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Magnetic and crystal structures of the honeycomb lattice $\text{Na}_2\text{IrO}_3$ and single layer $\text{Sr}_2\text{IrO}_4$\textsuperscript{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 $\text{Na}_2\text{IrO}_3$ [4]. The system orders magnetically below 18.1 K with $\text{Ir}^{4+}$ ions forming zigzag spin chains within the layered honeycomb network with ordered moment of 0.22 $\mu\text{B}$/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 $\text{Sr}_2\text{IrO}_4$, where new structural information and spin order are obtained that is not available from previous neutron powder diffraction measurement.


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