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

Loïc Journel, Tatiana Marchenko, Renaud Guillemin, Elie Kawerk, Matjaž Kavčič, Matjaž Žit-Nik, Klemen Bučar, Rok Bohinc, Marc Simon

To cite this version:

Loïc Journel, Tatiana Marchenko, Renaud Guillemin, Elie Kawerk, Matjaž Kavčič, et al.. Resonant X-ray Scattering of carbonyl sulfide at the sulfur K edge. Journal of Physics: Conference Series, 2015, 635 (11), pp.112109. 10.1088/1742-6596/635/11/112109 . hal-01203449

HAL Id: hal-01203449

https://hal.sorbonne-universite.fr/hal-01203449

Submitted on 28 Sep 2015

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Distributed under a Creative Commons Attribution 4.0 International License

IOPscience iopscience.iop.org

Home Search Collections Journals About Contact us My IOPscience

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

This content has been downloaded from IOPscience. Please scroll down to see the full text.

2015 J. Phys.: Conf. Ser. 635 112109

(http://iopscience.iop.org/1742-6596/635/11/112109)

View the table of contents for this issue, or go to the journal homepage for more

Download details:

IP Address: 134.157.80.136
This content was downloaded on 28/09/2015 at 08:23

Please note that terms and conditions apply.

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

Loïc Journel[*1], Tatiana Marchenko[*], Renaud Guillemin[*], Elie Kawerk[*], Matjaž Kavčič[†], Matjaž Žitnik[†], Klemen Bučar[†], Rok Bohinc[†] and Marc Simon[*]

[*]Sorbonne Universités, UPMC Université Paris 06 and CNRS, UMR 7614, Laboratoire de Chimie Physique-Matière et Rayonnement, F-75005, Paris, France
[†]J. Stefan Institute, Jamova 39, SI-1000, Ljubljana, Slovenia

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 (γ_1) and scattered (γ_2) 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 γ_1 and γ_2 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.

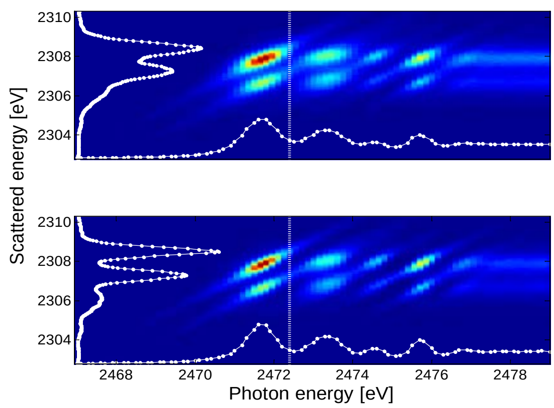

Figure 1. KL emission map before (top) and after deconvolution (bottom). X-ray emission spectra for an excitation energy indicated by the white dashed line are plotted on the left side of the maps.

References

[1] M. Simon *et al* 2006 *Phys. Rev. A* 73 020706(R).
[2] R. Guillemin et al 2012 Phys. Rev. A 86, 013407.
[3] S. Carniato *et al, 2012 J. Chem. Phys.* 137, 144303.
[4] R. P. Wayne 1991 *Chemistry of Atmospheres,* Oxford University Press, New York, USA.
[5] M. Kavcic *et al* 2012 *Rev. Sci. Instrum.* 83, 033113
[6] H. M. Adorf et al 1995, *Int. J. Imaging Syst. Technol.* 6, 339.
[7] T. Fister *et al* 2004 *Phys. Rev. B* 75, 174106.

[1] E-mail: loic.journel@upmc.fr

Content from this work may be used under the terms of the Creative Commons Attribution 3.0 licence. Any further distribution of this work must maintain attribution to the author(s) and the title of the work, journal citation and DOI.
Published under licence by IOP Publishing Ltd