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Experiment Report Form

The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF. Once completed, the original report should be sent, together with 5 reduced (A4) copies, to the User Office.

In addition, please send a copy of your file as an e-mail attachment to reports@esrf.fr**,** using the number of your experiment to name your file. This will enable us to process your report for the ESRF Annual Report.

Reports accompanying requests for additional beam time

If your report is to support **a new proposal**, the orginal report form should be sent with the new proposal form, and a copy of your report should be attached to each copy of your proposal. The Review Committees reserve the right to reject new proposals from groups who have not reported on the use of beam time allocated previously.

Reports on experiments relating to long term projects

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

Published papers

All users must give proper credit to ESRF staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to the Joint ESRF/ ILL library the complete reference and the abstract of all papers appearing in print, and resulting from the use of the ESRF.

Should you wish to make more general comments on the experiment, please note them on the User Evaluation Form, and send both the Report and the Evaluation Form to the User Office.

Deadlines for submission of Experimental Reports

- 1st March for experiments carried out up until June of the previous year;
- 1st September for experiments carried out up until January of the same year.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report, in English.
- include the reference number of the proposal to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.
- bear in mind that the report will be reduced to 71% of its original size. A type-face such as "Times", 14 points, with a 1.5 line spacing between lines for the text, produces a report which can be read easily.

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ESRF	**Experiment title:** Surface-induced conformational changes of planar aromatic molecules on metals	**Experiment number**: SI-634
Beamline: ID 32	**Date of experiment**: From: Nov.10, 2000 to: Nov. 20, 2000	**Date of report**: March 2, 2001
Shifts: 18	**Local contact(s)**: J. Zegenhagen / B. C. C. Cowie	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

*Frank Schreiber, *Kenneth A. Ritley, Bärbel Krause, Arndt Dürr,
Helmut Dosch
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Report:

As outlined in the proposal, this experiment has focussed on an x-ray standing wave (XSW) and x-ray photoelectron spectroscopy (XPS) study of an important compound used in molecular electronics, namely F16CuPc (perfluorinated Cu-phthalocyanine, C32F16N8Cu) on Ag(111).
The full quantitative analysis is not yet finished, but the qualitative features of the data lead us to following tentative conclusions:

1) We could successfully determine the bonding distance, d, of the F16CuPc molecule and small differences between the different atomic species within the molecule.
This is of importance for the understanding of this van-der-Waals-driven epitaxy and the electron transfer at the interface.

2) The coherent fraction appears to be relatively high, which is presumably due to the rigid nature of the molecule.

3) After exploiting the substrate (111) reflection, we also studied the XSW signal from the (222) reflection. Despite the difficult experimental conditions (including the need to apply a bias voltage to the sample for the detection of C(1s) photoelectrons and the low XPS cross-section for higher-energy x-rays), we were able to record data sets. This proof of principle, i.e., that the electron analyzer at ID32 is able to detect high-energy photoelectrons (up to about 4500 eV in kinetic energy) is very important for the planned future developments of high-energy XPS and exploiting higher-order reflections in XSW.

4) The XSW and XPS studies were performed at different temperatures,
and small, but important differences in the bonding configuration were found (thermally-induced chemisorption mediated by the pi-electrons of these otherwise predominantly van-der-Waals-bonded molecules).

5) We have detected differences in the XPS- and the Auger-detected XSW signals to address the question of non-dipolar contributions to the XPS cross-section (F. Schreiber et al., Surf. Sci. Lett., in print (2001)). After the proof of principle of this approach we intend to address the issue of the non-dipolar contributions systematicall in a future experiment.

We also wish to acknowledge the excellent collaboration with the ESRF scientists B.C.C. Cowie and J. Zegenhagen.