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Magnetic and crystal structures of the honeycomb lattice Na_2IrO_3 and single layer Sr_2IrO_4[1]

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5d based iridates have recently attracted great attention due to the large spin-orbit coupling (SOC). It is now recognized that the SOC that competes with other relevant energies, particularly the on-site Coulomb interaction U, and have driven novel electronic and magnetic phases [1-3]. Combining single crystal neutron and x-ray diffractions, we have investigated the magnetic and crystal structures of the honeycomb lattice Na_2IrO_3 [4]. The system orders magnetically below 18.1 K with Ir^{4+} ions forming zigzag spin chains within the layered honeycomb network with ordered moment of 0.22 μB /Ir site. Such a configuration sharply contrasts the Neel or stripe states proposed in the Kitaev-Heisenberg model. The structure refinement reveals that the Ir atoms form nearly ideal 2D honeycomb lattice while the IrO_6 octahedra experience a trigonal distortion that is critical to the ground state. The results of this study provide much-needed experimental insights into the magnetic and crystal structure crucial to the understanding of the exotic magnetic order and possible topological characteristics in the 5d-electron based honeycomb lattice. Neutron diffraction experiments are also performed to investigate the magnetic and crystal structure of the single layer iridate Sr_2IrO_4, where new structural information and spin order are obtained that is not available from previous neutron powder diffraction measurement.

[1] B. J. Kim *et al.*, Phys. Rev. Lett. 101, 076402 (2008).
[2] B. J. Kim *et al.*, Science 323, 1329 (2009).
[3] A. Shitade *et al.*, Phys. Rev. Lett. 102, 256403 (2009).
[4] F. Ye, *et al.*, Phys. Rev. B 85, 180403(R) (2012)

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