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Theoretical and Experimental Vibrational Characterization of Biologically Active Nd(III) Complex

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Abstract: The neodymium(III) complex of orotic acid (HOA) was synthesized and its structure determined by means of analytical and spectral analyses. Detailed vibrational analysis of HOA, sodium salt of HOA, and Nd(III)–OA systems based on both the calculated and experimental spectra confirmed the suggested metal–ligand binding mode. Significant differences in the IR and Raman spectra of the complex were observed as compared to the spectra of the ligand. The calculated vibrational wavenumbers, including IR intensities and Raman scattering activities, for the ligand and its Nd(III) complex were in good agreement with the experimental data. The vibrational analysis performed for the studied species, orotic acid, sodium salt of orotic acid, and its Nd(III) complex helped to explain the vibrational behaviour of the ligand's vibrational modes, sensitive to interaction with Nd(III). In this paper we also report preliminary results about the cytotoxicity of the investigated compounds. The cytotoxic effects of the ligand and its Nd(III) complex were determined using the MTT method on different tumour cell lines. The screening performed revealed that the tested compounds exerted cytotoxic activity upon the evaluated cell lines.

Keywords: Nd(III) complex; orotic acid; IR; Raman; DFT; cytotoxicity

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1. Introduction

Lanthanide complexes are of great interest because of their various potential applications. Due to the unique nature of lanthanide ions, such as their large radius and high coordination number, the assembly of lanthanide complexes possessing novel structures and special properties offers great challenges and opportunities in terms of controlling their shapes and dimensions. The selection of an appropriate organic ligand along with different synthetic methods is a key step in the construction of lanthanide complexes with the desired features. Ligands containing a combination of nitrogen and oxygen donor atoms demonstrate flexible coordination modes during the formation of coordination frameworks, which is why the studied lanthanide(III) complexes of biologically active derivatives of orotic acid deserve to be examined.

The coordination chemistry of orotic acid (2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylic acid, vitamin B_{13}, or HOA) and its sodium salt (NaOA) (see Figure 1) has been an area of great interest [1–5], ranging from bioinorganic to pharmaceutical and materials chemistry.

Metal orotates are widely applied in medicine [6], with platinum, palladium, and nickel orotate complexes being screened as potential therapeutic agents for cancer [7]. More recent interest has focused on the proposed biological function of orotic acid and its corresponding anions in binding biogenic metal ions, which is held responsible for the successful application of orotate complexes in curing syndromes associated with a