



	Experiment title: Local structural correlations in heavy rare-earth zirconates $A_2Zr_2O_7$	Experiment number: HC-4856
Beamline: BM23	Date of experiment: from: 08/09/2022 to: 12/09/2022	Date of report: 20/09/2022 <i>Received at ESRF:</i>
Shifts: 12	Local contact(s): João Elias RODRIGUES	
Names and affiliations of applicants (* indicates experimentalists): RNDr. Milan Klicpera, Ph.D.* Dr. Ross H. Colman Mgr. Daniel Staško* Mgr. Kristina Vlášková, Ph.D.* Charles University, Faculty of Mathematics and Physics, Department of Condensed Matter Physics, Ke Karlovu 5, 121 16 Prague 2, Czech Republic		

Report:

The powder samples from the $A_2Zr_2O_7$ family, where A = rare-earth element, were investigated employing the BM23 beamline and EXAFS technique. During the span of 4 days (12 shifts), 10 different $A_2Zr_2O_7$ samples was investigated. The energy was tuned to reach the absorption edge of Zr (K-edge) and rare-earth element (L3-edge). That is, the two sets of data were measured for each composition. Zr foil and rare-earth oxides A_2O_3 were used as reference samples. EXAFS was measured at 10 K for all investigated samples. In addition, temperature development of EXAFS was measured on selected samples ($A = La, Gd, Er, Yb$). The total amount of data gathered exceeded our expectations. The data are of sufficient quality for presentation and publication.

The measured data were analyzed only partially. So far, one week after the experiment, we processed the data and started to fit them with models: pyrochlore structure-based model enabled good description of data measured on light rare-earth members. Heavy rare-earth members crystallize in defect-fluorite and/or rhombohedral structure. Their spectra are thus more challenging to be correctly fitted.

Data processing is still ongoing, with the hope of precise identification of local structure of investigated oxides. The data are planned for publication in the near future and will be invaluable in the interpretation of our bulk and other microscopic (pair-distribution-function) results.