ESRF	**Experiment title:** X-ray absorption and inelastic scattering from sulfuric acid - water solutions	**Experiment number**: **CH-3914**
Beamline: ID20 ID26	**Date of experiment**: from: 6/11/13 to: 12/11/13 from: 05/12/13 to: 09/12/13	**Date of report**: 18/02/14
Shifts: ID20: 18 ID26: 9	**Local contact(s)**: Roberto Verbeni (email: verbeni@esrf.fr) Jean daniel Cafun (email: jean-daniel.cafun@esrf.fr)	*Received at ESRF:*

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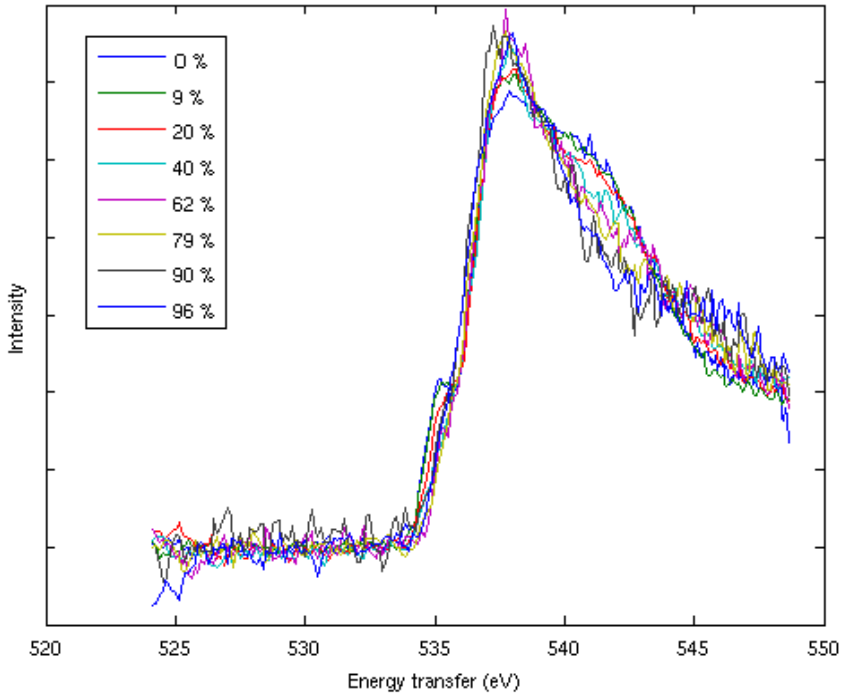
Report:

The beamtime application consisted of two separate experiment sessions on which
(i) O1s and S2p X-ray Raman Scattering (XRS) spectra
(ii) S1s Resonant Inelastic X-ray Scattering (RIXS) spectra
were recorded from H2SO4 (aq) solutions of concentrations 0-96 mass-%. The experiment aimed to characterize the core spectra of the samples and to be combined with theoretical simulations of the liquids. During the experiment, chemistry laboratory of ESRF and the help of Dr. Harald Müller was essential for success.

H2SO4 is fundamental driving force in atmospheric nucleation and subsequent formation of aerosols and droplets that affect the climate greatly, but whose effects are poorly understood. This beamtime application aimed to take a molecular microsope view on the solvation structure and protonation of sulfuric acid and the spectral fingerprints related. The experimental spectra are simulated using state-of-the-art computational methods and the whole study aims at giving a complete interpretation of bulk H2SO4(aq) and the X-ray fingerprints related.

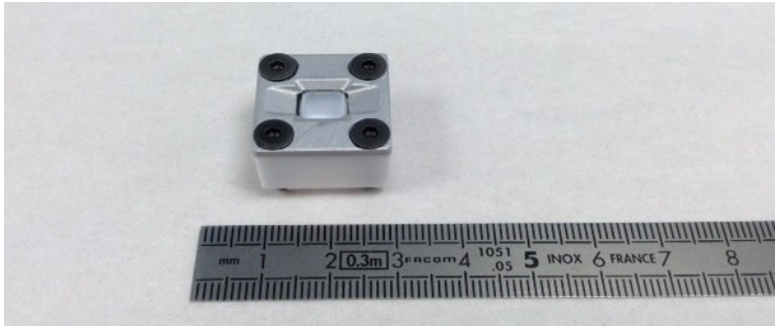
The beamtime at ID20 was used to record O1s and S2p spectra of numerous H2SO4 concentrations. As a sample of obtained results we present recorded spectra at O1s edge.



O1s spectra of sulfuric acid - water solutions recorded at ID20.

The O1s and S2p spectra were recorded in close-to-dipole transition regime and also at high momentum-transfer regime, manifesting higher multipole transitions, showing dramatic effects in the S2p spectra. The analysis is however onway.

The ID26 beamtime was made in collaboration with a group (M.Kavčič, M. Žitnik, and M.Petric) from Joseph Stefan institute Ljubljana, Slovenia. The group provided a RIXS spectrometer in which the liquid cell was placed and RIXS experiments were performed. Both Sulphur-K-alpha and Sulphur-K-beta RIXS spectra were recorded and the results will are interpreted using first-rpinciples simulations. The treatment of the experimental data is onway.



Liquid sample cell, made in Helsinki and used in the RIXS experiment at ID26, allowed studying liquid sulfuric acid experiments in a spectrometer requiring vacuum for operation.

So far it can be stated that the experiments proved to be successful. The extensive calculations performed proved to be able to produce the pure water and pure sulphuric acid spectra but there appears to be some error in energetics of oxygen core holes when the atom is in different molecule. The experiment therefore proved to be very useful in linking the simulations to reality. We are, however, very optimistic our further analysis to allow achieving all the goals of this proposal.