

**Experiment title:**

Hydrogen induced changes in electronic structure of CeTX compounds (T= Co, Ru, Mn and X= Si, Ge)

Experiment number:
CH2367**Beamline:**

BM30b

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Shifts:**Local contact(s):**

H. Palancher

*Received at ESRF:***Names and affiliations of applicants (* indicates experimentalists):**

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*Present affiliation : Institut Néel CNRS / Univ. J. Fourier***Report:**

Due to problems on the experiment of the previous users, our experiment has been allocated 1 day less than scheduled.

X-ray absorption spectroscopy (XAS) measurements were carried out at the L_3 edge of cerium (5.7 keV) both on $CeCo_{12-x}Fe_xB$ compounds where $x = 0, 2, 4$ and 8 and on hydrogenated and non-hydrogenated CeTX compounds where T=Co, Ru, Mn and X= Si, Ge.

I. $CeCo_{12-x}Fe_xB$ compounds

In this kind of R-T-B phases (R for a rare earth element and T for Co or Fe), the magnetic properties of the 3d transition metal atoms are strongly sensitive to their local atomic environment. The presence of boron as near-neighbour can for instance lead to the reduction of the magnetic moment through an hybridisation between orbitals of the metalloid and of the 3d metal [1-3]. Recently it has been shown that the rare earth element could also exhibit peculiar behaviour and more generally that the electronic state of R element has a strong influence on the magnetism of the 3d sublattice. This effect was highlighted with thorium [4, 5] that have a different oxidation degree than the common lanthanoids.

Concerning cerium, several electronic states can be obtained in intermetallic compounds. They can be discriminated from the position and the shape of the absorption spectra at an L-edge.

We measured the Ce absorption edge in transmission and fluorescence mode with rather long counting time because of the poor quality of the data, especially in transmission mode. This problem arises from the chemical composition of our sample where some elements are giving rise to fluorescence. Due to time constrains, the EXAFS signals were not measured and we concentrated on the XANES signals. Some of the measurements are presented in Fig. 1.

It is clear that the absorption spectrum is typical of intermediate valence state for all the studied $\text{CeCo}_{12-x}\text{Fe}_x\text{B}$ compounds. Nevertheless the Fe for Co substitution induces a significant evolution of the Ce valence state from 3.15 to 3.19. We indeed determined the contributions of both $4f^0$ and $4f^1$ electronic states in measured absorption spectra. To achieve this aim we fitted the spectra using the method described by J. Röhler [6]. One example of fitted curve is presented in Fig. 2 and the evolution of the valence state is presented in Fig. 3.

This study is a part of the thesis of M. H. Mayot [7] to be defended in 2007.

II. CeTX and corresponding CeTXH compounds

The hydrogen-induced changes in Ce electronic structure of this compounds has been investigated. We measured the Ce absorption edge in transmission and fluorescence mode once more with rather long counting time.

Whereas in most compounds H induces an evolution of the Ce valence state toward a more trivalent state, this evolution is found to be very sensitive to the nature of the T and X elements. Our measurements clearly show the expected effect of H on the valence of Ce (Fig. 4). The same fitting procedure than above will now be undertaken in order to quantify this evolution as regard to T and X elements.

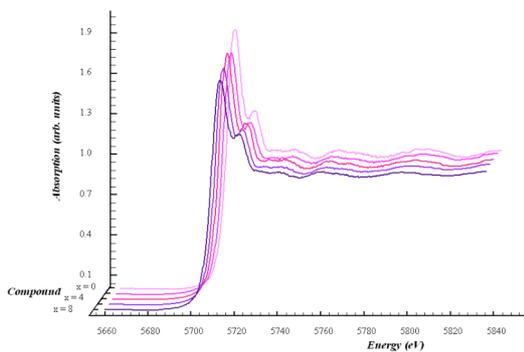


Fig. 1 : Absorption spectra in fluorescence mode of $\text{CeCo}_{1-x}\text{Fe}_x\text{B}$ compounds measured with an incoming beam around the Ce L_{III} edge.

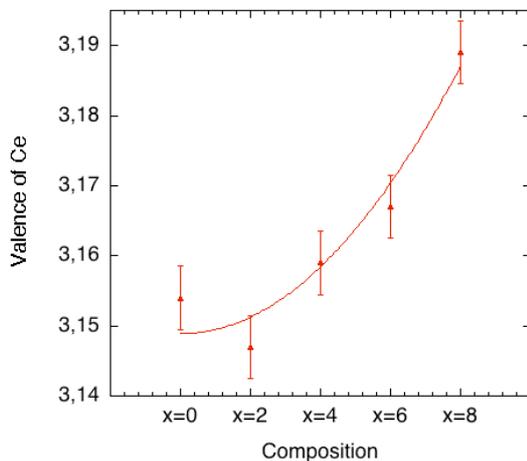


Fig. 3 : Fitted valence of cerium in the $\text{CeCo}_{12-x}\text{Fe}_x\text{B}_6$ compounds. Continuous line is a guide to the eyes.

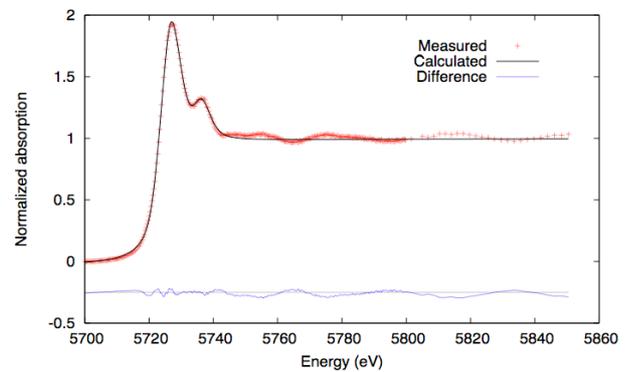


Fig. 2 : Best fit of the measurement on the $\text{CeCo}_{12}\text{B}_6$ compound.

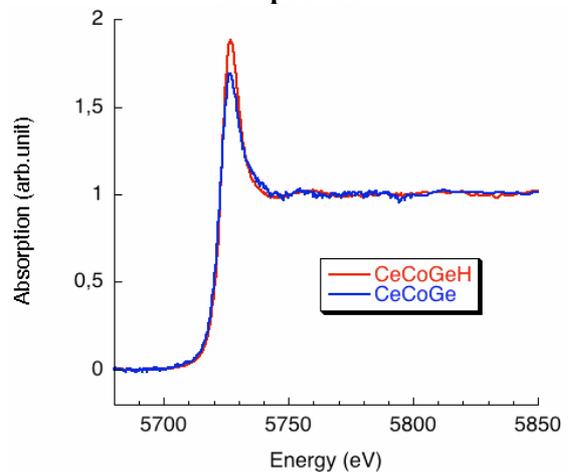


Fig. 4 : Absorption spectra of CeCoGe and CeCoGeH compounds measured with an incoming beam around the Ce L_{III} edge.

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