Poster Presentation

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Displacement Parameter Restraints for Dealing with Limited Data

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Standard crystallographic structure refinements employ anisotropic displacement parameters (ADPs) to represent the probability distribution of a scattering atom. Such distributions may be due to thermal motion of the atom and / or a spatial average of multiple discrete atomic positions. An anisotropic description of an atomic distribution requires six parameters, and - in cases where data is limited or poor quality - the optimal values of these parameters may be ill-defined. Application of restraints and constraints can impose some physical and chemical reality on the set of displacement parameters. Examples include those based on the Hirshfeld Rigid Bond Test [1], and more recently SHELXL’s RIGU [2]. We have implemented these and other a.d.p. restraints in CRYSTALS [3], for introducing reasonable relationships amongst common arrangements of anisotropic atoms. Use of a priori information in the form of restraints must always be justified, and we present an assessment of the applicability of the new restraints against a large data set of high quality crystal structure determinations.


Keywords: anisotropic displacement parameters, least-squares, restraints