ESRF	**Experiment title:** Substrate Induced Bending of Pi-Conjugated Molecules Studied by XSW	**Experiment number:** SI-1185
Beamline: ID 32	**Date of experiment:** from: 23/08/2005 to: 30/08/2005	**Date of report:** 07/02/2006
Shifts: 18	**Local contact(s):** Dr. J rg Zegenhagen	*Received at ESRF:*

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Report:

1. Introduction

As outlined in the proposal the purpose of the project was to gain insight into the adsorption behaviour of complex organic molecules on nobel metal substrates. In particular their binding distances, as they can be determined from experimental X-ray standing wave (XSW) data, are a key ingredient for the under-standing of the substrate-absorbate interaction.

As result of a previous XSW experiment we found that within the first monolayer the perfluorinated copper phthalocyanines show a surprising molecular distortion on Cu(111) and Ag(111) surfaces [1]. Since the character of the binding to the substrate should depend on chemical modifications of the molecules, we used FeCl and GaCl phthalocyanine (Pc) molecules in this experiment, see Fig. 1. From these new XSW measurements we hope to derive essentially the ñ atural" binding distance of the Pc core on the noble metals. In combination with earlier results these measurements should improve our understanding of the adsorption geometry of π-conjugated molecules.

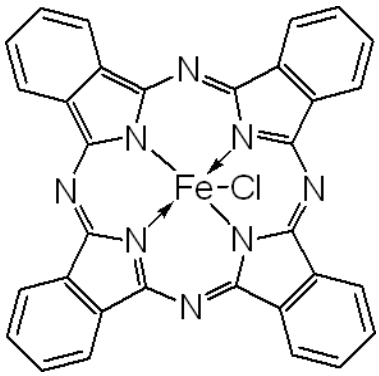

Figure 1: FeCl Phthalocyanine

Below we give a short summary of results from the beamtime at ID32.

2. XPS measurements on monolayers of FeCl and GaCl phthalocyanines

The relatively weak photoelectron signals from a sub monlayer of FeCl Pc and GaCl Pc required relatively long integration times. Since the stability of the monochromator allowed only for short XSW scans of approximately 30 minutes, we generally took several XSW scans which can be added later.
Several films of FeCl Pc and GaCl Pc with different coverages in the monolayer regime were prepared using the quarz crystal microbalance the XPS signal as thickness monitor.

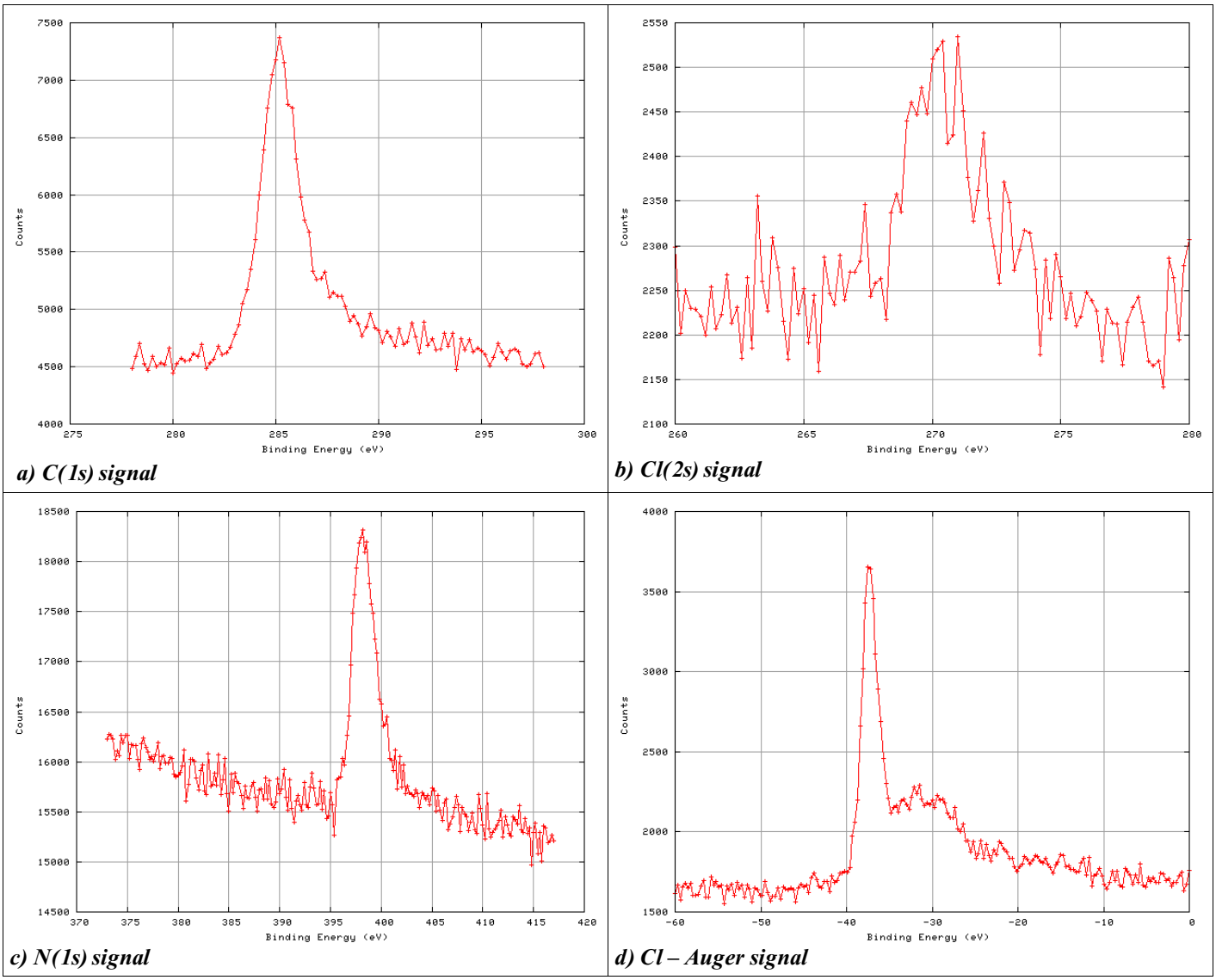

Figure 2: XPS signals from a submonolayer of FeCl phthalocyanines

On the basis of the XPS spectra we found no evidence of significant beam damage of the adsorbed phthalocyanine molecules.

3. XSW measurements on monolayers of FeCl and GaCl phthalocyanines

Our new Cu(111) substrate turned out to be of high quality, with the normal incidence rocking width of <= 0.90 eV close to the intrinsic value, see Fig 3a. First, the XSW signal from the clean copper surface (Fig. 3b) was measured to characterize the substrate. After evaporation of the organic molecules we obtained high qualitiy XSW data from both FeCl Pc and GaClPc monolayers.
By comparison of the N(1s) and the Cl(2s) signal (Fig. 3c and 3d) already their different shape indicates that the chlorine is located above the molecular plane of the phthalocyanine. From the fit to the photoyield we obtain the coherent position of the carbon, nitrogen and chlorine atoms in the molecule.

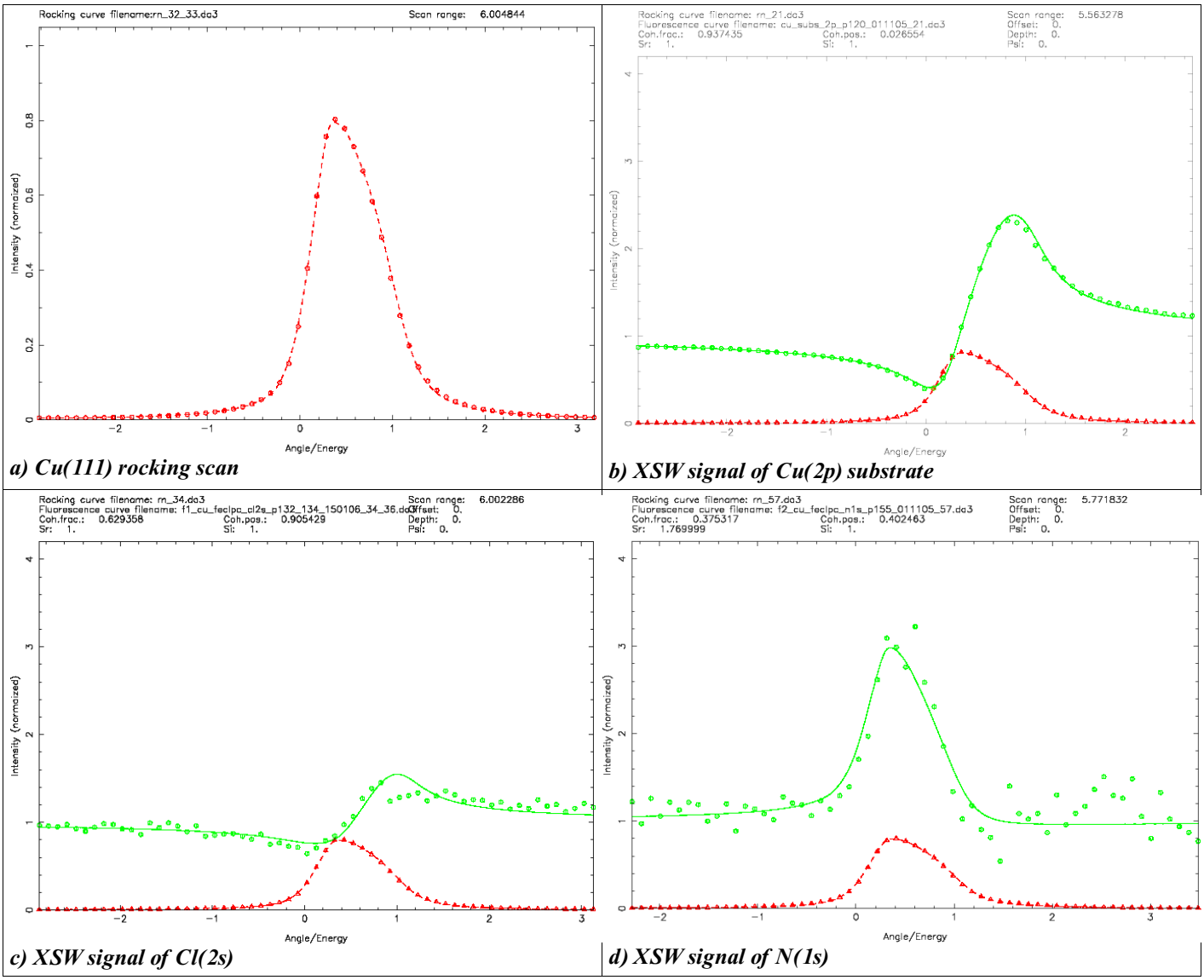

Figure 3: XSW from signals from a submonolayer of FeCl phthalocyanines

By heating the samples to different temperatures between T=30 ^{0}C and T=350 ^{0}C we studied annealing effects within the Pc monolayers. We generally found that coherent fraction derived from the XSW fits increase with the annealing temperature thus indicating an pronounced a higher order in the adsorbate layer.

4. Summary

Overall the experiment was very successful and we are currently working on the further analysis of the data. A comprehensive publication of the binding distances of different phthalocyanines is intended shortly.

We wish to acknowledge the excellent support from our local contact, as always on ID32.

5. References

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[2] N. Koch, S. Duhm, J. P. Rabe, S. Rentenberger, R. L. Johnson, J. Klankermayer, F. Schreiber, *Tuning the Hole Injection Barrier Height at Organic/Metal Interfaces With (Sub-) Monolayers of Electron Acceptor Molecules,* Appl. Phys. Lett. 87 (2005) 101905

[3] F. Schreiber, K. A. Ritley, I. A. Vartanyants, H. Dosch, J. Zegenhagen, and B. C. C. Cowie, *Non-dipolar contributions in XPS-detection of x-ray standing waves*, Surf. Sci. Lett. 486 (2001) 519