<b>ESRF</b>	<b>Experiment title:</b> <i>SORPTION OF Cd-CYSTEINE COMPLEXES BY KAOLINITE AND SMECTITE</i>	Experiment number: 08 01 623
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## **Report:**

The purpose of the present study is to examine the influence of cysteine  $(H_2NCH(CH_2SH)CO_2H)$  on Cd(II) interaction with well- and poorly-ordered kaolinite and smectites characterized by different layer-charge location (montmorillonite and vermiculite) in order to predict the mobility of Cd(II) and S-containing amino acids in a clay minerals rich environment.

The experimental method can be ideally divided into the following steps: *i*) adsorption of Cd and cysteine by smectites; *ii*) determination of Cd adsorbed species and of their reaction products; *iii*) application of Extended X-ray Absorption Fine Structure (EXAFS) analysis to gain insight into the structure of adsorbed Cd species.



Cd K-edge EXAFS data for Cd treated montmorillonite. Inverse Fourier-filtered scattering curve spectra. Solid lines indicate experimental data and circles indicate the fit curve obtained using CdO (monteponite) as reference compound.

The following are the principal conclusions of the study. i) The structural order substantially modifies the adsorption kinetic of the Cd-cysteine complex both on kaolinite and smectite samples. ii) EXAFS spectra obtained on both Cd-exchanged smectites agree with a first-shell coordination number of six oxygen atoms surrounding Cd at a distance of about 2.2 Å, with neighboring Cd atoms at about 3.2 Å. These Cd-Cd distances suggest the formation of dimers adsorbed on the mineral edge sites; iii) EXAFS spectra of Cd-

montmorillonite and Cd-vermiculite complexed with cysteine exhibit several individual contributions from Cd centers; the first coordination shell in Cd-cysteine-montmorillonite is characterized by a strong contribution from S atoms and data refinement suggest a Cd-S distance of 2.43 Å; an analogues situation can be found in Cd-cysteine-vermiculite with Cd-S distances of 2.49 Å. The experimental spectra well fit with CdS (hawleyte) calculated spectra even if a good agreement can be observed also considering Bis(S-methyl-L-cysteinato)cadmium(II) model compound, an organometallic molecules in which Cd atom is tetrahedrally coordinated by four sulfur atoms.



Cd K-edge EXAFS data for Cd and cysteine treated montmorillonite. Inverse Fourier-filtered scattering curve spectra. Solid lines indicate experimental data and circles indicate the fit curve obtained using CdS (hawleite) as reference compound.

For any further information and details please see:

Daniele Malferrari (2003) "Studio di complessi organo-metallici in fillosilicati" PhD Thesis, Dipartimento di Scienze della Terra, Università degli Studi di Modena e Reggio Emilia, L.go S.Eufemia 19, I-41100 Modena (Italy). Dottorato di ricerca in Mineralogia, Petrologia e Cristallografia XV Ciclo – I Ciclo Nuova Serie. Further information will be provided through an article which was submitted for publication.