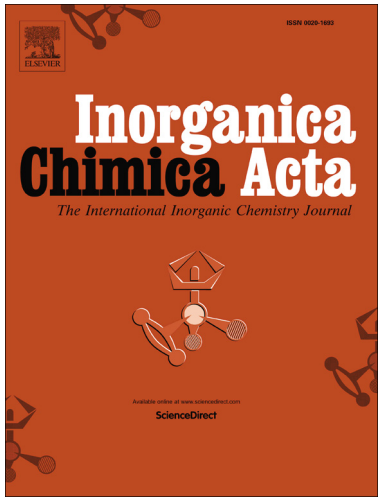

Research paper

Complexes of Zn(II) and Cd(II) with 2-acetylpyridine-aminoguanidine – syntheses, structures and DFT calculations

Mirjana M. Radanović, Marko V. Rodić, Ljiljana S. Vojinović-Ješić, Stevan Armaković, Sanja J. Armaković, Vukadin M. Leovac

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Complexes of Zn(II) and Cd(II) with 2-acetylpyridine-aminoguanidine – syntheses, structures and DFT calculations

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Abstract
The reaction of 2-acetylpyridine-aminoguanidine dihydrogenchloride (L·2HCl) with Zn(II) and Cd(II) ions, in the presence of deprotonating agent (LiOAc) and without it, yielded two types of complexes, *i.e.* neutral $[Zn(L)Cl_2]\cdot H_2O$ and $[Cd(L)Cl_2]$ and anionic complexes $[H_2L][ZnCl_4]\cdot H_2O$ and $[H_2L]_2[Cd_2Cl_8(H_2O)_2]$, respectively. In the latter two compounds, 2-acetylpyridine-aminoguanidine does not coordinate the metal and has the role of counter ion. Complexes are characterized by elemental analysis, IR spectroscopy, conductometric measurements and single crystal X-ray analysis. In the neutral complexes, chelating ligand is coordinated in an expected tridentate N_3 coordination mode *via* pyridine, azomethine, and nitrogen atom of the imino group of the aminoguanidine residue. Density functional theory (DFT) calculations have been used in order to investigate local reactivity properties of the newly synthesized complexes. Charge transfer within molecule as a consequence of light absorption has been investigated employing the time dependent DFT calculations and formalism of natural transition orbitals. DFT calculations have been also used in order to evaluate fundamental optoelectronic properties.

***Keywords*:** Zinc(II), cadmium(II), complexes; 2-acetylpyridine-aminoguanidine; crystal structure; DFT; TD-DFT; optoelectronics

1. Introduction

In the last decade, due to the resistance that microorganisms started to show towards the drugs used, significant efforts have been made with the aim to synthesize new antimicrobial drugs with enhanced activity and safer application [1]. Among those, Schiff bases, in particular those containing N donors, and their metal complexes stand out [2]. Besides, these compounds have widespread application as OLED materials, catalysts, pesticides, etc. [1].

Schiff bases of aminoguanidine and their metal complexes represent a well-known class of compounds due to the possibility of innumerous pharmacological applications (antiviral, antimalarial, anticoagulant, antileukemic, cardiotonic, anticancer agents, etc.) [3]. However, besides their mentioned biological and medicinal importance these compounds are very interesting for the use in organic synthesis, but also as catalysts and superbases [4].

Some time ago Schiff bases of 2-acetylpyridine and their metal complexes achieved the attention due to their substantial in vitro activity against various human tumor lines [5,6]. Besides, recent results show that transition, as well as non-transition metal complexes with 2-acetylpyridine-derived Schiff bases, have significant cytotoxic activity against some solid tumor and leukemia cells [7]. On the other hand, group 12 metal complexes are nowadays very interesting, because they usually show high photoluminescence and have potential applications as optoelectronic devices [8].

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