

CHARGE-FLIPPING STRUCTURE SOLUTION FROM SINGLE CRYSTAL AND POWDER DIFFRACTION DATA

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Charge flipping is an iterative method for ab initio reconstruction of electron densities from diffraction data [1]. Although originally developed with the focus on single crystal data, the structure solution algorithm was applied with especial vigour to more the specialized fields of modulated structures [2] and powder data [3,4].

The method has several attractive properties that make it the method of choice in many cases as it does not require any information about atom types, chemical composition or any information on the space group symmetry. Apart from the routine solution of all types of organic and inorganic structures, charge flipping is the preferred approach for structure solution of structures with ambiguous space group or with unknown composition.

The time required to setup a Charge Flipping run is minimal, maybe a few minutes at maximum. Structures that can be solved with Charge Flipping will usually solve in seconds up to a few minutes, where classic methods may take hours or even days for the same task with the same data.

An overview on this fascinating new development will be given. Capabilities and limits will be discussed using the sample data of the 3rd structure determination by powder diffractometry round robin [5].

References

- [1] G. Oszlányi and A. Süto *Acta Cryst.* (2004) **A60** 134-141
- [2] L. Palatinus, *Acta Cryst.* (2004) **A60** 604-610
- [3] J. Wu, K. Leinenweber, J. C. H. Spence, M. O'Keefe, *N. Mat.* (2006) **5** 647 - 652
- [4] C. Baerlocher, L. B. McCusker and L. Palatinus, *Z. Kristallogr.* (2007) **222** 47-53
- [5] A. Le Bail and L.M.D Cranswick (2008). <http://www.cristal.org/SDPDRR3/index.html>