ROBL-CRG	**Experiment title:** **Structural and magnetic properties of ternary uranates at low temperatures**	**Experiment number**: **20-01-651**
Beamline: BM 20	**Date of experiment**: from: 03.10.05 to: 07.10.05	**Date of report**: 18.01.2007
Shifts: 12	**Local contact(s):** A. Scheinost	*Received at ROBL:* 18.01.2007
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Report:

Soldatov, A.V., Lamoen, D., Konstantinovic, M.J., Berghe, S.V.d., Scheinost, A.C., and Verwerft, M. *Local structure and oxidation state of uranium in some ternary oxides: X-ray absorption analysis* Journal of Solid State Chemistry **180** (2007) 53-60

We investigated the local atomic and electronic structures of two related systematic sets of ternary uranium oxides, $NaUO_3$ - KUO_3 - $RbUO_3$ and $BaUO_3$ - $Ba_2U_2O_7$ - $BaUO_4$, by measuring the X-ray absorption near edge structure (XANES). The results are compared with calculations based on self-consistent real space full multiple scattering analysis. We found a very good agreement between measured and calculated spectra, which indicates that the uranium ions are in pure U^{5+} oxidation state in these compounds. The low energy shoulder observed in the U L_3 edge XANES is an intrinsic feature of the uranium unoccupied 3d electronic state of the U^{5+} ions. Specific double shoulder features in the higher energy range of the U L_3 edge XANES can be interpreted as indicative of the pure cubic perovskite structure.

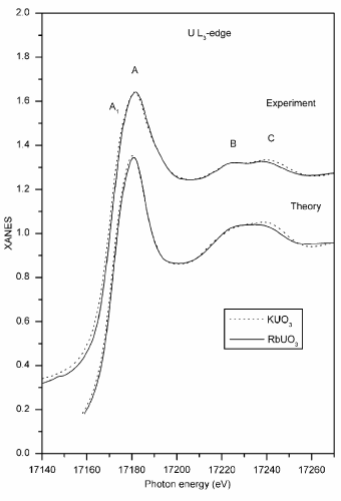

Fig. 1. Comparison of the experimental U L_3 edge XANES in KUO_3 and $RbUO_3$ with the theoretical spectra.

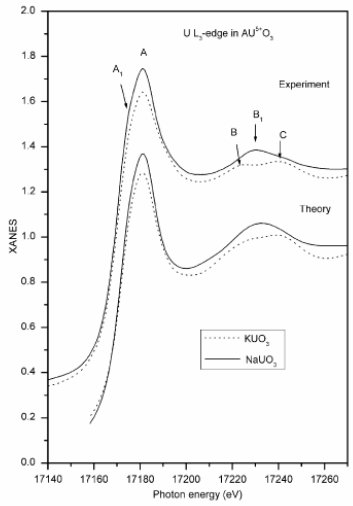

Fig. 2. Comparison of the experimental U L_3 edge XANES in KUO_3 and $NaUO_3$ with the theoretical spectra.

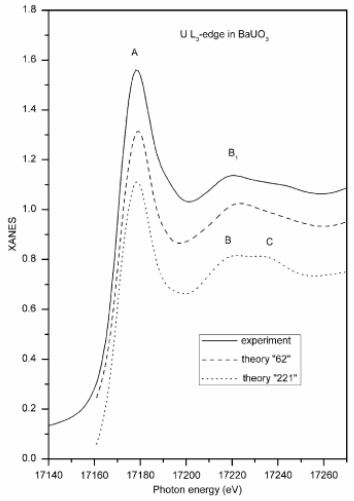

Fig. 3. Comparison of the experimental U L_3 edge XANES in $BaUO_3$ with the theoretical spectra. Calculated for two possible structural models (see text).

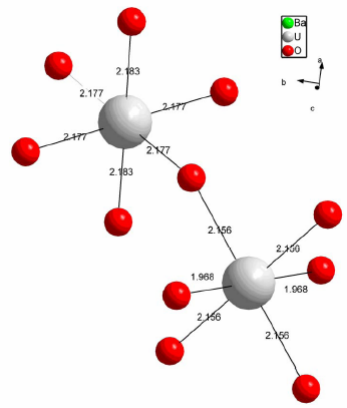

Fig. 4. Local structure around two nonequivalent uranium sites in $Ba_2U_2O_7$.

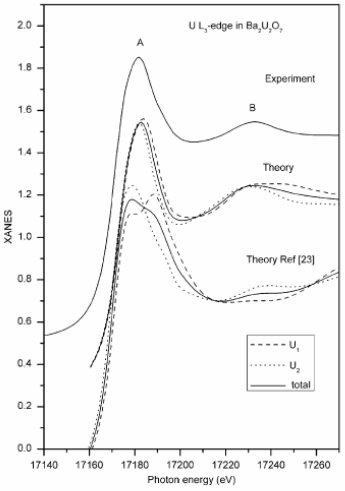

Fig. 5. Comparison of the experimental U L_3 edge XANES in $Ba_2U_2O_7$ with the theoretical spectra.

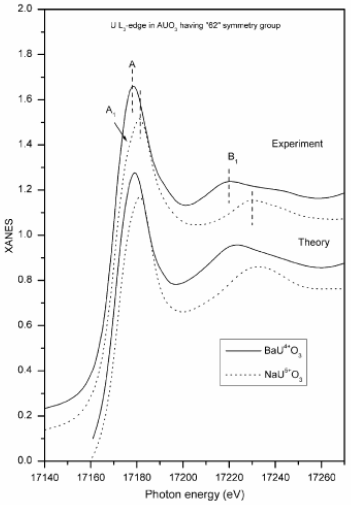

Fig. 6. Comparison of the experimental U L_3 edge XANES in $BaUO_3$ and $NaUO_3$ with the theoretical spectra.

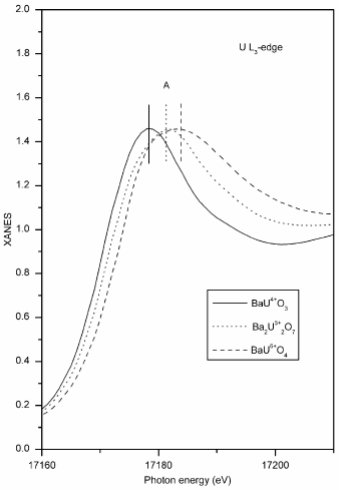

Fig. 7. Comparison of the renormalized (see text) experimental U L_3 edge XANES in $BaUO_3$, $Ba_2U_2O_7$ and $BaUO_4$.

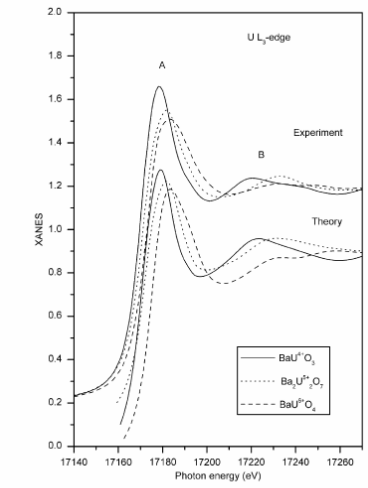

Fig. 8. Comparison of the experimental U L_3 edge XANES in $BaUO_3$, $BaUO_4$ and $Ba_2U_2O_7$ with the theoretical spectra.