MS19-04 | Crystal Structure and Isotope Effect in Quantum Liquid $H_3LiIr_2O_6$

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The search for realisations of the Kitaev model on a honeycomb lattice has recently led to the discovery of $H_3LiIr_2O_6$, lacking long-range order down to 50 mK and displaying experimental signatures consistent with a spin liquid ground state. Although the Ir-O network and its distortions are fundamental to the bond-dependent interactions on the honeycomb lattice, theoretical work suggests the inter-layer hydrogen and its ordering is crucial to understanding the intriguing behaviour of $H_3LiIr_2O_6$. Upon deuterium substitution, the antiferromagnetic couplings are enhanced but the liquid state remains robust. Structural studies to date have relied on X-ray diffraction which is unable to locate hydrogen / deuterium ions in the presence of heavy iridium, requiring the intuiting of possible positions based on crystal chemistry and knowledge of similar layered materials. Recently we have used the isotope effect on $H_3LiIr_2O_6$ to study the effect of the inter-layer species. In addition, we have taken advantage of recent developments in the use of ^{193}Ir enrichment. The structures of $H_3{}^7Li^{193}Ir_2O_6$ and $D_3{}^7Li^{193}Ir_2O_6$ have been elucidated using high resolution neutron diffraction, allowing the crucial determination of the hydrogen/deuterium positions and studies of disorder. The results of these detailed structural studies and their link to the isotope effect on physical properties will be discussed within the context of recent theoretical work and future materials design.