	Experiment title: Study of the crystal field strength in $M_xU_yO_z$ compounds by resonant inelastic X-ray scattering	**Experiment number**: CH-6255
Beamline: BM20	**Date of experiment**: from: 5.04.2022 to: 11.04.2022	**Date of report**: 13.09.2022
Shifts: 18	**Local contact(s)**: Elena Bazarkina & Kristina Kvashnina	*Received at ESRF:*

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Report:

The crystal field strength in KUO_3, $NaUO_3$ and $RbUO_3$ was investigated by means of high-energy-resolution fluorescence detected (HERFD) X-ray absorption spectroscopy (XAS) at the U L_3-edge.
We compared the substantial gain in resolution achieved by collecting the $L\beta_5$ emission line with the ROBL emission spectrometer coupled to the Si(311) monochromator, compared to the $L\alpha_1$ emission line collected with the Si(111) monochromator. The obtained spectra are shown in Figure 1.

Thanks to the gain in resolution, we have access to a very detailed uranium electronic structure as a function of the U surrounding geometry, varying from an almost perfect oxygen octahedra in KUO_3 to a distorted one in $NaUO_3$, and longer U-O distances in $RbUO_3$. Experimental spectra are now being interpreted using state of the art Density Functional Theory (DFT) calculations (FDMNES code). As shown in Figure 2, those calculations reproduce well the expeirmental features and they will provide a complete assessment on the uranium electronic structure and its behavior as a function of the geometrical changes in oxygen octahedra surrounding U, as previously demonstrated for KUO_3 in ref. [1]. For example, a direct evaluation of the crystal field was performed, providing a key parameter for accurate and predictive theoretical models in 5f chemistry.

In addition to the direct HERFD-XANES collection, we measured also the RIXS map using the Lb5 emission line. Example results for KUO_3 are shown in Figure 3. The RIXS maps are supporting the HERFD-XANES results, by demosntrating that the observed sharp features are indeed related to XANES and not to RIXS effects.

Those results are now being compiled and their interpretation finalized as a first scientific paper [2], as part of Simon Orlat PhD thesis.

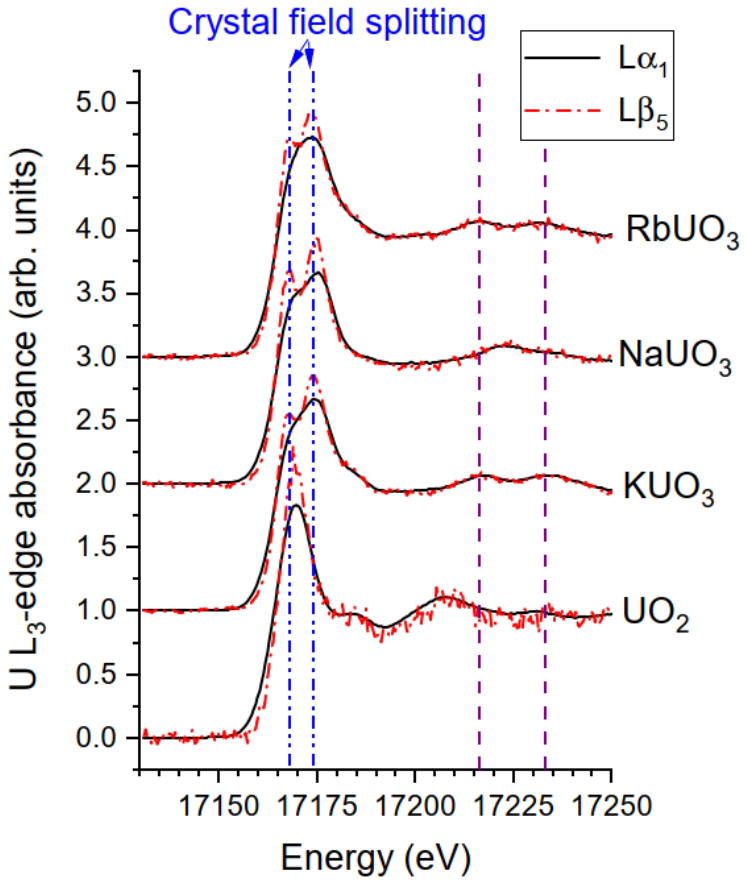

Figure 1. Comparison of Uranium L_3-edge HERFD-XANES collected at the La_1 and the Lb_5 emission lines for UO_2, KUO_3, $NaUO_3$ and $RbUO_3$ samples. The blue vertical dashed lines are showing the changes in crystal field splitting of the U-6d shells, while the violet dashed vertical lines are indicating the changes in the XANES features.

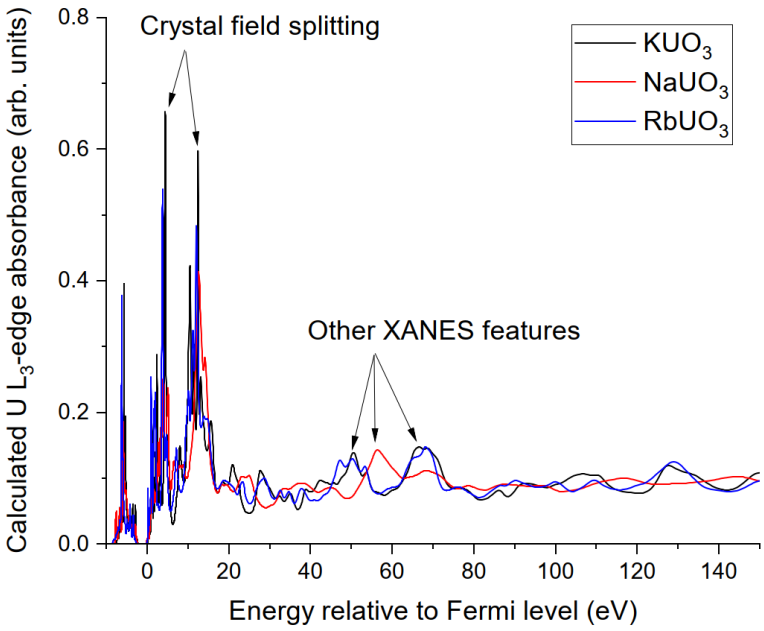

Figure 2. FDMNES calculated spectra for KUO_3, $NaUO_3$ and $RbUO_3$

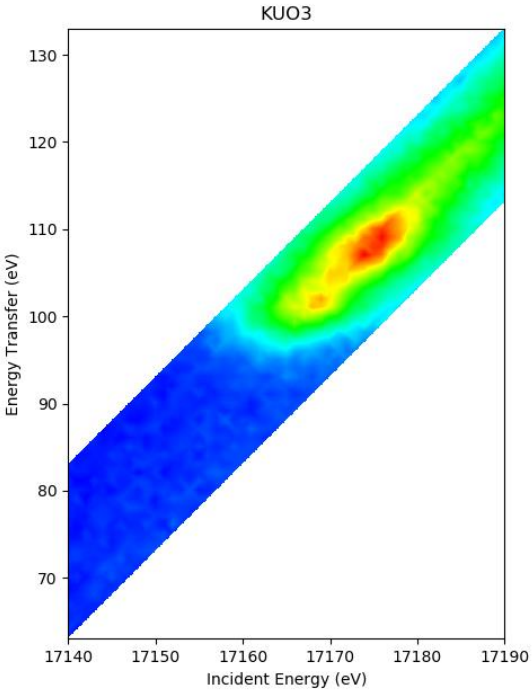

Figure 3. RIXS map of KUO_3 collected using the Lb5 emission line.

References:

[1] René Bes, Gregory Leinders and Kristina Kvashnina, Journal of synchrotron radiation 29 (2022).
[2] Simon Orlat, Igor Prozheev, Ine Arts, Gregory Leinders, Kristina Kvashnina and René Bes, Uranium 6d-states crystal field splitting in KUO3, NaUO3 and RbUO3. In preparation.