

Accepted Manuscript

Research paper

New NMR investigation of $[\text{RuF}_5\text{NO}]^{2-}$ anion.

L. Diana Castañeda Trujillo, Jorge L. Jios, Carlos A. Franca, Jorge A. Güida

PII: S0020-1693(17)31830-3
DOI: <https://doi.org/10.1016/j.ica.2018.03.010>
Reference: ICA 18155

To appear in: *Inorganica Chimica Acta*

Received Date: 30 November 2017
Revised Date: 8 February 2018
Accepted Date: 9 March 2018

Please cite this article as: L.D.C. Trujillo, J.L. Jios, C.A. Franca, J.A. Güida, New NMR investigation of $[\text{RuF}_5\text{NO}]^{2-}$ anion., *Inorganica Chimica Acta* (2018), doi: <https://doi.org/10.1016/j.ica.2018.03.010>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



New NMR investigation of $[\text{RuF}_5\text{NO}]^{2-}$ anion.

L. Diana Castañeda Trujillo¹, Jorge L. Jios², Carlos A. Franca¹ and Jorge A. Güida*^{1, 3, 4}

¹ CEQUINOR, Facultad de Ciencias Exactas, Universidad Nacional de La Plata, (CONICET-CCT La Plata), Boulevard 120 N° 1465, La Plata (1900), Argentina.

² UNIDAD PLAPIMU-LASEISIC (UNLP-CIC), Departamento de Química, Facultad de Ciencias Exactas, Universidad Nacional de La Plata, 47 esq. 115, 1900 La Plata, Argentina.

³ Departamento de Ciencias Básicas, Facultad de Ingeniería, Universidad Nacional de La Plata, La Plata, Argentina.

⁴ Departamento de Ciencias Básicas, Universidad Nacional de Luján, Luján, Argentina.

Corresponding author: guida@quimica.unlp.edu.ar

Abstract

The ^{15}N shift value is the main distinctive parameter to distinguish linear than angular MNO in transition metal nitrosyls by NMR spectroscopy. To get insight into the spectroscopic properties of a simple ruthenium-nitrosyl complex, the $[\text{RuF}_5\text{NO}]^{2-}$ anion, was reinvestigated. Their ^{15}N and ^{19}F nuclear magnetic resonance spectra (NMR) were analyzed and compared with the behavior observed for the geometrically related (C_{4v}) $[\text{Fe}(\text{CN})_5\text{NO}]^{2-}$ (^{15}N and ^{13}C enriched) ion. The different *splitting and coupling constants observed* in both systems were attributed to the small change in angles and atomic distances. These results highlight the sensitivity of this spectroscopy to detect small geometrical distortion in transition metal complexes. DFT calculations predicted for both systems, shifts and coupling constant values in good agreement with the experimental results. The DFT calculations predicted for both systems chemical shifts and coupling constants in good agreement with the experimental values.

Key words ^{19}F , ^{15}N NMR, $[\text{RuF}_5\text{NO}]^{2-}$, DFT Calculations, ruthenium nitrosyl

Download English Version:

<https://daneshyari.com/en/article/7750521>

Download Persian Version:

<https://daneshyari.com/article/7750521>

[Daneshyari.com](https://daneshyari.com)