The response of ROY polymorphs to high pressure

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The 'ROY' family of polymorphs that describe the organic molecule 5-methyl-2-[(2-nitrophenyl)amino]-3-thiophenecarbonitrile, encompasses at least 10 crystallographically-distinct forms adopting colours on the red → yellow region of the visible spectrum. The molecule exhibits flexibility about a torsion angle relating its cyclic endgroups where conjugation between these gives rise to its strong colouration (Figure 1).[1] Thus all the different forms are also conformational polymorphs. An additional complicating factor in its phase behavior is the simultaneous appearance of numerous polymorphs on crystallization. Its unusually complicated phase behavior has led to it becoming a model structure in computational structure prediction and crystallization control studies.[2]

Despite the wide attention the ROY system receives, the influence of non-ambient conditions on its structure remains relatively unknown. This, coupled with the propensity for pressure to drive transitions, probe energy landscapes, and manipulate intramolecular geometry where flexibility exists, led us to investigate the structures of members of the ROY family at high pressures and low temperatures.[3,4]

This talk will detail single crystal and powder experiments using X-ray and neutron diffraction on some of the ROY polymorphs. We show that careful DFT-assisted guidance of the refinement procedure produces usable structural models from limited data sets. From these models, we discuss the structural responses seen in the context of lattice- and intermolecular-energy calculations.

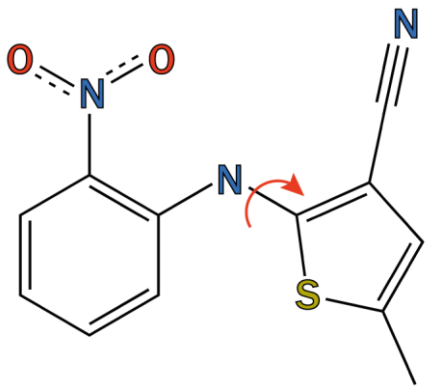

Figure 1. The molecular structure of ROY. The flexible SCNC torsion is indicated by the arrow.

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