Synthesis, structural and spectroscopic studies of two new Cd(II)-methyl lactate complexes in aqueous solution

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Abstract
Cadmium is one of the most important environmental pollutants. The involvement of Cd(II) in toxic manifestations and pathological aberrations in lower and higher organisms entails interactions with low and high molecular mass biological targets. Methyl-lactate is an \( \alpha \)-hydroxy substituted carboxylic compound with important medical and pharmaceutical applications. It is also an excellent chelator in several interaction systems with metal ions, resulting in the formation of several complexes. To understand the relevant chemistry in aqueous media as well as the biological consequences of Cd(II) toxicity, we have launched pH-dependent synthetic efforts targeting the structural speciation of the related binary Cd(II)-hydroxy carboxylate systems.

Keywords: cadmium, methyl-lactate, \( \alpha \)-hydroxy-isobutyric acid.

Introduction
As a toxic metal ion, Cd(II) is absorbed by the liver, ultimately finding its way to the kidney, the critical organ from the toxicity point of view.\(^1\) It is believed that Cd(II) accumulation in the human body over extended periods of time contributes to the toxic manifestation of the observed physiological aberrations in humans.

\( \alpha \)-Hydroxy-substituted carboxylic acid compounds have been used as inhibitors of harmful oxidation biochemical processes.\(^2\) Important research is also ongoing to develop new materials based on biodegradable polymers, derived from these compounds that can be used for reconstruction of biological tissues and organ transplantation.\(^3\) The presence of methyl-lactate in many biological systems as well as its interactive linkage with several metal ions, including Cd(II), has prompted us to study in depth the interactions of Cd(II) with methyl-lactate aqueous media.

Experimental
The synthesis of complexes 1 and 2 was achieved expediently by reacting cadmium nitrate and \( \alpha \)-hydroxy-isobutyric acid in water. Addition of aqueous sodium hydroxide in 1 and ammonium solution in 2 raised the pH of the solutions to appropriate values and concurrently provided the necessary counterions for the subsequently derived complexes. The resulting colorless solutions were treated with ethanol at 4 °C and afforded efficiently colorless crystalline materials. The overall stoichiometric reactions leading to complexes 1 and 2 are shown schematically below:

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The crystalline products were isolated and characterized analytically, spectroscopically and structurally by the following techniques: FTIR (Figure 1), X-Ray Crystallography, and $^{13}$C-MAS NMR (Figure 2).

**Figure 1.** FT-IR spectra of complexes 1 and 2.

**Figure 2.** $^{13}$C-MAS spectrum of complex 1.
**Conclusions**

In the course of the herein presented research, the ability of methyl lactate acid to promote complexation chemistry with Cd(II) was examined. Our studies were carried out in aqueous media and in a wide pH range. Addition of aqueous sodium hydroxide and ammonium solution, respectively, in appropriate amounts raised the pH and afforded formation the complexes 1 and 2. The products were isolated in a crystalline form and were characterized structurally and spectroscopically. The observed reactivity pointed to structural features borne by Cd(II)-methyl lactate species in aqueous media. The potential relevance of such low molecular mass species to biological events may ride on their physicochemical characteristics discovered in the course of this investigation.

Chemical reactivity experiments and biological studies to determine the toxicity of such compounds, which is one of the basic targets of our research, are currently ongoing.

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**References**