Magnetic Structure Analysis of $NiPS_{3-x}Se_x$

Mr Mario Lopez[1], Dr Ryan Stadel[1], Dr Efrain E Rodriguez[1]
[1]*University of Maryland*
mlopez95@umd.edu

Using neutron powder diffraction, we report the nuclear and magnetic structure of some nickel chalcophosphate compounds ($NiPS_{3-x}Se_x$) where x = 0.05 - 0.66. We observe a certain disorder where the Ni atoms and P-P dimers "swap" positions. Furthermore, this disorder reduces as more Se is incoporated into the [P2Q6]4- anion. Our rietveld refinemnets indicate that magnetic space group for these compounds could either be PA21/C or PC21/m since the refining parameters are all similar. However, because the largest reflection is indexed as (-110), which is plane that is geometrically more aligned to the c-axis, all our refinements indicate that the magnetic moments have a perference for the c-axis or out-of-plane direction. This result is at odds with current literature that state that the moments are aligned in the ab-plane or in-plane direction. Lastly, all our refinemnts indicate a magnetic moment size decreases as selenium concentration increases.