Neutron Laue diffraction allows for rapid data collections of crystalline molecular species using modestly sized samples. As such, the technique allows for systematic studies of hydrogen-bonding supramolecular systems to take advantage of the accurate hydrogen atomic position afforded by neutron scattering. Several systems will be highlighted for which neutron diffraction has provided valuable insight.

- Water squares holding together octahedral coordination complexes provide strong hydrogen bonding that causes axial distortion of the coordination sphere. Determination of the hydrogen positions showed a distortion of the complex and provided the basis model for calculations of the hydrogen bond strengths [1].

- Nitrile groups (R-C≡N) are not typically considered to be strong hydrogen bond acceptors. A systematic study has shown the orientational preferences of donor groups around the nitrile acceptor [2].

- Triazinones are good building blocks for supramolecular systems, acting as both hydrogen bond acceptor/donor species that are analogues of di-substituted urea. The substituent at the nitrogen can play a significant role in affecting the planarity of the ring system and the positions of the NH donor groups [3].

- Oxime/oximate systems have been studied in which the anionic form is isolated alongside the neutral molecule with an apparent shared proton. The hydrogen position can be determined by neutron diffraction and lies close to, but not at, the midpoint between the two oximate sites and therefore represents a highly unusual hydrogen bond.

![Figure 1](image-url)  
*Figure 1. A water square between octahedral complexes (left) and a hydrogen-bonded oxime system (right).*

