

## Experiment Report Form

**The double page inside this form is to be filled in for each experiment at the Rossendorf Beamline (ROBL).** This double-page report will be reduced to a one page, A4 format, to be published in the Bi-Annual Report of the beamline. The report may also be published on the Web-pages of the HZDR. If necessary, you may ask for an appropriate delay between report submission and publication.

Should you wish to make more general comments on the experiment, enclose these on a separate sheet, and send both the Report and comments to the ROBL team.

### Published papers

All users must give proper credit to ROBL staff members and the ESRF facilities used for achieving the results being published. Further, users are obliged to send to ROBL the complete reference and abstract of papers published in peer-reviewed media.



### Deadlines for submission of Experimental Report

Reports shall be submitted not later than 6 month after the experiment.

### 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 / experiment 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.
- bear in mind that the double-page report will be reduced to 71% of its original size, A4 format. A type-face such as "Times" or "Arial" , 14 points, with a 1.5 line spacing between lines for the text produces a report which can be read easily.

Note that requests for further beam time must always be accompanied by a report on previous measurements.

  ROBL-CRG	<b>Experiment title:</b> Round Robin Test for interlaboratory comparison of EXAFS data	<b>Experiment number:</b> <b>20-01-740</b>
<b>Beamline:</b> BM 20	<b>Date of experiment:</b> from: 12-Mar-14 to 14-Mar-14  24-Sep-14 to 26-Sep-14	<b>Date of report:</b> 07-March-17
<b>Shifts:</b> 11	<b>Local contact(s):</b> André Rossberg	<i>Received at ROBL:</i>
<b>Names and affiliations of applicants (* indicates experimentalists):</b>  André Rossberg <sup>1*</sup> , Jörg Rothe <sup>2</sup> , Christophe Den Auwer <sup>3</sup> , Katharina Mueller <sup>1</sup> , Robin Steudtner <sup>1</sup> , Andreas C. Scheinost <sup>1</sup>  <sup>1</sup> Helmholtz-Zentrum Dresden-Rossendorf, Institute of Resource Ecology, Dresden, Germany <sup>2</sup> Karlsruher Institut für Technologie, Institut für Nukleare Entsorgung, Karlsruhe, Germany <sup>3</sup> University of Nice Sophia Antipolis, Nice Chemistry Institute, Nice, France		

## Report

Within the framework of the workshop “Advanced Techniques in Actinide Spectroscopy 2014” (ATAS 2014) a inter-laboratory Round Robin Test (RRT) was aimed for comparison of molecular information obtained from several spectroscopic (TRLFS, vibrational spectroscopy, EXAFS, NMR, ESI-MS) and theoretical methods. Information about the reproducibility of XAS raw data and the precision in the calculated EXAFS structural parameter was investigated and compared. Three EXAFS beamlines participated in the RRT: ROBL (ESRF), INE-Beamline(BL) (Anka), MARS-BL (Soleil).

## Results

U-L<sub>III</sub> edge EXAFS spectra were measured at room temperature in transmission mode for four aqueous solutions with 0.025 M U(VI) and 0.95 M acetic acid, at pH 1.0, 2.0, 2.5 and 3.5.

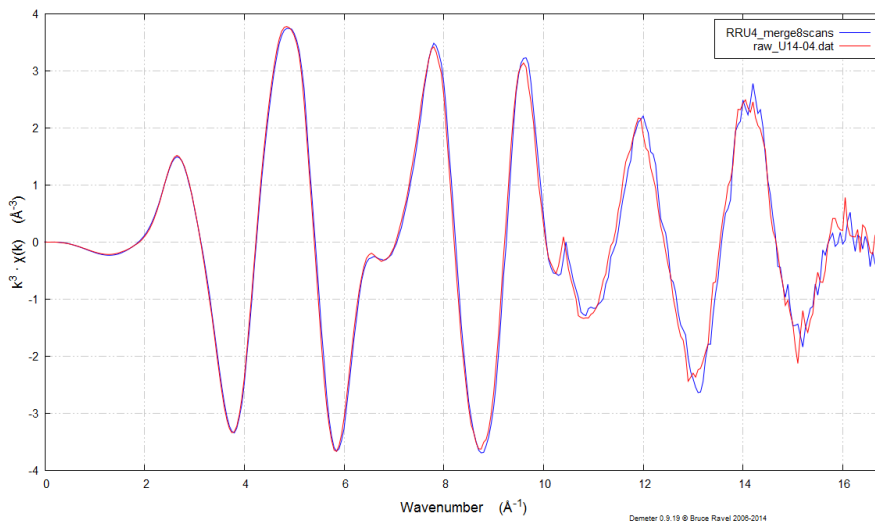


Figure 1: EXAFS spectra measured for the sample at pH 3.5 at ROBL (red) and the INE-BL (blue).

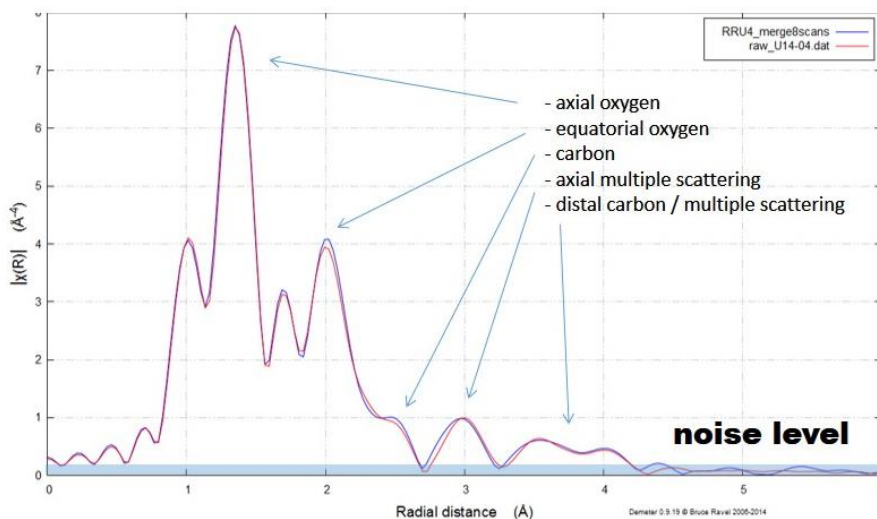


Figure 2: Fourier-transforms of the EXAFS spectra shown in Fig. 1 with experimental error (blue bar). Determined uranium interactions and scattering contributions.

The data quality, i.e. the experimental error, is for all four samples, measured at ROBL and at the INE-BL, equivalent. As an example Fig. 1 shows the comparison of the EXAFS spectra of the sample at pH 3.5 measured at the two BL's, while in Fig. 2 the corresponding Fourier-transforms (FT) are shown together with the experimental error. Both BL's identified the same structural features as shown for the sample at pH 3.5 (Fig. 2), but also for the other samples. The spectra were shell fitted, while the received structural parameters are unambiguously confirmed by all three teams better than within the typical EXAFS error margins [1]. Note that at the MARS-BL only the sample at pH 1 was measured. Deviations occurred only and necessarily, if for the shell fit of the spectra different shell fit models were taken.

#### References:

[1] Li, G. G., Bridges, F. & Booth, C. H. (1995). Physical Review B 52, 6332-6348.