**MS27-2-4 Estimating completeness in single-crystal high-pressure diffraction experiments**
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**Abstract**
The invention of Diamond anvil cell (DAC) has revolutionised many fields of science by providing a way to introduce high pressure (HP) while keeping the sample accessible to radiation. [1] Any decent single crystal can be encased inside a DAC, pressurised, and investigated by the means of X-ray diffraction (XRD) without a need for additional equipment or software. Structure factors collected in this way can be used to identify and solve numerous crystal structures, but their quality and quantity are never quite on par with even routine ambient-condition experiments. [2–6]
The geometry of a modern symmetrical DAC can be described using just a single parameter called the opening angle. Anvil cells commonly feature an opening angle of 35° or less, rendering up to 97% of otherwise collectable reflections inaccessible to the XRD experiment. Consequently, diffraction patterns collected in HP conditions are routinely incomplete, especially so in materials with low internal symmetry, which as a result are under-represented in HP studies. [7] Furthermore, this limitation affects the applicability of quantum-crystallographic techniques, as they often require abundant information on the reciprocal space. [8–10]
The above issue can be circumvented in two different ways: either by merging datasets collected on multiple crystals or by utilising the inherent symmetry of one crystal. The first approach, while innately simpler, requires special infrastructure such as well-focused incident beam or a gas membrane cells to avoid merging problems. [11,12] Meanwhile, the other solution calls only for a precise control over crystal orientation, which to some degree can be performed in any laboratory. [13]
In present work, a potency – maximum attainable completeness of collected data – was numerically calculated as a function of crystal orientation, DAC opening angle, resolution, and incident radiation wavelength. Static figures and tables describing the most common experimental set-ups were prepared and general conclusions were drawn. Crystal orientation was found to influence the potency far more than the opening angle or wavelength. In particular, it was shown that an unfortunately placed cubic sample can offer lower percent of data than a well-oriented crystal belonging to the orthorhombic system.
The exact values of potency vary between individual anvil cells and samples. In order to easily evaluate every diffraction set-up and predict best experimental strategies in each case, a dedicated python library was prepared. [14] A web-server “hikari-toolkit” was launched to allow every user to easily calculate the potency of their experimental set-up with ease.

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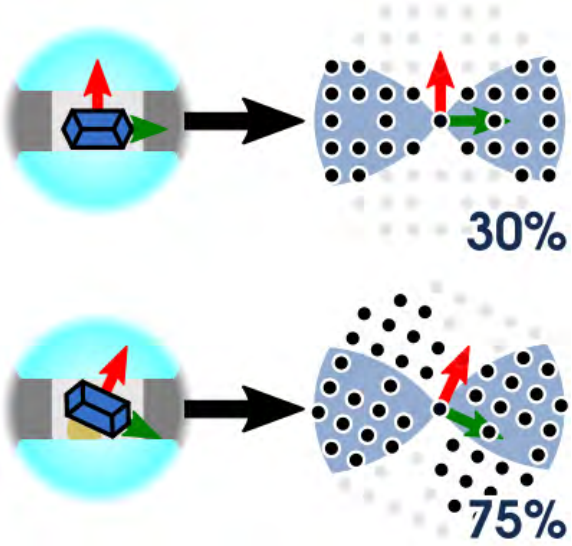
Crystal orientation affects potency in HP XRD




Potency as a function of crystal orientation