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

Deadlines for submission of Experimental Reports

Experimental reports must be submitted within the period of 3 months after the end of the experiment.

Experiment Report supporting a new proposal ("relevant report")

If you are submitting a proposal for a new project, or to continue a project for which you have previously been allocated beam time, you must submit a report on each of your previous measurement(s):

- even on those carried out close to the proposal submission deadline (it can be a "preliminary report"),

- even for experiments whose scientific area is different form the scientific area of the new proposal,

- carried out on CRG beamlines.

You must then register the report(s) as "relevant report(s)" in the new application form for beam time.

Deadlines for submitting a report supporting a new proposal

- > 1st March Proposal Round 5th March
- > 10th September Proposal Round 13th September

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.

Instructions for preparing your Report

- fill in a separate form for <u>each project</u> or series of measurements.
- type your report in English.
- include the experiment number 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: Investigation of photoreaction pathways of gold halide series	Experiment number: CH6650
Beamline:	Date of experiment:	Date of report:
ID09	from: 2023.4.25 to: 2023.4.30	2023.9.9
Shifts:	Local contact(s):	Received at ESRF:
18	Mikhail KOZHAEV	
Names and affiliations of applicants (* indicates experimentalists):		
Hyotcherl IHEE, Department of Chemistry, KAIST, Daejeon, Republic of Korea		
* Jungmin KIM, Department of Chemistry, KAIST, Daejeon, Republic of Korea		
* Jun HEO, Department of Chemistry, KAIST, Daejeon, Republic of Korea		
* Seunghwan EOM, Department of Chemistry, KAIST, Daejeon, Republic of Korea		
* Doyeong KIM, Department of Chemistry, KAIST, Daejeon, Republic of Korea		

* Jeong Hoon LEE, Department of Chemistry, KAIST, Daejeon, Republic of Korea

* Jungho MOON, Department of Chemistry, KAIST, Daejeon, Republic of Korea

Report:

The halogen ligands coordinated to the metal center are known for their remarkable polarity and abundant charge, particularly for their ability to increase the electron density around the metal ion. These properties have been extensively studied in our group through time-resolved X-ray solution scattering experiments, notably in the case of K[Au(CN)₂], a gold atom compound that has shown unique scientific phenomena. K[Au(CN)₂] exists in various oligomeric forms in the ground state, driven by aurophilic interactions, and has been analyzed to undergo a dynamic transition from trimers to tetramers under a 267 nm laser.

In order to investigate the influence of halogen ligands on the structural dynamics of the trimer-totetramer structural dynamics in K[Au(CN)₂], the researchers conducted time-resolved X-ray solution scattering experiments, known for their sensitivity to structural changes.

The experiments performed in this proposal involve 50 and 150 mM AuBr₂ and 50 mM AuI₂. To conduct this experiment, we utilized the 7/8+1 (192+8mA) bunch mode. We employed a 267 nm laser pulse as the pump and utilized X-ray scattering as the probe. The signal was detected using a Rayonix CCD detector. The time delay and difference scattering intensity are shown in **Figure 1**, as reported in the X-ray experimental results.



Figure 1. The difference scattering signals from conducted using time-resolved x-ray solution scattering at CH-6450 (A) 50 mM AuBr₂, (B) 50 mM AuI₂ and (C) 150 mM AuBr₂

In the difference scattering signal at 100 ps, we can observe that the signals of the previously studied K[Au(CN)₂], AuBr₂, and Aul₂ are all different (**Figure 2A**). Furthermore, we can also see that Aul₂ and AuBr₂ exhibit differences (**Figure 2B**). This explicitly confirms that the structural change signals vary in the presence of bromide and iodide ions compared to cyanide ions. The exact nature of the structural changes underlying these differences and the properties of the halogen ions responsible for these structural changes are currently being analyzed and will be addressed in the ongoing analysis and paper writing



Figure 2. The comparison between difference scattering signal at 100 ps time delay (A) The comparison between 50 mM AuBr₂, 150 mM AuBr₂ and K[Au(CN)₂] and (B) The comparison between Aul₂ and AuBr₂.