



Contribution ID: 66

Type: not specified

Neutron diffraction study of double tungstates $\text{Li}_2\text{M}^{II}(\text{WO}_4)_2$ (M=Co and Ni)

Neutron diffraction study of double tungstates $\text{Li}_2\text{M}^{II}(\text{WO}_4)_2$ (M=Co and Ni)

The isostructural $\text{Li}_2\text{Co}(\text{WO}_4)_2$ and $\text{Li}_2\text{Ni}(\text{WO}_4)_2$ crystallize in the triclinic structure (space group P-1, Z = 1). The crystal structures can be viewed as alternating layers of WO layers and Li-MO layers along the b-axis. The WO layers built up of edge-sharing WO₆ octahedra forming infinite zigzag chains along the a-axis as in many other tungstates. The edge-sharing LiO₆ octahedrons also form infinite chains extending along the c-axis. The divalent ions, Co²⁺ and Ni²⁺, are locating in the octahedral oxide environment, in the mesh forming by crossing LiO and WO chains, isolated from each other. Due to the lack of direct connection of the MO₆ octahedral, the magnetic coupling between the nearest neighboring M cannot through the strong M-O-M superexchange path (SE). Nevertheless the magnetic coupling can be achieved through more complex pathways, which is bridging by the oxygen ions in LiO₆ or WO₆. In $\text{Li}_2\text{M}^{II}(\text{WO}_4)_2$ the weak M-O-O-M pathways, known as super-superexchange (SSE) form complex network with magnetic frustrations, gives rise to complex magnetic behaviors.

The temperature dependent magnetic susceptibility and heat capacity clearly mark the two magnetic transition temperatures of each of the two compounds. In $\text{Li}_2\text{Ni}(\text{WO}_4)_2$ the two magnetic transition temperatures are TN₁ = 12.8 K and TN₂ = 17.5 K, whereas the slightly lower TN₁ = 7.2 K and TN₂ = 9.5 K for $\text{Li}_2\text{Co}(\text{WO}_4)_2$. The magnetic structures have been determined from neutron powder diffraction measurement conducted on Wombat and Echidna at ANSTO. For both compounds the magnetic correlation develops below TN₁, as an incommensurate modulation and the magnetic moments order into commensurate super cells below TN₂. Both compounds possess collinear antiferromagnetic spin configurations in the magnetic order phases. Surprisingly the magnetic unit cells of the two isostructural compounds are different. The magnetic unit cell of $\text{Li}_2\text{Ni}(\text{WO}_4)_2$ is (2a b 2c), and the magnetic moment of Ni²⁺ at 3 K is 1.925 B, roughly pointing along the a direction. Whereas a much larger magnetic unit cell of (2a 4b 4c) is realized in $\text{Li}_2\text{Co}(\text{WO}_4)_2$ below TN₂. Co spins in the {+ + - -} sequence are observed when moving to the neighboring magnetic sites along b and c-axis. The magnetic moment of Co²⁺ is 2.836 B at 5.5 K closely align along the a-axis as well. The different magnetic ground states in the two compounds might be resulted from the slight differences in the crystal structure and magnetic couplings.

Primary author: Dr WANG, Chin-Wei (National Synchrotron Research Center)

Co-authors: Prof. CHOU, F. C. (Center For Condensed Matter Science, National Taiwan University); Dr SANKAR, Raman (Center For Condensed Matter Science, National Taiwan University); Dr KARNA, Sunil (Center For Condensed Matter Science, National Taiwan University)

Presenter: Dr WANG, Chin-Wei (National Synchrotron Research Center)