Poster Presentation

IT.P06

Displacement Parameter Restraints for Dealing with Limited Data

R. Cooper[1], J. Arnold[1]

[1]*University of Oxford, Department of Chemistry, Oxford, UK*

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.

[1] *Hirshfeld F. L. (1976) Acta Cryst. A32, 239–244,* ***[2]*** *Thorn A., Dittrich B. & Sheldrick G. M. (2012) Acta Cryst. A68, 448–451,* ***[3]*** *Betteridge P. W., Carruthers J. R., Cooper R. I., Prout K., & Watkin D. J. (2003) J. Appl. Cryst. 36, 1487*

Keywords: anisotropic displacement parameters, least-squares, restraints