The investigation of 5d transition metal oxides (TMOs) has resulted in the observation of various novel properties due to spin-orbit coupling (SOC) competition. Compared to the 3d TMO, the 5d system has extended in the electronic wave function radius, which increased the splitting of the $t_{2g}$ manifold. Consequently, a small Coulomb interaction can result in insulating behavior [1]. A common magnetic interaction mediated by a single anion is well established, but the investigation of materials with magnetic interaction through two anions is relatively new [2,3]. Ca$_3$LiRuO$_6$ containing extended superexchange magnetic interactions of a hexagonal Ru-O-O-Ru in the forms of a K$_4$CdCl$_6$-type crystal structure is characterized by neutron diffraction.

Neutron diffraction is a well-established technique to investigate the nature of the magnetic state, quantifying the ordered moment(s) and density of unpaired electrons that constitute the magnetic moments [4]. However, a considerable challenge is faced in identifying the magnetic structure of Ca$_3$LiRuO$_6$ due to the complexity of the crystal structure, atomic position, and magnetic ordering, which results in multiple solutions, i.e., several structures may give similar diffraction patterns. Here, we presented the systematic work of Ca$_3$LiRuO$_6$ magnetic structure determination by FullProf (nuclear and magnetic refinement), WinPLOTR (propagation vector determination), SARAh (magnetic structure determination), Z-Rietveld/Rietan-FP (maximum entropy method refinement) and 3DBVSMAPPER/PyAbstantia (bond valence sum) [5-9].

Reference