

MS50-O2 Crystallography in the Courtroom

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Over nearly the last twenty years there has been a major increase in the awareness of the intellectual property implications and manifestations of the existence of multiple solid forms (polymorphs, solvates, hydrates and amorphous) of commercially important materials (e.g. pharmaceuticals, pigments, high energy magterials), due in part, at least, to a number of high profile litigations involving some leading pharmaceutical products. The prosecution of these litigations involves the recruitment of expert witnesses, who are called by the opposing sides to inform the court of the scientific principles issues in the legal conflict as well as to provide evidence in support of the party that has retained them. Due to the nature of the subject matter, many crystallographer have been retained as witnesses. The scientific subjects often deal with fundamental questions on the definition of chemical and physical terms, the precision, accuracy and interpretation of various analytical methods employed in the identification and characterization of different crystal forms, and the similarities and differences in the *modus operandi* of scientists and lawyers. Quite often colleagues and friends can find themselves on the opposite sides of a courtroom, due to differences in scientific opinion or interpretation of data involed in the litigations. These discussions frequently involve legitimate differences in scientific opinion with the courts left to decide either on which side is "right", or perhaps which side is most convincing. A number of examples of these litigations will be described and discussed.

Keywords: patents, litigations, polymorphs, crystal forms, expert witnesses

MS50-O3 Absolute structure

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The presentation will cover the history, development and current best practices in the treatment of non-centrosymmetric crystal structures. A full text on this subject was prepared for the International Year of Crystallography (Flack, 2014).

The origins of absolute-structure determination, starting from Friedel's 1913 proof that the intensities of the opposites hkl and $-h-k-l$ are identical, are traced. The important structural principles derived from the study of chiral, but pseudo-mirror symmetric, methpyrylon are described. For the present time, the use of the average and difference intensities of the opposites hkl and $-h-k-l$ are stressed. This leads to the use of *Friedif*, $2AD$ and selected D plots, of R_{merge} and the D -Patterson.

Flack, H. D. (2014). *Chimia*, **68**, 26-30.

Keywords: Absolute configuration, Absolute structure, Flack parameter, Resonant scattering