EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

ESRF

Experiment Report Form

The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF.

Once completed, the report should be submitted electronically to the User Office via the User Portal:

https://wwws.esrf.fr/misapps/SMISWebClient/protected/welcome.do

Reports supporting requests for additional beam time

Reports can be submitted independently of new proposals – it is necessary simply to indicate the number of the report(s) supporting a new proposal on the proposal form.

The Review Committees reserve the right to reject new proposals from groups who have not reported on the use of beam time allocated previously.

Reports on experiments relating to long term projects

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

Published papers

All users must give proper credit to ESRF staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to the Joint ESRF/ ILL library the complete reference and the abstract of all papers appearing in print, and resulting from the use of the ESRF.

Should you wish to make more general comments on the experiment, please note them on the User Evaluation Form, and send both the Report and the Evaluation Form to the User Office.

Deadlines for submission of Experimental Reports

- 1st March for experiments carried out up until June of the previous year;
- 1st September for experiments carried out up until January of the same year.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report, in English.
- include the reference number of the proposal to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.

ESRF	**Experiment title:** RIXS, XES and HERFD-studies on the d-electron structure and ligand bonding of transition metal carbonyl clusters as model systems for heterogeneous and homogeneous catalysts	**Experiment number**: CH-3219
Beamline: ID26	**Date of experiment**: from: 08/09/2010 to: 15/09/2010	**Date of report**: 28/02/2013
Shifts: 18	**Local contact(s)**: Dr. Kristina Kvashnina	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

*Matthias Bauer, FB Chemie, TU Kaiserslautern, Erwin-Schrödinger-Str. 54, 67663 Kaiserslautern

Report:

A paper about the chemical sensitivity of HERFD-XANES towards substituent effects in Ferrocene complexes has been published under:

A. J. Atkins, Ch. R. Jacob, M. Bauer, Chem. Eur. J. 18, 7021 (2012)

Summary of the communication (no abstract available):

X-ray spectroscopy at the metal K-edge is an important tool for understanding catalytic processes and provides insight into the geometric and electronic structure of transition metal complexes. In particular, X-ray emission-based methods such as high-energy resolution fluorescence detection (HERFD) X-ray absorption near-edge spectroscopy (XANES) hold the promise of providing increased chemical sensitivity compared to conventional X-ray absorption spectroscopy. Here, we explore the ability of HERFD-XANES spectroscopy to distinguish substitutions beyond the directly coordinated atoms for the example of ferrocene and selected ferrocene derivatives. The experimental spectra are assigned and interpreted through the use of density functional theory (DFT) calculations. We find that the pre-edge peaks in the HERFD-XANES spectra are affected by substituents at the cyclopentadienyl ring containing π-bonds.