Experimental report

02/10/2021

Proposal: 5-21-1139 **Council:** 10/2019

Title: New Kitaev iridates prepared by the low-temperature ion exchange

Research area: Physics

This proposal is a new proposal

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Experimental team:

Local contacts: Clemens RITTER

Samples: CuIrO3
ZnIrO3
MgIrO3

Instrument	Requested days	Allocated days	From	To
D2B	2	2	02/09/2020	04/09/2020
D20	2	0		

Abstract:

CuIrO3, ZnIrO3, MgIrO3 are new chemical compounds obtained from the Kitaev iridate beta-Li2IrO3 by an ion-exchange reaction. We seek to collect neutron powder diffraction data and refine crystal structures of these new compounds. The structural information obtained therein will be essential for understanding the magnetic behavior and, in particular, the possible spin-liquid physics suggested by our thermodynamic measurements on the Cu and Zn compounds.

New Kitaev iridates prepared by the low-temperature ion exchange

Abstract

$CuIrO_3$, $ZnIrO_3$, $MgIrO_3$, and $Li_{2x}Mg_{1-x}IrO_3$ (where x = 0.3, further for short $(LiMg)IrO_3$) are new chemical compounds obtained from the Kitaev iridate beta-Li_2IrO_3 by an ion-exchange reaction. We seek to collect neutron powder diffraction data and refine crystal structures of these new compounds. The structural information obtained therein will be essential for understanding the magnetic behavior and, in particular, the possible spin-liquid physics suggested by our thermodynamic measurements on the Cu and Zn compounds. In the case of Mg compounds, it is essential to determine the ratio of magnesium atoms in the two partially occupied positions, as this may shed light on the nature of the structural phase transition in $MgIrO_3$.

Experimental results

For each compound two long scans at the room temperature (300 K) and at the base temperature (BT) of 1.5 K (except for $(LiMg)IrO_3$ at 20 K) were performed at the high-resolution instrument D2B. Based on the obtained data, the crystal structures of $ZnIrO_3$ (**Fig 1**), $MgIrO_3$ (**Fig 2**), and $(LiMg)IrO_3$ (**Fig 3**) were Rietveld refined with Jana2006.

The structure refinement of $ZnIrO_3$ demonstrated an absence of structural disorder and the robust nature of the Ir hyperhoneycomb lattice. The obtained results are in a good agreement with high-resolution electron microscopy data and the refinement of synchrotron powder diffraction data.

There are two different magnesium positions in the structure of $MgIrO_3$. Both positions are partially occupied. The occupancy of the Mg1 position in the octahedra is 0.516(5), the occupancy of the Mg2 position in the tetrahedra is 0.484(5). Both values are almost equal to each other, whereas we could expect a significant change in the occupancies for the high-temperature (**HT**) and low-temperature (**LT**) phases of $MgIrO_3$. In contrast, at BT the ratio between Mg1 and Mg2 only slightly differs from the initial ratio at 300 K, *i.e.* for the **LT** phase the occupancies of Mg1 and Mg2 are 0.516(8) and 0.484(8), respectively; for the **HT** phase the occupancies of Mg1 and Mg2 are 0.407(19) and 0.593(19), respectively.

The crystal structure of $(LiMg)IrO_3$ is similar to the $MgIrO_3$ one and shows partially occupied Mg1 and Mg2 positions, but now containing also lithium atoms. The best fit of the data reveals an almost uniform distribution of magnesium and lithium between the Mg1 and Mg2 positions: 0.377(6) of Mg and 0.379(6) of Li in position Mg1; 0.313(6) of Mg and 0.240(3) of Li in position Mg2.

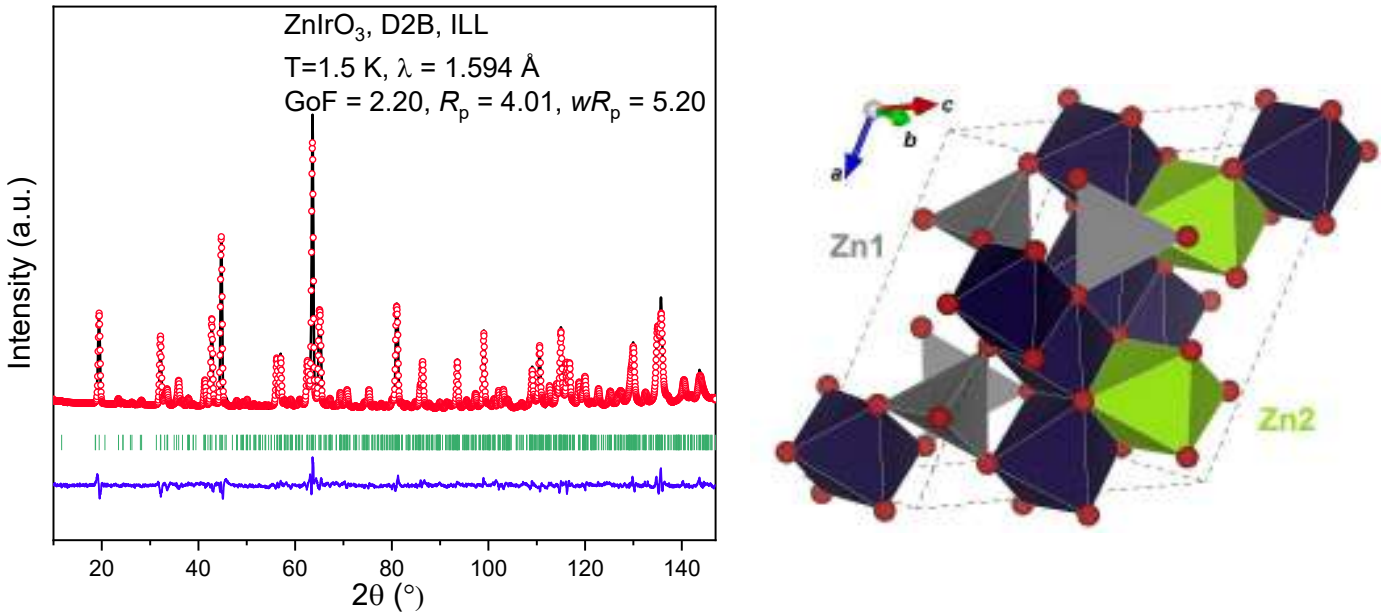

Fig 1. Rietveld refinement of the powder neutron diffraction data (left), and the crystal structure (right) of $ZnIrO_3$. Dark blue octahedra represent the motif of IrO_6 polyhedra, Zn1 positions are labeled by light green octahedra, Zn2 positions are labeled by grey tetrahedra.

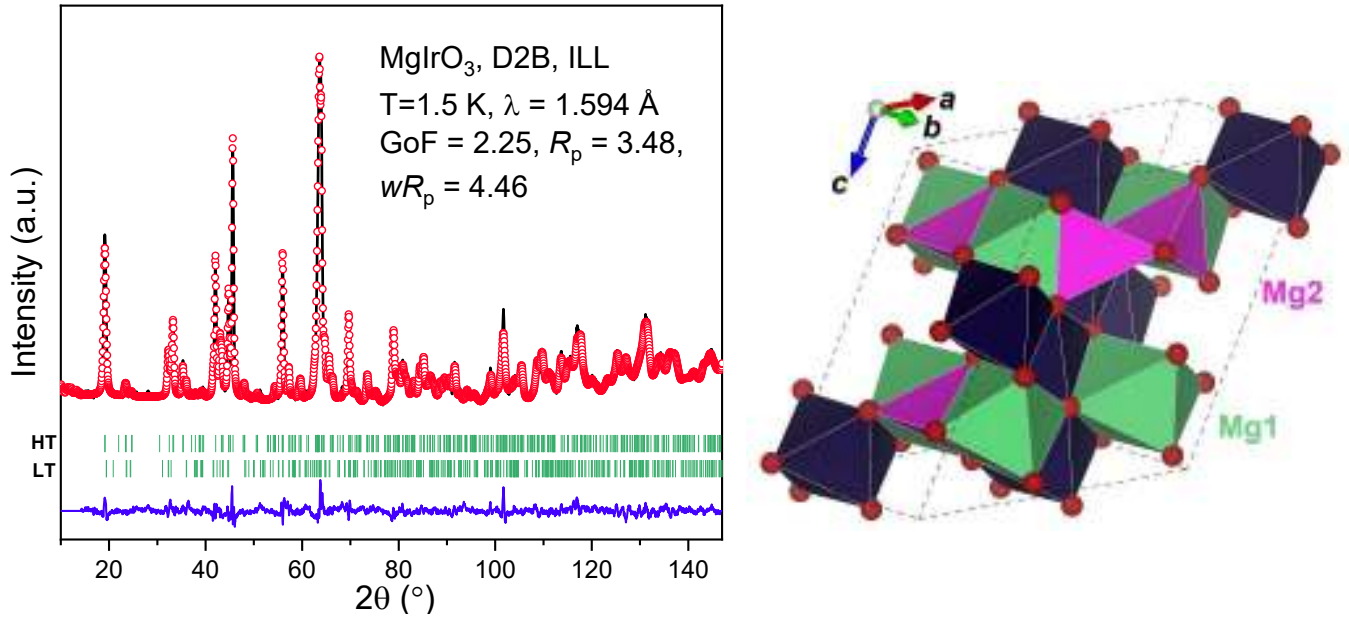

Fig 2. Rietveld refinement of the powder neutron diffraction data (left), and the crystal structure (right) of the low temperature (**LT**) phase of $MgIrO_3$. Dark blue octahedra represent the motif of IrO_6 polyhedra, Mg1 positions are labeled by green octahedra, Mg2 positions are labeled by pink tetrahedra.