



	Experiment title: Solving the puzzle of lineshape symmetries in La L _{4,5} absorption spectra	Experiment number: HE-3311
Beamline: ID16 (IXS)	Date of experiment: from: 21/4/2010 to: 27/4/2010	Date of report: 2/3/2015
Shifts: 18	Local contact(s): Simo Huotari	<i>Received at ESRF:</i>
Names and affiliations of applicants (* indicates experimentalists): Edlira Suljoti*1, Frank de Groot2, Simo Huotari*3 1 – Helmholtz Zentrum Berlin, Germany 2 – University of Utrecht, The Netherlands 3 – ESRF		

Report:

The results of this experiment have been approved for publication in New Journal of Physics (accepted 26/2/2015).

Title: High-resolution non-resonant x-ray Raman scattering study on rare earth phosphate nanoparticles

Authors: S. Huotari, E. Suljoti, C. J. Sahle, S. Rädels, G. Monaco, and F.M.F. de Groot

Abstract: We report high-resolution x-ray Raman scattering studies on high-order multipole spectra of rare-earth 4d - 4f excitations (the N_{4,5} absorption edge) in nanoparticles of phosphates LaPO₄, CePO₄, PrPO₄, and NdPO₄. We also present corresponding data of La 5p - 5d excitations (the O_{2,3} edge) in LaPO₄. The results are compared to those from calculations by atomic multiplet theory and for the dipole contribution to the La 4d - 4f transition from a calculation using time-dependent density functional theory (TDLDA). The agreement for the high-order multiplet spectra with the atomic multiplet calculations is remarkable in the case of the N_{4,5} spectra. In contrast, we find that the shallow O_{2,3} semicore excitations in LaPO₄ manifest a relatively broad band and an apparent quenching of 5p spin-orbit splitting. The more sophisticated TDLDA, which has earlier been found to explain dipolar spectra well in Ba compounds, is less satisfactory here in the case of La.