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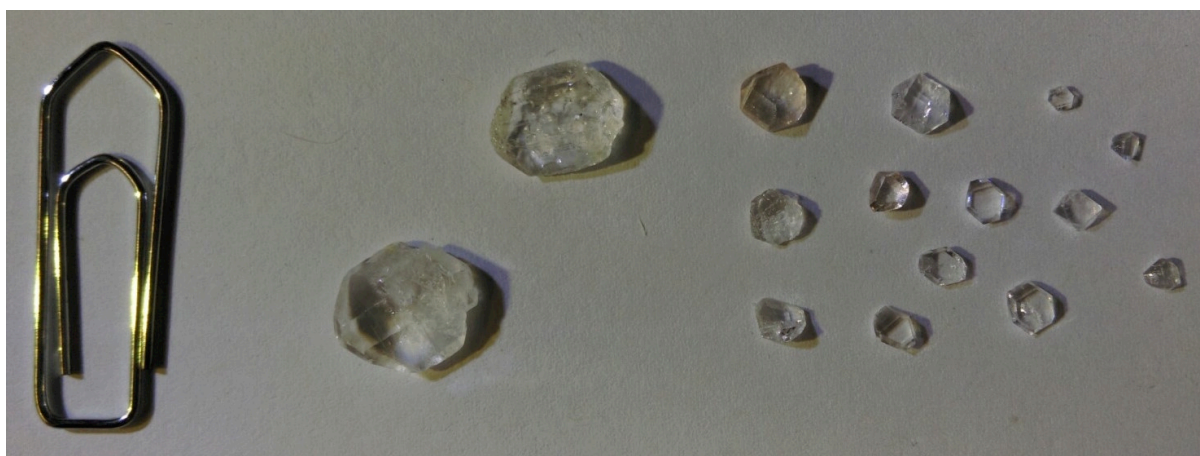


Figure S1 Crystals of HacacPy, **1** cover a wide range of sizes.

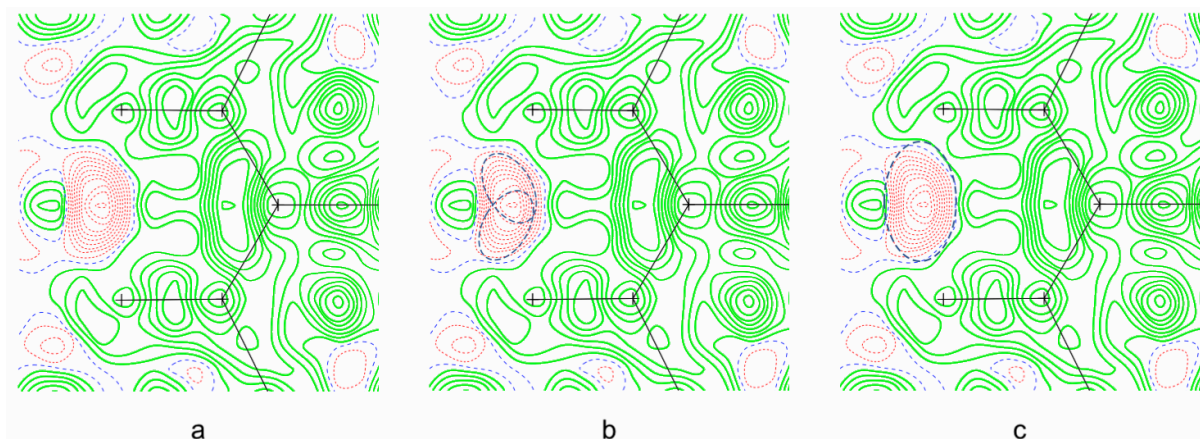


Figure S2 Difference nuclear density plot for **1α** before inclusion of the bridging H atom, and its alternative interpretations as superposition of disordered (b), or as ordered (c) arrangement. Contour lines have been drawn at $0.05 \text{ fm}\text{\AA}^{-3}$.

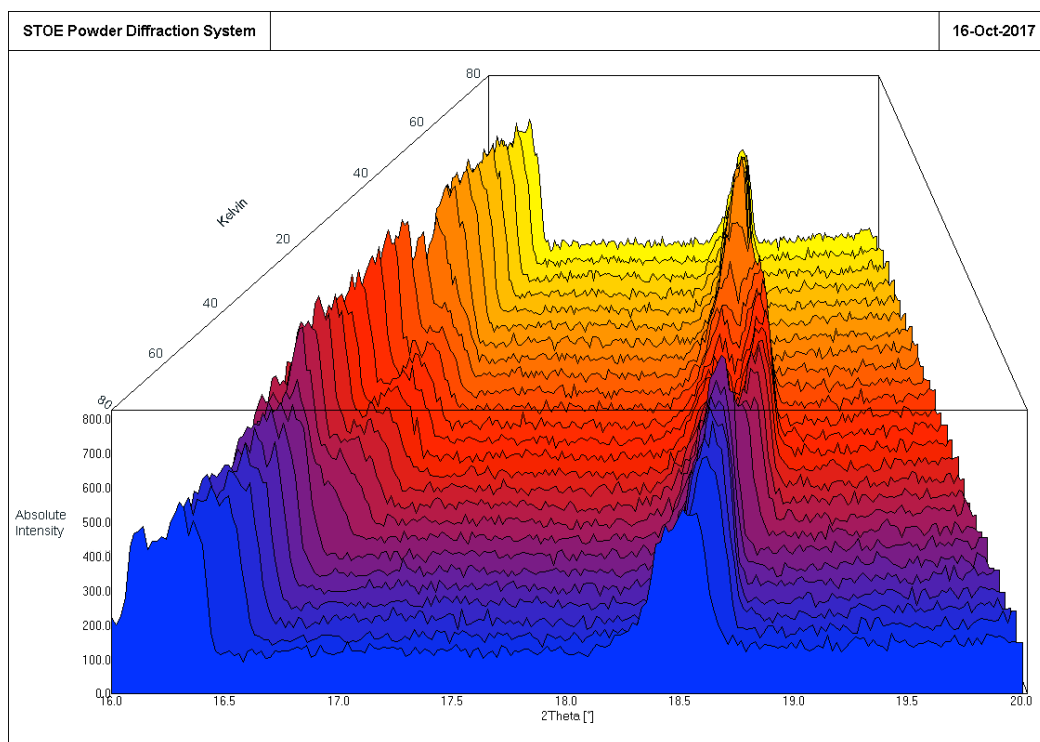
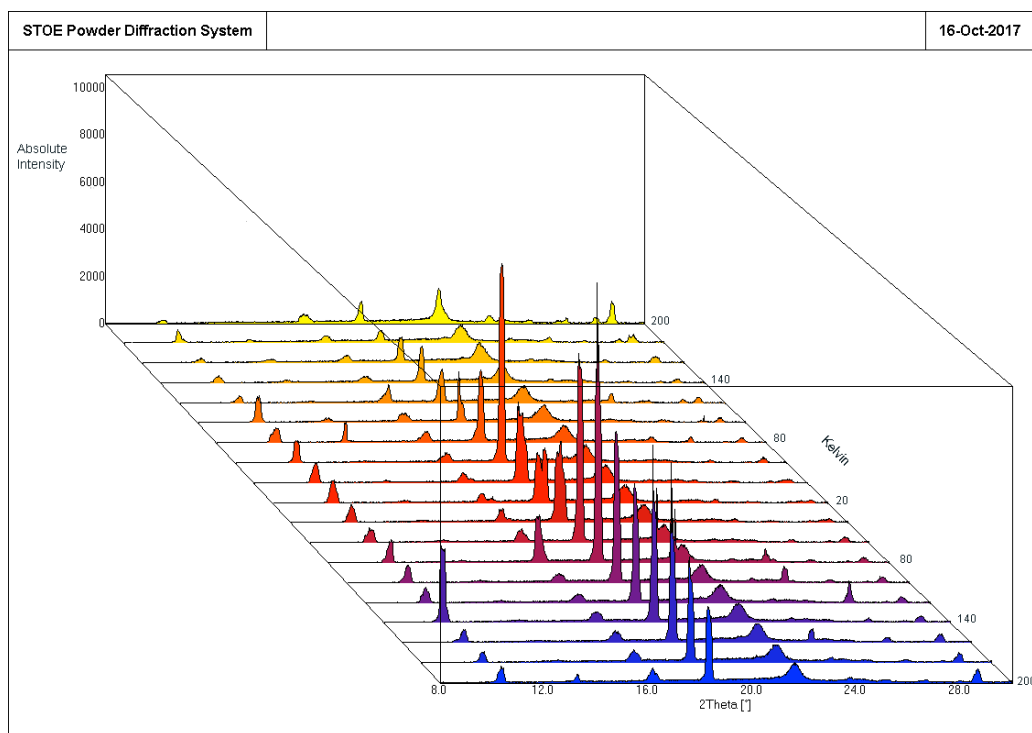
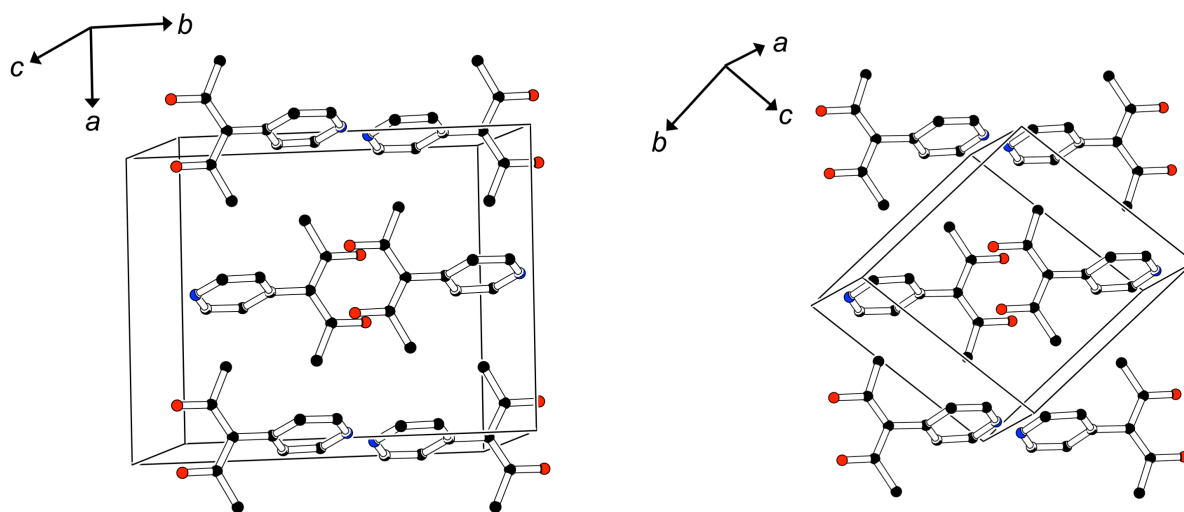


Figure S3 Variable temperature powder diffraction results for **1**. Diffractograms have been collected at temperature intervals of 20 K (top) and 5 K (bottom); in either case, a series of experiments first at decreasing and then at increasing temperature was performed.



Packing diagrams for **1 α** (left) and **1 β** (right) show the close relationship between the structures

Figure S4 Packing diagrams for **1 α** and **1 β** .