

W0213

An Elementary Approach for Determining Small Molecule Twinned Crystal Structures. James C. Fettinger, Chemistry, Univ. of California, Davis, Davis, CA 95616 USA.

An elementary and pseudo-straightforward procedure will be demonstrated for the determination and elucidation of small molecule twinned crystal structures. A series of examples will be shown implementing the SHELXTL suite of programs along with several additional utilities and the procedures used to determine the twin law, reduce and optimize the data and finally determine and refine the crystal structure.

With the advent of area detectors the recognition of a 'twinned' crystal is almost immediate. What is envisaged frequently on a data frame is occasionally more than one would prefer to 'see' but frequently the sample is all there is, air-sensitive and a 'must-have' so data collection commences and shortly thereafter the 'de-twinning' of the resulting structure begins.