8	6	7	5	4	3	4	3	2	3	2	1	0	1	2	3	3	4	5	6	7	7	7
9	8	9	8	7	8	6	7	5	4	3	4	3	2	3	2	1	2	2	2	1	0	1	2	3	4	5	6
10	9	10	9	8	9	7	8	6	5	4	5	4	3	2	3	2	3	3	2	1	0	1	1	2	3	4	5
11	10	11	10	9	10	8	9	7	6	5	6	5	4	3	4	4	4	3	2	1	0	2	3	4	5	6	6
11	10	11	10	9	10	8	9	7	6	5	6	5	4	3	4	4	4	3	2	1	2	0	1	2	3	4	4
12	11	12	11	10	11	9	10	8	7	6	7	6	5	4	5	5	5	4	3	2	3	1	0	1	2	3	3
13	12	13	12	11	12	10	11	9	8	7	8	7	6	5	6	6	6	5	4	3	4	2	1	0	1	2	2
14	13	14	13	12	13	11	12	10	9	8	9	8	7	6	7	7	6	5	4	5	3	2	1	0	1	1	1
15	14	15	14	13	14	12	13	11	10	9	10	9	8	7	8	8	8	7	6	5	6	4	3	2	1	0	2
15	14	15	14	13	14	12	13	11	10	9	10	9	8	7	8	8	8	7	6	5	6	4	3	2	1	2	0

Distance eigenvalues are

$$\begin{aligned} \rho_1 &\approx -80.965104, \quad \rho_2 \approx -31.702258, \quad \rho_3 \approx -9.5215078, \quad \rho_4 \approx -7.9149158, \quad \rho_5 \approx -6.4426906, \\ \rho_6 &\approx -5.0592994, \quad \rho_7 \approx -3.9149309, \quad \rho_8 \approx -2.9344665, \quad \rho_9 \approx -2.5787602, \quad \rho_{10} \approx -2., \\ \rho_{11} &\approx -1.8932615, \quad \rho_{12} \approx -1.585795, \quad \rho_{13} \approx -1.410641, \quad \rho_{14} \approx -1.2323891, \quad \rho_{15} \approx -1.1295526, \\ \rho_{16} &\approx -0.9899751, \quad \rho_{17} \approx -0.6998932, \quad \rho_{18} \approx -0.6764288, \quad \rho_{19} \approx -0.5902276, \quad \rho_{20} \approx -0.5200699, \\ \rho_{21} &\approx -0.4795013, \quad \rho_{22} \approx -0.4664063, \quad \rho_{23} \approx -0.3453248, \quad \rho_{24} \approx -7.340D - 15, \quad \rho_{25} \approx -5.545D - 15, \\ \rho_{26} &\approx 3.350D - 15, \quad \rho_{27} \approx 9.502D - 15, \quad \rho_{28} \approx 165.0534. \end{aligned}$$

Distance energy of vitamin D₃ is

$$\begin{aligned} \text{DE}(\text{C}_{27}\text{H}_{44}\text{O}) = & -80.965104 + -31.702258 + -9.5215078 + -7.9149158 + -6.4426906 + -5.0592994 + \\ & -3.9149309 + -2.9344665 + -2.5787602 + -2. + -1.8932615 + -1.585795 + \\ & -1.410641 + -1.2323891 + -1.1295526 + -0.9899751 + -0.6998932 + -0.6764288 + \\ & -0.5902276 + -0.5200699 + -0.4795013 + -0.4664063 + -0.3453248 + -7.340D - 15 + \\ & -5.545D - 15 + 3.350D - 15 + 9.502D - 15 + 165.0534. \end{aligned}$$

Distance energy of vitamin D₃ is 330.1068.

V. HARARY ENERGY

The concept of Harary energy was introduced by A. DilekGungor and A. Sinan Cevik [6]. The Harary matrix of G is the square matrix of order n whose (i, j)-entry is $\frac{1}{d_{ij}}$ where d_{ij} is the distance between the vertices v_i and v_j . Let $\rho_1, \rho_2, \dots, \rho_n$ be the eigenvalues of the Harary matrix of G. The Harary energy, HE(G) is defined by

$$HE(G) = \sum_{i=1}^n |\rho_i|. \text{ Further studies on Harary energy can be found in [7].}$$

Theorem 5.1. The Harary energy of vitamin D₃ is 35.865886.

Proof. Harary matrix of vitamin D₃ is

$$H(\text{C}_{27}\text{H}_{44}\text{O}) =$$

0	1	1/2	1/3	1/4	1/5	1/3	1/2	1/4	1/5	1/6	1/7	1/8	1/9	1/8	1/9	1/7	1/8	1/9	1/9	1/10	1/11	1/11	1/12	1/13	1/14	1/15	1/15
1	0	1	1/2	1/3	1/4	1/2	1	1/3	1/4	1/5	1/6	1/7	1/8	1/7	1/8	1/6	1/7	1/8	1/8	1/9	1/10	1/10	1/11	1/12	1/13	1/14	1/14
1/2	1	0	1	1/2	1/3	1/3	1/2	1/4	1/5	1/6	1/7	1/8	1/9	1/8	1/9	1/7	1/8	1/9	1/9	1/10	1/11	1/11	1/12	1/13	1/14	1/15	1/15
1/3	1/2	1	0	1	1/2	1/2	1/3	1/3	1/4	1/5	1/6	1/7	1/8	1/7	1/8	1/6	1/7	1/8	1/8	1/9	1/10	1/11	1/11	1/12	1/13	1/14	1/14
1/4	1/3	1/2	1	0	1	1/2	1/2	1/3	1/4	1/5	1/6	1/7	1/6	1/7	1/5	1/6	1/7	1/7	1/8	1/9	1/10	1/10	1/11	1/12	1/13	1/13	1/13
1/5	1/4	1/3	1/2	1	0	1/2	1/3	1/3	1/4	1/5	1/6	1/7	1/8	1/7	1/8	1/6	1/7	1/8	1/8	1/9	1/10	1/10	1/11	1/12	1/13	1/14	1/14
1/3	1/2	1/3	1/2	1	1/2	0	1	1	1/2	1/3	1/4	1/5	1/6	1/5	1/6	1/4	1/5	1/6	1/6	1/7	1/8	1/9	1/10	1/11	1/12	1/12	1/12
1/2	1	1/2	1/3	1/2	1/3	1	0	1/2	1/3	1/4	1/5	1/6	1/7	1/6	1/7	1/5	1/6	1/7	1/7	1/8	1/9	1/10	1/10	1/11	1/12	1/13	1/13
1/4	1/3	1/4	1/3	1/2	1/3	1	1/2	0	1	1/2	1/3	1/4	1/5	1/4	1/5	1/3	1/4	1/5	1/5	1/6	1/7	1/8	1/9	1/10	1/11	1/11	1/11
1/5	1/4	1/5	1/4	1/3	1/4	1/2	1/3	1	0	1	1/2	1/3	1/4	1/3	1/4	1/2	1/3	1/4	1/4	1/5	1/6	1/7	1/8	1/9	1/10	1/10	1/10
1/6	1/5	1/6	1/5	1/4	1/5	1/3	1/4	1/2	1	0	1	1/2	1/3	1/2	1/3	1	1/2	1/3	1/3	1/4	1/5	1/5	1/6	1/7	1/8	1/9	1/9
1/7	1/6	1/7	1/6	1/5	1/6	1/4	1/5	1/3	1/2	1	0	1	1/2	1/3	1/4	1/2	1/3	1/4	1/4	1/5	1/6	1/7	1/8	1/9	1/10	1/10	1/10
1/8	1/7	1/8	1/7	1/6	1/7	1/5	1/6	1/4	1/3	1/2	1	0	1	1/2	1/3	1/4	1/3	1/4	1/4	1/5	1/6	1/7	1/8	1/9	1/10	1/10	1/10
1/9	1/8	1/9	1/8	1/7	1/8	1/6	1/7	1/5	1/4	1/3	1/2	1	0	1	1/2	1/3	1/4	1/3	1/4	1/4	1/5	1/6	1/7	1/8	1/9	1/9	1/9
1/8	1/7	1/8	1/7	1/6	1/7	1/5	1/6	1/4	1/3	1/2	1	0	1	1/2	1/3	1/4	1/2	1/3	1/2	1/3	1/4	1/5	1/6	1/7	1/8	1/8	1/8
1/9	1/8	1/9	1/8	1/7	1/8	1/6	1/7	1/5	1/4	1/3	1/2	1	0	1	1/2	1/3	1/4	1/2	1/3	1/2	1/3	1/4	1/5	1/6	1/7	1/7	1/7
1/7	1/6	1/7	1/6	1/5	1/6	1/4	1/5	1/3	1/2	1	0	1	1/2	1/3	1/2	1	1/2	0	1	1/2	1/2	1/2	1/3	1/4	1/5	1/6	1/6
1/8	1/7	1/8	1/7	1/6	1/7	1/5	1/6	1/4	1/3	1/2	1	0	1	1/2	1/3	1/2	1	0	1	1/2	1/3	1/4	1/5	1/6	1/7	1/8	1/8
1/9	1/8	1/9	1/8	1/7	1/8	1/6	1/7	1/5	1/4	1/3	1/2	1	0	1	1/2	1/3	1/2	1	0	1	1/2	1/3	1/4	1/5	1/6	1/7	1/7
1/9	1/8	1/9	1/8	1/7	1/8	1/6	1/7	1/5	1/4	1/3	1/2	1	0	1	1/2	1/3	1/2	1	0	1	1/2	1/3	1/4	1/5	1/6	1/6	1/6
1/10	1/9	1/10	1/9	1/8	1/9	1/7	1/8	1/6	1/5	1/4	1/3	1/2	1	0	1	1/2	1/3	1/2	1	0	1	1	1/2	1/3	1/4	1/5	1/5
1/11	1/10	1/11	1/10	1/9	1/10	1/8	1/9	1/7	1/6	1/5	1/4	1/3	1/2	1	0	1	1/2	1/3	1/2	1	0	1	1/2	1/3	1/4	1/5	1/6
1/11	1/10	1/11	1/10	1/9	1/10	1/8	1/9	1/7	1/6	1/5	1/4	1/3	1/2	1	0	1	1/2	1/3	1/2	1	1/2	0	1	1/2	1/3	1/4	1/4
1/12	1/11	1/12	1/11	1/10	1/11	1/9	1/10	1/8	1/7	1/6	1/5	1/4	1/3	1/2	1	0	1	1/2	1/3	1/2	1	1/2	0	1	1/2	1/3	1/3
1/13	1/12	1/13	1/12	1/11	1/12	1/10	1/11	1/9	1/8	1/7	1/6	1/5	1/4	1/3	1/2	1	0	1	1/2	1/3	1/4	1/2	1	0	1	1/2	1/2
1/14	1/13	1/14	1/13	1/12	1/13	1/11	1/12	1/10	1/9	1/8	1/7	1/6	1/5	1/4	1/3	1/2	1	0	1	1/2	1/3	1/4	1/5	1/6	1/7	1/7	1/7
1/15	1/14	1/15	1/14	1/13	1/14	1/12	1/13	1/11	1/10	1/9	1/8	1/7	1/6	1/5	1/4	1/3	1/2	1	0	1	1/2	1/3	1/4	1/5	1/6	1/7	1/7

Harary eigenvalues are

$$\begin{aligned}\rho_1 &\approx -1.5221772, \quad \rho_2 \approx -1.4541112, \quad \rho_3 \approx -1.4273649, \quad \rho_4 \approx -1.3709553, \quad \rho_5 \approx -1.3265694, \\ \rho_6 &\approx -1.2980024, \quad \rho_7 \approx -1.2647773, \quad \rho_8 \approx -1.2322377, \quad \rho_9 \approx -1.1836879, \quad \rho_{10} \approx -1.0535582, \\ \rho_{11} &\approx -0.9834721, \quad \rho_{12} \approx -0.7464322, \quad \rho_{13} \approx -0.6665951, \quad \rho_{14} \approx -0.6143564, \quad \rho_{15} \approx -0.5499178, \\ \rho_{16} &\approx -0.5, \quad \rho_{17} \approx -0.4335371, \quad \rho_{18} \approx -0.2832636, \quad \rho_{19} \approx -0.0219270, \quad \rho_{20} \approx 0.0757466, \\ \rho_{21} &\approx 0.3080583, \quad \rho_{22} \approx 0.6590555, \quad \rho_{23} \approx 0.6741518, \quad \rho_{24} \approx 0.8891766, \quad \rho_{25} \approx 1.3887831, \\ \rho_{26} &\approx 2.4965294, \quad \rho_{27} \approx 3.5878371, \quad \rho_{28} \approx 7.8536044\end{aligned}$$

Harary energy of vitamin D₃ is

$$\begin{aligned}HE(C_{27}H_{44}O) = & -1.5221772 + -1.4541112 + -1.4273649 + -1.3709553 + -1.3265694 + \\ & -1.2980024 + -1.2647773 + -1.2322377 + -1.1836879 + -1.0535582 + \\ & -0.9834721 + -0.7464322 + -0.6665951 + -0.6143564 + -0.5499178 + \\ & -0.5 + -0.4335371 + -0.2832636 + -0.0219270 + 0.0757466 + \\ & 0.3080583 + 0.6590555 + 0.6741518 + 0.8891766 + 1.3887831 + 2.4965294 + \\ & 3.5878371 + 7.8536044.\end{aligned}$$

The Harary energy of vitamin D₃ is 35.865886.

VI. MAXIMUM DEGREE ENERGY

In the year 2009 Prof. C. Adiga and M. Smitha [8] defined maximum degree energy of a graph. Let G be a simple graph of order n with vertex set $V = \{v_1, v_2, \dots, v_n\}$ and edge set E. The maximum degree matrix of G is the $n \times n$ matrix defined by $A_{MD}(G) = (a_{ij})$, where

$$a_{ij} = \begin{cases} \max\{d(v_i), d(v_j)\} & \text{if } v_i v_j \in E \\ 0 & \text{otherwise} \end{cases}$$

The characteristic polynomial of $A_{MD}(G)$ is denoted by $f_n(G, \rho) = \det(\rho I - A_{MD}(G))$. The maximum degree eigenvalues of the graph G are the eigenvalues of $A_{MD}(G)$. Since $A_{MD}(G)$ is real and symmetric, its eigenvalues are real numbers and we label them in non-increasing order $\rho_1 \geq \rho_2 \geq \dots \geq \rho_n$. The maximum

degree energy of G is defined as $MDE(G) = \sum_{i=1}^n |\rho_i|$

Theorem 6.1. The maximum degree energy of vitamin D₃ is 99.62787.

Proof. Maximum degree matrix of vitamin D₃ is,

$$\text{MD}(\text{C}_{27}\text{H}_{44}\text{O}) =$$

Maximum degree eigenvalues are

$$\begin{aligned} \rho_1 &\approx -8.7284841, \quad \rho_2 \approx -6.611508, \quad \rho_3 \approx -5.8901867, \quad \rho_4 \approx -5.362739, \quad \rho_5 \approx -4.7939456, \quad \rho_6 \approx -4.5816137, \\ \rho_7 &\approx -3.609993, \quad \rho_8 \approx -3.2474791, \quad \rho_9 \approx -2.5669751, \quad \rho_{10} \approx -1.9728273, \quad \rho_{11} \approx -1.3108828, \quad \rho_{12} \approx -0.7630945, \\ \rho_{13} &\approx -0.3742057, \quad \rho_{14} \approx -3.649D-15, \quad \rho_{15} \approx 7.833D18, \quad \rho_{16} \approx 0.4821352, \quad \rho_{17} \approx 0.9310646, \quad \rho_{18} \approx 1.5278353, \\ \rho_{19} &\approx 1.9737317, \quad \rho_{20} \approx 2.3522699, \quad \rho_{21} \approx 3.3093884, \quad \rho_{22} \approx 3.3836386, \quad \rho_{23} \approx 4.5876091, \quad \rho_{24} \approx 4.7978695, \\ \rho_{25} &\approx 5.3407616, \quad \rho_{26} \approx 5.6391559, \quad \rho_{27} \approx 6.6094711, \quad \rho_{28} \approx 8.8790042. \end{aligned}$$

The Maximum degree of vitamin D₃

$$\text{MDE(C}_{27}\text{H}_{44}\text{O)} = | - 8.7284841 | + | - 6.611508 | + | - 5.8901867 | + | - 5.362739 | + | - 4.7939456 | + \\ | - 4.5816137 | + | - 3.609993 | + | - 3.2474791 | + | - 2.5669751 | + | - 1.9728273 | + \\ | - 1.3108828 | + | - 0.7630945 | + | - 0.3742057 | + | - 3.649D - 15 | + | 7.833D18 | + \\ | 0.4821352 | + | 0.9310646 | + | 1.5278353 | + | 1.9737317 | + | 2.3522699 | + \\ | 3.3093884 | + | 3.3836386 | + | 4.5876091 | + | 4.7978695 | + | 5.3407616 | + \\ | 5.6391559 | + | 6.6094711 | + | 8.8790042 |.$$

Maximum degree energy of vitamin D₃ is 99.62787.

VII. RANDIC ENERGY

It was in the year 1975, Milan Randic invented a molecular structure descriptor called Randic index [9] which is defined as $R(G) = \sum_{v_i v_j \in E(G)} \frac{1}{\sqrt{d_i d_j}}$. Motivated by this S.B.Bozkurt et al.[10] defined Randic matrix and

Randic energy as follows. Let G be graph of order n with vertex set $V = \{v_1, v_2, \dots, v_n\}$ and edge set E . Randic matrix of G is a $n \times n$ symmetric matrix defined by $R(G) := (r_{ij})$, where

$$r_{ij} = \begin{cases} \frac{1}{\sqrt{d_i d_j}} & \text{if } v_i v_j \in E(G) \\ 0 & \text{otherwise} \end{cases}$$

The characteristic equation of $R(G)$ is defined by $f_n(G, \rho) = \det(\rho I - R(G)) = 0$. The roots of this equation are called Randic eigenvalues of G . Since $R(G)$ is real and symmetric, its eigenvalues are real numbers and we label them in decreasing order $\rho_1 \geq \rho_2 \geq \dots \geq \rho_n$. Randic energy of G is defined as

$$RE(G) := \sum_{i=1}^n |\rho_i|$$

Further studies on Randic energy can be seen in the articles [11] and the references cited there in.

Theorem 7.1. The Randic energy of vitamin D₃ is 16.215777.

Proof. Randic matrix of vitamin D₃ is,

$$R(C_{27}H_{44}O) =$$

Randic eigenvalues are

$$\begin{aligned} \rho_1 &\approx -0.9908078, \rho_2 \approx -0.9823655, \rho_3 \approx -0.9332038, \rho_4 \approx -0.8747590, \rho_5 \approx -0.7531162, \rho_6 \approx -0.7193133, \\ \rho_7 &\approx -0.6855307, \rho_8 \approx -0.6153771, \rho_9 \approx -0.5210294, \rho_{10} \approx -0.4622779, \rho_{11} \approx -0.3096948, \rho_{12} \approx -0.1827637, \\ \rho_{13} &\approx -0.0776495, \rho_{14} \approx 1.632D - 17, \rho_{15} \approx 2.894D - 16, \rho_{16} \approx 0.1099013, \rho_{17} \approx 0.1980953, \rho_{18} \approx 0.3113099, \\ \rho_{19} &\approx 0.4400092, \rho_{20} \approx 0.5281061, \rho_{21} \approx 0.5608432, \rho_{22} \approx 0.6912916, \rho_{23} \approx 0.7175670, \rho_{24} \approx 0.7558095, \\ \rho_{25} &\approx 0.8505201, \rho_{26} \approx 0.9596414, \rho_{27} \approx 0.9847940, \rho_{28} \approx 1. \end{aligned}$$

The Randic energy of vitamin D₃ is

$$\begin{aligned} R(C_{27} H_{44} O) = & | -0.9908078 | + | -0.9823655 | + | -0.9332038 | + | -0.8747590 | + | -0.7531162 | + | -0.7193133 | + \\ & | -0.6855307 | + | -0.6153771 | + | -0.5210294 | + | -0.4622779 | + | -0.3096948 | + | -0.1827637 | + \\ & | -0.0776495 | + | 1.632D - 17 | + | 2.894D - 16 | + | 0.1099013 | + | 0.1980953 | + | 0.3113099 | + \\ & | 0.4400092 | + | 0.5281061 | + | 0.5608432 | + | 0.6912916 | + | 0.7175670 | + | 0.7558095 | + \\ & | 0.8505201 | + | 0.9596414 | + | 0.9847940 | + | 1 | . \end{aligned}$$

Randic Energy of vitamin D₃ is 16.215777.

VIII. LAPLACIAN ENERGY

The graph energy is defined in terms of the ordinary graph spectrum, that is, the spectrum of the adjacency matrix. Another well-developed part of algebraic graph theory is the spectral theory of the Laplacian matrix. The Laplacian matrix of an (n,m) - graph G is defined as $L(G) = \Delta(G) - A(G)$, where A is the adjacency matrix and Δ the diagonal matrix whose diagonal elements are the vertex degrees. Let $\mu_1, \mu_2, \dots, \mu_n$ be the eigenvalues of L(G). Laplacian energy was defined as $LE = LE(G) := \sum_{i=1}^n \left| \mu_i - \frac{2m}{n} \right|$.

Theorem 8.1. The Laplacian energy of vitamin D₃ is 60

Proof. Laplacian matrix of vitamin D₃ is

$$A = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 \end{bmatrix}$$

D =

$$(A - D)(C_{27}H_{44}O) =$$

Laplacian eigenvalues are

$$\begin{aligned}\rho_1 &\approx -5.595925, \rho_2 \approx -4.8642771, \rho_3 \approx -4.6883085, \rho_4 \approx -4.2685965, \rho_5 \approx -4.1553219, \rho_6 \approx -4.0808578 \\ \rho_7 &\approx -3.670488, \rho_8 \approx -3.5210049, \rho_9 \approx -3.3326348, \rho_{10} \approx -2.9701279, \rho_{11} \approx -2.7146822, \rho_{12} \approx -2.2692998 \\ \rho_{13} &\approx -2.0616344, \rho_{14} \approx -1.90502, \rho_{15} \approx -1.6655946, \rho_{16} \approx -11.5498536, \rho_{17} \approx -11.2070396, \rho_{18} \approx -1. \\ \rho_{19} &\approx -0.7698996, \rho_{20} \approx -0.7442639, \rho_{21} \approx -0.6111569, \rho_{22} \approx -0.5, \rho_{23} \approx -5281277, \rho_{24} \approx -0.4320534, \\ \rho_{25} &\approx -0.2828373, \rho_{26} \approx -0.0811915, \rho_{27} \approx -0.0298034, \rho_{28} \approx 2.880D - 16.\end{aligned}$$

$$\text{Average degree} = \frac{2m}{n} = \frac{2 \times 30}{28} = 2.142857.$$

The Laplacian energy of vitamin D₃ is,

$$\begin{aligned}\text{LE(C}_{27}\text{H}_{44}\text{O)} = & | -5.595925 - 2.142857 | + | -4.8642771 - 2.142857 | + | -4.6883085 - 2.142857 | + \\ & | -4.2685965 - 2.142857 | + | -4.1553219 - 2.142857 | + | -4.0808578 - 2.142857 | + \\ & | -3.670488 - 2.142857 | + | -3.5210049 - 2.142857 | + | -3.3326348 - 2.142857 | + \\ & | -2.9701279 - 2.142857 | + | -2.7146822 - 2.142857 | + | -2.2692998 - 2.142857 | + \\ & | -2.0616344 - 2.142857 | + | -1.90502 - 2.142857 | + | -1.6655946 - 2.142857 | + \\ & | -11.549853 - 2.142857 | + | -11.207039 - 2.142857 | + | -1 - 2.142857 | + \\ & | -0.7698996 - 2.142857 | + | -0.7442639 - 2.142857 | + | -0.6111569 - 2.142857 | + \\ & | -0.5281277 - 2.142857 | + | -0.4320534 - 2.142857 | + | -0.2828373 - 2.142857 | + \\ & | -0.0811915 - 2.142857 | + | -0.0298034 - 2.142857 | + | 2.880D - 16 - 2.142857 |.\end{aligned}$$

$$\text{LE(C}_{27}\text{H}_{44}\text{O)} = 118.77768.$$

IX. CONCLUSION

In this article, we have computed Energy, Seidel energy, Distance energy, Harary energy, Maximum degree energy, Randic energy, Laplacian energy of vitamin D₃.

REFERENCES

- [1]. I.Gutman, The energy of a graph, Ber. Math-Statist. Sekt. Forschungsz. Graz, 103(1978), 1-22.
- [2]. .Gutman, The energy of a graph: Old and New Results, ed. by A. Betten, A.Kohnert, R. Laue, A. Wassermann, Algebraic Combinatorics and Applications, Springer, Berlin, (2001), 196-211.
- [3]. Willem H.Haemers, Seidel Switching and Graph Energy, MATH Commun. Math. Comput. Chem., 68(2012), 653-659.
- [4]. R.L.Graham and H.O.Pollak, On the addressing problem for loop switching, Bell Labs Technical Journal, 50(1971),2495-2519.
- [5]. G.Indulal, I.Gutman and A.Vijayakumar, On distance energy of graphs, MATCH Communications in Mathematical and Computer Chemistry, 60(2008), 461-472.
- [6]. A.DilekGungor and A.SinanCevik, On the Harary Energy and Harary Estrada Index of a Graph, MATCH Commun.Math. Comput. Chem., 64(2010), 281-296.
- [7]. Zhihui Cui and Bolian Liu, On Harary Matrix, Harary Index and Harary Energy, MATCH Commun. Math. Comput.Chem., 68(2012), 815-823.
- [8]. C.Adiga and M.Smitha, On maximum degree energy of a graph, Int. J. Contemp. Math. Sciences, 4(8)(2009), 385-396.
- [9]. M.Randic, On Characterization of molecular branching, J. Amer. Chem. Soc., 97(1975), 6609-6615.
- [10]. S.B.Bozkurt, A.D.Gungor and I.Gutman, Randic spectral radius and Randic energy, Commun. Math. Comput. Chem.,64(2010), 239-250.
- [11]. K.C.Das, SezerSorgun and I.Gutman, On Randicenergy, Commun. Math. Comput. Chem., 73(2015), 81-92.

M. R. Rajesh Kanna. "Various Energies of Vitamin D3." IOSR Journal of Engineering (IOSRJEN), vol. 09, no. 02, 2019, pp. 53-63.