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Synchrotron light source to aid where traditional SCD experiments fall short

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The discovery of actuating materials, or materials that respond to external stimuli (light, heat, pressure etc.) has shed light on an entirely new area for exploration in the fields of crystal engineering and the chemistry of the solid state. Many of these actuating responses coincide with some sort of phase transformation or solid state reaction. Although the mechanisms of the transformations that result in the photosalient effect are fairly well understood, very little is known about the thermosalient effect and its causes.

Work done on 4-(dimethylamino)-benzonitrile (DMABN) showed a thermosalient event by hot stage microscopy (HSM) upon cooling at 240 K and the reverse upon heating at 290 K. DSC traces and VT-PXRD confirm this phase change. Additionally, cooling below 182 K showed crystals rolling under HSM, and a small change in the PXRD pattern appeared. However neither single crystal diffraction (SCD) nor DSC showed any indication of an event or change. A recent study by Klaser et al. suggested that, potentially, the thermosalient event may not have to correspond to a phase change but may simply be due to thermal expansion.1 However, when comparing the changes in the PXRD patterns collected from DMABN to the PXRD patterns corresponding to thermal expansion in the study by Klaser, it appears to be more than just thermal expansion. Due to methods employed to prevent a thermosalient crystal from jumping off the mount for a SCD experiment, solving the structure from VT-PXRD data may be more useful to elucidate the structural change causing the thermosalience.

Another area where conventional SCD instruments present limitations, however powerful modern ones have become, is the size of the incident X-ray beam. On an Incoatec microfocus IμS 3.0 source, a beam size of about 110 μm (Mo) can be expected. When trying to focus the analysis on a small area of a crystal, for example the bent area of a plastic/elastic molecular crystal, the beam is still too large to isolate studies on that area alone. In light of the above, we hope that the capabilities provided by a synchrotron light source may aid where traditional SCD falls short.

1 T. Klaser, J. Popović, J. Fernandes, S. Tarantino, M. Zema and Ž. Skoko, Crystals, 2018, 8, 301.

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