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The Mn(II) complex with 4-bromophenoxyacetic acid - X-ray absorption fine structure study

A. Wolska[1*], A. Drzewiecka-Antonik[1], P. Rejmak[1], M.T. Klepka[1] and W. Ferenc[2]

[1] *Institute of Physics, Polish Academy of Sciences, Al. Lotnikow 32/46, 02-668 Warsaw, Poland*
[2] *Faculty of Chemistry, Maria Curie-Skłodowska University, Plac Marii Curie-Skłodowskiej 2, PL-20031 Lublin, Poland*

*e-mail: wolska@ifpan.edu.pl

Manganese is one of the essential elements in the living organisms. In the human body, it is absorbed from food and water and is involved in many metabolic processes. In plants, manganese is taken from the soil and translocated to the sprouts. In soil, it can exist in eleven oxidation states: from -3 to +7, however, Mn(II) species are the most soluble and available ones. This divalent manganese, present in soil and plant tissues, interacts with anions as phenoxyacetate herbicides, forming metal-organic complexes. In order to get structural information about such compounds, we have synthesized analogous complexes in the laboratory conditions [1-3].

In this research, the Mn(II) complex with 4-bromophenoxyacetic acid was studied. To describe its molecular structure the X-ray absorption and X-ray diffraction techniques were applied. The XAFS measurements for the powdered complex were performed at ELETTRA synchrotron (Trieste, Italy). The X-ray diffraction intensities for the single crystal of the complex recrystallized from N,N-dimethylformamide (DMF) were collected at 120 K on SuperNova X-ray diffractometer using the mirror-monochromatized CuKα radiation [3].

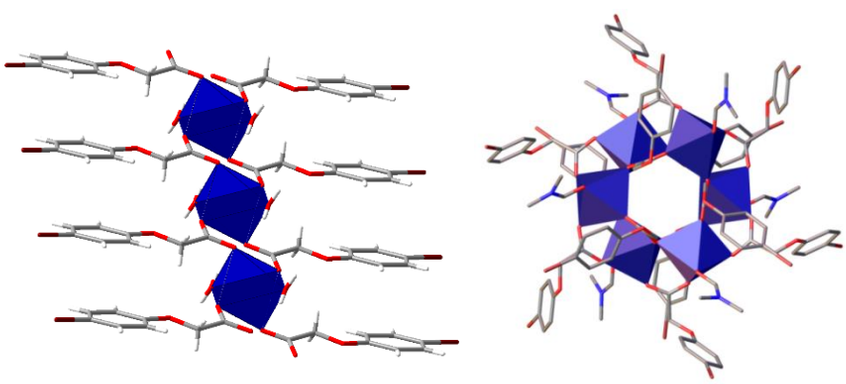

Figure 1. A polymeric structure of the complex from the XAFS analysis (left) vs. X-ray single crystal structure analysis (right).

The XAFS experiment was performed on the non-modified sample in a form of a microcrystalline powder. The analysis revealed that the complex forms a polymeric structure with 6 oxygen atoms bonded to Mn ion (see Fig.1). The oxygen atoms originate from 4 carboxylate groups and 2 water molecules. During recrystallization the coordination sphere of the metal center can be rearranged. In this case, the detachment of water molecules and attachment of the DMF molecules were observed. Due to the exchange of solvent molecules, the formation of hexanuclear manganese(II) carboxylate coordination clusters with a hydrophobic exterior was observed in the crystal.

References

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