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## Abstracts

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**DENSITY FUNCTIONAL THEORY:  
COMPUTER-ASSISTED STUDY OF <sup>1</sup>H  
AND <sup>13</sup>C NMR SPECTRA OF  
4-HYDROXY-3-(3'-METHYL-2'-  
BUTENYL)ACETOPHENONE  
ISOLATED FROM *SENECIO  
GRAVEOLENS* AND ITS  
MICROWAVE-ASSISTED SYNTHETIC  
DERIVATE, 4'-HYDROXY-3'-(3-  
METHYL-2-BUTENYL)CHALCONE**

**TEORÍA FUNCIONAL DE LA  
DENSIDAD: ESTUDIO ASISTIDO POR  
COMPUTADORA DE LOS  
ESPECTROS DE RMN <sup>1</sup>H Y <sup>13</sup>C DEL 4-  
HIDROXI-3-(3'-METIL-2'-  
BUTENIL)ACETOFENONA AISLADA  
DE *SENECIO GRAVEOLENS* Y SU  
DERIVADO SINTETIZADO POR  
MICROONDAS, 4'-HIDROXI-3'-(3-  
METIL-2-BUTENIL)CHALCONA**

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Full original article

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**Keywords:** NMR spectra, Spartan 19 software, Quantum chemistry, Chemical shifts.

**Palabras clave:** RMN espectros, Software Spartan 19, Química cuántica, Desplazamientos químicos.

**ABSTRACT**

The spectral computer-assisted study of <sup>1</sup>H and <sup>13</sup>C NMR chemical shifts ( $\delta$ ), and some other molecular properties of 4-hydroxy-3-(3-methyl-2-butenyl)acetophenone **1** and 4'-hydroxy-3'-(3-methyl-2-butenyl)chalcone **2** was carried out by using the density functional theory. Compound **1** was isolated from *Senecio graveolens* and its synthetic derivative **2** obtained by microwave irradiation of **1** with benzaldehyde, as previously published by the authors. The calculations yielded reliable results that are in good correlation with the corresponding experimental data. This is a good basis for collaboration between experimental and quantum chemists. Following current trends in NMR data description for small molecules, for its human- and computer-accessible 2D correlation data computer reading and storing, we summarized the 1D and 2D NMR experimental data of **1** and **2**.

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## PRIMARY REACTIONS OF HYDROGEN ABSTRACTION FROM TRANS-1,3-BUTADIENE BY USING RADICAL HYDROXYL

## REACCIONES PRIMARIAS DE ABSTRACCIÓN DE HIDRÓGENO DEL TRANS-1,3-BUTADIENO MEDIANTE RADICAL HIDROXILO

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**Keywords:** *Butadiene, hydrogen abstraction, conformers, DFT, theoretical study.*

**Palabras clave:** *Butadieno, extracción de hidrógeno, DFT, estudio teórico.*

### ABSTRACT

The abstraction channels of 1,3-butadiene ( $C_4H_6$ ) hydrogens by radical hydroxyl have been theoretically investigated, in their fundamental electronic state, in the gas phase and under normal conditions of pressure and temperature.

A study of the  $C_4H_6$  rotamers was performed, having found that the trans conformer is 12.3 kJ / mol more stable than the cis form. Three different  $C_4H_6$  hydrogen abstraction channels were determined, due to the presence of its three chemically non-equivalent protons. All molecular structures involved in each reactive channel were characterized, confirmed by their vibrational frequencies, intrinsic reaction coordinate (IRC) and transition vectors.

The density functional method (DFT) was used, with the hybrid functional B3LYP and Dunning base aug-cc-pVTZ, incorporated in the Gaussian 03 package. In all cases the energy was extrapolated to the base limit Complete (CBS) using an exponential method and applying zero point energy corrections (ZPE).

Negative activation energies are reported for the three reaction channels and the formation of post-reactive complexes.

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**MINERALOGICAL AND  
CRYSTALLO-CHEMICAL  
CHARACTERIZATION OF BOLIVIAN  
NATURAL ZEOLITES**

**CARACTERIZACIÓN  
MINERALÓGICA Y  
CRISTALOQUÍMICA DE ZEOLITAS  
NATURALES BOLIVIANAS**

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**Keywords:** *Clinoptilolite, Mordenite, Crystal-chemistry, Cation occupancy.*

**Palabras clave:** *Clinoptilolita, Mordenita, Química de cristales, Ocupación de cationes.*

**ABSTRACT**

Sampling, mineralogical characterization, and crystallo-chemical determination of two mineral samples of natural zeolites from the departments of Sucre and Oruro, Bolivia, have been carried out using powder X-ray diffraction techniques, scanning electron microscopy, dispersive energy spectroscopy and various refinement methods. The results indicate that the samples from Sucre have a high concentration in the potassium-type clinoptilolite phase zeolite. On the other hand, the mineral sample from Oruro turned out to be composed of a mordenite phase zeolitic phase with important montmorillonite clay contents and low quartz contents. Gravimetric separation and grain size techniques were used to isolate them from the zeolitic phase and perform crystallo-chemical characterization, reaching results of zeolite concentration of around 90%. The characterization results of these natural zeolites are of great interest for their potential applications in various fields.

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**VALIDATION OF THE X-RAY  
FLUORESCENCE (FRX-ED)  
ANALYTICAL METHOD FOR THE  
DETERMINATION OF METALS IN  
SOILS AT COLQUENCHA  
MUNICIPALITY**

**VALIDACIÓN DEL MÉTODO  
ANALÍTICO DE FLUORESCENCIA DE  
RAYOS X (FRX-ED) PARA LA  
DETERMINACIÓN DE METALES EN  
SUELOS DEL MUNICIPIO DE  
COLQUENCHA**

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**Keywords:** *Fluorescencia RX, Metales pesados, Suelos agrícolas, ISO 17025.*

**Palabras clave:** *X-R Fluorescence, Heavy metals, Agricultural soils, ISO 17025.*

**ABSTRACT**

The analytical method by the technique of X-ray Fluorescence with dispersive energy (FRX-ED) for the determination of the concentrations of Cu, Fe, Mn, Ni and Zn, has been validated with statistical tools in soil samples extracted from calicate soils of the Colquencha municipality. The FRX-ED technique does not require prior treatment in the preparation of standards, reference materials or soil samples, which are analyzed in the form of tablets. The quantification of the Cu, Fe, Mn, Ni and Zn metals is determined through the QXAS software and contrasted with the SOIL-7 certified reference material and the MAPEP-7 intercomparison material. Validated parameters for Cu, Fe, Mn, Ni and Zn compared to SOIL-7 and Ni and Zn compared to MAPEP-7 that include detection limit (LOD) and quantification (LOQ) are within the acceptance criteria. Reproducibility and repeatability have error values that are below 5% for Cu, Mn and Zn, while Fe showed values below 1%. The accuracy evaluated with the student t (one tail) does not present a significant difference for Cu, Mn and Zn, excepting Fe. The results obtained by FRX-ED showed us that the concentrations of the metals Cu, Fe, Mn and Zn in the soils are within the maximum permissible limits, according to the data reported in international studies, having established this, that the soils of the municipality of Colquencha are suitable for cultivation.

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