PONTIFICIA UNIVERSIDAD CATÓLICA DEL PERÚ

ESCUELA DE POSGRADO – MAESTRÍA EN QUÍMICA

Visita del Prof. Dr. Charles H. Lake

Indiana University of Pennsylvania
Department of Chemistry
Indiana, Pennsylvania (EE.UU.)

CONFERENCIA 1

Rietveld Analysis, Spallated Neutrons and Synchrotrons, the Crystal Structure of $Na_2(Zn,Co)SiO_4$

Fecha: Lunes 4 de junio
Hora: 5:30 pm
Lugar: Aula Q-102 (Sección Química)

Resumen

The solid-solution $Na_2(Zn,Co)SiO_4$ was synthesized by standard ceramic methods and investigated as a possible dilute magnetic semiconductor material. The compound possessed a band gap of 1.7 eV, which is clearly in the semiconductor region. Magnetic measurements revealed an antiferromagnetic transition at 5.7 K. X-ray powder diffraction data were collected at the Advanced Photon Source, Argonne National Laboratory. This data was used to elucidate and refine the crystal structure. Rietveld refinement converged to X^2 = 4.06 and R_p = 6.99 %, revealing a distorted tetrahedral structure. Major features left on the difference plot were shown to derive from peak shape issues as determined by a Le Bail extraction. Possible structural effects on the magnetic transition were investigated by collecting low temperature neutron diffraction data with the Orange Cryrostat at the Spallation Neutron Source, Oak Ridge National Laboratory. Neutron diffraction data were collected down to 2 K and revealed a structure transition which may be responsible for the antiferromagnetic transition.