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DISTINCT ENERGIES OF CHOLESTEROL

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Keywords:

Eigen values, Siedel energy, Maximum degree energy, Distance energy, Harary energy, Cholesterol

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ABSTRACT: Cholesterol is a waxy substance which is made in the body by the liver but is also found in some foods. It plays a vital role in how every cell works and is also needed to make Vitamin D, some hormones and bile for digestion. The concept of energy of a graph was introduced by I. Gutman in the year 1978. In this paper, we compute Siedel Energy, Maximum Degree Energy, Distance Energy, Harary Energy of Cholesterol.

INTRODUCTION: Cholesterol is a lipid with a unique structure consisting of four linked hydrocarbon rings forming the bulky steroid structure. There is a hydrocarbon tail linked to one end of the steroid and a hydroxyl group linked to the other end. The hydroxyl group is able to form hydrogen bonds with nearby carbonyl oxygen of phosphor lipid and sphingolipid head groups. Cholesterol is known as a sterol because it is made out of an alcohol and steroid. Cholesterol is present in most animal membranes with varying amounts but is absent in prokaryotes and intracellular membranes. Cholesterol is one of the basic sterols which occurs in all animal tissues and is of great importance to animal life.

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The thermodynamic properties of this material are, therefore, important in the study of the biochemical processes in which it is involved. It is one of the biomedical chemicals which is certified for purity and ordered as a standard reference material (SRM 9Ila) by the NBS Office of Standard Reference Materials. Since this material is of natural origin it is expected to be essentially free of sterol isomers.

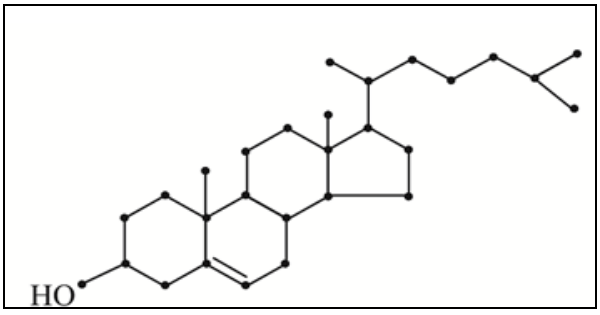


FIG. 1: STRUCTURE OF CHOLESTEROL

In 1927, Wieland and Adolf Windaus got Nobel Prize for cholesterol and bile acids structure. In 1932, Adolf Windaus clarified the structure of cholesterol. In 1964, Dr. Konrad Bloch received the

Nobel Prize for explaining the cholesterol synthesis. He showed HMG-CoA reductase was the enzyme in this complex synthesis. The cholesterol serves as a precursor for bile acids, sex hormones, and cortisol. Konrad Bloch and Feodor Lynen awarded Nobel Prize for cholesterol and fatty acids metabolism.

Cholesterol is a waxy substance which is made in the body by the liver but is also found in some foods. It plays a vital role in how every cell works and is also needed to make Vitamin D, some hormones and bile for digestion. Cholesterol is both our friend and foe - at normal levels, it is an essential substance for the body's normal functioning, but if levels in the blood get too high, it becomes a silent danger that puts us at risk of a heart attack.

Cholesterol is carried in the blood attached to proteins called lipoproteins. There are two main forms, LDL (low density lipoprotein) and HDL (high density lipoprotein). LDL cholesterol is often referred to as bad cholesterol" because too much is unhealthy. HDL is often referred to as good cholesterol because it is protective. Knowing the levels of these can help us to determine the risk of heart disease.

Molecules and molecular compounds are often modeled by molecular graph. A molecular graph is a representation of the structural formula of chemical compound in terms of graph theory, whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. Note that hydrogen atoms are often omitted. All molecular graphs considered in this paper are finite, connected, loop less, and without multiple edges. Let G = (V, E) be a graph with vertex set V and edge set E. The degree of a vertex u ϵ E is denoted by d_u and is the number of vertices that are adjacent to u. The edge connecting the vertices u and v is denoted by uv.

Let be a simple graph of order n with vertex set V = {v_1, v_2 ...., v_n} and edge set E.

The concept of energy of a graph was introduced by I. Gutman [1] in the year 1978.

Definition 1: The adjacency matrix of G is the n × n matrix defined by A (G) = (a_{ij}), where

$$a_{ij} = \begin{cases} 1 & if v_i v_j \in E \\ 0 & otherwise \end{cases}$$

The Eigen values $\lambda_1, \lambda_2 \ldots \lambda_n$ of A (G), assumed in none increasing order, are the Eigen values of the graph G. As A is real symmetric, the Eigen values of G are real with sum equal to zero. The energy E (G) of G is defined to be the sum of the absolute values of the Eigen values of G *i.e.*

$$E(G) = \sum_{i=1}^{n} |\lambda_i|$$

For details on the mathematical aspects of the theory of graph energy see the reviews [2], papers [3-5] and the references cited there in. The basic properties including various upper and lower bounds for energy of a graph have been established in [6-7], and it has found remarkable chemical applications in the molecular orbital theory of conjugated molecules [8-9]. Recently authors of this paper computed energy of Cholesterol [10].

In chemistry, the Eigen values represent the energy levels of the electrons in a molecule. The total π-electron energy E is the sum of the energies of all electrons in a molecule. The π-electron energy of a conjugated carbon molecule, computed using the Huckel theory, coincides with the energy as defined here. Hence results on graph energy assume special significance.

RESULTS AND DISCUSSIONS:

Siedel Energy: Let G be a simple graph of order n with vertex set V = {v_1, v_2 ...., v_n} and edge set E.

Definition 2: The Siedel matrix of G is the n × n matrix denoted by S (G):=(s_{ij}), where

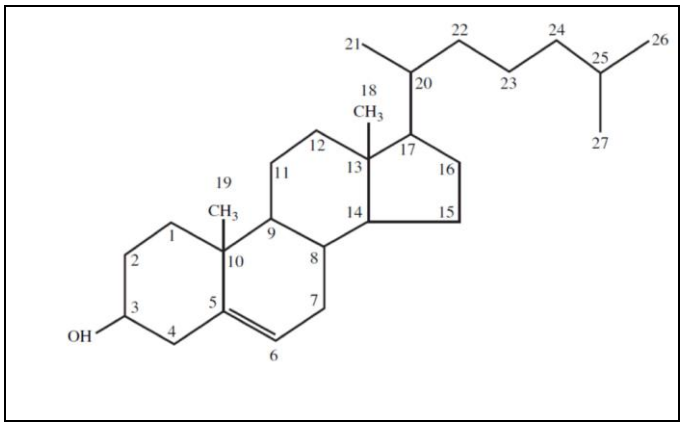
$$s_{ij} = \begin{cases} -1 & if v_i v_j \in E \\ 1 & if v_i v_j \notin E \\ 0 & if v_i = v_j \end{cases}$$

The characteristic polynomial of S (G) is denoted by $f_n(G, \lambda) = \det(\lambda I - S(G))$. The Seidel Eigen values of the graph G are the Eigen values of S (G). Since S (G) is real and symmetric, its Eigen values are real numbers. The Seidel energy 11 of G defined as

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

Theorem 1: The Seidel energy of cholesterol $C_{27}H_{46}O$ is 92.4048.

Proof: Consider a molecular graph of cholesterol $C_{27}H_{46}O$ as shown in the following figure. Here vertices are numbered from 1 to 27.



Siedel matrix S $C_{27}H_{46}O$ =

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

Seidel Eigen values are - 5.7653, -5.3085, -4.7155, -4.3272, -4.1246, -3.6630, -3.5870, -2.9693, 2.8077, -2.2836, -1.7611, -1.4999, -1.0000, -1.0000, -0.8582, -0.5314, 0.2864, 0.7493, 1.1671, 1.3602, 1.8557, 2.1002, 2.3920, 2.7396, 3.1094, 3.6053, 4.1364, 22.7008.

Seidel energy of a cholesterol is SE C27H46O = |-5.7653| + |-5.3085| + |-4.7155| + |-4.3272| + |4.1246| + |-3.6630| + |-3.5870| + |-2.9693| + |-2.8077| + |-2.2836| + |-1.7611| + |-1.4999| + |-1.0000| + |-1.0000| + |-0.8582| + |-0.5314| + |0.2864| + |0.7493| + |1.1671| + |1.3602| + |1.8557| + |2.1002| + |2.3920| + |2.7396| + |3.1094| + |3.6053| + |4.1364| + |22.7008| = 92.4048

Maximum Degree Energy: C. Adiga and M. Smitha [12] defined maximum degree energy of a graph. Let G be a simple graph of order n with vertex set V = {v_1, v_2 ...., v_n} and edge set E.

Definition 3: The maximum degree matrix of G is the n × n matrix defined by A_{MD} (G):= (a_{ij}), where

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

The characteristic polynomial of by AMD (G) is denoted by $f_n(G, \lambda) = \det(\lambda I - S(G))$. The maximum degree Eigen values of the graph G are the Eigen values of A_{MD} (G). Since A_{MD} (G) is real and symmetric, its Eigen values are real numbers and we label them in non-increasing order $\lambda 1 \geq \lambda 2 \geq ... \geq \lambda_n$. The maximum degree energy of defined as

$$E_{MD}(G) = \sum_{i=1}^{n} |\lambda_i|$$

Theorem 2: The maximum degree energy of cholesterol $C_{27}H_{46}O$ is 105.9520.

Proof: The maximum degree matrix of cholesterol is AMD $C_{27}H_{46}O$ =

$$\begin{bmatrix}
0&2&0&0&0&0&0&0&0&4&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
2&0&3&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&3&0&3&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&3\\
0&0&3&0&3&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&3&0&3&0&0&0&4&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&3&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&2&0&3&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&3&0&3&0&0&0&0&3&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&3&0&4&3&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
4&0&0&0&4&0&0&0&4&0&0&0&0&0&0&0&0&0&4&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&3&0&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&2&0&4&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&4&0&4&0&0&4&4&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&3&0&0&0&0&4&0&3&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&3&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&2&0&3&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&4&0&0&3&0&0&0&3&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&4&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&4&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&3&0&0&0&3&3&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&3&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&3&0&0&2&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&2&0&2&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&2&0&3&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&3&0&3&3&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&3&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&3&0&0&0\\
0&0&3&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0
\end{bmatrix}$$

Maximum degree Eigen values are -9.0371, -8.4868, -5.8588, -5.4042, -5.2821, -4.4786, -3.8268, -3.4847, -2.6850, -2.0074, -1.4005, -0.7548, -0.2692, -0.0000, 0.0000, 0.3403, 0.9849, 1.5335, 2.0806, 2.4522, 3.3577, 3.8326, 4.4780, 5.1679, 5.4000, 5.6746, 8.5682, 9.1054.

Maximum degree energy of a cholesterol is EMD ($C_{27}H_{46}O$) |-9.0371| + |-8.4868| + |-5.8588| + |-5.4042| + |-5.2821| + |-4.4786| + |-3.8268| + | -3.4847| + |-2.6850| + |-2.0074| + |-1.4005| +|-

0.7548| + | -0.2692| + |-0.0000| + |0.0000| + |0.3403| + |0.9849| + |1.5335| + |2.0806| + |2.4522| + |3.3577| + |3.8326| + |4.4780| + |5.1679| + |5.4000| + |5.6746| + |8.5682| + |9.1054| = 105.9520.

Distance Energy: Gopalapillai Indulal *et al.*, [13] defined distance energy of graphs. Let G be a simple graph of order n with vertex set V = {v_1, v_2 ...., v_n} and edge set E.

Definition 4: The distance matrix of G is the square matrix of order n whose (i, j) entry is the shortest distance between the vertices v_i and v_j. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the Eigen values of the distance matrix of G. The distance energy DE is defined as

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

Theorem 3: The distance energy of cholesterol $C_{27}H_{46}O$ is 328.3176.

Proof: The distance matrix of cholesterol is D $C_{27}H_{46}O$ =

$$\begin{bmatrix}
0 & 1 & 2 & 3 & 2 & 3 & 4 & 3 & 2 & 1 & 3 & 4 & 5 & 4 & 5 & 6 & 6 & 6 & 2 & 7 & 8 & 8 & 9 & 10 & 11 & 12 & 12 & 3 \\
1 & 0 & 1 & 2 & 3 & 4 & 5 & 4 & 3 & 2 & 4 & 5 & 6 & 5 & 6 & 7 & 7 & 7 & 3 & 8 & 9 & 9 & 10 & 11 & 12 & 13 & 13 & 2 \\
2 & 1 & 0 & 1 & 2 & 3 & 4 & 5 & 4 & 3 & 5 & 6 & 7 & 6 & 7 & 8 & 9 & 8 & 4 & 9 & 10 & 10 & 11 & 12 & 13 & 14 & 14 & 1 \\
3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 3 & 2 & 4 & 5 & 6 & 5 & 6 & 7 & 7 & 7 & 3 & 8 & 9 & 9 & 10 & 11 & 12 & 13 & 13 & 2 \\
2 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 2 & 1 & 3 & 4 & 5 & 4 & 5 & 6 & 6 & 6 & 2 & 7 & 8 & 8 & 9 & 10 & 11 & 12 & 12 & 3 \\
3 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 2 & 4 & 5 & 4 & 3 & 4 & 5 & 6 & 5 & 3 & 6 & 7 & 7 & 8 & 9 & 10 & 11 & 11 & 4 \\
4 & 5 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 4 & 3 & 2 & 3 & 4 & 4 & 4 & 4 & 5 & 6 & 6 & 7 & 8 & 9 & 10 & 10 & 5 \\
3 & 4 & 5 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 2 & 3 & 2 & 1 & 2 & 3 & 3 & 4 & 3 & 4 & 5 & 5 & 6 & 7 & 8 & 9 & 9 & 6 \\
2 & 3 & 4 & 3 & 2 & 3 & 2 & 1 & 0 & 1 & 1 & 2 & 3 & 2 & 3 & 4 & 4 & 4 & 2 & 5 & 6 & 6 & 7 & 8 & 9 & 10 & 10 & 5 \\
1 & 2 & 3 & 2 & 1 & 2 & 3 & 2 & 1 & 0 & 2 & 3 & 4 & 3 & 4 & 5 & 5 & 5 & 1 & 6 & 7 & 7 & 8 & 9 & 10 & 11 & 11 & 4 \\
3 & 4 & 5 & 4 & 3 & 4 & 4 & 2 & 1 & 2 & 0 & 1 & 2 & 3 & 4 & 5 & 3 & 3 & 3 & 4 & 5 & 5 & 6 & 7 & 8 & 9 & 9 & 6 \\
4 & 5 & 6 & 5 & 4 & 5 & 4 & 3 & 2 & 3 & 1 & 0 & 1 & 2 & 3 & 3 & 2 & 2 & 4 & 3 & 4 & 4 & 5 & 6 & 7 & 8 & 8 & 7 \\
5 & 6 & 7 & 6 & 5 & 4 & 3 & 2 & 3 & 4 & 2 & 1 & 0 & 1 & 2 & 2 & 1 & 1 & 5 & 2 & 3 & 3 & 4 & 5 & 6 & 7 & 7 & 8 \\
4 & 5 & 6 & 5 & 4 & 3 & 2 & 1 & 2 & 3 & 3 & 2 & 1 & 0 & 1 & 2 & 2 & 2 & 4 & 3 & 4 & 4 & 5 & 6 & 7 & 8 & 8 & 7 \\
5 & 6 & 7 & 6 & 5 & 4 & 3 & 2 & 3 & 4 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 4 & 5 & 3 & 4 & 4 & 5 & 6 & 7 & 8 & 8 & 8 \\
6 & 7 & 8 & 7 & 6 & 5 & 4 & 3 & 4 & 5 & 5 & 3 & 2 & 2 & 1 & 0 & 1 & 3 & 7 & 2 & 3 & 3 & 4 & 5 & 6 & 7 & 7 & 10 \\
6 & 7 & 9 & 7 & 6 & 6 & 4 & 3 & 4 & 5 & 3 & 2 & 1 & 2 & 2 & 1 & 0 & 2 & 6 & 1 & 2 & 2 & 3 & 4 & 5 & 6 & 6 & 9 \\
6 & 7 & 8 & 7 & 6 & 5 & 4 & 4 & 4 & 5 & 3 & 2 & 1 & 2 & 4 & 3 & 2 & 0 & 6 & 3 & 4 & 4 & 5 & 6 & 7 & 8 & 8 & 9 \\
2 & 3 & 4 & 3 & 2 & 3 & 4 & 3 & 2 & 1 & 3 & 4 & 5 & 4 & 5 & 7 & 6 & 6 & 0 & 7 & 8 & 8 & 9 & 10 & 11 & 12 & 12 & 5 \\
7 & 8 & 9 & 8 & 7 & 6 & 5 & 4 & 5 & 6 & 4 & 3 & 2 & 3 & 3 & 2 & 1 & 3 & 7 & 0 & 1 & 1 & 2 & 3 & 4 & 5 & 5 & 10 \\
8 & 9 & 10 & 9 & 8 & 7 & 6 & 5 & 6 & 7 & 5 & 4 & 3 & 4 & 4 & 3 & 2 & 4 & 8 & 1 & 0 & 2 & 3 & 4 & 5 & 6 & 6 & 11 \\
8 & 9 & 10 & 9 & 8 & 7 & 6 & 5 & 6 & 7 & 5 & 4 & 3 & 4 & 4 & 3 & 2 & 4 & 8 & 1 & 2 & 0 & 1 & 2 & 3 & 4 & 4 & 11 \\
9 & 10 & 11 & 10 & 9 & 8 & 7 & 6 & 7 & 8 & 6 & 5 & 4 & 5 & 5 & 4 & 3 & 5 & 9 & 2 & 3 & 1 & 0 & 1 & 2 & 3 & 2 & 3 \\
10 & 11 & 12 & 11 & 10 & 9 & 8 & 7 & 8 & 9 & 7 & 6 & 5 & 6 & 6 & 5 & 4 & 6 & 10 & 3 & 4 & 2 & 1 & 0 & 1 & 2 & 2 & 15 \\
11 & 12 & 13 & 12 & 11 & 10 & 9 & 8 & 9 & 10 & 8 & 7 & 6 & 7 & 7 & 6 & 5 & 7 & 11 & 4 & 5 & 3 & 2 & 1 & 0 & 1 & 1 & 1 \\
12 & 13 & 14 & 13 & 12 & 11 & 10 & 9 & 10 & 11 & 9 & 8 & 7 & 8 & 8 & 7 & 6 & 8 & 12 & 5 & 6 & 4 & 3 & 2 & 1 & 0 & 2 & 17 \\
12 & 13 & 14 & 13 & 12 & 11 & 10 & 9 & 10 & 11 & 9 & 8 & 7 & 8 & 8 & 7 & 6 & 8 & 12 & 5 & 6 & 4 & 2 & 2 & 1 & 2 & 0 & 16 \\
3 & 2 & 1 & 2 & 3 & 4 & 5 & 6 & 5 & 4 & 6 & 7 & 8 & 7 & 8 & 10 & 9 & 9 & 5 & 10 & 11 & 11 & 3 & 15 & 1 & 17 & 16 & 0
\end{bmatrix}$$

Distance Eigen values are -72.7700, -29.6860, -13.6556, -9.3113, -7.4864, -5.7116, -5.0599, -3.1580, -3.0693, -2.6724, -2.0821, -1.8804, -1.4986, -1.2677, -1.1933, -1.0229, -0.7876, -0.7063, -0.5414, -0.5001, -0.0978, -0.0000, 0.0880, 0.1681, 0.4935, 0.8872, 12.2914, 150.2307.

Distance energy of a cholesterol is DE $C_{27}H_{46}O$ = |-72.7700 | + | -29.6860| + |-13.6556| + |-9.3113| + |-7.4864| + |-5.7116| + |-5.0599| + |-3.1580| + |-3.0693| + |-2.6724| + |-2.0821| + |-1.8804| + |-1.4986| + |-1.2677| + |-1.1933| + |-1.0229| + |-0.7876| + |-0.7063| + |-0.5414| + |-0.5001| + |-0.0978| + |-0.0000| + |0.0880| + |0.1681| + |0.4935|+ |0.8872| + |12.2914| + |150.2307| = 328.3176.

Harary Energy: The concept of Harary was introduced by A. Dilek Güngör and A. Sinan Çevik [14]. Let G be a simple graph of order n with vertex set V = {v_1, v_2 ...., v_n} and edge set E.

Definition 5: The Harary matrix of G is the square matrix of order n whose (i, j) entry is $1/d_{ij}$ where d_{ij} is the distance between the vertices v_i and v_j. Let λ_1, λ_2. . . λ_n be the Eigen values of the Harary matrix of G. The Harary energy, HE (G) is defined by

$$HE(G) = \sum_{i=1}^{n} |\lambda_i|$$

Further studies on Harary energy can be found in[15].

Theorem 4: The Harary energy of cholesterol $C_{27}H_{46}O$ is 36.5093.

Proof: The Harary matrix of cholesterol is H ($C_{27}H_{46}O$) =

0 1 1/2 1/3 1/2 1/3 1/4 1/3 1/2 1 1/3 1/4 1/5 1/4 1/5 1/6 1/6 1/6 1/2 1/7 1/8 1/8 1/9 1/10 1/11 1/12 1/12 1/3
1 0 1 1/2 1/3 1/4 1/5 1/4 1/3 1/2 1/4 1/5 1/6 1/5 1/6 1/7 1/7 1/7 1/3 1/8 1/9 1/9 1/10 1/11 1/12 1/13 1/13 1/2
1/2 1 0 1 1/2 1/3 1/4 1/5 1/4 1/3 1/5 1/6 1/7 1/6 1/7 1/8 1/9 1/8 1/4 1/9 1/10 1/10 1/11 1/12 1/13 1/14 1/14 1
1/3 1/2 1 0 1 1/2 1/3 1/4 1/3 1/2 1/4 1/5 1/6 1/5 1/6 1/7 1/7 1/7 1/3 1/8 1/9 1/9 1/10 1/11 1/12 1/13 1/13 1/2
1/2 1/3 1/2 1 0 1 1/2 1/3 1/2 1 1/3 1/4 1/5 1/4 1/5 1/6 1/6 1/6 1/2 1/7 1/8 1/8 1/9 1/10 1/11 1/12 1/12 1/3
1/3 1/4 1/3 1/2 1 0 1 1/2 1/3 1/2 1/4 1/5 1/4 1/3 1/4 1/5 1/6 1/5 1/3 1/6 1/7 1/7 1/8 1/9 1/10 1/11 1/11 1/4
1/4 1/5 1/4 1/3 1/2 1 0 1 1/2 1/3 1/4 1/4 1/3 1/2 1/3 1/4 1/4 1/4 1/4 1/5 1/6 1/6 1/7 1/8 1/9 1/10 1/10 1/5
1/3 1/4 1/5 1/4 1/3 1/2 1 0 1 1/2 1/2 1/3 1/2 1 1/2 1/3 1/3 1/4 1/3 1/4 1/5 1/5 1/6 1/7 1/8 1/9 1/9 1/6
1/2 1/3 1/4 1/3 1/2 1/3 1/2 1 0 1 1 1/2 1/3 1/2 1/3 1/4 1/4 1/4 1/2 1/5 1/6 1/6 1/7 1/8 1/9 1/10 1/10 1/5
1 1/2 1/3 1/2 1 1/2 1/3 1/2 1 0 1/2 1/3 1/4 1/3 1/4 1/5 1/5 1/5 1 1/6 1/7 1/7 1/8 1/9 1/10 1/11 1/11 1/4
1/3 1/4 1/5 1/4 1/3 1/4 1/4 1/2 1 1/2 0 1 1/2 1/3 1/4 1/5 1/3 1/3 1/3 1/4 1/5 1/5 1/6 1/7 1/8 1/9 1/9 1/6
1/4 1/5 1/6 1/5 1/4 1/5 1/4 1/3 1/2 1/3 1 0 1 1/2 1/3 1/3 1/2 1/2 1/4 1/3 1/4 1/4 1/5 1/6 1/7 1/8 1/8 1/7
1/5 1/6 1/7 1/6 1/5 1/4 1/3 1/2 1/3 1/4 1/2 1 0 1 1/2 1/2 1 1 1/5 1/2 1/3 1/3 1/4 1/5 1/6 1/7 1/7 1/8
1/4 1/5 1/6 1/5 1/4 1/3 1/2 1 1/2 1/3 1/3 1/2 1 0 1 1/2 1/2 1/2 1/4 1/3 1/4 1/4 1/5 1/6 1/7 1/8 1/8 1/7
1/5 1/6 1/7 1/6 1/5 1/4 1/3 1/2 1/3 1/4 1/4 1/3 1/2 1 0 1 1/2 1/4 1/5 1/3 1/4 1/4 1/5 1/6 1/7 1/8 1/8 1/8
1/6 1/7 1/8 1/7 1/6 1/5 1/4 1/3 1/4 1/5 1/5 1/3 1/2 1/2 1 0 1 1/3 1/7 1/2 1/3 1/3 1/4 1/5 1/6 1/7 1/7 1/10
1/6 1/7 1/9 1/7 1/6 1/6 1/4 1/3 1/4 1/5 1/3 1/2 1 1/2 1/2 1 0 1/2 1/6 1 1/2 1/2 1/3 1/4 1/5 1/6 1/6 1/9
1/6 1/7 1/8 1/7 1/6 1/5 1/4 1/4 1/4 1/5 1/3 1/2 1 1/2 1/4 1/3 1/2 0 1/6 1/3 1/4 1/4 1/5 1/6 1/7 1/8 1/8 1/9
1/2 1/3 1/4 1/3 1/2 1/3 1/4 1/3 1/2 1 1/3 1/4 1/5 1/4 1/5 1/7 1/6 1/6 0 1/7 1/8 1/8 1/9 1/10 1/11 1/12 1/12 1/5
1/7 1/8 1/9 1/8 1/7 1/6 1/5 1/4 1/5 1/6 1/4 1/3 1/2 1/3 1/3 1/2 1 1/3 1/7 0 1 1 1/2 1/3 1/4 1/5 1/5 1/10
1/8 1/9 1/10 1/9 1/8 1/7 1/6 1/5 1/6 1/7 1/5 1/4 1/3 1/4 1/4 1/3 1/2 1/4 1/8 1 0 1/2 1/3 1/4 1/5 1/6 1/6 1/11
1/8 1/9 1/10 1/9 1/8 1/7 1/6 1/5 1/6 1/7 1/5 1/4 1/3 1/4 1/4 1/3 1/2 1/4 1/8 1 1/2 0 1 1/2 1/3 1/4 1/4 1/11
1/9 1/10 1/11 1/10 1/9 1/8 1/7 1/6 1/7 1/8 1/6 1/5 1/4 1/5 1/5 1/4 1/3 1/5 1/9 1/2 1/3 1 0 1 1/2 1/3 1/2 1/3
1/10 1/11 1/12 1/11 1/10 1/9 1/8 1/7 1/8 1/9 1/7 1/6 1/5 1/6 1/6 1/5 1/4 1/6 1/10 1/3 1/4 1/2 1 0 1 1/2 1/2 1/15
1/11 1/12 1/13 1/12 1/11 1/10 1/9 1/8 1/9 1/10 1/8 1/7 1/6 1/7 1/7 1/6 1/5 1/7 1/11 1/4 1/5 1/3 1/2 1 0 1 1 1
1/12 1/13 1/14 1/13 1/12 1/11 1/10 1/9 1/10 1/11 1/9 1/8 1/7 1/8 1/8 1/7 1/6 1/8 1/12 1/5 1/6 1/4 1/3 1/2 1 0 1/2 1/17
1/12 1/13 1/14 1/13 1/12 1/11 1/10 1/9 1/10 1/11 1/9 1/8 1/7 1/8 1/8 1/7 1/6 1/8 1/12 1/5 1/6 1/4 1/2 1/2 1 1/2 0 1/16
1/3 1/2 1 1/2 1/3 1/4 1/5 1/6 1/5 1/4 1/6 1/7 1/8 1/7 1/8 1/10 1/9 1/9 1/5 1/10 1/11 1/11 1/3 1/15 1 1/17 1/16 0

Harary Eigen values are -1.8471, -1.5175, -1.5014, -1.4253, -1.3437, -1.3132, -1.2673, -1.2141, -1.1722, -1.0569, -1.0071, -0.7066, -0.6466, -0.6106, -0.5231, -0.4968, -0.3526, -0.2341, -0.0184, 0.0336, 0.2585, 0.4867, 0.9153, 0.9361, 1.2310, 2.5362, 3.4653, 8.3920.

Harary energy of a cholesterol is HE ($C_{27}H_{46}O$) = |-1.8471| + |-1.5175| + |-1.5014| + |-1.4253| + |-1.3437| + |-1.3132| + |-1.2673| + |-1.2141| + |-1.1722| + |-1.0569| + |-1.0071| + |-0.7066| + |-0.6466| + |-0.6106| + |-0.5231| + |-0.4968| + |-0.3526| + |-0.2341| + |-0.0184| + |0.0336| + |0.2585| + |0.4867| + |0.9153| + |0.9361| + |1.2310| + |2.5362| + |3.4653| + |8.3920| = 36.5093.

CONCLUSION: In this paper, we compute Siedel energy, Maximum degree energy, Distance energy, Harary energy of cholesterol.

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