MS15-P15 | IN-SITU SINGLE CRYSTAL X-RAY DIFFRACTION STUDIES OF PROTON TRANSFER BEHAVIOUR UNDER AN APPLIED ELECTRIC FIELD ON I19, DIAMOND LIGHT SOURCE

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Hydrogen atoms (H-atoms) can exhibit the chemical phenomenal of transfer behaviour when part of a hydrogen bond (HB). This behaviour occurs related to the shape of the potential energy surface for H-atom motion for certain types of hydrogen bonds. Depending on HB characteristics, this transfer may be susceptible to external stimuli, such as temperature or pressure [1]. In ferroelectrics, proton shuttling may occur under an applied electric field facilitating the reversal of material polarity [2] or transitions between electric (ferro-para) states [3]. Materials such as these are of interest offering applications in sensing and data storage.

The electric properties of materials are typically determined from measuring dielectric constants [4] or polarisation-electric field loops [5] whilst structural effects can be elucidated using Bragg peak mapping [6]. In this work, we showcase a new electric field set up on I19, Diamond Light Source (U.K.) for in-situ single crystal X-ray diffraction measurements allowing full structure elucidation under an applied field. We describe the set-up and explore its potential in the study of proton transfer behaviour with the aim of discovering new candidates for electric field applications.

[1] D.M.S.Martins *et al.*, *J.Am.Chem.Soc.*, 2009, **131**, 3884-3893.
[2] I.A. Abronin, I.A.Koval'chuk and V.P.Sakun, *Russ.J.Phy.Chem.B*, 2016, **10**, 357-359.
[3] Z.-S.Yao *et al.*, *J.Am.Chem.Soc.*, 2016, **138**, 12005-12008.
[4] S.Horiuchi *et al.*, *Nat.Mater.*, 2005, **4**, 163.
[5] S.Horiuchi, R.Kumai and Y.Tokura, *J.Am.Chem.Soc.*, 2013, **135**, 4492-4500.
[6] H.Choe *et al.*, *J.Appl.Crystallogr.*, 2017, **50**, 975-977.