Getting the most out of your high pressure experiments!

Michael Ruf, Bruker AXS Inc., Madison WI, USA

Traditionally, high-pressure crystallography has been associated with the study of rocks and minerals from within the earth's crust. More recently, pharmaceutical development has benefitted from organic solid-state chemistry and its perspectives on structure and function in biologically-relevant molecules, with polymorphism being of critical importance. Of growing interest is the effect of pressure on drugs, since many solid drugs are exposed to mechanical manipulation during manufacturing.
The increased interest in high-pressure crystallography for the home lab has prompted the development of high-performance software solutions that address its particular challenges, elevating high-pressure crystallography into a powerful method that can be routinely used on modern diffractometers, such as the D8 QUEST or the D8 VENTURE.

We will report on an experiment, where advanced processing methods for Diamond Anvil Cell (DAC) data were put to the test, to produce results comparable in quality to standard single-crystal data, using the less common monoclinic polymorph of the sulfonium ylid.

The second experiment will address one of the challenges of high-pressure experiments: the limited accessibility of reciprocal space caused by geometrical limitations. Especially for lower-symmetry samples, the smaller number of available reflections can reduce the structure quality dramatically. Recent enhancements in hardware and software design have brought significant improvements in data acquisition and data processing quality both for high-pressure and multiple-domain-sample experiments. Here we explore a method for increasing the completeness of high-pressure experiments by mounting multiple samples in a DAC and measuring and processing data concurrently.