Structure Solution of Pharmaceutical Compounds from Powder Diffraction Data

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A significant part of contemporary medicine is based on the discovery and development of drugs, which are often molecules of ten to thirty non-hydrogen atoms. It is important to know the crystal structures of drug compounds and candidates for various reasons: fundamental understanding of structure and bonding vis-à-vis physiological action, the physical and chemical properties of polymorphs which are frequently encountered in drugs, and the relevance of polymorphism to patent protection and limits thereon. As it happens, many of these materials are available only as powders, and therefore any structural information must be obtained from powder diffraction.

Advances in instrumentation and data analysis techniques, both commercial and in the public domain, are proving equal to the task. However, judging from the literature, structure determination from powder data SDPD is still an obscure art, practiced by relatively few crystallographers. This is despite the outreach activities of a significant number of the innovators of SDPD, who have been working to develop and promulgate powder techniques.

I will review the state of the art and present some new results, such as the structures of chloramphenicol palmitate polymorphs.

Keywords: ab-initio powder structure determination, pharmaceutical structure determination, polymorphism