EUROPEAN SYNCHROTRON RADIATION FACILITY

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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 report should be submitted electronically to the User Office via the User Portal:

https://wwws.esrf.fr/misapps/SMISWebClient/protected/welcome.do

Reports supporting requests for additional beam time

Reports can be submitted independently of new proposals – it is necessary simply to indicate the number of the report(s) supporting a new proposal on the proposal form.

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.

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Experiment title: Lattice dynamics and hyperfine interactions for Os-monoarene complexes		Experiment number: LS-2334
Beamline: ID18 ID18	**Date of experiment**: from:19 Nov 2014 to:22 Nov 2014; from:04 Dec 2014 to:08 Dec 2014	**Date of report**: 27/02/2015
Shifts: 21 21	**Local contact(s)**: Dr. Aleksandr Chumakov (email: chumakov@esrf.fr) Dr. Rudolf Rueffer (email: rueffer@esrf.fr)	*Received at ESRF:*

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Report:

The aim of the allocated beamtime was to investigate the lattice dynamics and the hyperfine interactions on organometallic osmium monoarene complexes (99% enriched to ^{187}Os) with cancer cell cytotoxicity.

The whole beamtime was pleasant, the data acquisition procedure was smooth and the quality of the obtained data was exceptional.

The nuclear resonance of ^{187}Os was found at 9.778(3) keV. We determined the previously unknown nuclear quadrupole splitting of the excited state, $Q_{3/2}$= 1.46(10) barn, by measuring nuclear forward spectra from Os metal at room temperature. In addition, we precisely determined the lifetime of the first excited state of Os, which is 3.43(25) ns, see Fig. 1.

We designed a high resolution monochromator which we tested during the allocated beamtime. The provided energy band-pass was, 1.05(5) meV, in agreement with our theoretical design, see Fig. 2.

The obtained high resolution gave us the opportunity to carry out phonon spectroscopy. We first measured nuclear inelastic scattering spectra from Os metal and we extracted the density of phonon states as well as all the related thermodynamical properties. For example, the obtained Lamb-Mossbauer factor in Os metal is 0.95(1) at room temperature, the mean interatomic force constant is 335(5) N/m, the extracted speed of sound, 3.58(14) km/s, is in agreement with the macroscopically obtained value, 3.791 km/s. The preliminary data are include in a manuscript which is about to be submitted for publication.

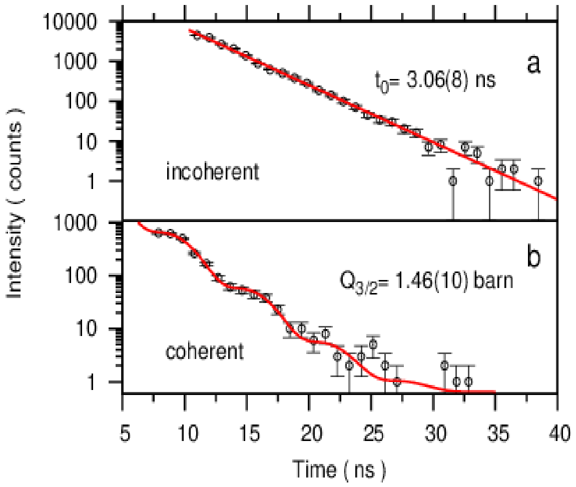

Fig. 1: The time distribution of the delayed incoherent (a) and of the coherent (b) scattering spectrum

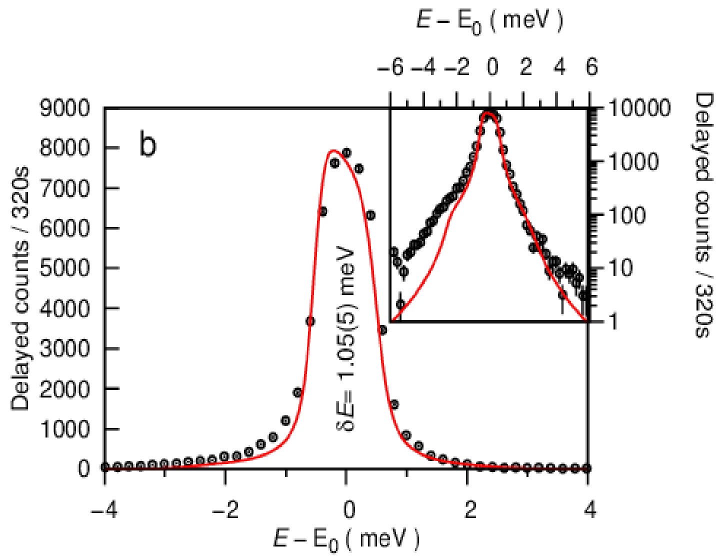

Fig. 2: The energy resolution of the high resolution monochromator in linear and logarithmic scale (points) and comparison to theory

More importantly we have collect good quality nuclear forward and inelastic scattering spectra on Os organometallics. Typical nuclear forward spectra are presented in Fig. 3. The corresponding nuclear inelastic scattering spectra are shown in Fig. 4.

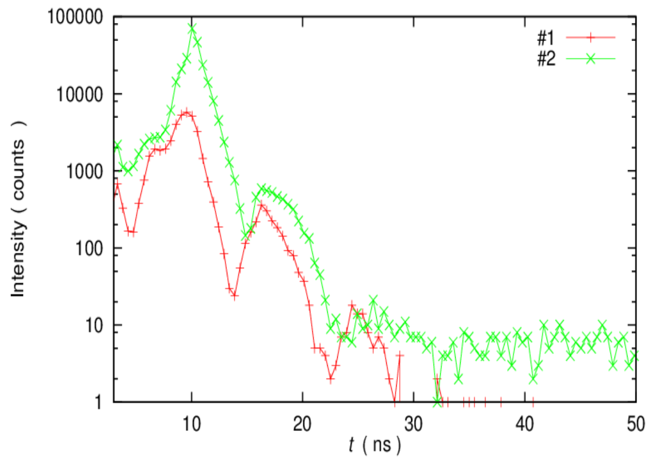

Fig. 3: The nuclear forward scattering spectra obtained in two different Os monoarene complexes.

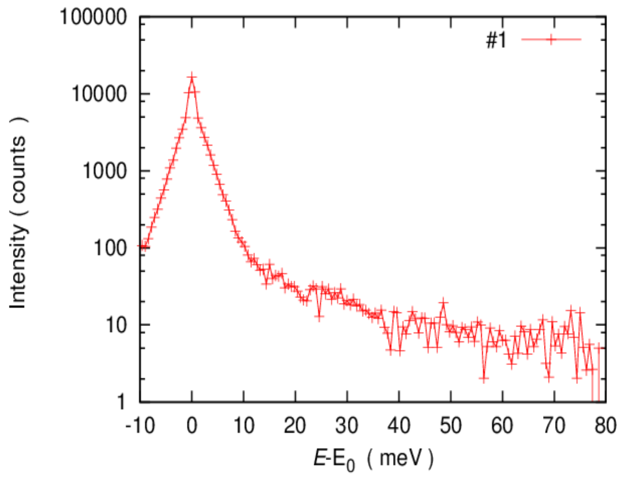

Fig. 4: The nuclear inelastic scattering spectrum obtained on the sample #1 depicted in Fig. 3

Combining the results obtained in this study with our further investigations, *i.e.*, first principle theoretical calculations, far-IR, *etc*, we are be able to correlate the difference in the interatomic bonding with respect to functionality of Os organometallics.