^{1}H NMR Spectroscopy of the New Xalapa Molecule

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August 30, 2021

Abstract

Proton nuclear magnetic resonance (^{1}H NMR) is the application of nuclear magnetic resonance in NMR spectroscopy with respect to ^{1}H within the molecules of a substance, in order to determine the structure of its molecules. The work focused on determining the ^{1}H NMR spectrum of the molecule here called Xalapa, in homage of the city of Xalapa, the capital city of the Mexican state of Veracruz and the name of the surrounding municipality. The ^{1}H NMR spectrum was obtained via computational methods *ab initio* Restricted Hartree-Fock. Optimization of molecular structure via UFF, followed by PM3, RHF/EPR-II and RHF/STO-6G, thus obtaining a stable structure, in STP, NMR via the GIAO (Gauge-Independent Atomic Orbital) method. The IUPAC name of the molecule was obtained, whose composition is C: 81.7%; H: 7.1%; N: 3.4%; O: 7.8%, formula weight: 411.53536 g, and molecular formula: $C_{28}H_{29}NO_2$. Limitations our study has so far been limited to computational simulation via quantum mechanics (QM) an applied theory. Our results and calculations are compatible with the theory of QM, but their physical experimental verification depends on experimental data that should be laboratory for experimental biochemical.

1 Introduction

The NMR (Nuclear Magnetic Resonance) spectroscopy is a spectroscopic technique to observe local magnetic fields around atomic nuclei. One magnetic field is placed in the sample and the NMR signal is produced by excitation of the nuclei sample with radio waves into nuclear magnetic resonance. The intramolecular magnetic field around an atom in a molecule changes the resonance frequency, thus giving access to details of the electronic structure of a molecule and its individual functional groups. As the fields are unique or highly characteristic to individual compounds, in modern organic chemistry practice, NMR spectroscopy is the definitive method to identify monomolecular organic compounds. [1]

Proton nuclear magnetic resonance (^{1}H NMR) is the application of nuclear magnetic resonance in NMR spectroscopy with respect to ^{1}H within the molecules of a substance, in order to determine the structure of its molecules. [2]

The work focused on determining the ^{1}H NMR spectrum of the molecule here called Xalapa, in homage of the city of Xalapa (often spelled Jalapa)

[0], the capital city of the Mexican state of Veracruz and the name of the surrounding municipality.

The ^{1}H NMR spectrum was obtained via computational methods*ab initio* Restricted Hartree-Fock [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0], GIAO (Gauge-Independent Atomic Orbital) methods [0, 0, 0, 0, 0].

The molecule was obtained experimentally in the laboratory of the University Autonomous of Campeche (Faculty of Chemical-Biological Sciences), Figure (1), Valverde et al. [0, 0, 0, 0, 0]
.

2 Methods

Its structure and chemical conformation and its ^{1}H NMR spectrum were obtained from computational chemistry calculations, using the GAMESS software. [0]

The methods used initially were UFF [0, 0, 0, 0, 0, 0, 0, 0, 0], obtaining the lowest energy molecular structure. Optimization of molecular structure via UFF, followed by PM3, RHF/EPR-II and RHF/STO-6G[1], thus obtaining a stable structure, in STP (Standard Temperature and Pressure) [0, 0, 0, 0, 0, 0, 0, 0, 0], and NMR via the GIAO method [0, 0, 0, 0, 0].

The properties keyword predicts NMR shielding tensors and magnetic susceptibilities using the Restricted Hartree-Fock (RHF) method, all DFT methods and the MP2 method NMR shielding tensors may be computed with the Gauge-Independent Atomic Orbital (GIAO) method [0, 0, 0, 0, 0].

The basis sets of *Barone*[2] which are optimized for the computation of hyperfine coupling constants. EPR-II is a double zeta basis set with a single set of polarization functions.

2.1 Hartree-Fock Method

Hartree-Fock Methods. [2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0]
The vast literature associated with these methods suggests that the following is a plausible hierarchy:

$$HF << MP2 < CISD < CCSD < CCSD(T) < FCI \quad (1)$$

[1]STO-nG basis sets are minimal basis sets, where *n* primitive Gaussian orbitals are fitted to a single Slater-type orbital (STO). The *n* originally took the values 2 – 6.

[2]V. Barone, *in Recent Advances in Density Functional Methods*, Part I, Ed. D. P. Chong (World Scientific Publ. Co., Singapore, 1996).

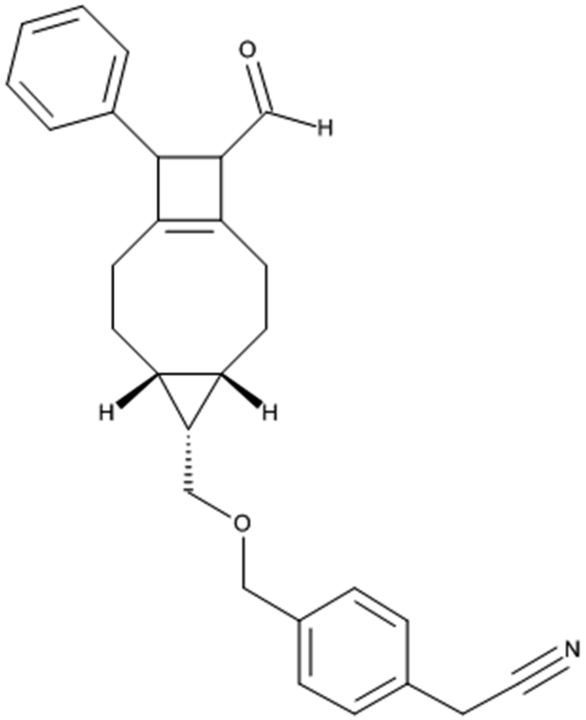

Figure 1: *Representation of the structure of the Xalapa molecule, obtained experimentally at the University Autonomous of Campeche (Faculty of Chemical-Biological Sciences) Valverde et al. [0, 0, 0, 0, 0].*

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 [2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0] in the case of FCI was due to the computational cost.

3 Hardware and Software

For calculations the computer used a Desktop with SUSE Linux Enterprise Desktop [31], AMD Ryzen 7 1800X processor [32], ASUS Prime A320M-K motherboard [33], 16GB of RAM, with 500GB SSD [34].

The *ab initio* calculations have been performed to study the equilibrium configuration of Xalapa molecule. The set of programs GaussView 5.0.8 [35], HyperChem 8.0.6 Evaluation [36]. are the advanced semantic chemical editor, visualization, and analysis platform and GAMESS [15, 35] is a computational chemistry software program and stands for General Atomic and Molecular Electronic Structure System [15, 35], BIOVIA Draw 2017 [37], CHARMM22 [38] set of programs were used.

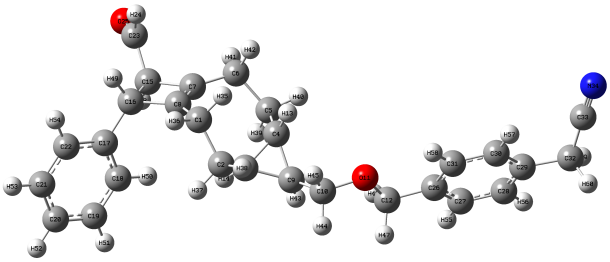

Figure 2: *Representation of the molecular structure of the Xalapa molecule, obtained after molecular optimization, using computational quantum chemistry methods, using the computer programs GAMESS [0, 0]. Subsequently, the UFF, PM3, ab initio RHF/EPR-II and RHF/STO-6G methods were used. Graphic edited in GaussView software [0].*

4 Results

The molecular structure of Xalapa molecule, were obtained through computationally calculated molecular dynamics, using the *ab initio* Restricted Hartree-Fock (RHF) method.

The name in Figure (1) of the new molecules obtained is 2-[4-[[rac-(4S,5S,6S,10R,11S)-10-formyl-11-phenyl-5-tricyclo[7.2.0.04,6]undec-1(9)-enyl]methoxymethyl]phenyl]acetonitrile.

4.1 Properties of Xalapa molecule

IUPAC name:
2-[4-[[rac-(4S,5S,6S,10R,11S)-10-formyl-11-phenyl-5-tricyclo[7.2.0.04,6]undec-1(9)-enyl]methoxymethyl]phenyl]acetonitrile;
PSA: 50.09;
ALogP: 4.892;
Stereo Center Count: 5;
Hydrogen Acceptor Count: 3;
Hydrogen Donor Count: 0
; Composition: C: 81.7%; H: 7.1%; N: 3.4%; O: 7.8%;
Formula Weight: 411.53536 g;
Exact Mass: 411.219829178001 g;
Molecular Formula: $C_{28}H_{29}NO_2$.
[0]

The Figure (1) representation of the structure of the Xalapa molecule, obtained experimentally at the University Autonomous of Campeche (Faculty of Chemical-Biological Sciences) Valverde et al.

The Representation of the molecular structure of the Xalapa molecule, Figure (2), obtained after molecular optimization, using computational quantum chemistry methods, using the computer programs GAMESS [0, 0]. Subsequently, the UFF, PM3, *ab initio* RHF/EPR-II and RHF/STO-6G methods were used. Graphic edited in GaussView software.

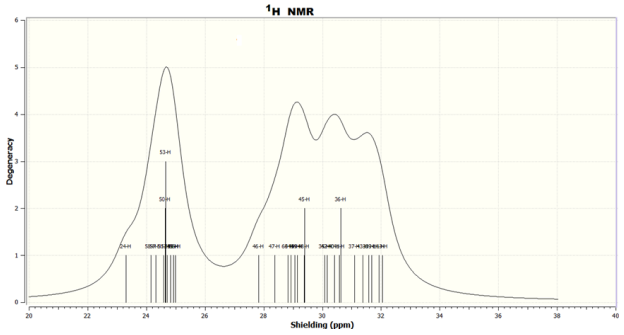

Figure 3: *Representation of Shielding from 20 to 40 ppm for Degeneracy of the ^1H NMR spectrum of the Xalapa molecule. Using computer programs GAMESS, the calculations obtained in the ab initio RHF, method NMR shielding tensors may be computed with the Gauge-Independent Atomic Orbital (GIAO) method.*

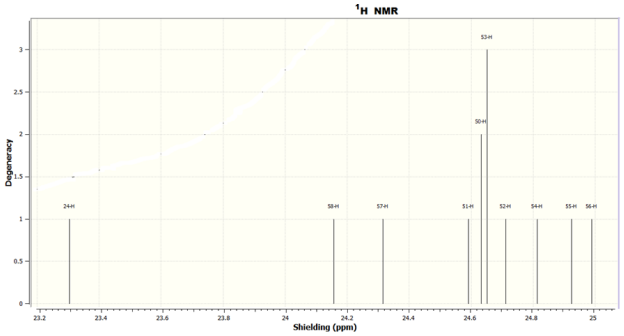

Figure 4: *Representation of from 23.2 to 25.05 ppm for Degeneracy of the ^1H NMR spectrum of the Xalapa molecule. Using computer programs GAMESS, the calculations obtained in the ab initio RHF, method NMR shielding tensors may be computed with the Gauge-Independent Atomic Orbital (GIAO) method.*

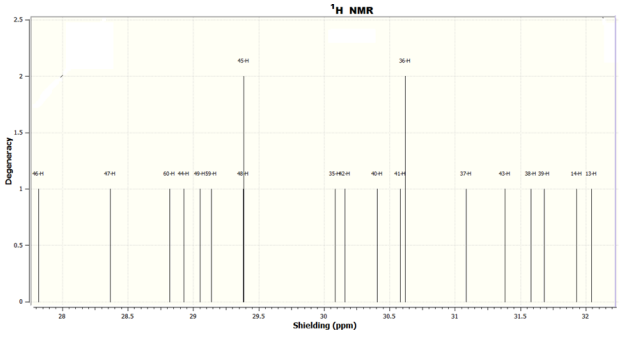

Figure 5: *Representation of from 27.5 to 32.5 ppm for Degeneracy of the ^1H NMR spectrum of the Xalapa molecule. Using computer programs GAMESS, the calculations obtained in the ab initio RHF, method NMR shielding tensors may be computed with the Gauge-Independent Atomic Orbital (GIAO) method.*

The Figure (3) representation of Shielding from 20 to 40 ppm for Degeneracy of the ^{1}H NMR spectrum of the Xalapa molecule, The Figure (4) representation of from 23.2 to 25.05 ppm for Degeneracy of the ^{1}H NMR spectrum of the Xalapa molecule and the Figure (5) representation of from 27.5 to 32.5 ppm for Degeneracy of the ^{1}H NMR spectrum of the Xalapa molecule. All Using computer programs GAMESS, the calculations obtained in the *ab initio* RHF, method NMR shielding tensors may be computed with the Gauge-Independent Atomic Orbital (GIAO) method.

The H50, H51, and H52 hydrogens of the aromatic ring are coupling with each other to form a triplet (1:2:1), Figures (3) and (4). The H53 hydrogen is not coupling with the other H atoms and appears as a singlet, Figures (3) and (4).

Hydrogen H45 from group CH_2 bonded to Oxygen O11 not coupling with the other H atoms, as well as Hydrogen H36 from group CH2 from aromatic ring C_9H_{10}, bonded to Carbon C1, Figures (3) and (5).

5 Conclusions

The ^{1}H NMR spectrum of the Xalapa molecule. was calculated, indicating the characteristic of the nano-molecule genesis. Characterized its ^{1}H NMR spectrum quantum calculated, accepted by quantum chemistry parameters, with *ab initio* methods, in the GIAO methods.

The molecule is named IUPAC 2-[4-[[rac-(4S,5S,6S,10R,11S)-10-formyl-11-phenyl-5-tricyclo[7.2.0.04,6]undec-1(9)-enyl]methoxymethyl]phenyl]acetonitrile; of composition: C: 81.7%; H: 7.1%; N: 3.4%; O: 7.8%, formula weight: 411.53536 g, and molecular formula: $C_{28}H_{29}NO_2$.

Limitations our study has so far been limited to computational simulation via quantum mechanics (QM) an applied theory. Our results and calculations are compatible with the theory of QM, but their physical experimental verification depends on experimental data that should be laboratory for experimental biochemical.

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