

Accepted Manuscript

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PII: S0022-2860(17)31351-0

DOI: [10.1016/j.molstruc.2017.10.020](https://doi.org/10.1016/j.molstruc.2017.10.020)

Reference: MOLSTR 24391

To appear in: *Journal of Molecular Structure*

Received Date: 15 May 2017

Revised Date: 25 August 2017

Accepted Date: 6 October 2017

Please cite this article as: A.Z. El-Sonbati, M.A. Diab, S. Morgan, H.A. Seyam, Supramolecular structures for determination and identification of the bond lengths in novel uranyl complexes from their infrared spectra, *Journal of Molecular Structure* (2017), doi: 10.1016/j.molstruc.2017.10.020.

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Supramolecular structures for determination and identification of the bond lengths in novel uranyl complexes from their infrared spectra

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Abstract

Novel dioxouranium(VI) heterochelates with neutral bidentate compounds (L_n) have been synthesized. The ligands and the heterochelates $[UO_2(L_n)_2(O_2NO)_2]$ were confirmed and characterized by elemental analysis, 1H NMR, UV.-Vis, IR, mass spectroscopy, X-ray diffraction and thermogravimetric analysis (TGA). IR spectral data suggest that the molecules of the Schiff base are coordinated to the central uranium atom (ON donor). The nitrate groups are coordinated as bidentate ligands. The thermodynamic parameters were calculated using Coats–Redfern and Horowitz–Metzger methods. The ligands (L_n) and their complexes (1-3) showed the ν_3 frequency of UO_2^{2+} has been shown to be an excellent molecular probe for studying the coordinating power of the ligands. The values of ν_3 of the prepared complexes containing UO_2^{2+} were successfully used to calculate the force constant, F_{UO} ($1n\ 10^8 N/\text{\AA}$) and the bond length R_{UO} (\AA) of the U-O bond. A strategy based upon both theoretical and experimental investigations has been adopted. The theoretical aspects are described in terms of the well-known theory of 5d-4f transitions. Wilson's, matrix method, Badger's formula, and Jones and El-Sonbati equations were used to calculate the U-O bond distances from the values of the stretching and interaction force constants. The most probable correlation between U-O force constant to U-O bond distance were satisfactorily discussed in term of Badger's rule and the equations suggested by Jones and El-Sonbati. The effect of Hammett's constant is also discussed.

Keywords: UO_2^{2+} complexes; X-ray diffraction; Badger's formula; Jones and El-Sonbati equations; DNA binding interaction.

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1. Introduction

Recently, there has been increasing interest in syntheses of heterocyclic compounds that have biological and commercial importance [1]. Antipyrine compounds play an important role in modern organic synthesis, not only because they

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