

Supplementary Material

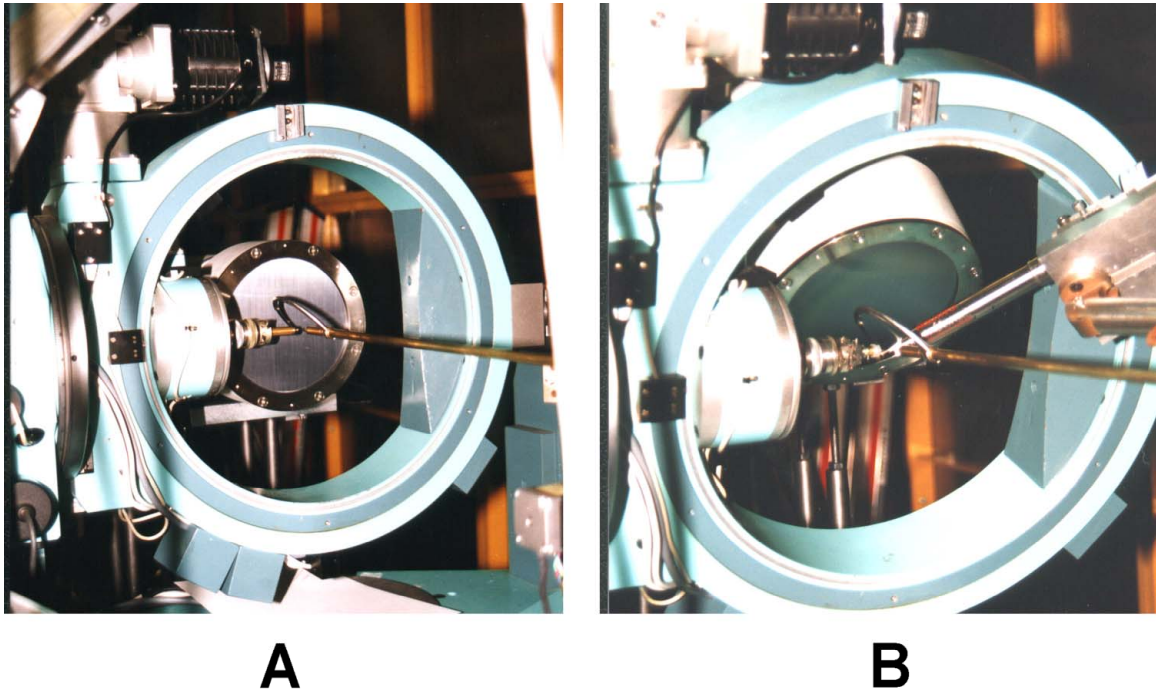


Figure S1: The experimental setup for the data collection at beamline PETRA1. A main element is the Huber six-circle goniometer. The thin brass tube from the right is the collimator delivering the beam, with a beamstop mounted on an arc. The CCD detector could be mounted in two positions, face-on (A) and with 45 degree inclination (B). In (B) the cryostat is visible (diagonal from top to right). Also, the χ -circle had to be rotated in order to accommodate the detector.

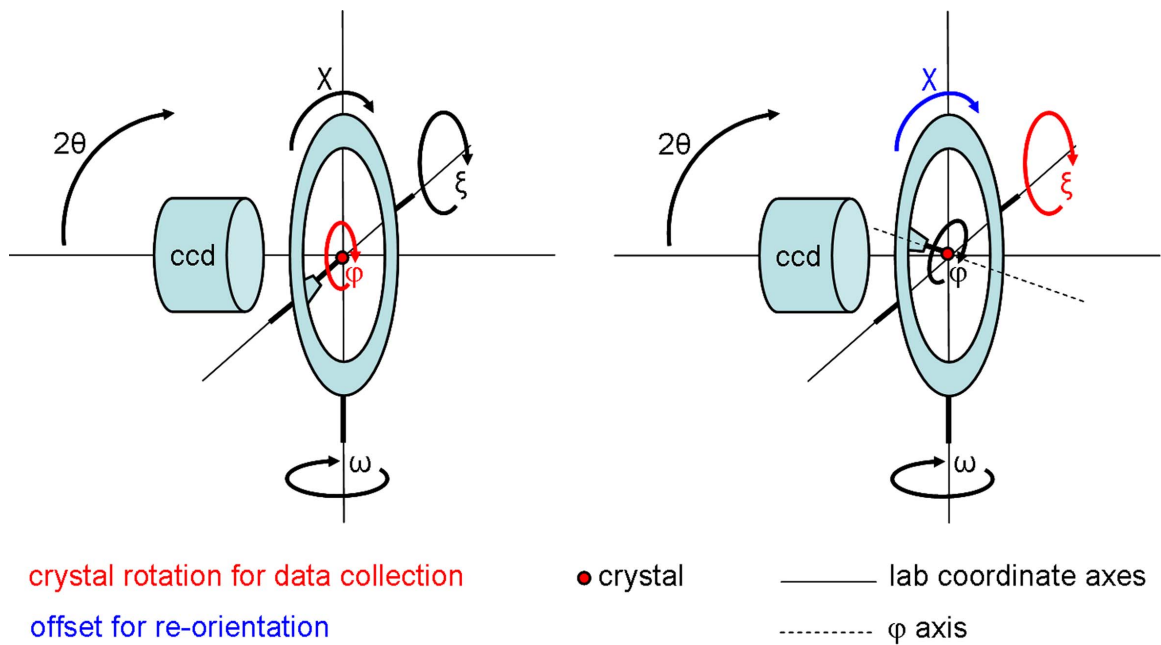


Figure S2: Schematic of the data collection setup at beamline PETRA1 (see also figure 4) with some of the rotation axes indicated. Re-orientation in kappa-fashion was impeded by the bulky χ circle and the cramped crystal environment. The 2θ setting was mimicked by mounting the detector inclined by 45 degrees, since normally that circle is in the horizontal plane.