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Resonant X-ray Scattering of carbonyl sulfide at the sulfur K edge

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Synopsis New results on free OCS molecules have been obtained using Resonant X-ray Inelastic Scattering spectroscopy. A deconvolution algorithm has been applied to improve the energy resolution spectra of which we can extract detailed information on nuclear dynamics in the system.

We present results obtained using Resonant Inelastic X-ray Scattering (RIXS) spectroscopy on isolated OCS molecules after sulfur K-shell photoexcitation. This technique has been demonstrated to be sensitive to both nuclear dynamics on a femtosecond timescale [1, 2] (the core-hole lifetime is used here as a characteristic time to probe nuclear rearrangements) and to the chemical environment of the molecule [3]. We present the first results obtained on free OCS molecules which is the most abundant sulfur compound naturally present in the atmosphere and is a significant compound of the global sulfur cycle [4].

We have recorded OCS KL RIXS map where the intensity is plotted as a function of incident (γ1) and scattered (γ2) photon energies (top of figure 1.). This map is composed of 87 consecutive spectra recorded at excitation energies ranging from 2467 to 2480 eV with 150 meV step. KL emission lines correspond to the filling of the S 1s hole by an electron of the 2p orbitals. The spectra were recorded at the ID26 beamline of the ESRF synchrotron using the X-ray spectrometer developed at the J. Stefan institute, Ljubljana [5]

In core-shell spectroscopies, like RIXS, image analysis is complicated due to the broadening induced by a number of physical or instrumental processes. The experimental broadening is mainly due to the limited bandwidth of the incident photon beam and energy resolution of the spectrometer. The measured image I as a function γ1 and γ2 is then the result of the convolution of the true 'physical' image O with a function P representing the effects of experimental broadening, i.e. I = P * O where * represents the convolution symbol. The problem of extracting the original image O from I has been the subject of many papers in different experimental fields (including deblurring images from Hubble space telescope [6]) and different methods have been applied to remove intrinsic broadening due to very short core-hole lifetime of heavy elements [7]. We have implemented iterative deconvolution algorithms (Richardson – Lucy method) and we will show that such algorithms provide an effective way to deconvolve instrumental broadening typical of RIXS data (see bottom of figure 1).

The main molecular features of x-ray emission characteristic of the OCS system obtained at high energy resolution after deconvolution procedure will be presented.

![Figure 1. KL emission map before (top) and after deconvolution (bottom). X-ray emission spectra for an excitation energy indicated by the white dashed line are plotted on the left side of the maps.](image)

References