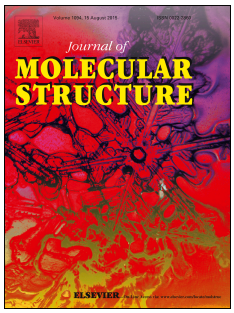
Accepted Manuscript



Synthesis, spectroscopy, crystal structure and DFT studies of cobalt(III) complexes featuring dimethylglyoximate and aniline or *p*-bromoaniline ligands

O. Berradj, A. Adkhis, H. Bougherra, G. Bruno, F. Michaud

PII: S0022-2860(16)31230-3

DOI: 10.1016/j.molstruc.2016.11.058

Reference: MOLSTR 23159

To appear in: *Journal of Molecular Structure*

Received Date: 8 September 2016

Revised Date: 19 October 2016

Accepted Date: 20 November 2016

Please cite this article as: O. Berradj, A. Adkhis, H. Bougherra, G. Bruno, F. Michaud, Synthesis, spectroscopy, crystal structure and DFT studies of cobalt(III) complexes featuring dimethylglyoximate and aniline or *p*-bromoaniline ligands, *Journal of Molecular Structure* (2016), doi: 10.1016/j.molstruc.2016.11.058.

Synthesis, spectroscopy, crystal structure and DFT studies of cobalt(III) complexes featuring dimethylglyoximate and aniline or *p*-bromoaniline ligands

O. BERRADJ[1], A. ADKHIS[1*], H. BOUGHERRA[1], G. BRUNO[2], F. MICHAUD[3]

[1]*Laboratoire de physique et chimie des matériaux, Université M. Mammeri, Tizi Ouzou Algérie.*

[2]*Département des Sciences Chimiques Viale F. Stagno D'Alcontres, 31 98166 Messina (Vill. S. Agata), Italy*

[3] *Université de Brest, France*

Abstract

Two new cobalt(III) compounds $[Co(Hdmg)_2(Ani)_2]NO_3.2H_2O$ (**I**) and $[Co(Hdmg)_2(Ani\text{-}Br)_2]NO_3.H_2O$ (**II**), where Hdmg is the dimethylglyoximate monoanion, Ani is aniline and Ani-Br is p-bromoaniline, were synthesized and characterized using spectroscopic techniques including IR, UV-Visible, and X-ray diffraction. In the octahedral Co(III) complexes, the two dimethylglyoximato ions are coordinated to a cobalt atom in a planar configuration and are connected by intramolecular O-H…O hydrogen-bonding. The nitrogen atoms of the two aniline ligands occupy the apical sites. A Density Functional Theory approach has been successfully used for the investigation of the nature of solid state interactions and determination of the whole molecular packing. It was found that the computational data are in good agreement with the experimental results.

Keywords : dimethylglyoxime, cobalt complexes, IR and UV-visible studies, DFT calculations, crystal structure

1. Introduction

Cobaloxime complexes are of interest from both chemical and biological point of view [1]. Because of similarities in structures and chemical behaviours, they are considered as vitamin B_{12} model compounds [2,3]. During the last decades a few ionic mononuclear *trans*-octahedral Co(III) complexes with the formula $[Co(Hdmg)_2A_2]X$, where Hdmg is dimethylglyoximate monoanion, A a neutral organic ligand, and X a counter-anion (Cl^-, Br^-, I^-, NO_3^-, BF_4^-…), have been studied. In the octahedral coordination sphere of the central cobalt atom, four coordination sites in the equatorial positions are occupied by nitrogen atoms of two dimethylglyoximate monoanions, and the other two sites are occupied by atoms of monodentate neutral ligands [4,5]. In these *trans*-octahedral complexes, the oxygen atoms of two dimethylglyoximates are connected by intramolecular O-H…O hydrogen bonding leading to a stable pseudo-macrocyclic system. Previous investigations on aniline-