EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

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.

ESRF	**Experiment title:** Resonant inelastic x-ray scattering of the new iridium compound Ba_2YIrO_6	**Experiment number**: HC 1523
Beamline: ID 20	**Date of experiment**: from: 24.9.2014 to: 30.9.2014	**Date of report**: 4.3.2015
Shifts: 16	**Local contact(s)**: Michael Krisch	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

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Report:

We performed resonant inelastic x-ray scattering (RIXS) measurements on the new iridate Ba_2YIrO_6. This compound realizes a lattice of Ir-sites in a $5d^4$ configuration, which exhibit a non-magnetic J=0 ground state in the free ion limit. These systems are hence expected to be non-magnetic. It was therefore a great surprise when we observed a paramagnetic response of Ba_2YIrO_6. The aim of this study was to clarify the microscopic origin of this unexpected magnetic response. To this end, we used RIXS at the Ir L_3-edge (11.217 keV) to determine the dispersion of the J=1 and J=2 excitations along various high-symmetry directions in reciprocal space. For the measurements π-polarized incoming photons were used and the scattering angle was chosen close to 2θ=90° in order to suppress the elastic scattering.

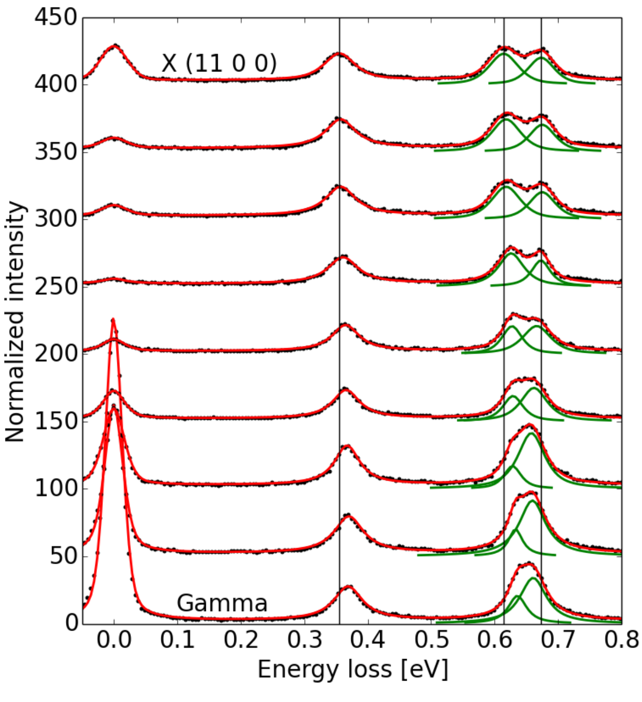

Figure 1: Dispersion of the J=1 and J=2 excitations along the Γ–X direction.

In Fig. 1, a representative data set of measurements along the Γ–X direction is presented. The spectra show three important features at energy losses fitting well to our theoretical model calculations, namely a J=1 triplet at ≈350 meV and a J=2 quintet at ≈650 meV. However, we also observe a feature which is not reproduced by the theoretical model at

around 1.2 eV (not shown in Figure 1). This excitation is much broader then the lower J=1,2 features and indicates a continuum of excitation. The J=1 and J=2 peaks show a downward dispersion towards the X-point, which is in accordance with our model calculations. However, the experimentally observed dispersions are by a factor of 10 smaller than those obtained by our previous model calculations. Most importantly, we do not observe any evidence of a magnetic instability due to a magnetic soft mode. As an immediate result of this study we can therefore exclude the theoretically predicted condensation of J=1 or J=2 excitations in Ba_2YIrO_6.

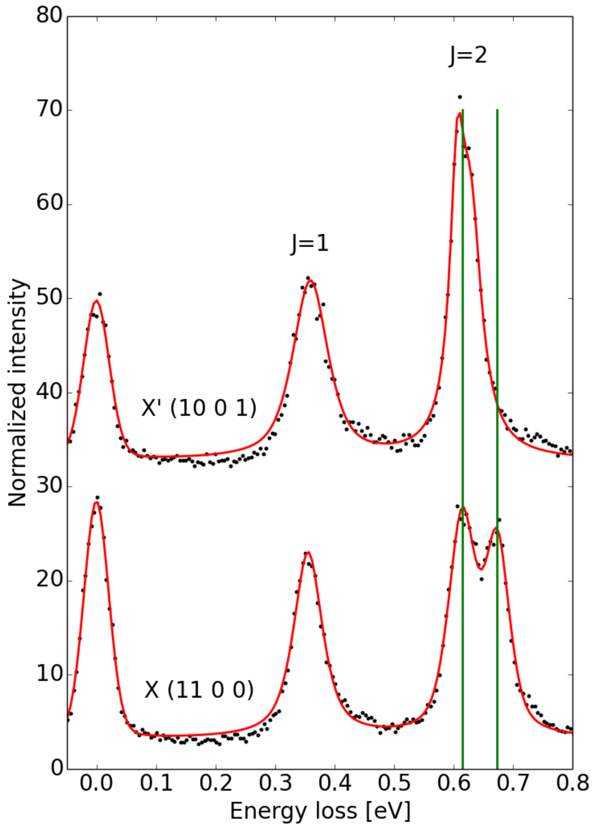

Figure 2: RIXS-spectra at different symmetrical equivalent points X and X'

We also discovered important selection rules that provide essential microscopic information. As shown in Fig. 2, the RIXS spectra at different but equivalent high-symmetry points can strongly differ. Particularly the feature assigned to the J=2 excitations in X is clearly split up into two branches, whereas in X' obviously one branch vanishes. We also performed measurements along the path X-W-K-W'-X' between these two points, to investigate the development of this effect. These selection rules contain direct information about the symmetry properties of the different quintet excitations. Currently we are in the process of comparing these results to numerical calculations on a quantitative level, taking into account the exact scattering geometry. This will enable us to extract details on the symmetry properties of the different excitations and to assign specific features in the RIXS spectra to them. In this way, these data will provide a very detailed characterization of the relevant energy scales for this magnetic system. We expect, that this will ultimately enable us to rationalize the unusual magnetic behavior of these $5d^4$-systems.