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Role of correlated disorder on lattice dynamics in negative thermal expansion material, Cadmium Cyanide.

Cubic cadmium(II) cyanide is amongst the most important isotropic negative thermal expansion (NTE) materials, with behavior more than twice as extreme as that of better known systems such as ZrW_2O_8. We investigate the relationship between the geometrically frustrated orientational order of the molecular CN^- anion the system's lattice dynamics. Inelastic neutron scattering (INS) is reported on the system approaching the cyanide order-disorder transition from above and displays non-trivial mode-softening over a wide range of temperatures associated with the correlated cyanide order. The simulation of lattice dynamics in systems with correlated disorder is involved: supercell lattice dynamics (SCLD) are used for simulations on a simple model system. Simplifying approximations are investigated towards the goal of reproducing the INS measured, and understanding the significance of correlated disorder in the NTE mechanism.

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