

Koala, a versatile single-crystal diffractometer

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KOALA is a versatile diffractometer for neutron single-crystal diffraction studies on a wide range of applications in chemistry, materials science and physics. Of the many user experiments published from KOALA data, we present two case studies related to materials science and physics.

The $S=\frac{1}{2}$ helical-honeycomb antiferromagnet $\text{-Cu}_2\text{V}_2\text{O}_7$ shows a broad peak in its magnetic susceptibility ~ 50 K followed by an abrupt increase below 33 K, indicative of a phase transition to a magnetically ordered state. Neutron diffraction reveals that $S=\frac{1}{2}$ Cu^{2+} spins are antiferromagnetically aligning with an ordered moment of 0.93(9) B, predominantly along the crystallographic a axis.

The photovoltaic materials MAPbX_3 ($\text{MA} = \text{CH}_3\text{NH}_3$; $\text{X} = \text{Cl, Br, I}$) are widely studied due to their high conversion efficiencies. NMR spectra indicates dynamic reorientation of the MA ion, suggesting tumbling within the perovskite cage with only the amine end of the group interacting with the inorganic network. Single-crystal neutron diffraction was used to refinement all three structures for comparison. In each case, the MA group is disordered and surrounded by halogen ions with anisotropic displacement ellipsoids. However, for the Br and Cl structures small anomalies were observed in the probability density of the lead ions, possibly indicating a ferroelectric-like behaviour or a subtle difference in symmetry.

Level of Expertise

Speakers Gender

Do you wish to take part in the poster slam

No

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