Neutron cryo-crystallography: methods, applications and challenges

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Neutron crystallography is an important complementary technique to X-ray crystallography since it provides details of the H-atom and proton positions in biological molecules and from crystals that are free from radiation damage. Historically, the use of neutron crystallography was limited because very large crystals of several cubic millimetres were required, due to the low fluxes of even the most intense neutron sources. In more recent years however, crystal volume requirements have been reduced via the use of new and improved neutron instrumentation, and the creation of dedicated deuteration facilities for the production of perdeuterated samples. These developments now allow crystals with volumes from ~0.1 – 1 mm^3 to be used for high-resolution neutron diffraction studies of biological macromolecules with unit-cell edges from ~ 50 - 150 Å, respectively [1]. Nevertheless, further reductions in crystal volumes are certainly required before the application of neutron crystallography can become commonplace. In this talk I will speak about progress in the development of neutron cryo-crystallography, which until recently had been rarely attempted [2, 3] and yet can allow smaller crystal volumes to be used than at room temperature, and permit a wider array of studies to be performed, such as cryo-trapping studies of enzyme reaction intermediates [4].

[1] Blakeley *et al.,* (2015) *IUCrJ* **2(4)**, 464-474.

[2] Blakeley *et al.,* (2004) *Proc. Natl. Acad. Sci. U.S.A.*, **101(47)**, 16405-16410.

[3] Myles *et al.,* (2012) *J. Appl. Cryst.*, **45(4)**, 686–692.

[4] Casadei *et al.,* (2014) *Science*, **345(6193)**, 193-197.