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ENERGY OF TRIGLYCERIDE

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ABSTRACT

Using Huckel molecular orbital (HMO) theory of total pi-electron energy, Prof Ivan Gutman conceived the idea of energy of a graph in the year 1978.A triglyceride is a chemical compound formed from one molecule of glycerol and three fatty acids.Its molecular formula is $C_{55}H_{98}O_6$.In this paper, we compute energy of Triglyceride.

Mathematics Subject Classification: 05C12, 05C90.

Keywords: Energy, Triglyceride.

1. INTRODUCTION

Triglycerides are a type of fat (lipid) found in our blood. When we eat, our body converts any calories it doesn't need to use right away into triglycerides. The triglycerides are stored in our fat cells. Later, hormones release triglycerides for energy between meals. If we regularly eat more calories than we burn, particularly "easy" calories like carbohydrates and fats, we may have high triglycerides (hypertriglyceridemia). A simple blood test can reveal whether our triglycerides fall into a healthy range. Triglycerides and cholesterol are separate types of lipids that circulate in our blood. Triglycerides store unused calories and provide our body with energy, and cholesterol is used to build cells and certain hormones. Because

triglycerides and cholesterol can't dissolve in blood, they circulate throughout our body with the help of proteins that transport the lipids (lipoproteins).

Triglycerides are chemically tri esters of fatty acids and glycerol. Triglycerides are formed by combining glycerol with three fatty acid molecules. Alcohols have a hydroxyl (HO–) group. Organic acids have a carboxyl (–COOH) group.

Triglycerides are esthers with three fatty acid chains, and it is the fatty acid chains that make them what they are.

If they are saturated, as are animal fatty acids, that means that they are long chains of carbon molecules completely surrounded by hydrogen atoms. They carry a great deal of chemical energy in the C-H bonds and they are slower to break down, so they are good storage molecules of energy.

Unsaturated fatty acid triglycerides are those which have double bonds along their length, making them have fewer hydrogen bonds per fatty acid molecule. These are plant fatty acids, and they are easy to break down but have fewer C-H bonds for storage of chemical energy.

Molecules and molecular compounds are often modeled by molecular graph. Amolecular graph is a representation of the structural formula of a 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, loopless, and without multiple edges.

ENERGY

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

The concept of energy of a graph was introduced by I. Gutman [4] in the year 1978.

Definition1.1. The adjacency matrix of G is the $n \times n$ 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 eigenvalues$\lambda_1,\lambda_2, \ldots ,\lambda_n$ of $A(G)$, assumed in non increasingorder, are the eigenvaluesofthe graph G.

As Aisrealsymmetric, the eigenvalues 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 eigenvalues 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 [5], papers [1,2,6] and the references cited there in. The basic properties including various upper and lower bounds for energy of a graph have

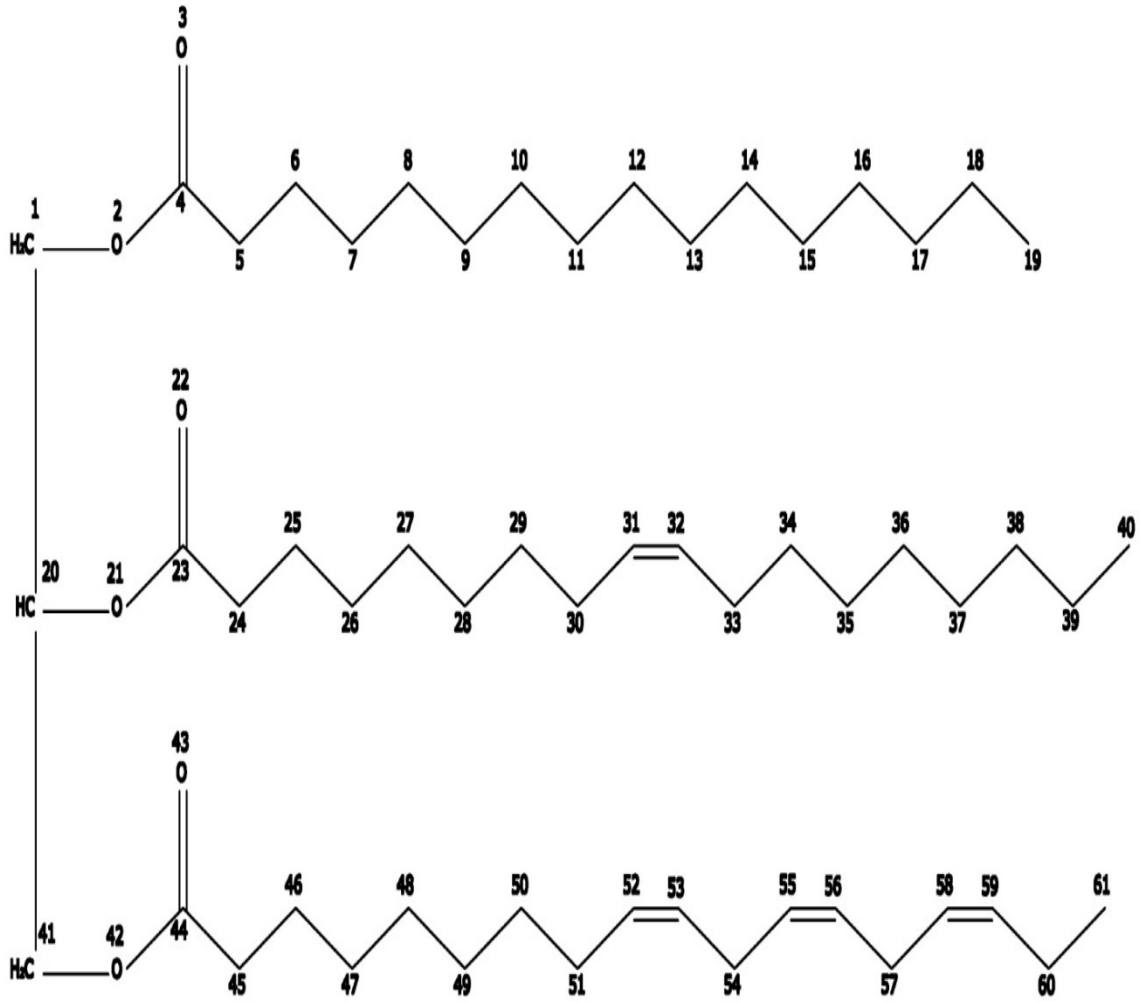
been established in [8,9], and it has found remarkable chemical applications in the molecular orbital theory of conjugated molecules [3,7]. Recently authors of this paper Computed of Energy of Cholesterol [10].

In chemistry, the Eigenvalues represents 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.

2. Main Results

Theorem 2.1. The Energy of a Triglyceride is 75.9770.

Proof. Consider a molecular graph of Triglyceride $C_{55}H_{98}O_6$ as shown in the following figure. Here vertices are numbered from 1 to 61.



The adjacency matrix of a Triglyceride is $A(C_{55}H_{98}O_6)$ =

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Eigenvalues are -2.1949, -2.0193, -2.0044, -1.9676, -1.9502, -1.9400, -1.8777, -1.8432, -1.8145, -1.7435, -1.6869, -1.6378, -1.5730, -1.4858, -1.4345, -1.3497, -1.2462, -1.2039, -1.0740, -0.9774, -0.9381, -0.7977, -0.6928, -0.6449, -0.5912, -0.3910, -0.3366, -0.3148, -0.2570, -0.0000, -0.0000, 0.0000, 0.2570, 0.3148, 0.3366, 0.3910, 0.5912, 0.6449, 0.6928, 0.7977, 0.9381, 0.9774, 1.0740, 1.2039, 1.2462, 1.3497, 1.4345, 1.4858, 1.5730, 1.6378, 1.6869, 1.7435, 1.8145, 1.8432, 1.8777, 1.9400, 1.9502, 1.9676, 2.0044, 2.0193, 2.1949

Energy of a Triglyceride is $E(C_{55}H_{98}O_6) =$

|-2.1949| + |-2.0193| + |-2.0044| + |-1.9676| + |-1.9502| + | -1.9400| + |-1.8777| + |-1.8432| + |-1.8145| + |-1.7435| + | -1.6869| + |-1.6378| + |-1.5730| + |-1.4858| + |-1.4345| + |-1.3497| + |-1.2462| + |-1.2039| + |-1.0740| + |-0.9774| + |-0.9381| + |-0.7977| + |-0.6928| + |-0.6449| + |-0.5912| + |-0.3910| + |-0.3366| + |-0.3148| + |-0.2570| + |-0.0000| + |-0.0000| + |0.0000| + | 0.2570| + |0.3148| + |0.3366| + |0.3910| + |0.5912| + |0.6449| + |0.6928| + |0.7977| + |0.9381| + |0.9774| + |1.0740| + | 1.2039| + |1.2462| + |1.3497| + |1.4345| + |1.4858| + |1.5730| + |1.6378| + |1.6869| + |1.7435| + |1.8145| + |1.8432| + | 1.8777| + | 1.9400| + | 1.9502| + | 1.9676| + |2.0044| + |2.0193| + |2.1949|
= 75.9770.

Conflict of interests: The authors declare that there is no conflicts of interests regarding the publication of this paper.

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