

Report on HE-3229: **"Structural and dynamical properties of chlorinated hydrocarbons in gaseous state studied by high resolution RIXS Cl-1s."**

We have successfully measured Cl K XANES and Cl RIXS  $K\alpha$  spectra of 11 different chlorohydrocarbon (HCC) gaseous targets using high resolution x-ray spectrometer of J. Stefan Institute of Ljubljana. The studied targets were 3 chloromethanes (single C atom: dichloromethane, chloroform, carbon tetrachloride), 4 chloroethanes (2 C atoms with a single bond: chloroethane, 1,1 dichloroethane, 1,2, dichloroethane and methyl chloroform), 3 chloroethenes (two C atoms with double bond: 1,2 dichlorethene cis, 1,2 dichlorethene trans and 1,1 dichlorethene) and chlorobenzene with a single chlorine atom attached to the benzene ring. Except for the gaseous chloroethane, the studied targets are liquids at room temperature with vapor pressure in the 10 - 500 mbar range. The experiments were performed with gas enclosed in stainless steel cell, sealed by 12.5 micron Kapton windows at about several tens of mbar pressure. Prior to the cell filling the air was removed from the source by a sequence of freezing, pumping and warming. The XANES spectra in the region of chlorine K edge were measured by a photodiode located at the same distance from the target as Si 111 crystal that was employed for diffraction of emitted x-rays towards the CCD camera. Several RIXS scans were also performed around the K edge, observing  $K\alpha$  and for some samples also the  $K\beta$  spectrum, depending on target sensitivity against the radiation damage. An example of chloroform XANES and RIXS  $K\alpha$  spectrum integrated over a small energy interval around the emission peak is shown in figure below. The trends are observed in XANES spectra for various targets depending on the number and configuration of chlorine atoms and on the carbon bond strength. High resolution RIXS spectra exhibit broadening of the first resonance linewidth at detuning which indicates that in HCC the dissociation is active on the time scale of an inner hole lifetime, similar to HCl. The experiment was ended by configuring the beamline mono to Si 311 crystal and the spectrometer mono to Si 220 in order to record Xe  $L_3$  RIXS spectrum at fixed energy below the  $L_3$  edge. Such a combination assured an overall energy resolution of emission in the range of 0.8 eV which is much better than the natural linewidth of  $L_3$  hole in Xe (2.8 eV) and also better from previously reported RIXS results.

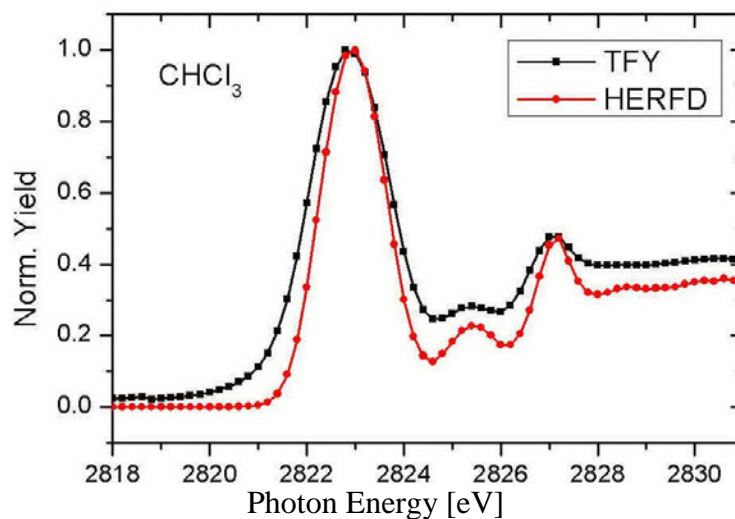


Figure 1. Total fluorescence yield (TFY) and integrated RIXS yield (HERFD) for chloroform (CHCl<sub>3</sub>).