

Pressure-induced localisation of the hydrogen-bond network in KOH-VI
Dataset

This data repository is organised as follows:

Figure-Data: contains the information used to produce the figures - either crystallographic information for structures that were shown, or data sets used to create the figures.

Neutron-Data: contains information on how to obtain the neutron diffraction pattern shown and refined in Figure 4.

VASP-Inputs: exemplary input files for structural optimisation of the various KOH phases, here for the I4/m phase at P=10GPa.

Andreas Hermann
a.hermann@ed.ac.uk
December 2015