	Experiment title: RIXS spectroscopy of sulfur containing molecules around the 1s threshold	Experiment number: HE 2788	
	Beamline: ID26	Date of experiment: from: 08/04/2008 to: 15/04/2008	Date of report: 1/10/2008 <i>Received at ESRF:</i>
	Shifts: 18	Local contact(s): Pieter GLATZEL	
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Introduction:

When monochromatic synchrotron light with photon energy close to the ionization threshold is used for the target excitation, the resonant inelastic x-ray scattering (RIXS) occurs. The process can be described as an inelastic scattering of the incident photon at a resonance energy of the target atom/molecule using the Kramers-Heisenberg formalism [1]. RIXS spectroscopy provides us opportunity to study atomic and molecular states which can be excited selectively by the monochromatic photon beam. In comparison with the more standard near edge x-ray absorption spectroscopy (XANES), RIXS measurements provide additional information since the final state energy is also defined by measuring the fluorescent decay channel. In experiments where total experimental resolution is narrower than the natural broadening, nuclear dynamics including nuclear rearrangement, geometry change and fast dissociation can be probed on the timescale given by the core-hole lifetime. In our experiment RIXS spectroscopy was applied for the study of different sulphur molecules. The series of 1s2p and 1s3p RIXS spectra were collected for the H₂S, SO₂ and SF₆ molecules with excitation energy tuned around the 1s ionization threshold of sulphur.

Experiment:

The 1s2p and 1s3p RIXS maps of studied S containing molecules in the region around sulphur 1s ionization threshold were measured with the high resolution crystal spectrometer of J. Stefan Institute. For the present experiment the spectrometer was equipped with the Si(111) crystal ($2d = 6.271\text{\AA}$) in Johansson geometry with the Rowland circle radius of 500 mm. The diffracted x-rays were detected with a back illuminated CCD camera consisting of 770×1150 pixels (pixel size = $22.5 \times 22.5 \mu\text{m}^2$) resulting in energy resolution of appr. 0.4 eV for the measured x-ray fluorescence. The spectrometer was installed in the first experimental hutch of the ID26 undulator beamline equipped with a double Si(111) crystal monochromator yielding a photon flux of high 10^{12} ph/sec, with 0.4 eV bandwidth. The incident photon beam was impinging on a stainless steel cylindrical target cell separated from the spectrometer vacuum chamber with 12.5 μm thick kapton windows.

The pressure in the target cell was 50-80 mbar. Even though relatively low target pressure was used, which is important to reduce self-absorption correction, high photon flux and good efficiency of our set-up enabled us to collect full RIXS maps for all studied samples for both 1s2p and 1s3p transitions. For the case of SO₂ and H₂S target we have collected a series of 1s2p and 1s3p emission spectra in the range of excitation energies from 2469 to 2490 eV, with 0.25 and 0.20 eV energy steps, respectively. In case of SF₆ target emission spectra were collected for the 2475 - 2495 eV energy range with 0.3 eV energy step.

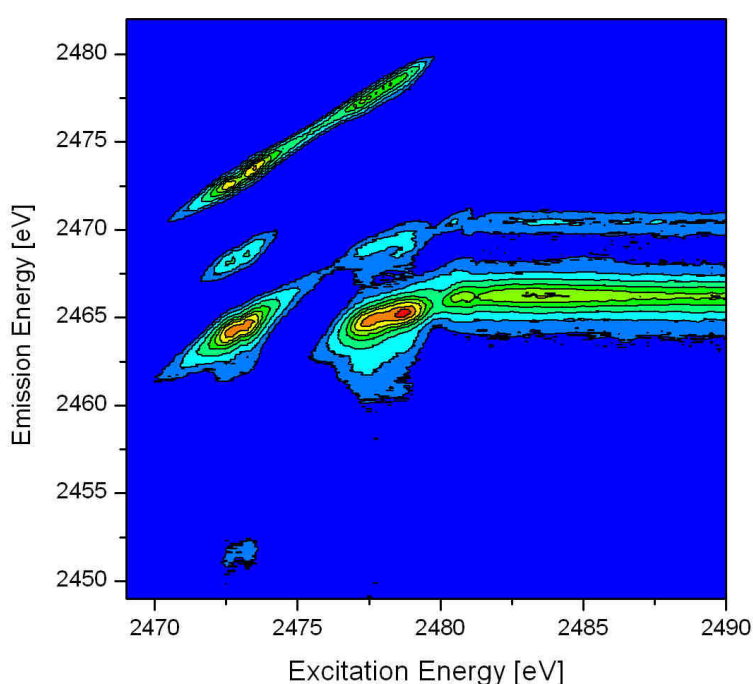


Figure 1: 1s3p RIXS map of SO₂ target around the sulphur K edge. The full scan consists of 85 K β emission spectra with 0.25 eV step in excitation energy.

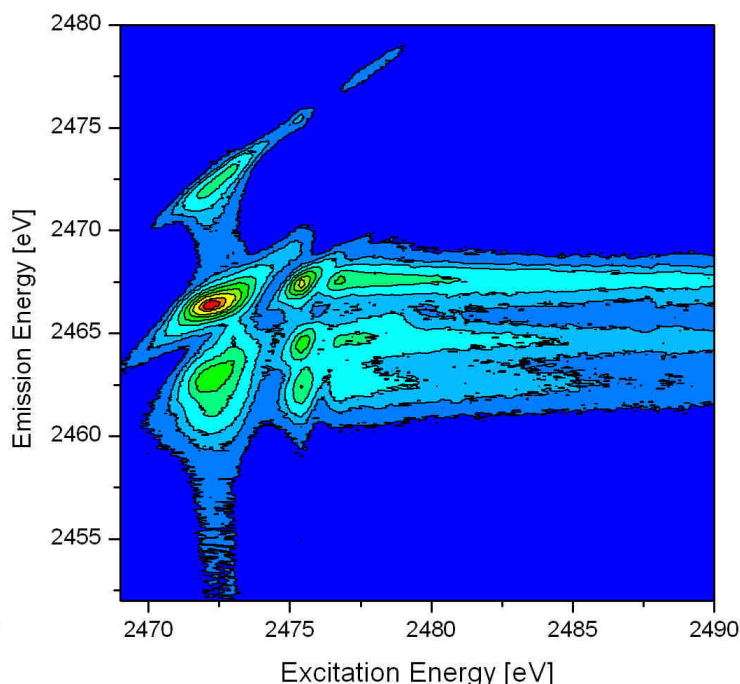


Figure 2: 1s3p RIXS map of H₂S target around the sulphur K edge. The full scan consists of 106 K β emission spectra with 0.2 eV step in excitation energy.

Data analysis:

For illustration the 1s3p RIXS maps collected for the H₂S and SO₂ targets are presented in Figs.1. and 2. The strongest resonances are clearly resolved in the presented plots followed by the edges typical for excitations into continuum. It is very interesting to note strong signal due to elastic scattering (emission energy equals excitation one). Since in our experiment the emission axis is perpendicular to the incoming beam (emission is in the direction of polarization), the contribution of Rayleigh scattering is negligible and the recorded elastic scattering is due to resonant excitations only. This is presented very clearly in Figs1. and 2 where strong elastic signal is recorded only on main resonances. The diagram K β emission line exhibit significant deviations from the straight linear dispersion typical for the resonant Raman scattering, which is a consequence of the fast nuclear processes. Even though the core-hole lifetime in this case is only in the order of 1 fs, nuclear dynamics can still be observed, similar as it was recently reported for the core excited HCl molecule [2]. On the other hand no such effect (or much less pronounced) is observed in the elastic peak, which is following very nicely the linear dispersion curve. More detailed analysis of the measured spectra is still in progress.

References:

- [1] A. Kotani, S. Shin, Rev. Mod. Phys. **73**, 203 (2001).
- [2] M. Simon et al., Phys. Rev. A **73**, 020706(R) (2006).