

"Structural DSC - exploiting time-resolved powder diffraction"

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Differential Scanning Calorimetry (DSC) is a powerful technique for the rapid identification of the number of polymorphs in a given sample of a pharmaceutical material. In a matter of minutes, DSC provides basic thermodynamic information that allows the determination of the temperatures of melting, dehydration and of polymorph transformations. While this knowledge is important, it is minimal in its information content compared, for example, with a full crystallographic knowledge of the molecular conformation and crystal packing of a pharmaceutical compound. It would therefore be highly beneficial to be able to monitor the temperature evolution of the crystal structure of a material at the speed of differential scanning calorimetry. Ideally, it should be possible to provide a good quantitative phase analysis and even attempt a low-resolution structure solution from high resolution X-ray powder diffraction patterns that have been collected in minutes rather than hours.

In this presentation, we discuss initial results of rapid high resolution diffraction measurements obtained from the ID31 powder diffractometer at the ESRF, Grenoble. These measurements allow us to determine the evolution of polymorphs and their structural variation as function of temperature. This structural DSC (Differential Scanning Crystallography) offers valuable additional complementary information to standard DSC.