ESRF	**Experiment title:** "The effect of structure on the magnetism of Ir double perovskites"	**Experiment number**: HC-3620
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Report:

In iridates the comparable energy scales of the SOC, U and CEF interactions create a delicately balanced ground state, which is largely sensitive to changes in local environment symmetry or dimensionality and drive complex magnetic and electric-transport behaviors. Moreover, the ability of Ir to exist in different oxidation states and the spatial extent of the 5d orbitals should also result in a wide range of electric and magnetic behaviors and a large sensibility to external stimuli. Double perovskites containing Ir seem an optimal playground to explore this. Very recent works suggest that the Ir-Ir interaction may be more critical than typically assumed [1]. Moreover, the application of physical pressure has been proved to play an important role by shrinking interatomic distances and changing B-O-Ir angles, leading to drastic changes on SOC and CEF interactions, which highly affects the magnetic ordering and transport properties [2]. However, the correlation between structural details and magnetic properties on these compounds is far from achieved. Consequently, a comprehensive work is necessary to clarify how the magnetic structure relates to structural details. Within this scenario, we are carrying out a broad investigation on the crystal and magnetic structures of Sr_2BIrO_6 compounds. Our results show a variety of complex magnetic behaviors that depend on the Ir oxidation state. Besides, the differences observed between samples with the same Ir valence suggest that the magnetization (the magnetic structure) is highly sensitive to small structural changes. For Sr_2NiIrO_6 XMCD under pressure also reveals a complex response as it first decreases under low applied pressure, but later the XMCD intensity increases under further physical pressure rise.

We have performed HP-EXAFS measurements to explore the local structure around Ir, especially bond distances and local distortions and angles. EXAFS measurements were carried out at the Ir L3 edge in the transmission mode at low temperature (T = 10 K) for pressures up to ~40 GPa. Two powdered double perovskite samples were measured: Sr2NiIrO6 (Ir6+) and Sr2YIrO6 (Ir5+). Nano-polycrystalline diamond anvils with ruby chips as pressure markers, provided through a scientific collaboration with Prof. Irifune, were used.

The Figure 1 shows the XANES spectra recorded at the Ir edge in both, Sr2NiIrO6 and Sr2YIrO6, samples. In both cases a shift towards higher energies is observed as the pressure increases: up to ~0.4 eV shift at ~45 GPa, indicating a clear reduction in the Ir-O bond distance. Similarly, the EXAFS range also reveals a gradual reduction of the Ir-O distance (see Figure 2). Under the maximum applied pressure, the Ir-O distance decreases ~0.1 Å in Sr2YIrO6 and ~0.05 Å in Sr2NiIrO6. The reduction observed in the intensity of the first peak of the FT also suggests that the IrO6 octahedra are gradually distorted only in Sr2YIrO6 compound.
Regarding longer-range order, Ir-O-Ir distances and angles, the preliminary analysis of the EXAFS spectra recorded on Sr2NiIrO6 indicate just a slight diminution of the distances. In Sr2YIrO6, however, the drastic intensity reduction observed in the corresponding Fourier Transforms seems to be better (mainly) explained by an increase of the structural disorder and/or a drastic reduction of the Ir-O-Ir tilting angles. We have also found that the changes obtained by high pressure are bigger than for chemical pressure.

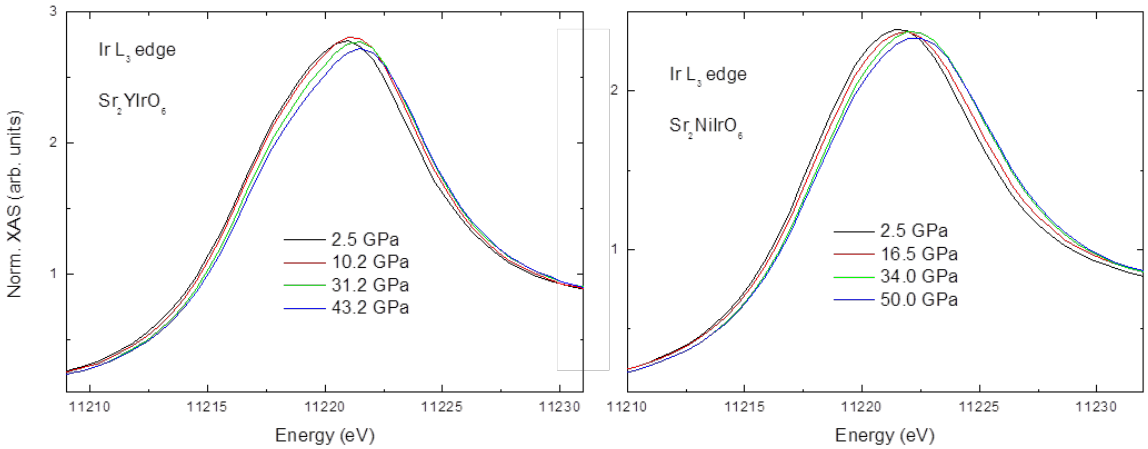

Fig. 1. Ir L3-edge XANES recorded at 10 K on Sr2YIrO6 (left) and Sr2NiIrO5 (right).

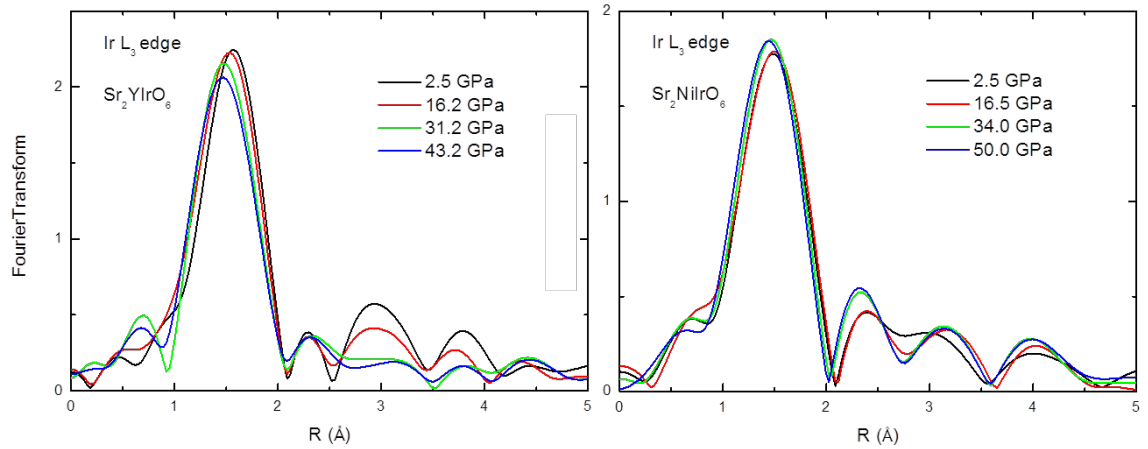

Fig. 2. Fourier transform of the EXAFS recorded at 10 K on Sr2YIrO6 (left) and Sr2NiIrO5 (right).

Therefore, we observe that the impact of hydrostatic pressure on the the crystal structure is quite different for the two studied double prerovskites. Nevertheless, further analysis is needded to fully understand the mechanisms behind the pressure induced magnetic changes.

References:

[1] X. Ou et al., Scientific Reports 4, 7542 (2014); R. Morrow et al., Chem Mater. 28, 3666 (2016).
[2] D. Haskel Phys. Rev. Lett. 109, 027204 (2012), C. Donnerer Phys. Rev. B 93, 174118 (2016), M.A. Laguna-Marco Phys. Rev. B 90, 014419 (2014).