THz Raman spectroscopy to probe lattice dynamics and phase transitions in molecular crystals

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Micro-Raman spectroscopy in the THz region is a powerful tool for the study of crystal packing, polymorphism and phase transitions of molecular materials. The intermolecular vibrations (lattice phonons), occurring at THz frequencies, reflect the intermolecular interactions and unit cell symmetry. The use of polarized light on oriented single crystals also gives phonon symmetry species, associated with directional information on the molecular displacements involved.
Approaching phase transitions, the role of lattice dynamics occurring along different directions can thus be assessed separately, revealing the mechanism of the transition. This methodology was successfully applied to molecular semiconductors showing ordered smectic mesophases. The mechanism of the transition from crystal to liquid crystal was reconstructed combining the separate temperature evolution of interlayer and in-plane polarized phonons.