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MS10 H-bonding & weak interactions in crystals: neutrons and X-rays

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MS10-O1 Nanoscale hydrogen bond network revealed by neutron scattering

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Neutron science is the science of everyday life, providing a microscopic view of the materials we rely on for modern life. Neutrons, similarly to X-rays, penetrate matter. However, unlike X-rays, neutrons interact with matter in a different manner, thus allowing the identification of elements with very low molecular weight, including hydrogen. Thus while X-rays is one of the most important characterization methods in solid state chemistry and materials science, neutron diffraction is more commonly used to provide information on proton distribution within the structure. For this reason, both X-rays and neutron diffraction, complemented by neutron spectroscopy, which brings information about hydrogen mobility, can contribute for better understanding of complex structures. In this talk I will discuss on this promising approach by presenting a couple of specific examples. The first is related to a number of differences in the structural and dynamical behavior of D-alanine when compared to L-alanine^[1] and the second to the interplay of molecular flexibility and hydrogen bonding manifested in the polymorphs of paracetamol.^[2] Finally I will give a brief overview in how this approach can extend to the study of highly intricate pore structures.^[3]

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