

Abstract Submitted
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Rigid Unit Modes; their energy and temperature dependence with aluminium phosphate ADAM BERLIE¹, The Bragg Institute, ANSTO, YUN LIU, Australian National University, DEHONG YU, GORDEN KEARLEY, The Bragg Institute, ANSTO, CHRIS LING, University of Sydney, RAY WITHERS, Australian National University — One of the problems within crystallography is the concept of the average structure where due to dynamical translations or librations the structure is not truly static. This type of behaviour is common within polyhedral based compounds such as AlPO_4 where, in this case, the rigid tetrahedra can move or tilt with respect to each other as a consequence of the instability of the 180° Al-O-P bond. We explore the energy and temperature dependence of these modes using inelastic neutron scattering and heat capacity measurements as well as using computational modelling to assign the observed behaviour to these rigid unit modes.

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