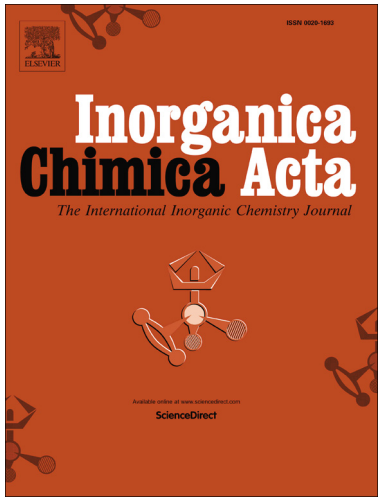

Research paper

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New NMR investigation of $[RuF_5NO]^{2-}$ anion.

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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 $[RuF_5NO]^{2-}$ 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}) $[Fe(CN)_5NO]^{2-}$ (^{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, $[RuF_5NO]^{2-}$, DFT Calculations, ruthenium nitrosyl