# Rietveld Refinement of organic molecules: investigation of hydrogen-bond patterns

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Over the past decade, organic molecules of increasing sizes are being solved from powder diffraction data using either direct methods or direct space methods. The quality of the diffraction data attained places the limit on the complexity of the structure to be solved. But when size of the molecule is not the critical issue, powder diffraction techniques can still address interesting structural problems of different nature. In this talk, examples of such applications will be discussed here using x-ray powder diffraction data collected on beam line ID31 at the ESRF. We will show the versatility of situ temperature controlled powder diffraction experiments to follow changes in the molecular conformation and the H-bond patterns of hydrate amino acids as they transit from room temperature to dehydration, melting and decomposition. We will also show the solution of the crystal structures of two N,S pro-ligands being used in biomimetic inorganic chemistry for the synthesis of “green” catalysts.