High Pressure Single-Crystal Neutron Diffraction of DKDP

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The initial results of a new initiative of the Paris-Edinburgh (PE) collaboration to develop single-crystal technology for high-pressure neutron diffraction are presented. Single-crystal neutron diffraction data have been collected from D_2KPO_4 at pressures up to 7.5 GPa. At 4.2 GPa it has been suggested by Endo [1] that the hydrogen bond lengths elongate and the proton centres in a single minimum between the two oxygen atoms. However, these results were obtained using x-rays which are insensitive to the scattering of light atoms and hence neutron diffraction data on a single crystal sample are essential in determining precisely the atomic co-ordinates during this possible transition. Previously only data up to 2.0 GPa have been collected using single crystal neutron diffraction. We present structures determined from a single crystal of 4 mm^3 using time-of-flight Laue diffraction on the SXD instrument at the ISIS Facility at Rutherford Appleton Laboratory in the UK.

[1] Endo S. et al, *Nature*, **340**, 452, 1989.

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