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SÜLEYMAN DEMİREL UNIVERSITY
GRADUATE SCHOOL OF NATURAL AND APPLIED SCIENCES

OPTIMIZING THE STRUCTURES OF GLYCERIC ACID MOLECULE BY MODERN OPTIMIZATION TECHNIQUES

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APPROVAL OF THE THESIS

"Optimizing the Structures of Glyceric Acid Molecule by Modern Optimization Techniques" submitted by **Ghassan QADERI** in partial fulfillment of the requirements for the **degree of Master of Science in Department of Mathematics**, Graduate School of Natural and Applied Sciences, Suleyman Demirel University.

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UNDERTAKE

I hereby declare that all information in this document has been obtained and presented in accordance with academic rules and ethical conduct. I also declare that, as required by these rules and conduct, I have fully cited and referenced all material and results that are not original to this work.

Ghassan QADERI

TABLE OF CONTENTS

ÖZET

Yüksek Lisans Tezi

MODERN OPİMİZASYON TEKNİKLERİ İLE GLYCERİC ACİD MOLEKÜLÜN YAPİSİNİ OPTİMİZE ETME

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Bu tezde, gliserik asit molekülünün enerji yapısını modellemek için bulanık mantık yaklaşımı uygulandı. Model, Gaussian Programında Yoğunluk Fonksiyonel Teorisi (DFT) yöntemiyile elde edilen teorik sonuçlara göre kurulmuştur.

İki torsiyon açısına bağlı olarak makul hesaplama maliyeti ve yüksek doğruluk ile minimum değer elde etmek için molekülün sürekli enerji yapısının inşa edilmesi amaçlanmaktadır. Başka metotlar ve deneylerden faylanarak elde edilmesi zahmetli ve zaman alan test edilmemiş koşullar için veriler, Bulanık Mantık yaklaşımı kullanılarak daha hızlı ve daha az hesaplamayla elde edilmiştir.

Elde edilen model, molekülü minimum enerjili en iyi açı çiftini belirlemek için kullanılmıştır. Son olarak, sonuçlar DFT ile elde edilen sonuçlarla karşılaştırılmıştır.

Anahtar Kelimeler: Optimizasyon, Düzgün Olmayan Modelleme, Bulanık Küme, Karar Verme, DFT, Gaussian.

2016, 64 sayfa

ABSTRACT

M.Sc. Thesis

OPTIMIZING THE STRUCTURES OF GLYCERIC ACID MOLECULE BY MODERN OPTIMIZATION TECHNIQUE

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In this thesis, we have been applied the fuzzy logic approach in order to model the energetic structure of glyceric acid molecule. The model has been set up according to theoretical results obtained by the Gaussian Program on the Density Functional Theory (DFT) method.

We aim to construct the continuous energy structure of the molecule depending on its two torsion angles and to obtain its minimum value with reasonable computational costs and high accuracy. Also, we got the results for the untested data, which are expensive and time consuming to be obtained by other methods and experimental.

The constructed model was used to determine the best angle value pairs that make the energy of the molecule minimum. Finally, the results are compared with those obtained by DFT.

Keywords: Optimization, Non-smooth Modelling, Fuzzy Sets, Making Decisions, DFT, Gaussian.

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Last but not the least, I would like to thank my family: my parents and my brothers and sister for supporting me spiritually throughout writing this thesis and my life in general. Very warm thanks go to my wife Joanna who always encouraged me and showed me great patience right to the end of the study. Thanks to my children Ahmed QADERI and Mohammed QADERI for their patience. Thanks to all my friends who have supported me and advised me.

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LIST OF FIGURES

LIST OF SYMBOLS

B3LYP	The hybrid of Becke's non-local three parameter exchange and correlation functional with the Lee-Yang-Parr functional
BOA	Bisector Of Area
CS	Crisp Set
DFT	Dinsity Function Theory
FCR	Fuzzy Control Rules
FIP	Fuzzy Inference Process
FIS	Fuzzy Inference System
FL	Fuzzy Logic
FLM	Fuzzy logic Modeling
FLV	Fuzzy linguistic Variables
FMR	Fuzzy Mapping Rules
FS	Fuzzy Set
FS	Fuzzy Singleton
FS	Fuzzy System
GA	Glyceric Acid
LDA	Local Density Approximation
LOM	Largest Of Maximum
MF	Membership Functions
MOM	Mean Of Maximum
MSO	Molecular Structure Optimization
PES	Potential Energy Surface
SOM	Smallest Of Maximum

LIST OF TABLES

1. INTRODUCTION

1.1. Introduction to DFT

Traditional correlation methods are too expensive for the large molecules, density function theory (DFT) is the Kohn-Sham formulation (Parr and Yang, 1989; Labanowski and Andzelm, 1991), and has emerged in the past few years as a successful alternative to traditional methods using configuration expansion. The lasting popularity of DFT is because of many factors: the introduction of new, accurate exchange-correlation potentials (Lee et al.,1988;Becke,1988;Vosko Atal.,1980;Perdew et al., 1992), which yield substantially improved predictions; the introduction of analytical first derivatives (Fan et al.,1988;Fournier et al.,1989), the recent formulation (Fournier, 1990;Komornicki and Fitzgerald, 1993), and implementation (Johnson and Frisch, 1993) of analytical second derivatives; and finally the development of programs (Gill et al.,1992;Handny et al.,1992), which approach the numerical precision of traditional quantum chemistry methods.

An important advantage of the DFT method is that the convergence with respect to improvements in the basis set is quicker than in traditional correlation techniques since the principally set serves only to describe the strongly occupied molecular orbitals, not the highly oscillatory correlation orbital's (Rauhut and Pulay, 1995).

DFT-based methods ultimately derive from quantum mechanics research from the 1920's, especially the Thomas-Fermi-Dirac model, and from Slater's fundamental work in quantum chemistry in the 1950's. The density function theory DFT approach is based upon a strategy of modeling electron correlation across the general functional of the electron density.

The Hohenberg-Kohn theorems allow us to construct a rigorous many-body theory using the electron density as the fundamental quantity. These methods owe their modern origins to the Hohenberg-Kohn theorem, published in 1964 (Hohenberg and Kohn) which showed existence of a unique functional which determines the ground state energy and density exactly.

Kohn and Sham, (Kohn and Sham, 1965) suggested a route for how the hitherto unknown universal functional can be approached In order to alleviate the situation and realize that orbital-based approaches such as the Hartree-Fock method perform much better in this respect, Kohn and Sham introduced the idea of a non-interacting reference system based on the set of orbital (i.e., one electron functions) so that the major part of the kinetic energy can be computed to good accuracy. In a similar way to the exchange functional, a local correlation functional can also improve by adding a gradient correction.

The pure density function theory methods are defined by pairing an exchange functional. For example, the known BLYP functional pairs Becke's gradient-corrected exchange functional with the gradient-corrected correlation functional of Lee, Yang and Parr. Density function theory changed the way of approaching Quantum mechanics. Its accuracy and predictive power are comparable to those of other ab initio methods but a lot cheaper computationally. Thus DFT is conveniently used for molecular structure optimization (MSO) or even for dynamic exploration of the potential energy surface (PES).

The DFT based B3LYP functional has been widely utilized in exploring the electronic structure and spectral characteristics of various inorganic, bioinorganic, and organometallic chemistry (Siegbahn and Borowski, 2006; Lee et al., 1988; Becke, 1988; Becke, 1993). However, many attempts have been made to develop new exchange and correlation functions to enhance the quality of prediction and develop the applicability of computational DFT methods for different systems (Hohenberg and Kohn, 1964; Kohn and Sham, 1965). There is a large number of theoretical studies on the structures, and stability.

DFT calculations are used widely to compute structures and relative energies of tautomer's as well as protonation states, solvated structures, and vibrational spectra. (DFT) approaches, especially those using the hybrid fundamental have evolved become a strong and very reliable tool, being routinely used for the determination of different molecular properties.

B3LYP functional has been earlier shown to provide an excellent compromise between accuracy and computational efficiency for large and medium sized

molecules (Volkenstein et al., 1949; Chowdhry et al., 2003; Chis, 2004; Asensio et al., 2003).

1.2. Introduction to Fuzzy Logic

The history of Fuzzy Logic is beginning with Buddha, (who lived in India in about 500 B.C and founded the religion called Buddhism). Buddhist philosophy was based on the idea that the world is full of contradictions. Almost everything contains some of its opposite, or in other words, that things can be (A) and not (A) at the same time. This shows us a clear connection between Buddha's philosophy and modern fuzzy logic.

About 200 years later, the Greek scholar Aristotle developed binary logic. Unlike Buddha, he thought that the world was made up of opposites, everything has to be (A) or not (A), it can't be both. It was and still is acceptable and correct scientifically .Like many others, Russell tried to reduce math to logic.

When he discovered his paradox during work, he got scared himself. It did, however, give him the honor of being one of the fathers of fuzzy logic. After that in 1964, Professor Zadeh started wondering, if there wasn't a better logic to use in machinery. So, his idea is that if you could tell an air-conditioner to work a little more quickly when it gets hotter, or similar problems, it would be much more efficient than having to give a rule for each temperature. Also, he noticed that it is interesting that humans do not have sufficient capacity to deal with large amounts of numerical data and information, despite, his amazing ingenuity in making complex decisions.

On the other hand, computers can do more complex calculations in the fraction of a second while they are completely unable to do the most basic human activities unless it is a numerical representation. This human superiority is clear, and so, the inability of the numerical systems pushed Lofty A. Zadeh to research and access the theory of Fuzzy logic in 1965 (Zadeh, 1965;Zadeh, 1975;Zadeh, 1978;Zadeh , 1976). Also, he had observed that conventional computer logic couldn't manipulate data that represented subjective or vague ideas, so he established fuzzy logic to allow computers to determine the distinctions among data with shades of gray, similar to the process of human reasoning. In spite of the fact that, the innovation was presented in the U.S., U.S. and European

scientists and researchers largely ignored it for years, maybe because of its unconventional name. They refused to consider important something that sounded so childlike. Some mathematicians claimed that fuzzy logic was merely probability in disguise. But fuzzy logic was easily accepted in Japan, China and other Asian countries.

The largest number of fuzzy logic researchers today are found in China, with over 10,000 scientists. Japan, though considered at the leading edge of fuzzy studies, has fewer people engaged in fuzzy Iogig research.

Fuzzy logic was not a suitable theory for the researchers at that time because it contained vagueness in the engineering field. However, since the 1970s, the approach of the set theory has been widely applied to control systems. The basics of fuzzy logic were used to control a steam engine by Mamdani from the University of London in 1974 (Mamdani, 1974). That study was a milestone for fuzzy logic.

The first industrial application of fuzzy logic was a cement kiln built in Denmark in 1975. Fuji Electric applied the fuzzy logic theory to the control of a water purification operation in the 1980. In Japan, as a challenging engineering project, in 1987, Sendai Railway system that had automatic train operation control that was built with fuzzy logic principles.

Fuzzy control techniques were used in all the critical operations in the control of the train, such as accelerating, stopping operations, and breaking. In 1987, Takeshi Yamakawa used fuzzy control in an inverted pendulum experiment, which is a classical control problem.

After these successful applications using fuzzy logic, not only engineers but also social scientists applied it in different areas. In technology now a days, many companies use fuzzy logic in their engineering projects for example, air conditioners, video cameras, washing machines, televisions, medical diagnoses, bus time tables, antilock braking system, etc. Since its inception in 1965, fuzzy set theory has been advanced to a powerful mathematical theory. It has been applied to many mathematical areas such as, analysis, algebra, control theory, graph theory, measure theory Optimization, topology, operations research, and so on. It

has also been applied both, alone and in combination with classical approaches as the principle dish in practice in various disciplines, such as control, data processing, decision support, engineering, logistics, medicine, and others. It is particularly well suited as a bridge between natural language and formal models. There are many studies which use the fuzzy logic approach (Sahiner et al., 2013; Sahiner et al., 2014; Sahiner et al., 2015).

To model the problem at hand, Fuzzy logic now a days is used in washing machines (Sahiner and Qaderi, 2015). The modelling techniques based on fuzzy inference systems (FIS) are attractive and found many successful applications in different fields (Zhao et al., 2013; Song Atal, 2013; GAO et al, 2012). Compared with the other prediction approaches, the fuzzy approaches have the following features: 1) rule-based structures able to capture the dependency between inputs and outputs of a system; 2) the fuzzy linguistic variables (FLV) availability to deal with uncertainties in natural way; 3) they are capable of modelling nonlinear systems; 4) the singular and linguistic outputs can be easily formed; 5) they are insensitive to random noise.

In this thesis we have used the fuzzy logic approach (BY MATLAB PROGRAM) to model the energetic structure of the glyceric acid molecule in order to obtain the best torsion angle values which make the energy of glyceric acid minimum. This distinguishes this study from other studies. Therefore, we can make the data continuous and get the results for the untested data.

1.3. Goal of Thesis

There are a lot of misconceptions about fuzzy logic (FL). In the first place, fuzzy logic is an accurate logic of imprecision and approximate reasoning. There are two of remarkable human capabilities: first, the capability to talk, reason and make rational decisions in an environment of imprecision, uncertainty, incompleteness of information, conflicting information, partiality of truth and partiality of possibility, more specifically, in an environment of missing

information, and second, the capability to perform a wide variety of physical and mental tasks without any measurements and any computations.

Fuzzy logic is close to the function of human thought. Applications of fuzzy logic are rapid and cost effective. The application process does not require a mathematical model, and it is quite easy. Uncertain and indefinite information can be used with cheap sensors, it brings flexibility to the measurement of the process, which allows the definition of concepts or correctness values in a graded way. As well, it is widespread from the other techniques, therefor, the goal of my thesis to apply the fuzzy logic approach in order to model the energetic structure of glyceric acid molecule.

The model has been set up according to the theoretical results obtained by the Gaussian Program using the Density Functional Theory (DFT)/B3LYP/ 6-31/G (d). By using fuzzy logic control, we have been able to determine the minimum energy value of the glyceric acid molecule depending on the two torsion angles (SC1=O3C1C2O5), (SC2=C1C2C6O7), compared with the results obtained by DFT method. As well as aiming to make the data continuous we have also obtained the results for the untested data.

2. BASIC DEFINITIONS AND TERMINOLOGY FOR DFT

2.1. Gaussian

Is a computer program for computational chemistry initially released in 1970 by John Pople (Gaussian70: Written by John Pople's group at Carnegie-Mellon University in the 1970s. John Pople was awarded the Nobel Prize in 1998 for his development of computational methods in quantum chemistry) (Pople, 2004; pople and gaussian, 2004), and his research group at Carnegie-Mellon University (CMU) as Gaussian 70 (Hehre et al., 1970). It has been continuously updated since then (David, 2001).

The name originates from Pople's use of Gaussian orbitals to speed up calculations compared to those using Slater-type orbitals, a choice made to improve performance on the limited computing capacities of then-current computer hardware for Hartree–Fock calculations.

The current version of the program is Gaussian 09 (Frich et al., 2003). Originally available through the Quantum Chemistry Program Exchange, it was later licensed out of CMU, Starting from the basic laws of classical or quantum mechanics Gaussian predicts the energies, molecular structures, and vibrational frequencies of atomic or molecular systems, side by side with many of the molecular properties derived from these basic computation types. So, it can be used by chemists, chemical engineers, physicists, biochemists and other scientists for research in established and emerging areas of chemical interest. It allows to perform virtual chemistry with a reasonable cost and save much experimental time in the laboratory.

2.2. The job types available in Gaussian

1. **SP:** Single point energy.
2. **Scan:** Potential energy surface scan.
3. **Freq**: Frequency and thermochemical analysis.
4. **Opt**: Geometry optimization.
5. **IRC:** Reaction path following.
6. **IRCMax**: Find the maximum energy along a specific reaction path.
7. **Polar:** Polarizabilities and hyper polarizabilities.
8. **Density=Checkpoint** Recomputed population analysis only.

9. **Stable:** Test wave function stability.
10. **ADMP and BOMD:** Direct dynamics trajectory calculation.
11. **Guess=Only:** Print initial guess only; recomputed population analysis.
12. **Rear chive:** Extract archive entry from checkpoint file only.

2.3. The Following Basis Sets That Stored Internally In the Gaussian Program

- STO-3G.
- 3-21G.
- 6-31G.
- 6-311G.

Single first polarization functions can also be requested using the usual * or ** notation. Note that (d, p) and ** are synonymous - 6-31G** is equivalent to 6-31G (d, p), for example-and that the 3-21G* basis set has polarization functions on second row atoms only. The + and ++ diffuse functions are available with some basis sets, as are multiple polarization functions. The keyword syntax is best illustrated by example: 6-31+G (3df, 2p) designates the 6-31G basis set supplemented by diffuse functions, 3 sets of d functions and one set of (f) functions on heavy atoms, and supplemented by 2 sets of p functions on hydrogens.

Adding a single polarization function to 6-311G (i.e. 6-311G (d)) will result in one d function for first and second row atoms and one f function for first transition row atoms, since d functions are already present for the valence electrons in the latter. Similarly, adding a diffuse function to the 6-311G basis set will produce one's, one p, and one d diffuse functions for third-row atoms.

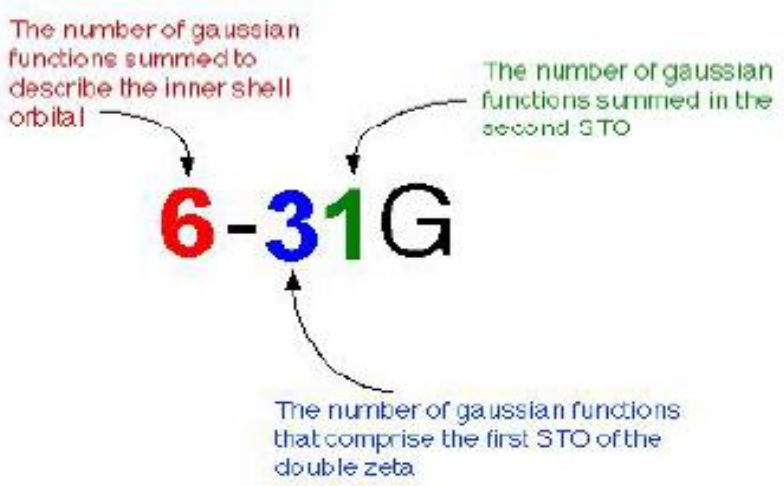

Figure 2.1. Graphical explain 6-31 G.

2.4. B3LYP

B3LYP is one of the energy functional of the density functional methods, the energy is reported in DFT calculations in a form similar to that of Hartree-Fock calculations.

That means: the hybrid of Becke's non-local three parameter exchange and correlation functional with the Lee-Yang-Parr functional (Lee et al., 1988; Becke, 1933; Parr and Yang, 1989).

2.5. Density Functional Theory (DFT)

DFT is an approach to the electronic structure of atoms and molecules and states that all the ground-state properties of a system are function of the charge density. Namely, the electron density is the basic variable, instead of the wave function. This reduces the computational burden of treating electron-electron interaction terms, which are treated explicitly as a functional of the density. This method combines the capacity to incorporate exchange-correlation effects of electrons with reasonable computational costs and high accuracy (Kohn and Sham, 1965; Parr et al., 1989; Dreizler and Gross, 1990; Koch and Holthausen, 2001; Fiolhais et al., 2003; Sholl and Steckel, 2009).

The exact exchange energy functional is expressed in terms of the Kohn–Sham orbitals rather than density, so it is termed an implicit density functional. One of the most commonly used versions is B3LYP, which stands for Becke, 3-parameter, Lee-Yang-Parr.

DFT is a computational quantum mechanical modelling method used in physics, chemistry and materials science to investigate the electronic structure (principally the ground state) of many-body systems, in assigned atoms, molecules, and the condensed phases. By using this theory, characteristics of a many-electron system can be determined by using functional, i.e. functions of another function, which in this case is the spatially dependent electron density. Consequently the name (DFT) comes from the use of the functional of the electron density. The density function theory is among the most popular and flexible methods available in condensed-matter physics, computational chemistry, and computational physics.

The density functional theory has been very popular for calculations in solid-state physics since the 1970s. However, DFT was not considered accurate enough for calculations in quantum chemistry until the 1990s, when the approximations used in the theory were greatly refined to ideal as a model for the exchange and correlation interactions. In many cases the results of DFT calculations for solid-state systems agree quite satisfactorily with experimental data. DFT computational costs are relatively low when compared to traditional methods, such as Hartree–Fock theory and its descendants based on the complex many-electron wave function.

Despite recent improvements, there are still difficulties in using DFT to properly describe intermolecular interactions (of critical importance to understanding chemical reactions), especially van der Waals forces (dispersion); charge transfer excitations; transition states, global potential energy surfaces, dopant interactions and some other strongly correlated systems; and in calculations of the band gap and ferromagnetism in semiconductors (Assadi et al. 2013). Its incomplete treatment of dispersion can adversely affect the accuracy of DFT (at least when used alone and uncorrected) in the treatment of systems which are

dominated by dispersion (e.g. interacting noble gas atoms) (Mourik Atal., 2002), or where dispersion competes significantly with other effects (e.g. in biomolecules) (Vondrášek et al., 2005). The development of new DFT methods designed to overcome this problem, by alterations to the functional and inclusion of additional terms to account for both core and valence electrons (Grimme, 2006), or by the inclusion of additive terms, (Zimmerli et al., 2004; Grimme, 2004; Von Lilienfeld et al., 2004; Tkatchenko and Scheffleris, 2009), is a current research topic.

2.6. Methods in DFT

Method in DFT Are Complex and Varying, but Can Roughly Be Divided Into Three Varieties:

1. The first verity is methods that use the local density approximation (LDA) determined solely based on the characteristics of the electron density. The critical proposition of this approximation is that, for a molecule with so many electrons in a gaseous state, density is uniform throughout the molecule. This is not the case for molecules, where the electron density is decidedly non-uniform. This approach does, however, work well with electronic band structures of solids, showing the range of energies in which electrons are permitted or not permitted. Aside from this application, however, local density approximations are not very satisfactory.
2. The second variety is methods that bring together electron density calculations with a gradient correction factor. The gradient A in mathematics is a function which measures the rate of change of some property. In this case, the gradient looks to calculate the non-uniformity of the electron density, so is known as gradient-corrected. Another term for this is non-local.
3. The third variety is methods that are a combination of a Hartree-Fock approximation to the energy exchange and a density function theory approximation to the exchange energy, all combined with a functional that includes electron correlation. These methods are known as hybrid methods. This is the most common and popular DFT method used in practice. Therefor we used this method in my thesis.

2.7. How to Build Molecule Using Gaussian?

1. Open the Gaussian program.
2. Go to icon (file) L-click + chose (NEW) + create molecule group.
3. Press the “Element Fragment” icon (the 6C icon). This opens a window displaying the periodic table of the elements.
4. Choose the desired atom using the L-click. Make sure that the atom or fragment you want to add is the one that is marked on the lower part of the periodic table. You can view the fragment you choose, before adding it, in the main Gaussian.
5. After that, place the fragment, using the L-click, in the small blue window.
6. After adding all desired atoms (excluding hydrogens) you can start bonding them as you wish using the “Modify Bond” option in the “Builder”. You do this by pressing the “Modify Bond” icon then choosing two atoms by L-clicking on them in the small blue window. The two chosen atoms change color and are marked as (1) and (2). Note that it is essential to press the “OK” push button after choosing the bond.
7. After connecting all the main atoms in the desired way, you can add hydrogen atoms by using the “Add Valence” option on the “Builder” window. Press the “Add Valence” using the L-click then press on one of the atoms in the small blue window. Each L-click used in this way adds one hydrogen atom.
8. You can remove atoms from the structure by using the “Delete Atom” icon on the “Builder” window. L-click this icon, then L-click the atom that you wish to remove.

   After all atoms are placed in the small blue (structure) window, L-click the “Clean” button in the “Builder” window in order to adjust molecular geometry according to a predefined set of rules.

9. Go to icon (EDIT) L-click + chose (REDUNDANT COORDINATES EDITOR) to choose our angles.
10. Save the data file that you created in this way in your directory. It may be used as an input file for Gaussian calculation.
11. L-click on the "calculation" option in the Gaussian window menu.

12. After click calculation show us list (job type, method…etc).

13. Select "Job Type" option. Here you may choose the type of calculation you want to perform, e.g. energy calculation, structure optimization, NMR, etc.

14. Next go to the "Method" option, Here you choose the level of calculation, e.g., Hartree-Fock, DFT, etc. You may choose a restricted or unrestricted calculation, and, if you chose the DFT option a new options 'inside field' will pop-up for choosing the DFT functional, e.g. B3LYP. Here you also choose the basis set you wish to use.

15. The next option is the "Title" it is not necessary to write a title, but it is highly recommended. Later, when looking at the results, the title may help you remember what was going on and if there is something important.

16. The "Link 0" option is not relevant to us.

Next is the "General" option, where here you may specify certain information, e.g. if you want additional (than the usual) printing, or should Gaussian ignore symmetry or use it. Usually it is helpful to use symmetry to reduce the calculation time; however, it can be sometimes problematic.

17. The Guess, NBO and PBC options in the upper toolbar are not relevant to us at this point.

18. The last options in the upper toolbar is 'Solvation'. If calculation in a solvent, instead of vacuum, is desired you can do it here. You may choose the different salvation approximation method, the solvent or alternatively the associated dielectric constant.

19. After we specified all we need from Gaussian and our "input" is ready we need to send the Job using the "Submit" option in the lower toolbar. L-click on the "Submit" will open Gaussian after saving the input file.

20. A Gaussian window is now open and it should be "working" until it is finished, it is now possible to see the Gaussian or close it and only see the output.

21. It is now possible to open the output file and analyze the results you have obtained.

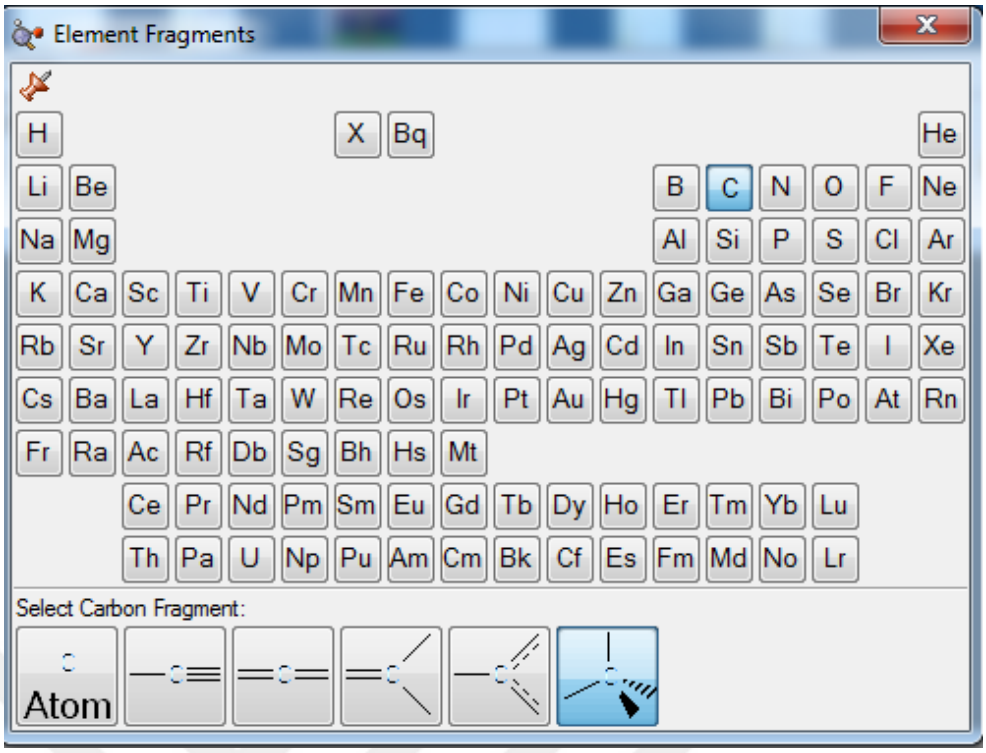

Figure 2.2. Graphical show element fragments.

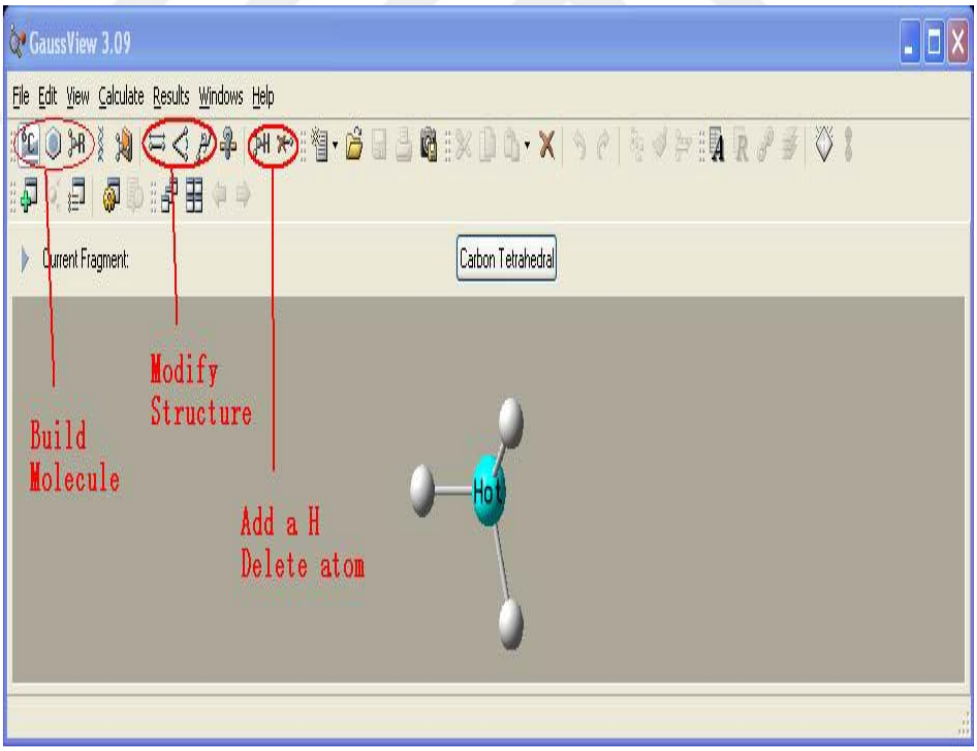

Figure 2.3. Graphical show (build molecule, modify structure and ad H delete atom).

2.8. Advantages of DFT

1. DFT is a general-purpose computational chemistry method and as such, can be applied to most systems.
2. The most important advantage of the DFT methods is the large increase in computational accuracy without the additional increase in computing time.
3. DFT methods with B3LYP/6-31G (d) are oftentimes considered to be a standard model chemistry for many applications.
4. DFT with B3LYP methods clearly provide better results for reaction chemistry calculations.

2.9. Disadvantages of DFT

1. The one of the main disadvantages of Density Function Theory (DFT) methods is the challenge in determining the most convenient way for a particular application.
2. The practitioner should, prior to choosing a DFT method, consult the literature to determine the suitability of that choice for that particular problem or application. In this way, Density Function Theory usage tends to favor the more sophisticated user.
3. The other disadvantage is that when you use DFT to calculate the energy it is not calculated at all points.
4. Also, when you use DFT to calculate the energy it gives us discontinuous data.
5. DFT methods are considered by some people, to produce unacceptable results for weak hydrogen bonding interactions.

2.10. Historical Application of DFT

In 1920: Introduction of the Thomas-Fermi model.

In 1964: Hohenberg-Kohn paper proving existence of exact DFT.

In 1965: Kohn-Sham scheme introduced.

In 1970s and early 80s: LDA. DFT becomes useful.

In 1985: Incorporation of DFT into molecular dynamics (Car-Parrinello).

In 1988: Becke and LYP functionals. DFT useful for some chemistry.

In1998: Nobel Prize awarded to Walter Kohn in chemistry for development of DFT.

3. BASIC DEFINITIONS AND TERMINOLOGY FOR FUZZY LOGIC

3.1. Fuzzy Logic Approach

It is well known that the concept of fuzzy sets was introduced by Zadeh (Zadeh, 1967). And the main idea of fuzzy set theory is: instead of select the exact boundaries as in an ordinary set, a fuzzy set allows no sharply deed boundaries because of generalization of a characteristic function to a membership function (Sakawa, 1993). Fuzzy logic starts with concept of a fuzzy set which is a set without crisp, clearly deed boundary. After that Zadeh developed many of the methods of fuzzy logic based on this simple idea. It took a couple of decades for the rationale of fuzzy sets to be understood and applied by other scientists. So, fuzzy set is defined as:

$S = \{(x, \mu s(x)) : x \in X, \mu s(x) \in [0,1]\}$. (Altinok et al., 2009).

The traditional way to represent elements u of a set A is through the characteristic function:

1- $\mu_A(u) = 1$, if u is an element of the set$A$.

2- $\mu_A(u) = 0$, if u is not an element of the set$A$.

That is, an object either belongs or does not belong to a given set.

In fuzzy sets an object can belong to a set partially. The degree of membership is defined through a generalized characteristic function called membership function:

$$\mu_A(x): \boldsymbol{U} \rightarrow [\mathbf{0}, \mathbf{1}]$$

Where $\boldsymbol{U}$ is called the universe, and A is a fuzzy subset of $\boldsymbol{U}$.

The values of the membership function are real numbers in the interval [0, 1], where 0 means that the object is not a member of the set and 1 means that it belongs entirely. Each value of the function is called a membership degree.

Fundamental differences between the classical and fuzzy logic

Classical	Fuzzy
A or not A	A and not A
Certain	Partially
All or nothing	In specific degrees
0 or 1	Continuity between 0 and 1
Binary Units	Fuzzy Units

Table 3.1. The differences between classical logic and fuzzy logic.

3.2. The Relation between Universal Set and Fuzzy Set

If there are a universal set and a crisp set, we consider the set as a subset of the universal set. Therefore, in the same way, we consider a fuzzy set A as a subset of universal set$x$.

The crisp set (CS) v.s. the fuzzy set (FS)

The CS is defined in such a way as to partition the individuals in some given universe of discourse into two parts: members or non-members. But, many classification concepts do not exhibit this characteristic. For example, expensive cars, or sunny days and the set of tall people.

FS can be defined mathematically by assigning for everybody possible in the universe of discourse a value representing its grade of membership in the FS.

For example, a FS representing our perception of sunny weather might assign a degree of membership of 1 to a cloud cover of 0%, 0.8 to a cloud cover of 20%, 0.4 to a cloud cover of 30%, and also 0 to a cloud cover of 75%.

3.3. Some Definitions about Fuzzy Logic

Definition 3.3.1. Convexity

A fuzzy set A is convex if and only if

$$\forall x_1, x_2 \in X \wedge \forall \lambda \in [0,1], \mu_A[\lambda x_1 + (1-\lambda)x_2] \geq \min\{\mu_A(x_1), \mu_A(x_2)\}.$$

Instead of this, A is convex if all its α-level sets are convex. Note that the definition of convexity of a fuzzy set is not as strict as the common definition of convexity of a function. Indeed, it corresponds to the definition of quasi-concavity of a function.

Definition 3.3.2. Convex fuzzy set

A convex fuzzy set is described by a membership function whose membership values are strictly monotonically increasing, or strictly monotonically decreasing, or strictly monotonically increasing then strictly monotonically decreasing with increasing values for elements in the universe. In another worlds, if for any elements *x*, *y*, and *z* in a fuzzy set A, the relation $x < y < z$ implies

$$\mu_A(y) \geq \min[\mu_A(x), \mu_A(z)]$$

then A is said to be a convex fuzzy set .

Definition 3.3.3. Fuzzy Number (FN)

The FN is a fuzzy set with the following conditions (Çolak et al., 2009; Çolak et al., 2011; Hazarika and Savas, 2007)

1- Convex fuzzy set.

2- Normalized fuzzy set.

3- Its membership function is piecewise continuous.

4- It is defined in the real number.

Definition 3.3.4. Equality of fuzzy sets

Let A and B be fuzzy subsets of a classical set X. A and B are said to be equal, symboling $A=B$, if $A \subset B$ and $B \subset A$. We note that $A = B$ if and only if $A(x) = B(x) for\ x \in X$.

Definition 3. 3.5. Empty fuzzy set

The empty fuzzy subset of X is defined as the fuzzy subset $\emptyset \; of \; X$ such that $\emptyset(x) = 0$ for each$x \in X$. It is easy to see that $\emptyset \; C \; A$ holds for any fuzzy subset $A \; of \; X$.

Definition 3.3.6. The largest fuzzy set in X

This is called universal fuzzy set in X, denoted by$1x$, is defined by $1x(t) = 1, \forall t \in X$. It is easy to see that $A \; C \; 1x$ holds for any fuzzy subset$A \; of \; X$.

Definition 3.3.7. Normal fuzzy set

A fuzzy subset A of a classical set X is called normal if there exists $x \in X$ such that $A(x) = 1$, otherwise A is subnormal.

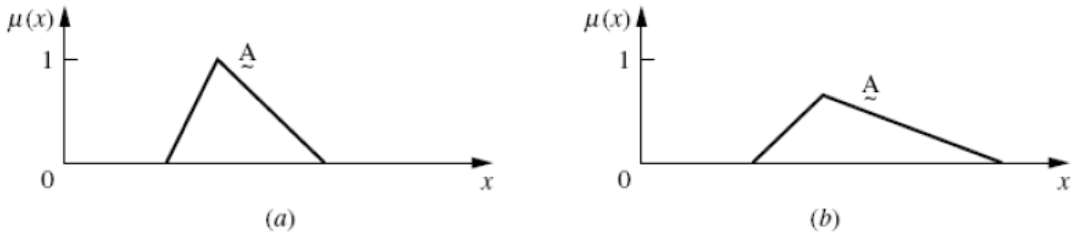

Figure 3.1. Fuzzy set that are normal (a) and subnormal (b).

Definition 3.3.8. Complement

We can find the complement set of fuzzy set A also in a crisp set. We denote the complement set of A as Ã. Membership degree can be calculated as following:

$$\mu_{\tilde{A}}(x) = \mu(NOT\ A)$$

$$= 1 - \mu_A(x).$$

Definition 3.3.9. Union

Membership value of member x in the union takes the greater value of membership between A and B

$$(A \cup B)_X = max[A(x), B(x)].$$

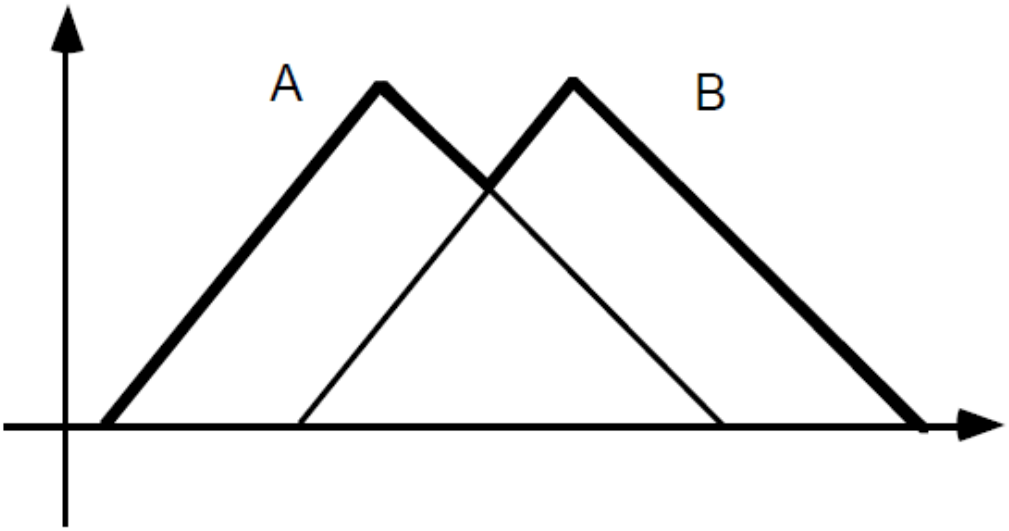

Figure 3.2. Union of two triangular fuzzy numbers.

Definition 3.3.10. Intersection

Intersection of fuzzy sets A and B takes a smaller value of membership function between A and B

$$(A \cap B)_X = min[A(x), B(x)].$$

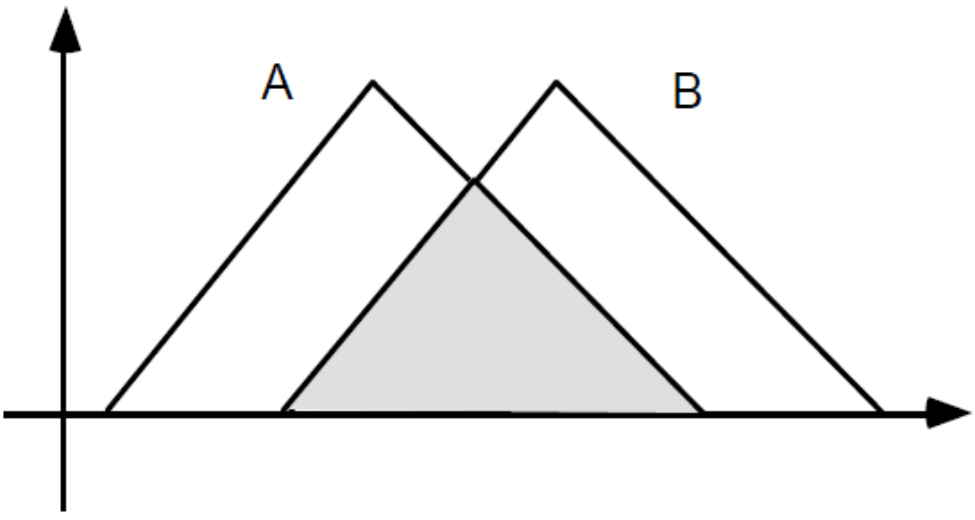

Figure 3.3. Intersection of two triangular fuzzy numbers.

Definition 3.3.11. Core

The core of a membership function for some fuzzy set A is defined as that region of the universe that is characterized by complete and full membership in the set A. That is, the core comprises those elements x of the universe such that $\mu_A(x) = 1$.

Definition 3.3.12. Support

The support of a membership function for some fuzzy set A is defined as that region of the universe that is characterized by nonzero membership in the set A. That is, the support comprises those elements x of the universe such that $\mu_A(x) > 0$.

Definition 3.3.13. Boundaries

The boundaries of a membership function for some fuzzy set $A$are defined as that region of the universe containing elements that have a nonzero membership but not complete membership.

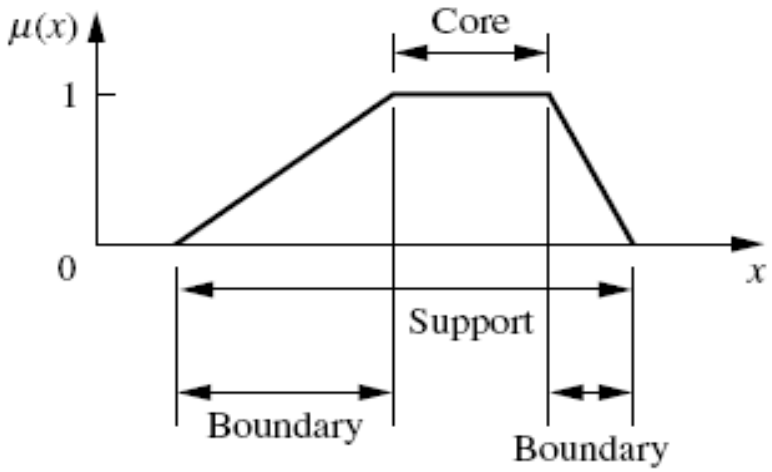

Figure 3.4. Graphical examples for **(**core**,** Support**,** Boundaries**).**

Definition 3.3.14. Fuzzy point

Let A be a fuzzy number. If $\sup(A) = \{x_0\}$ then A is called a fuzzy point and we use the notation$A = \bar{X}_O$.

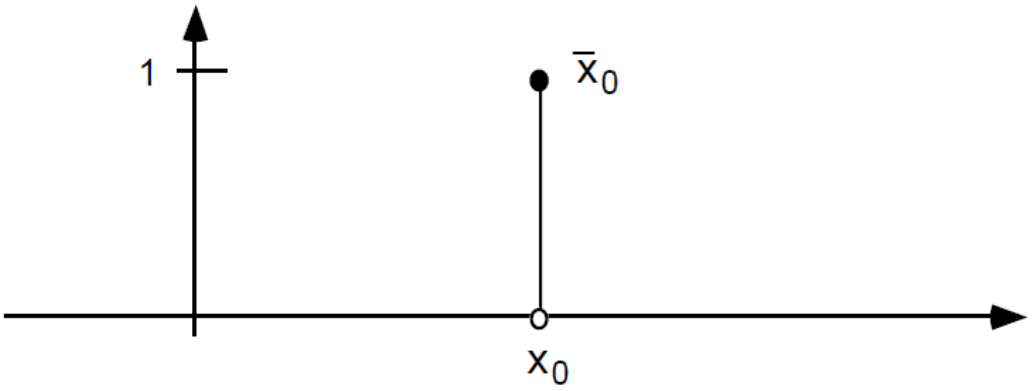

Figure 3.5.Graphical show fuzzy point.

Let $A = \bar{X}_O$ be a fuzzy point. It is easy to see that $A\gamma = [x_0, x_0] = \{x_0\}, \forall\gamma$.

Definition 3.3.15. Crossover points

The crossover points of a membership function are defined as the elements in the universe for which a particular fuzzy set A has values equal to 0.5, i.e., for which $\mu_A(x) = 0.5$.

Definition 3.3.16. ∝*-Cut, strong* ∝*-cut*

The **∝-cut** or **∝**-level set of a fuzzy set A is a crisp set defined by $A\propto = \{x \in X \mid \mu_A(x) \geq \propto\}$. Strong **∝**-cut or strong **∝**-level **se**t are defined similarly: $A'\propto = \{x \in X \mid \mu_A(x) > \propto\}$.

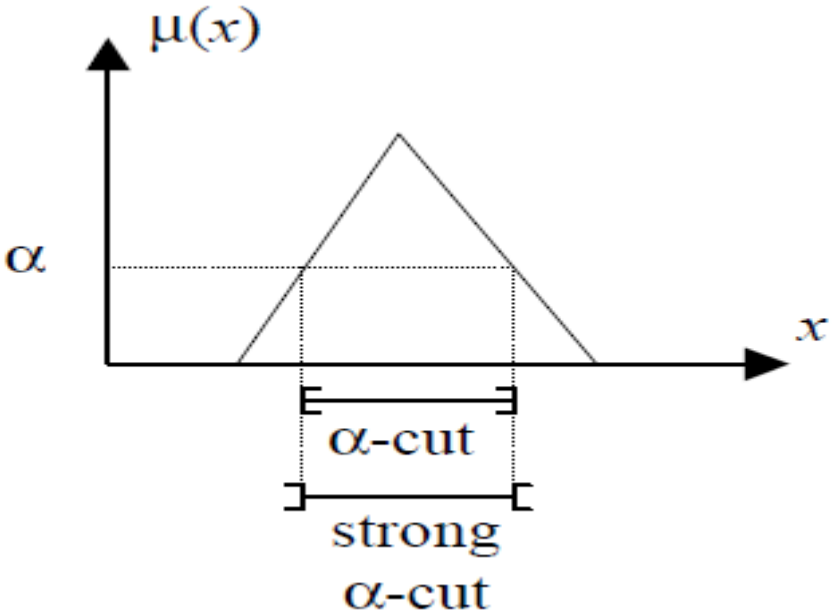

Figure 3.6. Graphical examples for $(\alpha - cut, strong\ \alpha - cut)$.

Definition 3.3.17. Fuzzy singleton (FS)

A fuzzy set whose support is a single point in X with $\mu_A(x) = 1$ is called a fuzzy singleton.

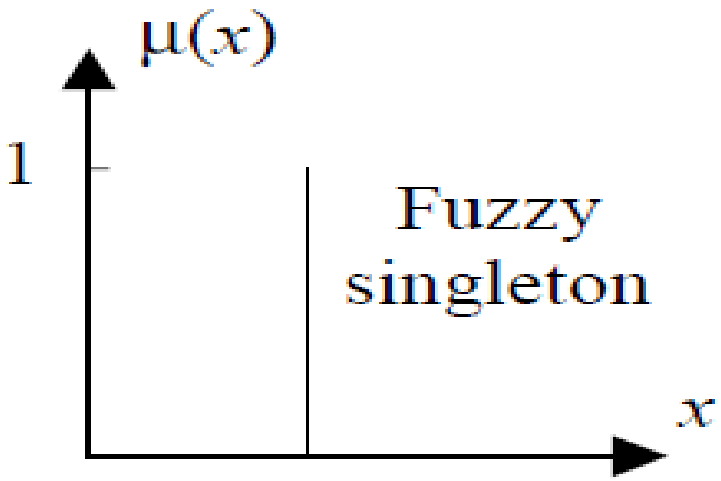

Figure 3.7. Graphical example of a fuzzy singleton.

Definition 3.3.18. Subset hood

Let A and B be fuzzy subsets of a classical set X. We say that A is a subset of$B$ if $A(t) \leq B. \forall t \in X$.

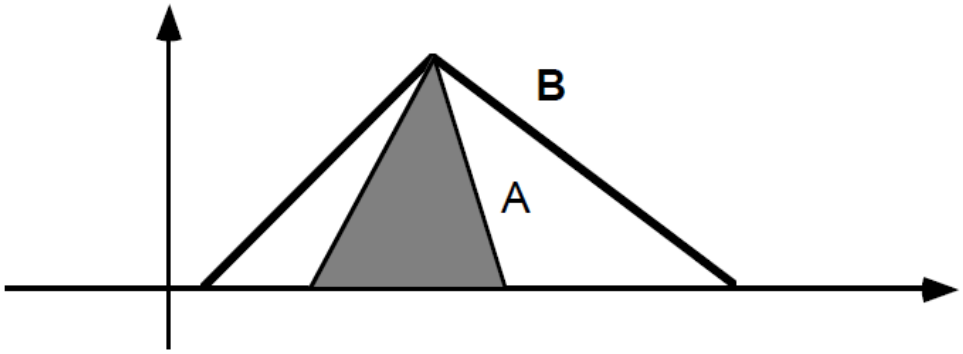

Figure 3.8. Graphical show A is subset of B.

Definition 3.3.19. Fuzzy rules

In 1973, Lotfi Zadeh published his second most influential paper. This paper outlined a new approach to analysis of complex systems, in which Zadeh suggested capturing human knowledge in fuzzy rules.

Definition 3.3.20. Linguistic variables

In daily contact we often use short sentences that are carrying the same amount of information as their longer counterparts. If we say that “the man is tall” we actually mean that “the man's height belongs to the tall men (very long) category.” Even if we knew that the height of man was exactly (190 cm), in everyday communication we would prefer saying that “the man is tall” as we would assume that there is a common understanding what a very tall man is according to the classification length terms. The term tall may denote two different values: numerical (190 cm) and linguistic (very long). Variables, for which values are words or sentences, rather than numbers, are called linguistic variables. Therefore, this strategy is expressed in the form of IF–THEN rules, which contain linguistic variables - usually the names of inputs and outputs, rather than their concrete values (numbers). As mentioned by Zadeh, linguistic variables may assume different linguistic values over a specified universe of discourse. This means that linguistic values defined by an appropriate semantic rule represent nothing but attributes properties about the physical values in a part of a specified universe of discourse.

3.4. Fuzzy Inference System

The fuzzy set is an effective tool and allows us to represent things or members in a vague or ambiguous way. The fuzzy set also offers a way that is similar to a human being’s concepts and thinking process. However, just the fuzzy set itself cannot lead to any useful and practical products until the fuzzy inference process (FIP) is applied. To apply fuzzy inference to a real product or to solve an actual problem, three consecutive steps are needed, which are:

3.4.1. Fuzzification

Is the first step to apply a fuzzy inference system (FIS). Most variables existing in the real world are crisp or classical variables. One needs to convert those crisp variables (both input and output) to fuzzy variables, and then apply fuzzy inference to process the data to obtain the desired output. At the end, in most cases, the fuzzy outputs need to be converted back to crisp variables to complete the desired control objectives. In general, this step includes two processes: derive the membership functions for input and output variables and represent them with linguistic variables. This process is equivalent to converting or mapping a classical set to a fuzzy set to varying degrees.

3.4.2. Fuzzy Control Rules (FCR)

Can be considered as the knowledge of an expert in any field of application. The fuzzy rule is represented by a sequence of the form IF-THEN, leading to algorithms describing what action or output should be taken in terms of the currently observed information, which includes both the fuzzy input and feedback if a closed-loop control system is applied. The law to design or build a set of fuzzy rules is based on a human being's knowledge or experience, which is dependent on each different practical application. A fuzzy IF-THEN rule associates a condition described using linguistic variables and fuzzy sets to an output or a conclusion. The 'IF' part is mainly used to capture knowledge by using the elastic conditions and the 'THEN' part can be used to give the conclusion or output in linguistic variable form. This IF-THEN rule is widely used by the fuzzy inference system to compute the degree to which the input data matches the condition of a rule. There are two types of real applications:

3.4.2.1. Fuzzy Mapping Rules

Fuzzy mapping rules submit a functional mapping between the input and the output using linguistic variables. The basis of a fuzzy mapping rule is a fuzzy graph, which describes the relationship between the input and the output. Sometimes, in real applications, it is very hard to conclude a certain relationship between the fuzzy input and the fuzzy output, or the relationship between those inputs and outputs are very complicated even when that relationship is developed. Fuzzy mapping rules are a very good solution for those cases. FMR work in a similar way to human intuition or insight, and each fuzzy mapping rule only approximates a limited number of elements of the function, so the entire function should be approximated by a set of fuzzy mapping rules.

3.4.2.2. Fuzzy Implication Rules

A fuzzy implication rule describes a general logic implication relationship between the fuzzy inputs and the fuzzy outputs. The establishment of a fuzzy implication rule is the narrow sense of fuzzy logic (John and Reza, 1999). Fuzzy implication rules are related to classical two-valued logic and multiple valued logic.

3.4.3. Defuzzification

The conclusion or control output derived from the combination of input, output membership functions and fuzzy rules is still a vague or fuzzy element, and this process in called fuzzy inference. To make the conclusion or fuzzy output available to real applications, a defuzzification process is needed. The defuzzification process is meant to convert the fuzzy output back to the crisp or classical output of the control objective. Knowing that the fuzzy conclusion or output is still a linguistic variable, this linguistic variable needs to be converted to the crisp variable by the defuzzification process. We have different types of methods such as centroid, bisector, middle of maximum, smallest of maximum, and largest of maximum.

3.4.3.1. Centroid of area

This method returns the output by calculating the centroid of area formed by the aggregated fuzzy sets of the consequents as follow:

$$x_{COA} = \frac{\int \mu A(x) x \mathrm{d}x}{\int \mu A(x) \mathrm{d}x}$$

where $\int \mu A(x) \mathrm{d}x \neq 0$, for all μ_A.

3.4.3.2. Bisector of area (BOA)

The vertical line corresponding to the output generated by BOA splits the aggregated fuzzy sets into two sub-regions of equal area. This operation can be expressed as follow:

$$\int_{a}^{y_{\mathbf{BOA}}} \mu_B(y) dy = \int_{y_{\mathbf{BOA}}}^{\beta} \mu_B(y) dy$$

where $\propto = \min\{ v/v \in V\}, \beta = \max\{v/v \in V\}$.

Note that the value resulted from this method is sometimes coincidently identical to that generated from COA.

3.4.3.3. Smallest of maximum (SOM)

This method generates the crisp output by taking the smallest value that gives the maximum membership degree of the aggregated fuzzy set

$$y_{\mathbf{SOM}} = min\{y | \mu_B(y) = \max(\mu_B(y))\}.$$

3.4.3.4. Largest of maximum (LOM)

Instead of smallest value as SOM, LOM takes the largest value corresponding to the maximum membership degree to yield the final crisp output.

$$y_{\mathbf{LOM}} = max\{y | \mu_B(y) = \max(\mu_B(y))\}.$$

3.4.3.5. Mean of maximum (MOM)

In this defuzzification, the mean of maxima is taken as the crisp output.

$$y_{\text{MOM}}=\frac{y_{SOM}+y_{LOM}}{2}$$

Note that if the aggregated membership function has a unique maximum degree, rather than a range (i.e., a plateau at the maximum value), the crisp outputs generated by SOM, LOM, and MOM are all identical. The consequent yi corresponding to the i th rule (M rules in total) in the Sugeno type of FIS is a function of inputs rather than a fuzzy set in the Mamdani type of FIS.I prefer centroid types of these methods in my thesis.

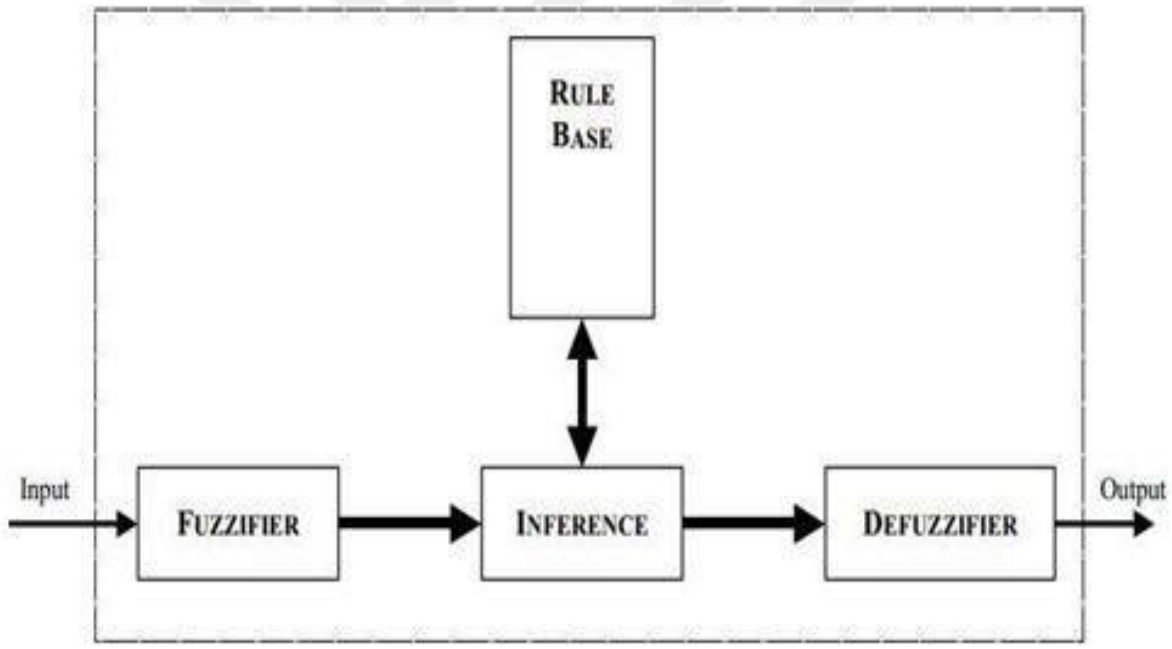

Figure 3.9. Basic structure of Fuzzy Inference System.

Therefore, in fuzzy logic system (FIS), there are different types of membership functions: (triangular, trapezoidal, Z-shaped, Gaussian, sigmoidal, S-shaped, bell-shaped). The exact type depends on the actual applications. For those systems that need significant dynamic variation in a short period of time, a triangular or trapezoidal should be used For those system that need very high control accuracy, triangular and trapezoidal membership functions were selected for my

thesis. The triangular membership function is a function of a vector, x and depends on three scalar parameters, a, b and c

$$\mu(x;a,b,c) = \begin{cases} 0 & , \quad x \le a \\ \frac{x-a}{b-a} & , \quad a \le x \le b \\ \frac{c-x}{c-b} & , \quad b \le x \le c \\ 0 & , \quad c \le x \end{cases}$$

or more compactly, by

$$\mu(x;a,b,c) = \max\left(\min\left(\frac{x-a}{b-a}, \frac{c-x}{c-b}\right), 0\right).$$

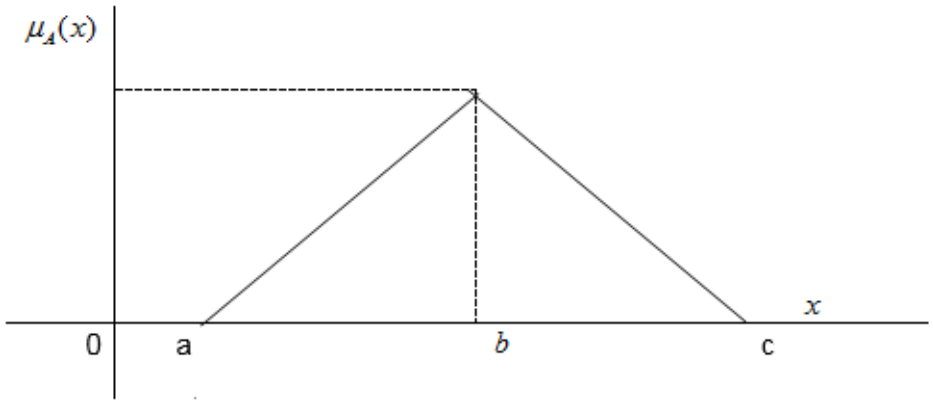

Figure 3.10**.** Graphical show triangular membership function.

The trapezoidal curve is a function of a vector, x, and depends on four scalar parameters a, b, c and d, as given by

$$\mu(x;a,b,c,d) = \begin{cases} 0 & , \quad x \le a \\ \frac{x-a}{b-a} & , \quad a \le x \le b \\ 1 & , \quad b \le x \le c \\ \frac{d-x}{d-c} & , \quad c \le x \le d \\ 0 & , \quad d \le c \end{cases}$$

$$\mu(x;a,b,c,d) = \max\left(\min\left(\frac{x-a}{b-a}, 1, \frac{d-x}{d-c}\right), 0\right).$$

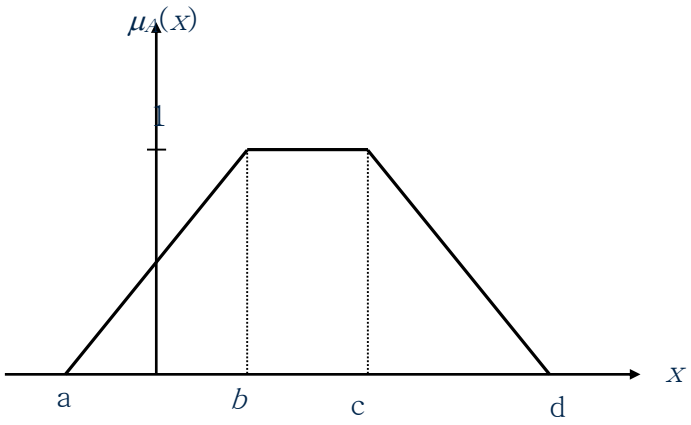

Figure 3.11. Graphic showing trapezoidal membership function.

3.5. How to build a fuzzy system?

There are six steps needed for building a fuzzy system

- Step 1. Determine the values of the input and output variables.
- Step 2. Fuzzify the variables: create fuzzy sets to represent the different values of the input variables. Fuzzification is the process of making a crisp quantity fuzzy.
- Step 3. Create the fuzzy sets for the output variables of the system.
- Step 4. Generate a set of fuzzy rules based on the input and output fuzzy sets.
- Step 5. Choose a defuzzification method and apply it to the results obtained from the rules that are satisfied.
- Step 6. The crisp value obtained from steps 5 is the answer to your problem.

- **3.6. Some of the basic characteristics of fuzzy systems (FS)**

1. Membership functions (MF) are numerical representations of the linguistic concepts; they can be built either through learning from data, or through experts opinion, or through both.
2. Fuzzy concepts have to have linguistic meaning; they need to be articulated.
3. Fuzzy rules can be represented by vague, ambiguous or contradictory knowledge.

4. Fuzzy systems are robust; even if some rules are removed from the rule map, it means that the system still work properly; fuzzy systems are also robust toward changing conditions in the environment.
5. Fuzzy systems are simple to build, easy to realize, and easy to explain.
6. These characteristics of fuzzy systems make them suitable for solving practically some of the generic problems.

In fact there two fuzzy inference systems Mamdani and Sugeno. Each of the systems contain the same number of inputs with the same type of membership functions. They even contain the same rules. They differ, however, in the output generation process from the fuzzy inputs. The most fundamental difference between Mamdani FIS and Sugeno FIS is the way the crisp output is generated from the fuzzy inputs (Jassbi et al., 2007). Mamdani FIS uses the technique of defuzzification of a fuzzy output, Sugeno FIS uses weighted average to compute the crisp output. Therefore in Sugeno FIS the defuzzification process is bypassed.

3.7. Comparison between Mamdani FIS and Sugeno FIS

Mamdani fuzzy inference system (FIS)	**Sugeno fuzzy inference system (FIS)**
Has output membership function	Does not have output membership function
Crisp result obtained through defuzzification of rules' consequent	No defuzzification: crisp result is obtained using weighted average of the rules' consequent
Less flexibility in the system design	More flexibility in the system design; more parameters in the output
MISO and MIMO systems	Only MISO systems
Expressive power and interpretability rule consequents	Loss of interpretability
Non-continuous output surface	Continuous output surface
Output distribution	No output distribution only 'resulting action' Mathematical combination of the rule strength and the output

Table 3.2. Comparison between Mamdani FIS and Sugeno FIS.

According to the previous, there are some advantages of using either Mamdani FIS or Sugeno FIS.

3.8. The advantages of using Mamdani FIS

• Expressive power.

• Easy formalization and interpretability.

• Reasonable results with relatively simple structure.

• Intuitive and interpretable nature of the rule base.

For this reason Mamdani FIS is widely used in particular for decision support application.

• Can be used for both MISO and MIMO systems.

• Output can either be fuzzy or a crisp output.

3.9. The advantages of using Sugeno FIS

• There are algorithms which can be used to automatically optimize the Sugeno FIS. One of the tools that can calibrate the weights of the Sugeno FIS output is MATLAB's ANFIS.

• Better processing time since the weighted average replaces the time consuming defuzzification process.

• Computational efficiency and accuracy.

• More robust when in presence of noisy input data such as sensor data?

• Rules consequents can have as many parameters per rule as input values allowing more degrees of freedom and more flexibility in the design.

• Adequate for functional analysis because of the continuous structure of output function same inputs do not originate substantially different outputs.

4. Application of Gaussian DFT /B3LYP/ 6-31 G (d)

4.1. Glyceric Acid

Is a natural three-carbon sugar acid. Salts and esters of glyceric acid are known as glycertes. Glycerol after reacting with gym-an oxygen giving reagent (such as KMnO4+H2SO4) produces glyceric acid:

KMnO4+3H2SO4=K2SO4+3H20+5[O] CH2OH-CHOH-CH2OH+ [O]
=CH2OH-CHOH-COOH+H2O.

Chemical formula: C3H6O4.

The two dimension structure of gleceric acid is shown in Figure 4.1.

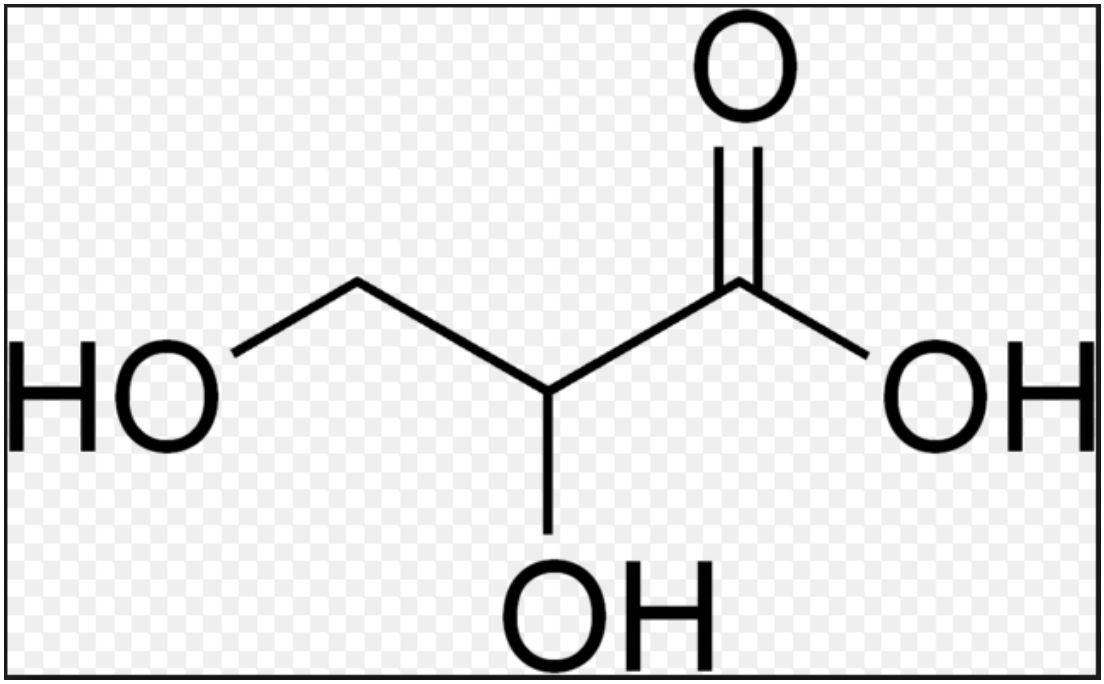

Figure 4.1: The two dimension structure of gleceric acid.

Also the three dimension of glyceric acid is shown in Figure 4.2

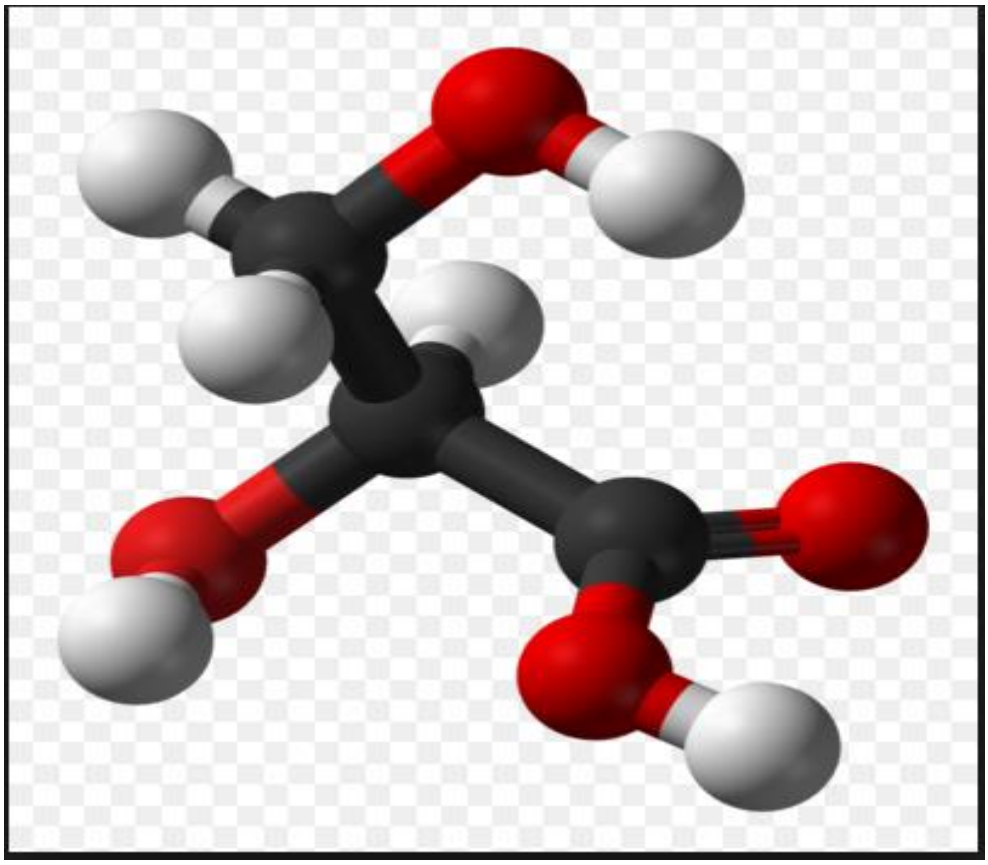

Figure 4.2. The three dimension structure of glyceric acid.

Glycolic acid (GA) is a small-molecule hydroacetic acid that is colorless, odorless and hydroscopic. These characteristics make GA a suitable ingredient for keratolysis (exfoliation) and anti-aging applications (stimulation of tissue production and hydration). GA is also water soluble, making it versatile for dermatologic and cosmetic formulations.

GA is used in the textile industry as a dyeing and tanning agent, (Kempiak and Uebelhoer, 2008). In the food industry it is used as a flavoring agent and as a preservative. It is also used in adhesives and plastics (Briden et al., 2007). GA is often included in emulsion polymers, solvents and additives for ink and paint for improving flow properties and imparting gloss. Also it is used in surface treatment products to increase the coefficient of friction on tile flooring.

GA is available in varying concentrations and grades, depending on the intended use. Industrial-grade GA applied at more than 70% concentrations is not

considered to a hazardous material for rust removal and textiles. Pharmaceutical-grade GA undergoes a complex series of filtration and purification processes. For skin applications, GA is used in concentrations ≤70%, with clinical use above 50% concentration.

In addition, it has been shown to be effective in minimizing acne scars and stimulating dermal regeneration. Also, it is effective in enhancing the Archaeology of other products to reduce acne flare ups and infection (Kempiak and Uebelhoer, 2008; Briden et al., 2007; Effron et al., 2009; Dreno et al., 2007). The glyceric acid molecule consists from six angles, so we choose only two angles that make the lowest energy values for the molecule.

The molecular structure of glyceric acid was optimized by using the spin-unrestricted DFT (B3LYP) method with 6-31 G (d) basis set and, given together with the atoms as numbered in Fig 3 (Miertus et al., 1981; Cammi et al., 1995). All the calculations were performed using the Gaussian 03 package (Frisch et al., 2003), and Gauss-View molecular visualization programs (Frish et al., 2001), on the personal computer. In the calculations, after opening Gaussian view 05 shows us the main Gaussian and a small blue window.

Click the "Element Fragment" icon (the 6C icon) is clicked, it shows us the periodic table of elements, I chose glyceric acid. After that the fragment is placed on the small blue window. After that adding all required atoms (excluding hydrogens) are added. After pressing the "Modify Bond" icon two atoms are chosen by L-clicking on them in the small blue window.

The two chosen atoms change color and are marked as (1) and (2). After connecting all the main atoms in the desired way, you can add hydrogen atoms by using the "Add Valence" option on the "Builder" window.

Click the "Add Valence" using the L-click then press on one of the atoms in the small blue window. Each L-click used in this way adds one hydrogen atom, as shown in Figure 4.3.

Then I chose REDUNDANT COORDINATES EDITOR to choose the tow torsion angles from the icon ''edit''. I chose the dihedral method to obtain Potential

Energy Surface (PES). The first angle is ''3,1,2,5'', by increasing 40^0 and scan coordinate 18. So we obtain the SC1 (O3C1C2O5). And the second angle is ''1,2,6,7'', by increasing 40^0 and scan coordinate 18. Also the SC2 (C1C2C6O7) is obtained as shown in Figure 4.3.

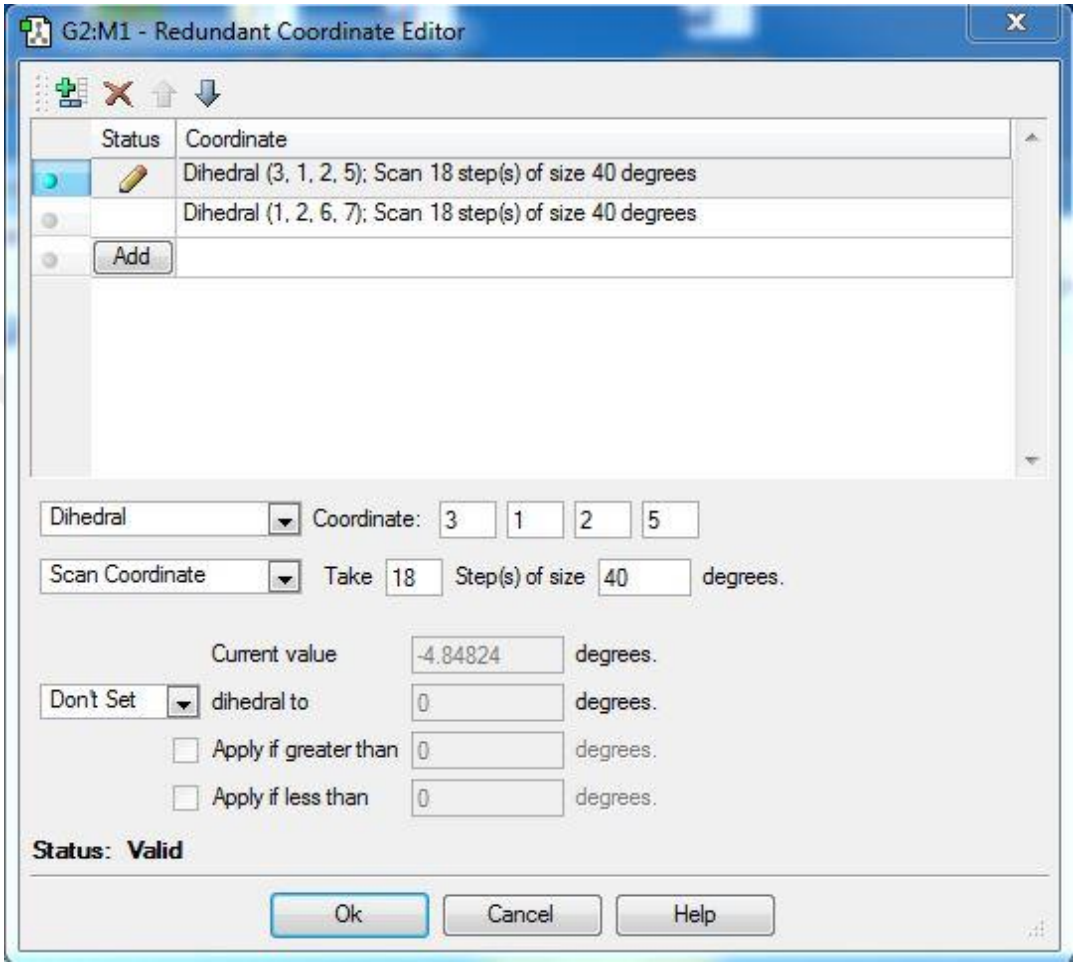

Figure 4.3. Redundant Coordinates Editor to Choose The Angles.

On the small blue window it pressed R- click and chose "VIEW" and "labels" to show us all of the oxygen, carbon, hydrogen, The red ball is oxygen, the green ball is carbon and the white ball is hydrogen as shown in Figure 4.4.

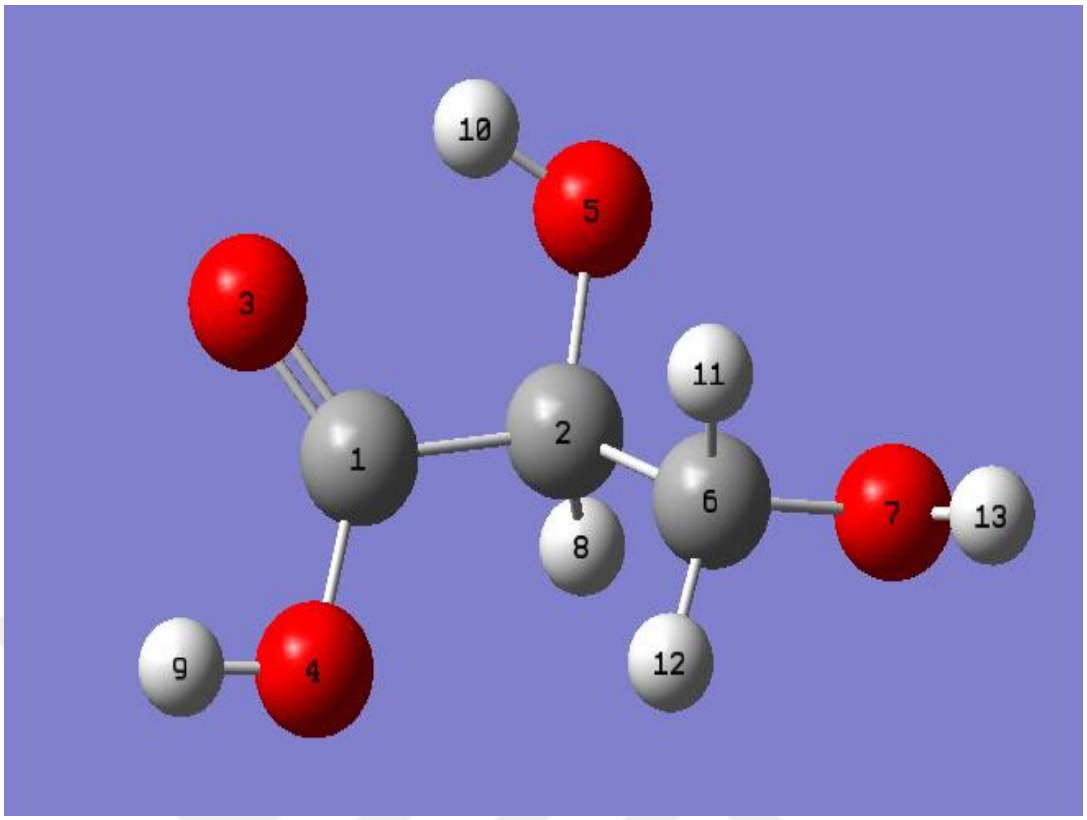

Figure 4.4. Optimized Structure of the Glyceric Acid Molecule.

Then one must L-click on the "calculation" option in the Gaussian window menu, and choosen "calculation" to show us the list (job type, method…etc) from the "Job Type" option. Here you may chose the type of calculation you want to. So it chose "energy" because I want to obtain the minimum energy of the glyceric acid molecule, as shown in Figure 4.5.

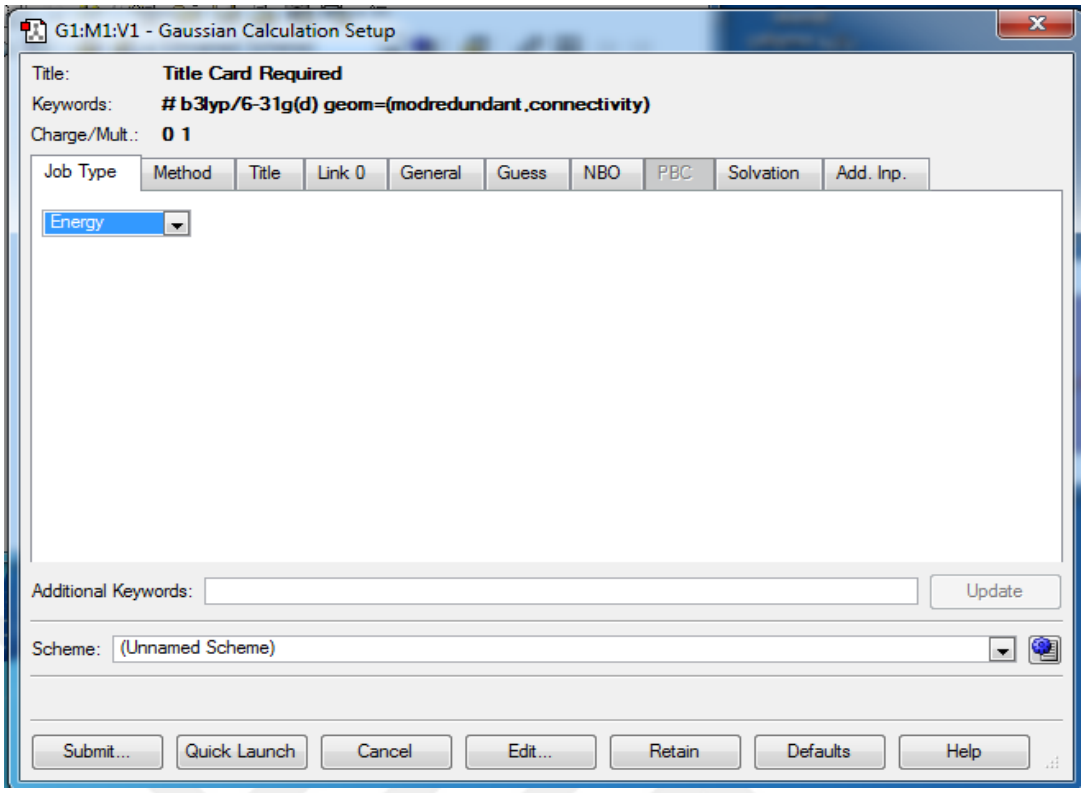

Figure 4.5. Figure show how to chose the type of calculation.

After that in "Method" option. I have chosen "Ground state", "DFT", "Defaut spin" , "B3LYP", with basic set "6 -31 G (d)" as shown in Figure 4.6.

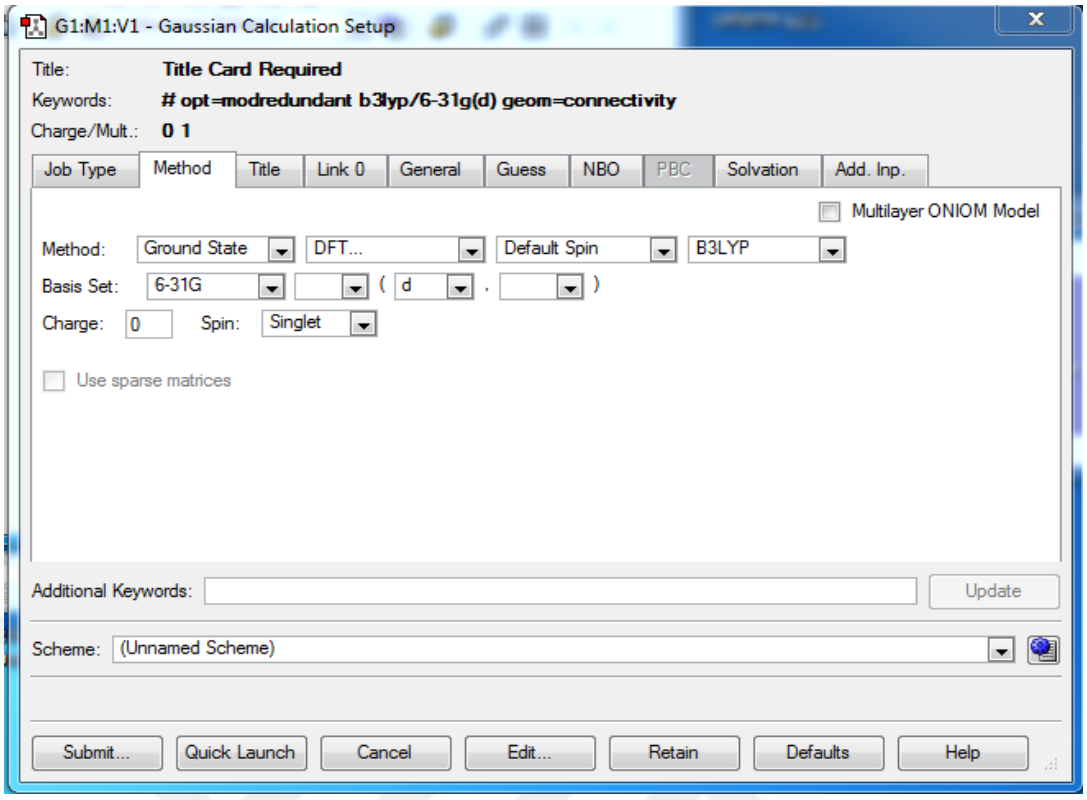

Figure 4.6. Figure Show How To Choose Our Method.

The next option is the "Title". It is not necessary to write a title, but it is highly recommended. Latter, when looking at the results, the title may help you remember what was going on and if there is something important.

The "Link 0" option is not relevant to us. Next is the "General" option, where you may specify certain information. The "Guess", "NBO" and "PBC" options in the upper toolbar are not relevant to us at this point. The last option in the upper toolbar is ''Solvation'' as shown in Figure 4.7.

After that I chosen "submit" to calculate. The program then asked me to save it and waite until it was completed.

In the end we obtained the two dimensional PES graph of a glyceric acid molecule as shwon in figure 4.7.

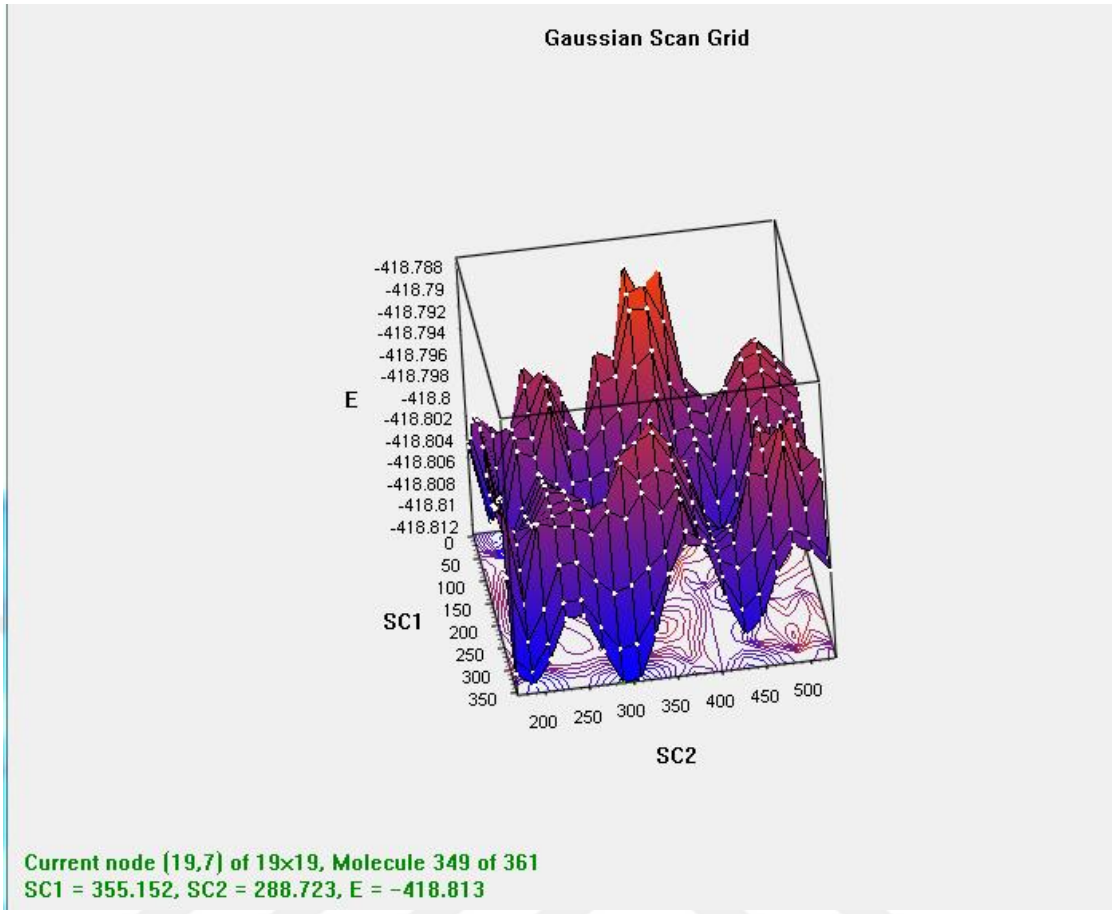

Figure 4.7. Two dimensional PES graph of glyceric acid molecule. E= Energy, SC1=O3C1C2O5 and SC2= C1C2C6O7.

As we see the Figure 4.7, the data is not continuous and there are some untested data. The minimum energy is "-418.813" Hartree/particle obtained from the SC1 at the point "355.152 ^{0}", and SC2 at the point "288.732 ^{0}".

After that we can see the Gaussian calculation summary by clicking the result in the Gaussian window menu and choosing "summary" as shown in Figure 4.8.

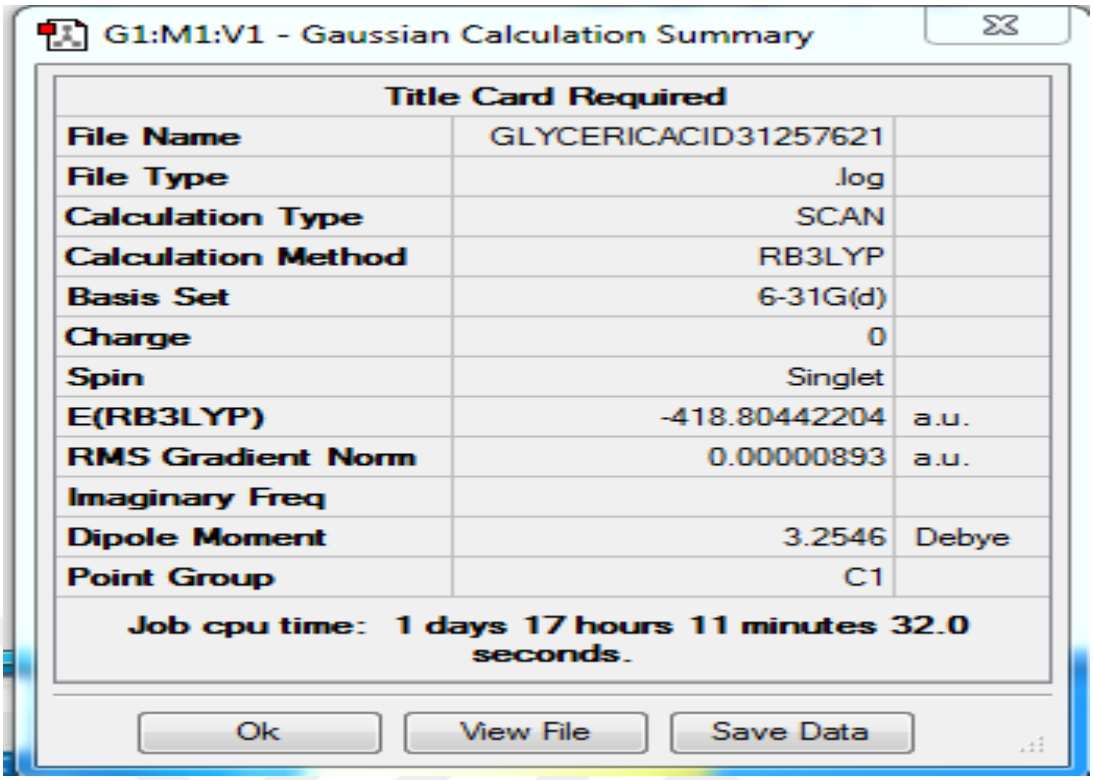

Figure 4.8. Figure shows the Gaussian calculation summary.

To set up a model, we built a fuzzy logic model by using two inputs and one output. Our inputs in this study as I said before are "SC1=O3C1C2O5", "SC2=C1C2C6O7" and our output is the energy of the molecule changing with respect to the dihedral angles, SC1 and SC2. The membership functions are; the first input variable "SC1", the second input variable "SC2" the energy of the molecule as our output variable are given in Figure 4.9 -11, respectively.

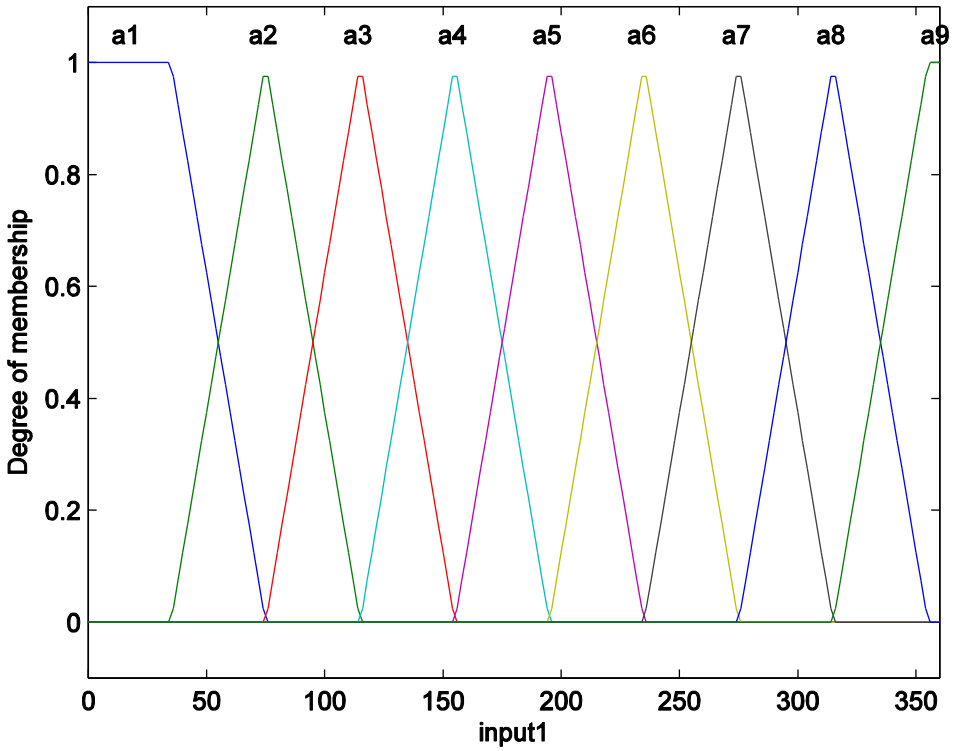

Figure 4.9. Membership functions for the SC1.

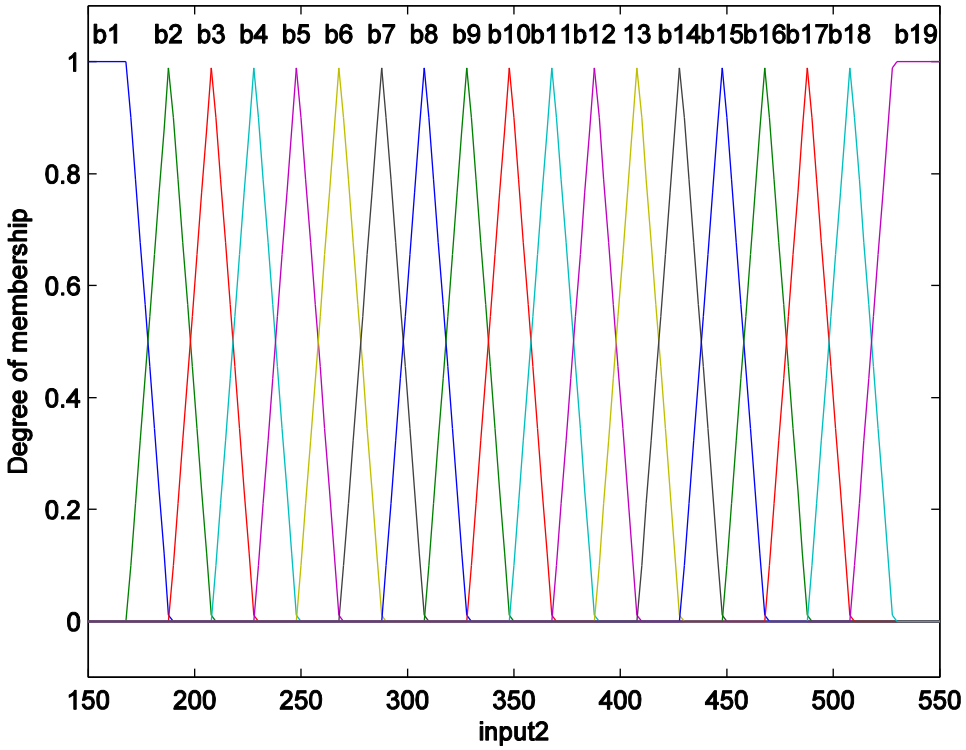

Figure 4.10. Membership functions for the SC2.

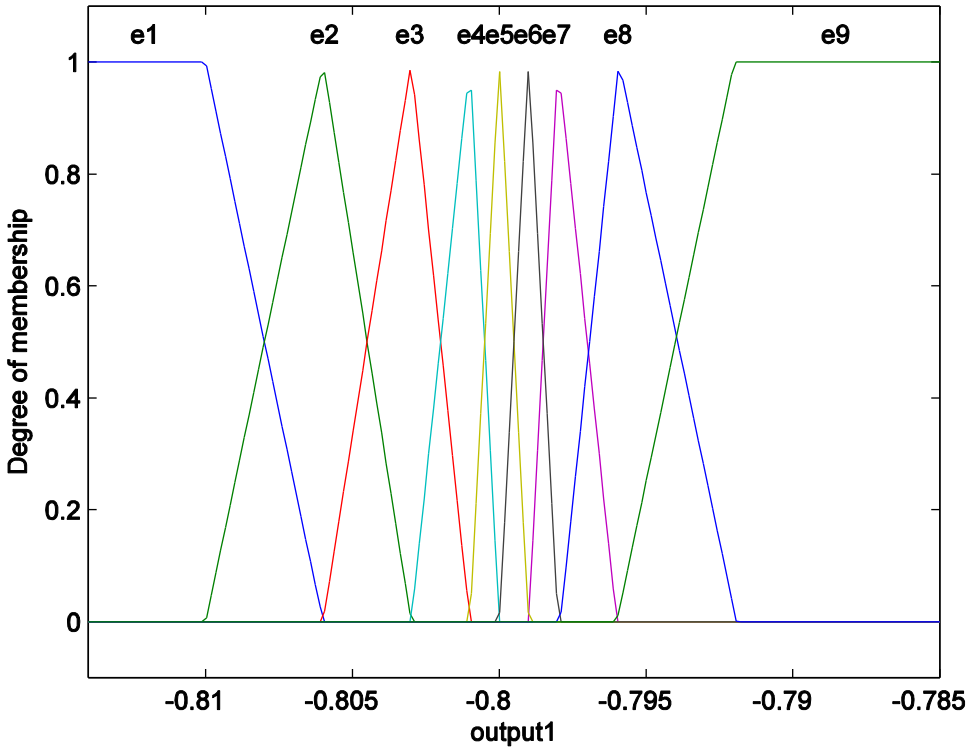

Figure 4.11. Membership functions for the energy.

The first angle value is increased by a step of 40^0 starting with 35.15^0 and ending with 355.15^0 while the second angle value is again increased by the step of 40^0 starting with 168.723^0 and ending with 528.723^0. Therefore, we have nine fuzzy numbers for the first input and seventeen for the second input for two torsion angles.

The first angle values $(a1, a2, \dots, a9)$ the second angle values $(b1, b2, \dots, b19)$ are considered as input data and the energy values of the molecule $(e1, e2, \dots, e9)$ is considered as output data in our model.

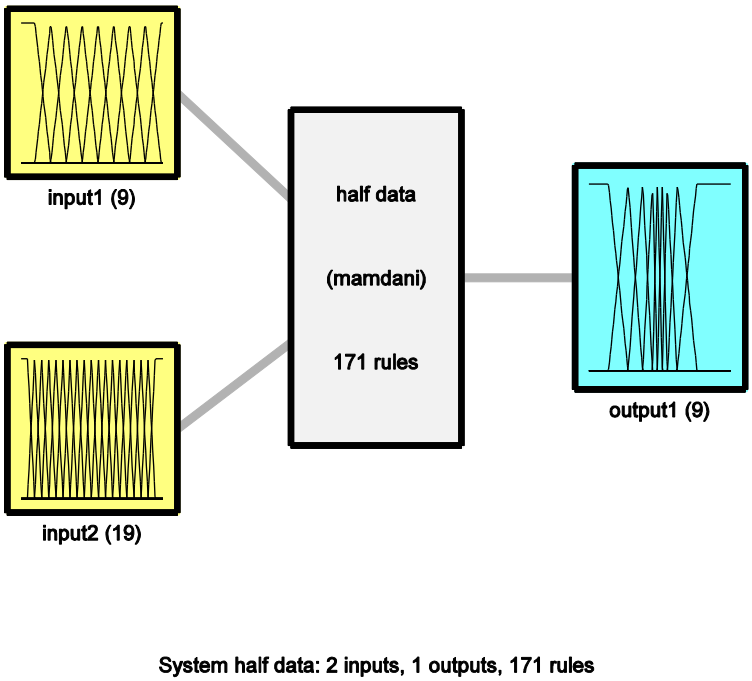

Figure 4.12. General structure of Fuzzy Inference System.

The rule structure is designed based on how the experts interpret the characteristics of the variables of the system. It is possible to write down "if-then" fuzzy rules. Some of the rules used in the model are as the following

- If (Angle1 is $a1$) and (Angle2 is $b9$) then (Energy is $e5$) (1)
- If (Angle1 is $a2$) and (Angle2 is $b9$) then (Energy is $e4$) (1)
- If (Angle1 is $a3$) and (Angle2 is $b9$) then (Energy is $e3$) (1)
- If (Angle1 is $a7$) and (Angle2 is $b9$) then (Energy is $e4$) (1)
- If (Angle1 is $a2$) and (Angle2 is $b9$) then (Energy is $e1$) (1)
- If (Angle1 is $a15$) and (Angle2 is $b17$) then (Energy is $e5$) (1)
- If (Angle1 is $a18$) and (Angle2 is $b8$) then (Energy is $e4$) (1)

⋮

The surfaces of the energy values of the molecule is a function of "SC1=O3C1C2O5" and "SC2=C1C2C6O7" which are obtained by using centroid methods in defuzzification stage, represented in Figure 4.13.

Using the fuzzy logic approach we have modelled the relation between the input and output data. In fact, the fuzzy logic approach sets the continuous function between input variables and output.

If we want to know the best values of the inputs that give the minimum value of the output we have to make local searches around the local minima that can be seen from the model surfaces. Since the number of the local minima is finite, it is easy to find the global minimum of the energy for the molecule, accurately. We have seen that, if we check the possible values of the minimum energy for the molecule, we see that it is possible to find the deeper energy values as a global minimum of the molecule by making arrangements on the elements of fuzzy inference system.

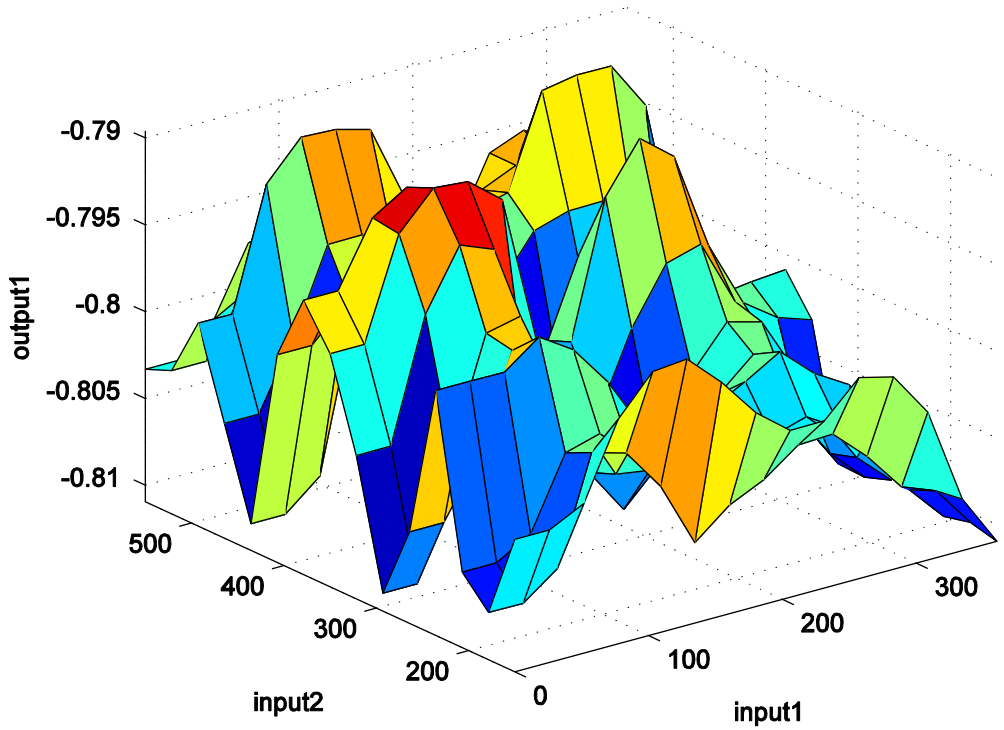

Figure 4.13. Surfaces of Fuzzy Inference System.

By using fuzzy logic, we have modelled the relationship between input and output data. Actually, the fuzzy logic approach sets the continuous function between input SC1and SC2 and output the energy.

The correlation coefficient R^2, which is obtained by regression analysis shows that the experimental results and fuzzy logic results are close to the rate of 95.88%, as shows in Figure 4.14.

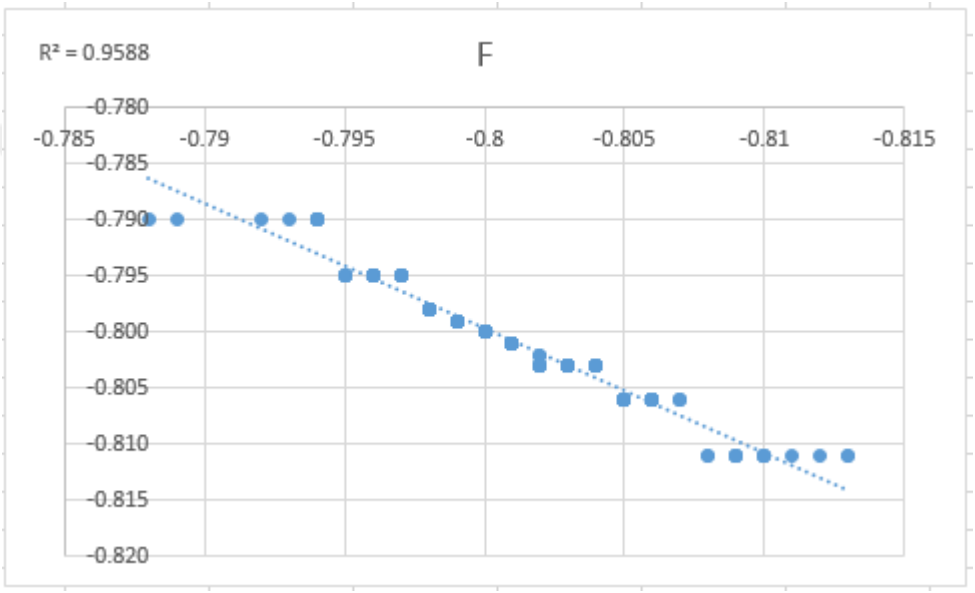

Figure 4.14. Comparison of the DFT values and Mamdani type FLM predictions.

4.2. Tables of Data

SC1	SC2	ENERGY	FUZZY
15	168	-0.802	-0.803
75	168	-0.798	-0.798
115	168	-0.798	-0.798
155	168	-0.799	-0.799
195	168	-0.801	-0.801
235	168	-0.800	-0.800
275	168	-0.797	-0.795
315	168	-0.798	-0.798
355	168	-0.805	-0.806
15	188	-0.800	-0.800
75	188	-0.796	-0.795
115	188	-0.796	-0.795
155	188	-0.795	-0.798
195	188	-0.796	-0.800
235	188	-0.801	-0.795
275	188	-0.803	-0.795
315	188	-0.799	-0.801
355	188	-0.794	-0.803
15	208	-0.794	-0.799
75	208	-0.796	-0.790
115	208	-0.799	-0.790
155	208	-0.798	-0.795
195	208	-0.794	-0.799
235	208	-0.794	-0.798
275	208	-0.802	-0.790
315	208	-0.802	-0.790
355	208	-0.796	-0.803
15	228	-0.795	-0.803
75	228	-0.798	-0.795
115	228	-0.801	-0.795
155	228	-0.795	-0.798
195	228	-0.796	-0.801
235	228	-0.801	-0.795
275	228	-0.804	-0.795
315	228	-0.806	-0.801
355	228	-0.799	-0.803
15	248	-0.797	-0.806
75	248	-0.803	-0.799
115	248	-0.806	-0.795
155	248	-0.804	-0.803
195	248	-0.799	-0.806
235	248	-0.804	-0.803
275	248	-0.809	-0.799
315	248	-0.808	-0.803
355	248	-0.800	-0.811

15	268	-0.801	-0.811
75	268	-0.806	-0.800
115	268	-0.809	-0.801
155	268	-0.805	-0.806
195	268	-0.804	-0.811
235	268	-0.805	-0.806
275	268	-0.810	-0.803
315	268	-0.800	-0.806
355	268	-0.799	-0.811
15	288	-0.800	-0.800
75	288	-0.801	-0.799
115	288	-0.806	-0.800
155	288	-0.805	-0.801
195	288	-0.805	-0.806
235	288	-0.804	-0.806
275	288	-0.806	-0.806
315	288	-0.797	-0.803
355	288	-0.792	-0.806
15	308	-0.801	-0.795
75	308	-0.803	-0.790
115	308	-0.800	-0.801
155	308	-0.800	-0.803
195	308	-0.802	-0.800
235	308	-0.803	-0.800
275	308	-0.801	-0.802
315	308	-0.796	-0.803
355	308	-0.788	-0.801
15	328	-0.793	-0.795
75	328	-0.799	-0.790
115	328	-0.800	-0.790
155	328	-0.797	-0.799
195	328	-0.798	-0.800
235	328	-0.798	-0.795
275	328	-0.800	-0.798
315	328	-0.799	-0.798
355	328	-0.789	-0.800
15	348	-0.794	-0.799
75	348	-0.801	-0.790
115	348	-0.800	-0.790
155	348	-0.794	-0.801
195	348	-0.797	-0.800
235	348	-0.803	-0.790
275	348	-0.803	-0.795
315	348	-0.803	-0.803
355	348	-0.795	-0.803
15	368	-0.798	-0.803
75	368	-0.802	-0.795
115	368	-0.801	-0.798

155	368	-0.796	-0.803
195	368	-0.798	-0.801
235	368	-0.804	-0.795
275	368	-0.809	-0.798
315	368	-0.800	-0.803
355	368	-0.794	-0.811
15	388	-0.799	-0.800
75	388	-0.805	-0.790
115	388	-0.803	-0.799
155	388	-0.797	-0.806
195	388	-0.796	-0.803
235	388	-0.806	-0.795
275	388	-0.813	-0.795
315	388	-0.810	-0.806
355	388	-0.802	-0.811
15	408	-0.801	-0.811
75	408	-0.807	-0.803
115	408	-0.809	-0.801
155	408	-0.804	-0.806
195	408	-0.799	-0.811
235	408	-0.806	-0.803
275	408	-0.813	-0.799
315	408	-0.806	-0.806
355	408	-0.798	-0.811
15	428	-0.801	-0.806
75	428	-0.805	-0.798
115	428	-0.806	-0.801
155	428	-0.801	-0.806
195	428	-0.800	-0.806
235	428	-0.805	-0.801
275	428	-0.810	-0.800
315	428	-0.801	-0.806
355	428	-0.795	-0.811
15	448	-0.795	-0.801
75	448	-0.802	-0.795
115	448	-0.802	-0.795
155	448	-0.800	-0.802
195	448	-0.800	-0.803
235	448	-0.803	-0.800
275	448	-0.806	-0.800
315	448	-0.797	-0.803
355	448	-0.796	-0.806
15	468	-0.800	-0.795
75	468	-0.801	-0.795
115	468	-0.800	-0.800
155	468	-0.800	-0.801
195	468	-0.800	-0.800
235	468	-0.803	-0.800

275	468	-0.806	-0.800
315	468	-0.806	-0.803
355	468	-0.800	-0.806
15	488	-0.799	-0.806
75	488	-0.804	-0.800
115	488	-0.803	-0.799
155	488	-0.803	-0.803
195	488	-0.801	-0.803
235	488	-0.807	-0.803
275	488	-0.810	-0.801
315	488	-0.809	-0.806
355	488	-0.801	-0.811
15	508	-0.805	-0.811
75	508	-0.808	-0.801
115	508	-0.807	-0.806
155	508	-0.803	-0.811
195	508	-0.805	-0.806
235	508	-0.810	-0.803
275	508	-0.812	-0.806
315	508	-0.802	-0.811
355	508	-0.799	-0.811
15	528	-0.797	-0.803
75	528	-0.798	-0.799
115	528	-0.801	-0.795
155	528	-0.801	-0.798
195	528	-0.798	-0.801
235	528	-0.804	-0.801
275	528	-0.811	-0.798
315	528	-0.795	-0.803
355	528	-0.796	-0.811

Table 4.1. Table of my data.

4.3. Comparison between Gaussian DFT and Fuzzy Logic

Gaussian DFT	FL
The function is not continuous	Continuous function
Does not pass all points within the period	Passing all points within the period
Easy Application	Difficult application
Application takes a long time up to 48 hours	Application takes less than DFT
You do not need to input and output in a table	You need input and output in a table
Less widespread and used commonly	More widespread and used more commonly
You can see the points of the local and Global minimum through the surface easily	You can see the points of the local and Global minimum through the surface may be the same or not

Table 4.2. Difference between DFT and Fuzzy Logic.

5. CONCLUSIONS AND FUTURE STUDIES

By using fuzzy logic control, we have been able to determine the minimum energy value of a glyceric acid molecule depending on the two torsion angles "SC1=O3C1C2O5" and "SC2=C1C2C6O7" to compare with the results obtained by DFT method. As well, we have aimed to make the data continuous and we have also obtained the results for the untested data.

For comparison with the results obtained by the DFT method we have also applied fuzzy logic to extend the data collection with the R^2 which is obtained by regression analysis. It shows that DFT and fuzzy logic results are close to the rate 95.88%.

On the other hand, we have observed that the some minimum energy values can be obtained at input variables "SC1 and SC2" such that the other method (such as DFT) may not catch these points, for example, the local minimum energy of the molecule is attained at the point "195.2^0, 428.7^0" as -418.811 Hartree/particle which may not be obtained by other methods. Also, the global minimum energy of the molecule is attained at the point "355.2 ^{o}, 288.7 ^{o}" which is the same point with the same value of -418.813 Hartree/particle calculated by the DFT method.

On the other hand, the points that made the global minimum energy of the molecule obtained from the fuzzy logic may or may not be the same as we have obtained from the Gaussian program but, must be very close to it.

In the end we see that fuzzy logic is suitable for the many physical, engineering, medical, chemical and mathematical problems. Finally, the results are compared with those obtained by DFT.

In the next studies we will use the quadratic Bezier curve in order to make some or all local minimum smoothing by choosing three or two control points (Malkevitch, 2004; Cevidanes et al., 2010).

In addition to modern techniques, it is possible to use some classical techniques such as filled function method (Ge, 1990; Ge, 1987). Smooth and descent method (Yilmaz and Sahiner, 2015; Yilmaz and Sahiner, 2014).

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