ESRF	<b>Experiment title:</b> Core level crossing and its consequences on the structural stability of Iridium	Experiment number: HC-3391
Beamline:	Date of experiment:	Date of report:
BM23 and ID15B	from: 08/11/2017 to: 14/11/2017 and	"relevant report"
	from: 08/02/2018 to: 11/02/2018	
Shifts: 15 and 12	<b>Local contact(s)</b> : Virginia Monteseguro Padrón and Gaston Garbarino	Received at ESRF:
Dr. Virginia I Dr. Vera Cua Dr. Catalin P Dr. Johan Jön	filiations of applicants (* indicates experimentalists): Monteseguro Padrón*, Universidad de Cantabria rtero Yague*, Universidad de Zaragoza opescu*, ALBA Synchrotron osson, Linköping University el Sans Tresserras*, Universidad Politécnica de Valencia	

## **Report:**

This beamtime has generated one published work.

## <u>Abstract</u>

The 5d transition metals have attracted specific interest for high-pressure studies due to their extraordinary stability and intriguing electronic properties. In particular, iridium metal has been proposed to exhibit a recently discovered pressure-induced electronic transition, the so-called core level crossing transition at the lowest pressure among all the 5d transition metals. Here, we report an experimental structural characterization of iridium by x-ray probes sensitive to both long- and short-range order in matter. Synchrotron-based powder x-ray diffraction results highlight a large stability range (up to 1.4 Mbar) of the low-pressure phase. The compressibility behaviour was characterized by an accurate determination of the pressure-volume equation of state, with a bulk modulus of 339(3) GPa and its derivative of 5.3(1). X-ray absorption spectroscopy, which probes the local structure and the empty density of electronic states above the Fermi level, was also utilized. The remarkable agreement observed between experimental and calculated spectra validates the reliability of theoretical predictions of the pressure dependence of the electronic structure of iridium in the studied interval of compressions.

## Full reference detail:

V. Monteseguro, J. A. Sans, V. Cuartero, F. Cova, Igor A. Abrikosov, W. Olovsson, C. Popescu, S. Pascarelli, G. Garbarino, H. Johan M. Jönsson, T. Irifune, and D. Errandonea. **Phase stability and electronic structure of iridium metal at the megabar range**. *Scientific Reports*, 9, 8940 (2019).