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Jumping molecular crystals: the role of molecular vibrations

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While we are familiar with the concept of the conversion of thermal energy to mechanical work, there is a little known class of materials known as thermosalient or jumping crystals which can spectacularly turn a small temperature change into a high speed leap, many times their own length.
These materials might lead to some exciting new options for the creation of microscopic machines. The jumping and other movement is usually associated with a rapid single crystal-single crystal phase transition. Unfortunately the confusing mix of explanations in the literature shows that this phenomenon is poorly understood, which hinders the crystal engineering required to explore technical applications.
The classic approach in studying such materials is to use diffraction to determine the crystal structure, however vibrational spectroscopy can be used to complement this information particularly from a dynamical aspect, revealing more about the nature of the phase transition.
In this presentation I will present a case study on the newly discovered jumping crystal, nickel dithiocarbamate (Ni:DTC). I will briefly outline the current thinking on SCSC phase transitions in molecular crystals. Measurements of phonon and intramolecular vibrational modes from the THz – Far Infrared beamline using the variable temperature cryostat will be presented. Interpretation was guided with Crystal17 modelling using periodic density functional theory so lattice modes could be calculated. Calculations were based on structures determined by single crystal diffraction.

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