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# Ab initio study of the main components of biodiesel derived from soybean oil

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**Estudo Ab initio dos principais componentes do biocombustível proveniente do óleo de soja**

**Resumo**: O presente trabalho foi realizado utilizando o pacote computacional Gaussian03, onde procurou-se mostrar algumas propriedades que envolvem as principais moléculas dos ésteres metílicos, derivados dos ácidos graxos presentes no óleo vegetal de soja. Foram analisados dados obtidos em relação a energia do sistema e cargas de Mulliken sobre os átomos investigados. Buscou-se expor a problemática dos combustíveis fósseis em decorrência dos impactos ambientais. Realizamos análises teóricas das moléculas dos ésteres resultantes da reação de transesterificação com metanol, utilizando o método ab initio, usando o conjunto de base 6-31G.

**Palavras chave**: Análise teórica, ab initio, óleo de soja, metil ésteres.

**Abstract**: The present study was conducted using the Gaussian 03 computational package to demonstrate properties involving the main molecules of methyl esters derived from fatty acids in soybean oil. The data were analyzed in terms of the energy of the system and Mulliken charges on the atoms investigated. The aim was to address the problem of fossil fuels with regard to environmental impact. Theoretical analysis of the ester molecules resulting from the transesterification reaction with methanol was performed based on the ab initio method using the 6-31G basis set.

**Key words**: Theoretical analysis, ab initio, soybean oil, methyl esters.

## Introduction

Computational simulations constitute a powerful tool for understanding molecular and atomic phenomena and considerable advances have been made in this field of research. Such simulations enable establishing a close link between theory and practice, contributing to the improvement of both. The use of this method can theoretically project the desirable properties of substances of interest, with the subsequent empirical investigation of only those that are potentially promising for research, which economizes both human and financial resources (Gavira 2003).

The methods most employed in studies include the ab initio method, which is derived from the Latin meaning "first principles", whereas the semi-empirical quantum method consists

of using empirical approximations to predict fundamental characteristics of atoms and molecules. The complex systems of molecular and atomic patterns need to be studied in a more in-depth manner. For such, this type of method can be used to analyze basic scientific principles that are not yet well founded (Rossetti 2006).

Considering this subject in terms of current problems, the present investigation addresses biodiesel derived from soybean oil, in which the synthesis process occurs through a transesterification reaction. These fuels are used in small percentages in diesel oil and could partially or completely replace petroleum diesel oil in internal combustion engines of vehicles and other types of machines. Together with ethanol, biodiesel constitutes an important alternative in the biofuel industry due to the fact that it is derived from biomass (organic matter of a vegetal or animal origin) (BRASIL 2007).

The need to study biofuels has led to the increasing production/creation of new forms of knowledge and, consequently, novel discoveries. However, the study of the biofuel-forming molecules in soybean oil, which is the primary objective of the present study, could provide knowledge on the energy and physiochemical characteristics of the molecules that compose biodiesel and contribute to the understanding of the intrinsic characteristics of biofuel derived from this oleaginous plant (Azevedo & Lima 2016). The present investigation was performed using the Gaussian 03 computational package to conduct a theoretical study using quantum calculations to explain properties of methyl ester molecules derived from fatty acids in soybean oil.

## Study of novel fuels

The quest for new sources of renewable energy has been an objective in both Brazil and the rest of the world due to the future scarcity of fossil fuels and the environmental impact of the burning of these substances, such as the greenhouse effect, acid rain and the harm caused to human health. As Guariero et al. (2011) point out: "[…] exposure to particles culminates in causes of premature death, chronic asthma and an increase in hospitalizations among children and seniors [...]".

Biofuels are renewable fuel alternatives and biodiesel in particular stands out, since it can be obtained through different raw materials of a vegetal or animal origin. According to REN21 (2017): "Liquid biofuels continue to account for a large share of the contributions of renewable energy to the transportation sector. In 2016, these fuels provided about 4% of fuel used in road transportation worldwide."

To contextualize the global situation, biofuels underwent a 7% increase in 2013, with 5% increase in ethanol and an estimated 11% increase in biodiesel, representing increases of 87.2 billion and 26.3 billion liters, respectively. North America was the region with the largest production and consumption of ethanol, followed by Latin America, but Europe was the continent the produced and consumed the largest portion of biodiesel in the world (REN21 2014).

According to Castellanelli (2016), many sources in Brazil that have a considerable potential for the production of biodiesel are either wasted or their potential is underpublicized. Some of these sources could contribute directly to the national and global energy sector, considerably diminishing the environmental impacts caused by the burning of petroleum-based products.

These new fuel alternatives offer environmental benefits and can assist in generating work and income in rural areas, supplementing the income of regions and individuals that depend mainly on family farming.

As Trzeciak *et al.* (2008) state:

> The introduction biofuels to the Brazilian energy matrix came about through Law n° 11097 of January 13th, 2005. According to this law, the use of B2 (2% biodiesel and 98% petroleum diesel) was optional from 2005 to the end of 2007, becoming mandatory in early 2008. Between 2008 and 2013, the use of

> B5 will be optional and will become mandatory after this period. The cultivated area needed to meet the 2% mixture of biodiesel to petroleum diesel is estimated at 1.5 million hectares, which is equivalent to 1% of the 150 million hectares available for agriculture in Brazil. Brazil has the greatest biological diversity in the world, with an estimated flora of 50.000 to 60.000 species.

The production of biodiesel from vegetal and/or animal oil is achieved through the transesterification processes. Depending on the type of alcohol used in the reaction, biodiesel can be a methyl ester stemming from the use of methanol or an ethyl ester stemming from the reaction of ethanol and both processes generate glycerin as a byproduct, which is a compound used in industry with a certain aggregated value (Prates *et al.* 2007).

The potentiality of the use of biodiesel depends on a gamut of factors, such as economic competitiveness, quality, acceptance, etc., indicating that as long as consumers do not see any real advantage over petroleum diesel, they are not likely to opt for biodiesel, which leads to a very restricted dissemination of novel fuels. It should be stressed that biodiesel does not require any modifications to the internal combustion engine and can therefore be used in all vehicles (Beneditti *et al.* 2006).

Recent studies have shown a quantity of relevant unsaturated fatty acids in soybean oil, accounting for approximately 86% of the constituents of the beans. The fatty acids found in this oil are palmitic acid (C16:0), the percentage of which ranges from 8 to 17%, stearic acid (C18:0; 3 to 30%), oleic acid (C18:1; 25 to 60%), linoleic acid (C18:2; 25 to 60%) and linolenic acid (C18:3; 2 to 5%). Depending on the concentration of particular fatty acids in soybean oil, such as high concentrations of esters from linolenic and linoleic acids, the oil may be inadequate for food processing due to its lower stability in the presence of oxidation (Melo 2009; Silva 2014) and may be used for other purposes.

## Ab initio method

The properties of materials are currently investigated using methods that can be divided in two special classes: the ab initio method, the aim of which is to obtain properties from an approximate solution of Schrödinger equation (**Equation 1**), and the semi-empirical method, the aim of which is to use experimental values in calculations (Hehre 1986; Levine 1991). In 1926, Austrian physicist Erwin Schrödinger introduced the equation used to describe the atom, which is known as Schrödinger's wave equation:

$$(\hat{H}\Psi = E\Psi) \tag{1}$$

in which $\hat{H}$ is the Hamiltonian operator, $\Psi$ is the wave function of the electron and E is the energy of the system. Currently, a broad class of practical technological applications can be modeled through analytical solutions and numeric simulations involving this equation as a basic tool.

## Mulliken charges

Mulliken population analysis is certainly one of the most traditional and widely disseminated methods among chemists. This method is based on molecular orbital theory, in which a set of molecular orbitals ($\psi_i$) is defined as a linear combination of k atomic orbitals, which is also known as a basis function, the coefficients of which are determined using the Hartree-Fock method. Mulliken population analysis owes is considerable popularity, in part, to its easy calculations. It should be stressed, however, that this method has important limitations and its use has been widely criticized. Mulliken population analysis assists in identifying momentary partial charges in a system derived from the readjustment of the electron cloud (Guadagnini & Bruns 1995).

## Material and Methods

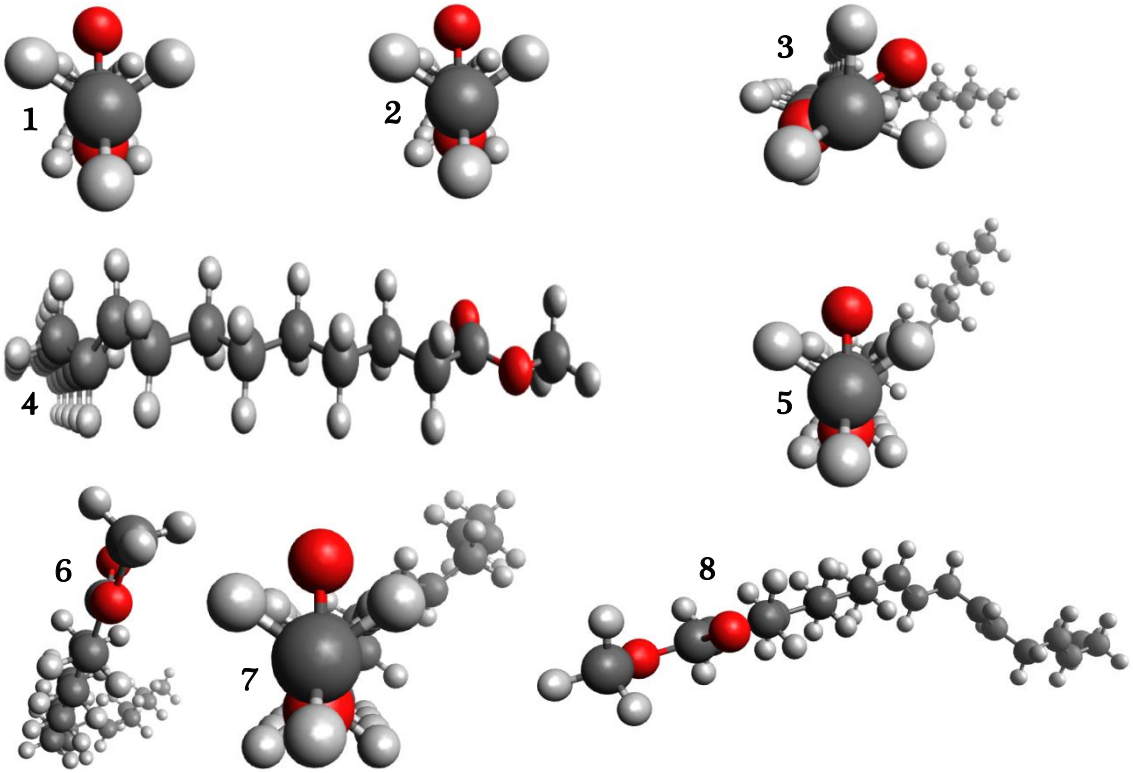
Hartree-Fock-Roothaan theory, which is an improvement on the Hartree-Fock method and is known as the self-consistent field method, was used to conduct a theoretical study on esters obtained from soybean oil. Deriving what is currently known as the Hartree Equation as an approximate solution of the Schrödinger Equation, Douglas Hartree required the final field calculated from the charge distribution to be "self-consistent" with the initially assumed field. Therefore, self-consistency is a requirement of the solution.

The atomic centers of the atoms studied (carbon, hydrogen and oxygen) were described using the 6-31G basis set. However, we used the STO-3G and 3-21G basis sets to diminish the computational cost. The STO-3G (Slater-type orbital) basis set was one of the first function sets successfully used to evaluate parameters related to species such as helium gas (H2) and the helium hydride ion (HeH+) (Szabo & Ostlund 1996; Oliveira 2010). The 3-21G and 6-31G basis functions are called divided valence basis functions, the main characteristic of which is the division of orbitals into two main regions: orbitals located closer to the nucleus and orbitals located in the outermost part.

All calculations were performed with the aid of the Gaussian 03 computational package. We used the free software Avogadro version 1.1.1 to create the optimized molecular structures. The GIMP software was used to insert the numeration of some of the atoms of some molecules. The software programs were executed in the GNU/Linux environment (Avogadro 2012; Gimp 2017).

## Results and Discussion

The most stable three-dimensional structures of the esters derived from the transesterification reactions of triglycerides are illustrated in **Figures 1–8**, which were optimized to locate the minimum energy structure using the method Hartree-Fock (HF) in the Gaussian 03 software and modeled with the Avogadro program. The molecules derive from the transesterification reaction of soybean oil with methanol.




**Figures 1–8**. Conformational analysis: **1**. Front view of C16:0; **2**. Front view of C18:0; **3**. Front view of C18:1; **4**. Front view after unsaturation of C18:1; **5**. Front view of C18:2; **6**. Peripheral view of C18:2; **7**. Front view of C18:3; **8**. Peripheral view of C18:3.

Star conformations were obtained in all esters, as seen clearly in the eight figures above. These conformations reduce the energy of the system, forming much more stable conformations.

The figures below show the methyl esters derived from the transesterification reactions of the triglycerides. **Figure 9**: methyl ester containing 16 carbon atoms and no unsaturation, IUPAC name: methyl hexadecanoate; **Figure 10**: methyl ester containing 18 carbon atoms and no unsaturation, IUPAC name: methyl octadecanoate; **Figure 11**: methyl ester containing 18 carbon atoms and one unsaturation, IUPAC name: methyl (9E)-octadec-9,12-enoate; **Figure 12**: methyl ester containing 18 carbon atoms and two unsaturations, IUPAC name: methyl (9E,12E)-octadec-9,12-dienoate; **Figure 13**: methyl ester containing 18 carbon atoms and three unsaturations, IUPAC name: methuyl (9E,12E,15E)-octadec-9,12,15-trienoate. The numbers of atoms in the figures show the atoms investigated. The carbon 1 atom and oxygen 2 and 4 atoms are seen in **Figures 9–10**.

For the esters oleic, linoleic and linolenic acids (C18:1, C18:2 and C18:3, respectively), which are illustrated in **Figures 11–13**, the prevailing isomerism is E in preference over Z, which has less repulsion between the groups, thereby diminishing the energy of the molecule and contributing to minimize the energy of the system. More carbon atoms are seen in **Figures 11–13**, since these have unsaturations.

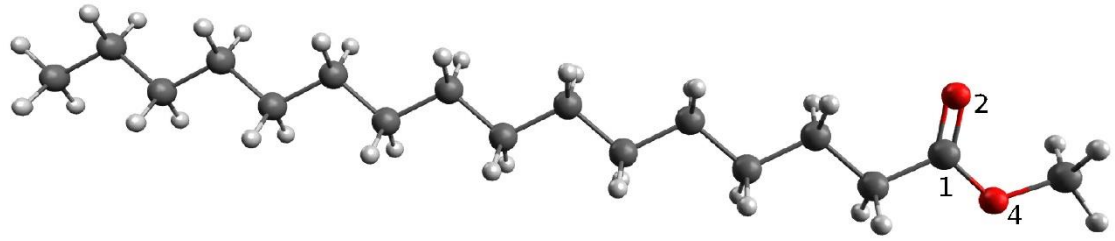



**Figure 9**. Methyl ester derived from palmitic acid containing 16 carbon atoms and no unsaturation, methyl hexadecanoate [C16:0].

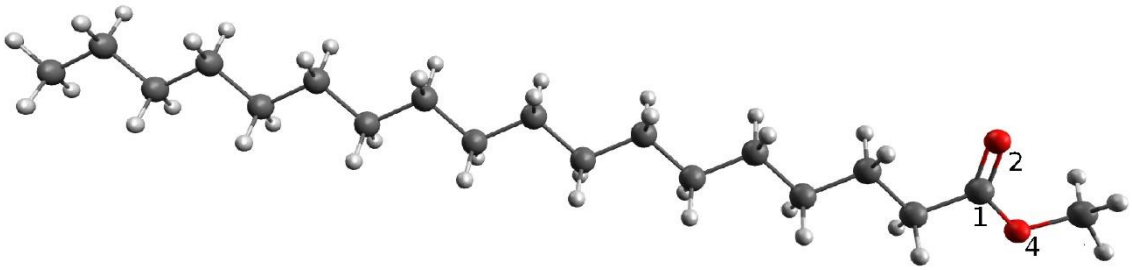



**Figure 10**. Methyl ester derived from stearic acid containing 18 carbon atoms and no unsaturation, methyl octadecanoate [C18:0].

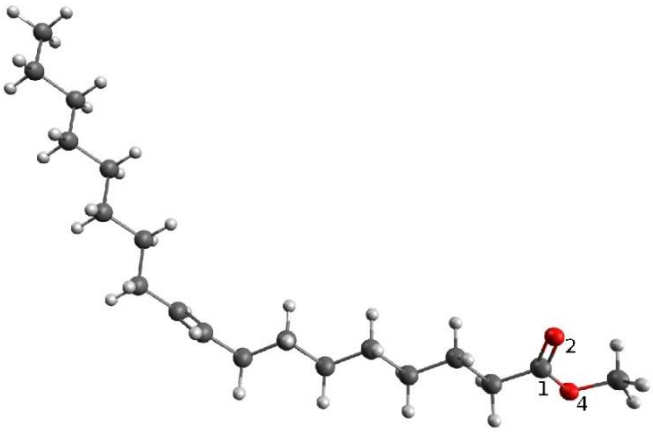



**Figure 11**. Methyl ester derived from oleic acid containing 18 carbon atoms and one unsaturation, methyl (9E)-octadec-9,12-enoate [C18:1].

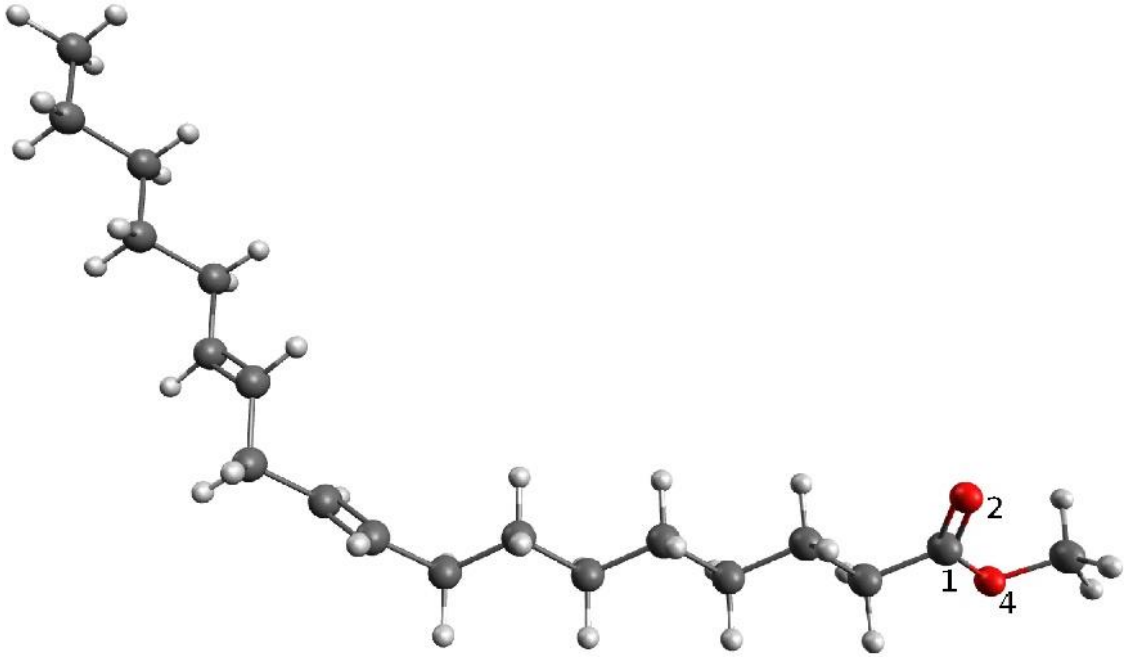



**Figure 12** - Methyl ester derived from linoleic acid containing 18 carbon atoms and two unsaturations, methyl (9E,12E)-octadec-9,12-dienoate [C18:2].

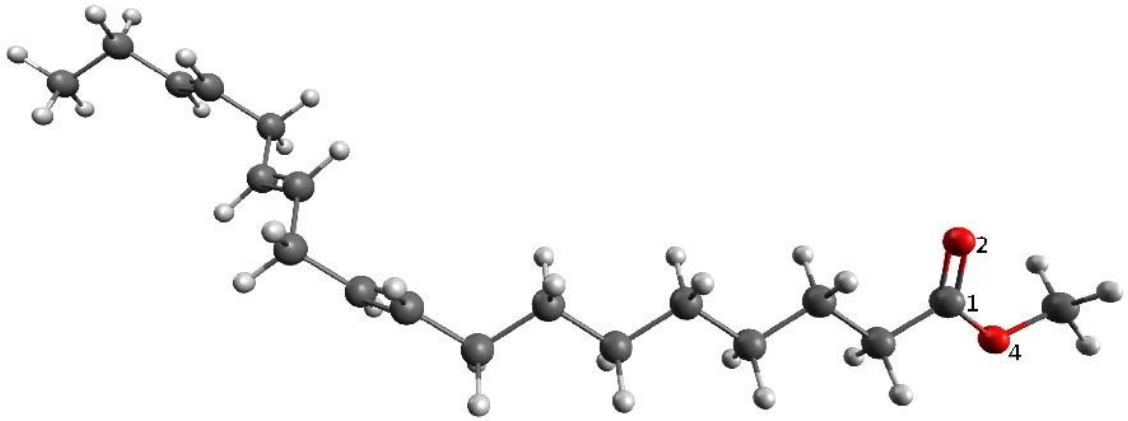



**Figure 13** - Methyl ester derived from linolenic acid containing 18 carbon atoms and three unsaturations, methyl (9E,12E,15E)-octadec-9,12,15-trienoate [C18:3].

## Analysis of Mulliken charges

**Table 1** displays the Mulliken charges on the atoms studied (1, 2 and 4) taking into consideration that the atoms analyzed are oxygen and carbon forming C−O and C=O bonds. The presence of oxygen in these bonds causes the displacement of the electrons of the bond in the direction of this atom, leading to polarity in the molecule and, consequently, a positive charge density in Atom 1 and negative charge density in Atoms 2 and 4. Analyzing the results displayed in the table, Atom 4 has a more negative charge density than Atom 2, which may be due to the electron-donating methyl group linked to Atom 4.

In comparison of the results for esters C16:0 and C18:0 displayed in Table 1, there is a decrease in the content of positive charge of Atom 1 caused by the increase in the carbon chain. This increase leads to a reduction in the positive charge density on the atom due to the fact that the ethyl group (~$C_2H_5$) that was added to the chain is an electron donor, thereby rearranging the electrons in Atom 1 such that its positive charge content is diminished. Moreover, analyzing the values related to the increase in unsaturations, Atom 1 of ester C18:0 basically has the same

value as Atom 1 of the ester C18:3. We can therefore conclude that the increase in unsaturations does not have any affect regarding the charge density in this atom.

Concerning Atom 2 of ester C18:0, the insertion of an unsaturaiton led to a small increase in the negative charge content. However, the values remained nearly constant with the increase in the number of unsaturations. The same occurred for Atom 4.

**Table 1**. Mulliken charge values for some atoms analyzed in systems investigated.

| MULLIKEN CHARGES<br>Basis set: 6-31G | | | | | |
|---|---|---|---|---|---|
| **ATOMS** | **C16:0** | **C18:0** | **C18:1** | **C18:2** | **C18:3** |
| **A1** | 0.777400 | 0.771780 | 0.783578 | 0.783575 | 0.783577 |
| **A2** | -0.569213 | -0.566491 | -0.578046 | -0.578016 | -0.577998 |
| **A4** | -0.727174 | -0.709870 | -0.730817 | -0.730824 | -0.730821 |

## Analysis of energy

The graph in **Figure 14** displays the results of the energy analysis, illustrating several aspects related to the energy of the system and enabling some considerations regarding the stability of the compounds analyzed.

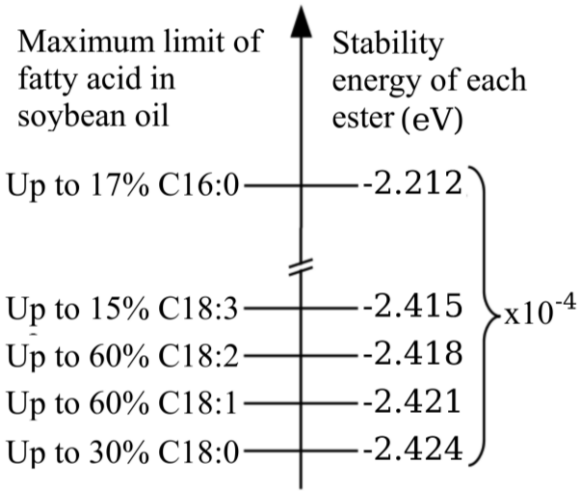



**Figure 14**. Graph of methyl ester energy in increasing order using HF/6-31G basis set and information on maximum amount of fatty acid in soybean oil.

**Figure 14** shows that the most stable molecule of the biodiesel is that of ester C18:0 and the least stable is that of ester C16:0. Regarding the increase in the number of unsaturations of the molecules with 18 atoms, an increase in stability was found in the following order: C18:0 > C18:1 > C18:2 > C18:3. Comparing the energies of the molecules with 18 carbon atoms, the energy of the system increases with the increase in unsaturations. The molecule with no unsaturations (linear) has the least energy, since it does not undergo the repulsion action of any group, in comparison to those with unsaturations in the carbon chain, especially when the unsaturation is found in the middle of the chain. This may occur due to the effects of steric impediment (molecules with unsaturations tend to form angles), as shown in **Figure 15**. A lower angle **A** translates to greater repulsion of the groups and, consequently, greater energy. Taking this factor into account, the molecule with the largest number of unsaturations has more energy.

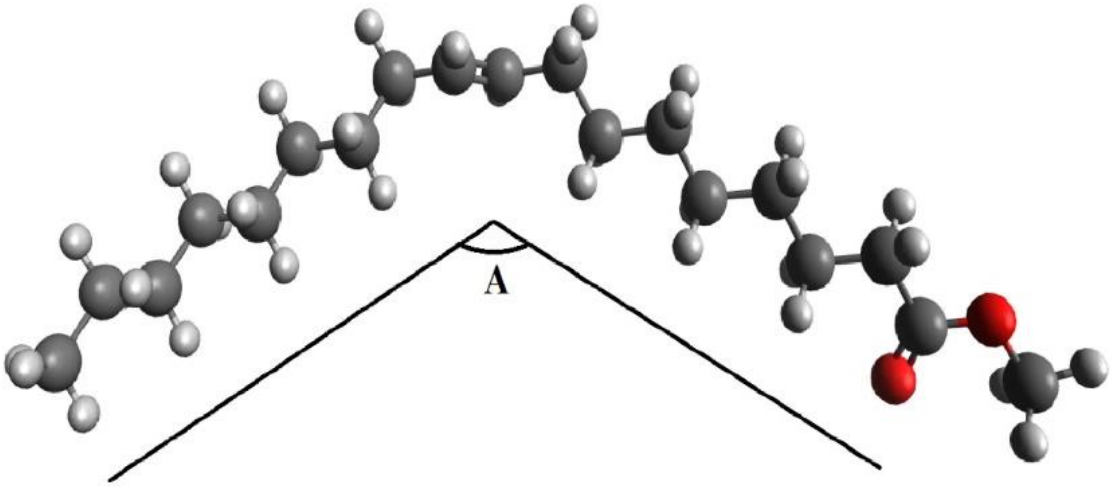



**Figure 15**. Angle caused by unsaturation in molecule of C18:1.

## Conclusions

In the present study, HF/6-31G was capable of determining parameters of the substances studied, which is in agreement with the principles of chemistry. The analysis of Mulliken charges enabled the precise determination of the positive center of the molecules studied. Therefore, this analysis can assist in the study of reactions in which molecules may participate.

Considering the stability of the systems investigated, we may conclude that the most stable molecule is the ester C18:0. However, this ester is not that which is contained in a greater percentage of the soybean oil. Thus, the analysis shows that, to some extent, the esters obtained from soybean oil have certain instability, demonstrating that this substance may undergo the effects of oxidation.

Analyzing the energy graph, one may conclude that the biodiesel obtained from soybean oil is an unstable substance, since the percentage of unstable compounds in its composition is greater for the molecules of the methyl esters C18:1 and C18:2. This finding is in agreement with data described by previous authors, who state that soybean biodiesel tends to undergo oxidation reactions easily (Melo 2009; Silva 2014). Therefore, this biofuel should be stored well and not be exposed due to its oxidative instability.

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## References

AVOGADRO (2012) AVOGADRO: An open-source molecular builder and visualization tool. Version 1.1.1, Marcus D.H. *et al*. Avogadro: An advanced semantic chemical editor, visualization, and analysis platform. *Journal of Cheminformatics*.

Azevedo A.N.G. & Lima B.G.A. (2016) Biocombustíveis: desenvolvimento e inserção internacional. *Revista Direito Ambiental e Sociedade*, 6(1): 77–100.

Benedetti O., Plá J.A., Rathmann R. & Padula A.D. (2006) Uma proposta de modelo pra avaliar a viabilidade do biodiesel no Brasil. *Teoria e evidência econômica*, 14(edição especial): 82–107.

BRASIL (2007) Biocombustíveis: 50 perguntas e respostas sobre este novo mercado. Brasília: Ministério das Minas e Energia. 44 p. Available in: https://www.agencia.cnptia.embrapa.br/Repositorio/matprima1_000g7pcetcc02wx5ok0wtedt32e6jis7.pdf (Accessed on: 07/07/2018).

Castellanelli C.A. (2016) Desenvolvimento sustentável: aproveitamento de resíduos e oleaginosas alternativas para a produção de biocombustível. *Revista Observatório de la Economía Latinoamericana*: 1–16.

Gaussian 03, Revision B.04, Frisch M.J., Trucks G.W., Schlegel H.B., Scuseria G.E., Robb M.A., Cheeseman J.R., Montgomery J.A., Vreven Jr. T., Kudin K.N., Burant J.C., Millam J.M., Iyengar S.S., Tomasi J., Barone V., Mennucci B., Cossi M., Scalmani G., Rega N., Petersson G.A., Nakatsuji H., Hada M., Ehara M., Toyota K., Fukuda R., Hasegawa J., Ishida M., Nakajima T., Honda Y., Kitao O., Nakai H., Klene M., Li X., Knox J.E., Hratchian H.P., Cross J.B., Adamo C., Jaramillo J., Gomperts R., Stratmann R.E., Yazyev O., Austin A.J., Cammi R., Pomelli C., Ochterski J.W., Ayala P.Y., Morokuma K., Voth G.A., Salvador P., Dannenberg J.J., Zakrzewski V.G., Dapprich S., Daniels A.D., Strain M.C., Farkas O., Malick D.K., Rabuck A.D., Raghavachari K., Foresman J.B., Ortiz J.V., Cui Q., Baboul A.G., Clifford S., Cioslowski J., Stefanov B.B., Liu G., Liashenko A., Piskorz P., Komaromi I., Martin R.L., Fox D.J., Keith T., Al-Laham M.A., Peng C.Y., Nanayakkara A., Challacombe M., Gill P.M.W., Johnson B., Chen W., Wong M.W., Gonzalez C. & Pople J.A. Gaussian, Inc., Pittsburgh PA, 2003.

Gavira M.O. (2003) Simulação computacional como uma ferramenta de aquisição de conhecimento. Dissertação de Mestrado, Escola de Engenharia de São Carlos. Universidade de São Paulo, São Carlos.

GIMP (GNU Image Manipulation Program, 2017). Available in: https://www.gimp.org (Accessed on: 06/01/2018).

Guadgnini P.H. & Bruns R.E. (1995) Cargas atômicas em moléculas. *Química Nova*, 19(2): 148–155.

Guarieiro L.L.N., Vasconcellos P.C. & Solci M.C. (2011) Poluentes Atmosféricos Provenientes da Queima de Combustíveis Fósseis e Biocombustíveis: Uma Breve Revisão. *Revista Virtual Química*, 3(5): 434–445.

Hehre H.J. (1986) Ab initio molecular orbital theory. New York: John Wiley & Sons. 576 p.

Levine I.N. (1991) Quantum chemistry. Englewood Cliffs: Prentice Hall. 675 p.

Mello M.A.R. (2009) Monitoramento da Estabilidade Oxidativa no Armazenamento de Biodiesel Metílico de Soja/Mamona e Blendas em Recipientes de Vidro. Dissertação de Mestrado, Programa de pós-graduação em Química. Universidade Federal da Paraíba, João Pessoa, Paraíba.

Oliveira J.P.C. (2018) Estudo ab initio da estrutura hiperfina de sistemas moleculares em interação com metais. Dissertação de Mestrado, Programa de Pós-Graduação em Física. Universidade Federal da Bahia, Salvador, Bahia.

Prates C.P.T., Pierebon E.C. & Costa R.C. (2007) Formação do Mercado de biodiesel no Brasil. *BNDES Setorial*, 25: 39–64.

REN21 (2014) Global Status Report, Paris: REN21 Secretariat, 2014. Available in: http://www.ren21.net/Portals/0/documents/Resources/GSR/2014/GSR2014_full%20report_low%20res.pdf (Accessed on: 03/2018).

REN21 (2017) Renewables Global Status Report, Paris: REN21 Secretariat.2017. Available in: <http://www.ren21.net/wp-content/uploads/2017/06/17-8399_GSR_2017_ Full_Report_0621_Opt.pdf (Accessed on: 03/2018).

Rino J.P. & Studart N. (2001) Um potencial de interação para o estudo de materiais e simulações por dinâmica molecular. *Química Nova*, 24(6): 676–682.

Rossetti H.L. (2006) Utilização de métodos de modelagem molecular para caracterização do sistema $(nBuCp)_2Zr(CH_3)_2$ imobilizado em sílica e ativado com MAO. Dissertação de Mestrado, Programa de Pós-Graduação em Química. Universidade Federal do Rio Grande do Sul, Porto Alegre, Rio Grande do Sul.

Silva M.V.D. (2012) Modelagem molecular aplicada a reações de produção do biodiesel. Dissertação de Mestrado, Programa de Pós-Graduação em Engenharia Química. Universidade Federal de Uberlândia, Uberlândia, Minas Gerais.

Silva L.C.M. (2014) Processo de produção de biodiesel e análise de parâmetros de qualidade. Dissertação de Mestrado, Escola Superior de Tecnologia e Gestão do Instituto Politécnico de Bragança. Instituto Politécnico de Bragança, Bragança Paulista, São Paulo.

Silva P.R.F. & Freitas T.F.S. (2008) Biodiesel: o ônus e o bônus de produzir combustível. *Ciência Rural*, 38(3): 843–851.

Szabo A.E. & Ostlund N.S. (1996) Modern quantum chemistry: introduction to advanced electronic structure theory. New York: Dover Publications. 480 p.

Trzeciak M.B., Neves M.B., Vinholes P.S. & Villela F.A. (2008) Utilização de sementes de espécies oleaginosas para produção de biodiesel. *Informativo ABRATES*, 18(1-3): 30–38.