Diffuse Scattering in Small Molecule Crystallography and Beyond.

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Diffuse scattering has been known and studied since the earliest days of X–ray crystallography over 100 years ago but has largely remained the realm of a relatively few specialist research groups because of its generally very low intensity and the diversity of effects that can give rise to it. Diffuse scattering occurs in the diffraction patterns of all real crystalline materials from the simplest, (e.g. NaCl), to the most complex macromolecules (e.g. proteins). Despite much early interest and research (e.g. the first issue of Acta Crystallographica in 1948 contained numerous articles on diffuse scattering [1,3]) progress in the development of the field was slow, particularly at a time when enormous advances were being made in conventional crystal structure determination.

With the advent of synchrotron sources, latest high-resolution and high dynamic range X-ray pixel detectors and powerful computers for analysis and modelling, the problems that limited development of diffuse scattering methods have now largely been solved for small molecule crystallography. With current methods virtually any disorder problem can be tackled to yield details of structure and dynamics that goes far beyond the confines of the average unit cell description of structure [4, 5].

We have been involved in the development of methods for recording, interpreting and analysing diffuse scattering for approximately 50 years. In this talk we describe the advances that have been made in analysing diffuse scattering in small molecule crystallography during this time with a view to informing the development of methods in macromolecular crystallography in which there has been a resurgence of interest in recent years [6,7].

References

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