[MS33-04] Pressure-induced polymorphism in small molecule acrylic acids. Ian B. Hutchison, Amit Delori, Iain D.H. Oswald.

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Polyacrylic acid (PAA) and polymethacrylic acid (PMA) are used in a wide range of research and industrial applications, ranging from superabsorbent materials to drug delivery vehicles. Traditionally PAA and PMA are synthesised using both thermal and photo polymerisation methods from the corresponding monomers acrylic and methacrylic acid. Over the past ten years, Raman spectroscopy has been used to investigate the polymeristion of simple unsaturated compounds such as acrylamide,[1] and ethylene[2] through the application of pressure. Further studies have investigated the effect of pressure and laser irradiation on compounds such as acetylene, butadiene and propene.[3] Recently Murli and Song used Raman Spectroscopy to investigate the application of pressure to a monomer capable of hydrogen bonding, acrylic acid. The induced initiator-free polymerisation of acrylic acid was investigated by compressing pure acrylic acid to approximately 8 GPa.[4] They observed two crystalline phases (I and II) of acrylic acid with Phase I representing a low-temperature configuration whilst Phase II was suggested to enhance molecular interactions towards polymerisation, albeit that they did not determine the crystal structure for this phase. Murli and Song stated that 'In-situ high-pressure X-ray or neutron diffraction measurements would be helpful to monitor the changes in bond lengths of acrylic acid as a function of compression…'4 Previous work by the group has characterised the crystal structures acrylic acid (A) and its derivative methacrylic acid (B) under high-pressure conditions using X-ray single-crystal diffraction in order to provide further insight into this system.[5] High pressure polymorphs of both compounds were characterised but further insight into the pressure behaviour of these two molecules has been investigated using neutron diffraction. Herein we present the results of this study.

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