Infrared spectrum for derivative steroid with potential to treat breast cancer

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Abstract—This study applies Density Functional Theory (DFT), using the B3LYP functional, and via ab initio Restrict Hartree-Fock (RHF) methods, to study the infrared spectrum of steroid 17-Iodo-androst-16-ene. The spectrum was obtained via computational methods ab initio RHF and DFT. Optimization of molecular structure via UFF (Universal Force Field), followed by PM3 (Parametric Method 3), with geometric optimization, obtaining the spectrum of other basis sets of steroid 17-Iodo-androst-16-ene. The study this steroid was chosen because it can could act as aromatase enzyme inhibitors and this phenomenon could be translated as good compounds to treat breast cancer.

The B3LYP functional always presents the lowest thermal energy than the RHF in all calculated bases, however the RHF always presents the highest Entropy than the B3LYP, in all the calculated basis sets. The normalized spectrum calculated in the B3LYP/SVP functional/basis set have harmonic frequency with peaks 3,241.83 cm⁻¹, 100% and 3,177.535 cm⁻¹ at 43.304% absorbance. The study has so far been limited to computational methods compatible with the theory of quantum chemistry.

Index Terms—Hartree-Fock method, DFT, B3LYP, UFF, PM3, Infrared spectroscopy, Cancer.

I. INTRODUCTION

This study applies Density Functional Theory (DFT), using the B3LYP functional, and via ab initio Restrict Hartree-Fock (RHF) methods, to study the infrared spectrum of steroid 17-Iodo-androst-16-ene derived.[14].

The spectrum was obtained via computational methods ab initio RHF and DFT. [1], [2], [3], [4], [5], [6], [7], [8], [9], [10], [11], [12], [13] Optimization of molecular structure via UFF (Universal Force Field), followed by PM3 (Parametric Method 3) [1], [2], [3], [4], [5], [6], [7], [8], [9], [10], [11], [12] with geometric optimization, obtaining the spectrum of other basis sets of steroid 17-Iodo-androst-16-ene derived[14].

A steroid (named after the steroid cholesterol) is a biologically active organic compound with four fused rings arranged in a specific molecular configuration. Steroids have two principal biological functions: as important components of cell membranes that alter membrane fluidity and as signaling molecules. Hundreds of steroids are found in plants, animals and fungi. All steroids are manufactured in cells from the sterols lanosterol (opisthokonts) or cycloartenol (plants). Lanosterol and cycloartenol are derived from the cyclization of the triterpene squalene. [16]

The steroid nucleus (core structure) is called gonane (cyclopentanoperhydrophenanthrene). It is typically composed of seventeen carbon atoms, bonded in four fused rings: three six-member cyclohexane rings (rings A, B and C in the first illustration) and one five-member cyclopentane ring (the D ring), Figure (1). Examples include anabolic steroids, the lipid cholesterol, the sex hormones estradiol and testosterone, and the anti-inflammatory corticosteroid drug dexamethasone. [16]

Some aromatase enzyme inhibitors drugs have been used to treat cancer; however, their interaction with aromatase is not clear. Evaluated the interaction of steroid 17-Iodo-androst-16-ene derivatives with aromatase enzyme surface using 3eqm protein. The results showed differences in the aminoacid residues involved in the interaction of steroid

1The steroid [16] 17-Iodo-androst-16-ene derived of testosterone. Testosterone is the primary male sex hormone and anabolic steroid in males [15].
derivatives interact with 3eqm protein surface Arg115; Phe134; Trp224; Ala306; Thr110; Val370; Met374; Leu127. The steroid derivatives could act as aromatase enzyme inhibitors and this phenomenon could be translated as good compounds to treat breast cancer. [17]

The ab initio and DFT [12] [13] [14] [16] [15] [16] [17] [18] calculations have been performed to study the equilibrium configuration, and calculation of its Infrared Spectrum (IR), its Entropy (S), Heat capacity (C<sub>v</sub>), chemical and molecular structure of steroid derived, via GAMESS. [19]

II. METHODS

A. Hartree-Fock Methods

The molecular Hartree-Fock [1] [2] [3] [4] [7] [8] [9] [10] [11] [12] wave function is written as an antisymmetrized product (Slater determinant) of spin-orbitals, each spin-orbital being a product of a spatial orbital φ<sub>i</sub> and a spin function (either α or β).

The expression for the Hartree-Fock molecular electronic energy E<sub>HF</sub> is given by the variation theorem as

\[ E_{HF} = \langle D|\hat{H}_{el}|D\rangle \]  
(1)

where D is the Slater-determinant Hartree-Fock wave function and \( \hat{H}_{el} \) and \( V_{NN} \) are given by

\[ \hat{H}_{el} = -\frac{\hbar^2}{2m_e} \sum_i \nabla_i^2 - \sum_i \sum_{i>j} Z_{\alpha\beta} e^{'2} / r_{ij} + \sum_i \sum_{i>j} e^{'2} / r_{ij} \]  
(2)

\[ V_{NN} = \sum_{\alpha} \sum_{\beta>\alpha} Z_{\alpha\beta} e^{'2} / r_{\alpha\beta} \]  
(3)

Since \( V_{NN} \) does not involve electronic coordinates and D is normalized, it has to

\[ \langle D|V_{NN}|D\rangle = V_{NN} \langle D|D\rangle = V_{NN} \]  
(4)

The operator \( \hat{H}_{el} \) is the sum of one-electron operators \( \hat{f}_i \) and two-electron operators \( \hat{g}_{ij} \); it has to

\[ \hat{H}_{el} = \sum_i \hat{f}_i \sum_{j>i} \hat{g}_{ij} \]  
(5)

it has to here

\[ \hat{f}_i = -\frac{1}{2} \nabla_i^2 + \sum_{i>j} Z_{\alpha\beta} e^{'2} / r_{ij} \]  
(6)

and

\[ \hat{g}_{ij} = -1/r_{ij} \]  
(7)

The Hamiltonian \( \hat{H}_{el} \) is the same as the Hamiltonian \( \hat{H} \) for an atom except that

\[ \sum_{\alpha} \sum_{\alpha} / r_{i\alpha} \]  
(8)

replaces \( Z/r_i \) in \( \hat{f}_i \). Hence

\[ E = \langle D|\hat{H}|D\rangle = 2 \sum_{i} (\phi_i(1)|\hat{f}_i|\phi_i(2)) \]  
(9)

\[ + \sum_{j=1}^{n/2} (2\hat{J}_{ij} - \hat{K}_{ij}) \]  

where

\[ \hat{J}_{ij} = \langle \phi_i(1)|\phi_j(2)|e^{'2}/r_{12}|\phi_i(1)|\phi_j(2) \rangle \]  
(10)

and

\[ \hat{K}_{ij} = \langle \phi_i(1)|\phi_j(2)|e^{'2}/r_{12}|\phi_i(1)|\phi_j(2) \rangle \]  
(11)

\[ \hat{f}_i = -(h^2/2m_e) \nabla_i^2 - Ze^{'2}/r_i \]  
(12)

can be used to give \( D|\hat{H}_{el}|D \).

Therefore, the Hartree-Fock energy of a diatomic or polyatomic molecule with only closed shells is

\[ E_{HF} = 2 \sum_{i} \hat{H}_{i\alpha}^{\text{core}} + \sum_{j} \sum_{j>i} \hat{V}_{\alpha\beta} (1/2) \sum_{\alpha} Z_{\alpha\beta} e^{'2}/r_{\alpha\beta} \]  
(13)

\[ \hat{H}_{i\alpha}^{\text{core}} = \langle \phi_i(1)|\hat{H}_{i\alpha}^{\text{core}}(1)|\phi_i(1) \rangle \]  
(14)

\[ \hat{J}_{ij} = \langle \phi_i(1)|\phi_j(2)|1/r_{12}|\phi_i(1)|\phi_j(2) \rangle \]  
(15)

and

\[ \hat{K}_{ij} = \langle \phi_i(1)|\phi_j(2)|1/r_{12}|\phi_i(1)|\phi_j(2) \rangle \]  
(16)

where the one-electron-operator symbol was changed from \( \hat{f}_i \) to \( \hat{H}_{i\alpha}^{\text{core}}(1) \). [6]

The vast literature associated with these methods suggests that the following is a plausible hierarchy:

\[ HF << MP2 < CISD < CCSD < CCSD(T) < FCI \]

The extremes of ‘best’, FCI, and ‘worst’, HF, are irrefutable, but the intermediate methods are less clear and depend on the type of chemical problem being addressed. The use of HF [1], [2] [3] [4] [7] [8] [9] [10] [11] [12] [18] [21] [22] [19], [20] in the case of FCI was due to the computational cost.
B. DFT

Density-functional theory (DFT) is a computational quantum mechanical modelling method used in physics, chemistry, and materials science to investigate the electronic structure of many-body systems, in particular atoms, molecules, and the condensed phases. Using this theory, the properties of a many-electron system can be determined by functional, i.e. functions of another function. In the case of DFT, these are functional of the spatially dependent electron density. DFT is among the most popular and versatile methods available in condensed-matter physics, computational physics, and computational chemistry.

As usual in many-body electronic structure calculations, the nuclei of the treated molecules or clusters are seen as fixed (the Born–Oppenheimer approximation), generating a static nuclei of the treated molecules or clusters are seen as fixed.

The Figures (2) show the plot of the normalized spectrum.

\[
E_{XC}^{B3LYP} = (1 - a)E_x^{LSDA} + aE_x^{HF} + b\Delta E_x + (1 - c)E_c^{LSDA} + cE_c^{LYP}, \quad (18)
\]

where: \(a = 0.20, \ b = 0.72, \) and \(c = 0.81.\) \(E_x^{B}\) is a generalized gradient approximation: the Becke 88 exchange functional and the correlation functional of Lee, Yang, and Parr for B3LYP, and \(E_c^{LSDA}\) is the VWN local spin density approximation to the correlation functional.

The three parameters defining B3LYP have been taken without modification from Becke’s original fitting of the analogous B3PW91 functional to a set of atomization energies, ionization potentials, proton affinities, and total atomic energies.

III. HARDWARE AND SOFTWARE

Computer used for was a Desktop AMD Ryzen 7 1800X processor, 16GB of RAM, with 500GB SSD, with SUSE Linux Enterprise Desktop.

The \(ab\ initio\) and B3LYP calculations have been performed to study the equilibrium configuration, for the calculation of chemical and molecular structure, its IR, S, and \(C_V\) of the steroid. The set of programs GaussView 5.0.8, GAMESS, BIOVIA Draw 2017, and CHARMM22 were used.

IV. RESULTS

A. Properties

IUPAC name: rac-(5R,8S,9R,10S,13S,14S)-17-iodo-10,13-dimethyl-2,3,4,5,6,7,8,9,11,12,14,15-dodecahydro-1H-cyclopenta[a]phenanthrene

Dipole Moment: 1.8778 Debye

Degree of freedom: 141

Molecular Formula: \(C_{139}H_{230}\)

E(B3LYP) = -7660.8047960 a. u.; \(19, 20\)

Polarizability (\(\alpha\)) = 218.035129 a. u.; \(19, 20\)

E (Thermal) = 288.606 KCal/Mol; \(19, 20\)

Heat Capacity \(\left(C_V\right) = 72.217\) Cal/Mol-Kelvin; \(19, 20\)

Entropy = 132.406 Cal/Mol-Kelvin; \(19, 20\)

B. Analyses, Figures and Tables

The Figure (1) show Molecular structure of steroid steroid 17-Iodo-androst-16-ene derived.

The Figure (2) show the plot of the normalized spectrum calculated in the B3LYP/SVP functional/basis set, for harmonic frequency peaks 3,241.83 cm\(^{-1}\), 1.0 and 3,177.53
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Fig. 1: Molecular structure of steroid steroid 17-Iodo-androst-16-ene derived, via B3LYP/SVP [7], [16] [15], [17] [18], [21] [19], [22] functional /basis sets, via GAMMES, Gaussview. Represented in gray is Carbon, in white is Hydrogen and in purple is Iodine. Source: Authors.

\[ \text{cm}^{-1} \] at 0.43304 absorbance.

The Table (1) has the \( E_T \) (Thermal), Heat Capacity \( (C_V) \) and Entropy \( (S) \) for basis set calculated.

The Table (2) represented the Harmonic frequencies \( (\text{cm}^{-1}) \) for Intensity \( \text{(km/mol)} \) of the steroid 17-Iodo-androst-16-ene [15] molecule via B3LYP functional [7], [16] [15], [17] [18], [21] [19], [22] SVP basis set for the infrared spectrum.

The lowest \( E_T \) (Thermal Energy) calculated is 288.606 KCal/Mol in the B3LYP/SVP functional /basis sets and the highest 344.895 KCal/Mol in the RHF/STO-3G method/basis sets.

The lowest Entropy \( (S) \) calculated is 110.839 Cal/Mol-Kelvin in the B3LYP/CEP-4G functional/basis sets and the highest 138.035 Cal/Mol-Kelvin in the RHF/def2SV method/basis sets.

The Heat Capacity \( (C_V) \) calculated is 54.211 Cal/Mol-Kelvin in the B3LYP/CEP-4G functional/basis sets, and the highest 73.614 Cal/Mol-Kelvin in the RHF/SVP method/basis sets.

It can be seen that for the given molecule, the B3LYP functional always presents the lowest thermal energy than the RHF in all calculated bases, however the RHF always presents the highest Entropy than the B3LYP, in all the calculated basis sets. Better bases were not used because they are out of reach for the Iodine atom.

As expected, both RHF and B3LYP functional show similar results on the STO-3G and LanL2MB basis sets.

Table 1: \( E_T \) (Thermal)(KCal/Mol), Heat Capacity \( (C_V)(\text{Cal/Mol-Kelvin}) \) and Entropy \( (S)(\text{Cal/Mol-Kelvin}) \) for basis set calculated. [19], [20]

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<th>Basis Set</th>
<th>( E_T )</th>
<th>( C_V )</th>
<th>( S )</th>
</tr>
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<td>344.895</td>
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<td>292.533</td>
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<td>131.878</td>
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Source: Authors.
Table 2: Table containing the harmonic frequencies (cm\(^{-1}\)) for Intensity (km/mol) of the steroid 17-Iodo-androst-16-ene ([15] molecule via B3LYP functional, [7], [16] [15], [17], [18], [21] [19], [22] SVP basis set for the infrared spectrum.

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<th>I (km/mol)</th>
<th>(\nu) (cm(^{-1}))</th>
<th>I (km/mol)</th>
<th>(\nu) (cm(^{-1}))</th>
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Source: Authors.
V. Conclusions

The study this steroid was chosen because it could act as aromatase enzyme inhibitors and this phenomenon could be translated as good compounds to treat breast cancer.

The normalized spectrum calculated in the B3LYP/SVP functional/basis set have harmonic frequency with peaks 3,241.83 cm\(^{-1}\), 100\% and 3,177.53 cm\(^{-1}\) at 43.304\% absorbance.

It can be seen that for the given molecule, the B3LYP functional always presents the lowest thermal energy than the RHF in all calculated bases, however the RHF always presents the highest Entropy than the B3LYP, in all the calculated basis sets. Better bases were not used because they are out of reach for the Iodine atom.

The study has so far been limited to computational ab initio methods. The results are compatible with the theory of quantum chemistry.

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References