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Proton Dynamics in Potassium Dihydrogen Phosphate (KDP) at Pressures up to 2.5 GPa by Inelastic Neutron Scattering

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In the crystal structure of KDP (KH2PO4) the phosphate tetrahedra are linked together by a net of O-H-O hydrogen bonds. At ambient pressure and temperature protons are disordered in a two-minimum potential along the bonds. At a temperature of 123 K a ferroelectric phase transition takes place related to the locking of protons in one of these two energy minima. We used inelastic neutron scattering to follow pressure and temperature variation of bond-stretching and bond-bending vibrations of hydrogen. A compact high-pressure cell of a generic "piston-cylinder" type has been designed in order to make use of a special scattering geometry of the neutron spectrometer IN1-Lagrange at ILL with large solid angle open for scattered neutrons. The most informative energy range for hydrogen bond vibrations stays above the vibration range of the cell materials what makes the consequences of trade-off on sample volume and attainable pressure experimentally less penalising. The proton vibration spectra in KDP up to quasi-hydrostatic pressures of 25 kbar and temperatures around the phase transition have been recorded and analysed in the model of double-well interatomic potential with varied oxygen-hydrogen distance.

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