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The Use of Advanced Refinement Techniques to Model Whole Molecule Disorder: Examples of Applications in Chemical Crystallography. Charles Campana, Bruker AXS Inc., 5465 East Cheryl Pkwy., Madison, WI 53711.

There are numerous examples of chemically important crystal structures for which chemically and crystallographically acceptable results are not easily obtained, even though the crystalline specimens are of excellent quality and the experimental data are collected carefully and correctly. These problems are usually tractable with the use advanced features of generally available programs, combined with some practical experience.

The diagnosis and treatment of problem crystal structures requires a logical, step-wise approach. We first look for symptoms which will reveal systematic errors in data, incorrect unit cells and/or space groups, twinning or incommensurate structures. Each of these problems has a treatment and a cure.

If none of the above conditions exist, and there is still a problem in solving and refining the structure, we may be able to analyze the structure and to refine it using disorder models and advanced refinement techniques.

We will present a series of chemically interesting structures to illustrate the method we have successfully used to analyze and refine complex disorders, including whole molecule disorders. All of the examples utilize advanced features available in the public-domain SHELXL program.