

has been applied to a large set of small and medium size crystal structures, included small proteins.

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Missing data in a modified charge flipping

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Missing data is a general hindrance for all *ab initio* structure determination methods. Charge flipping [1,2] is no exception, and the problem is more exposed, due to the dual-space nature of the iterative algorithm.

Two publications have already appeared addressing this issue. These either fill the missing data by making the Patterson function positive and smooth with the maximum entropy method and then run the original iteration process [3], or correct phases by the tangent formula and use charge flipping with drastically increased perturbations [4].

Here we offer a third approach that is easier to implement and still works well for structures of usual complexity. Our solution is constructed from the following elements:

- i. Normalized data, where normalization means division by the scattering factor of the heaviest atom in the structure.
- ii. Freely floating moduli of unobserved structure factors within the observed resolution sphere.
- iii. A set of utilized structure factors extended to higher than observed resolution.
- iv. Special treatment of extinctions everywhere.
- v. A modified iteration scheme that simultaneously increases perturbation in reciprocal space and includes full negative feedback. No extra parameters beyond the dynamical density threshold are introduced. Extended resolution acts as a damping factor.
- vi. Figure-of-merits checked in an auxiliary step of the iteration process.

To show the efficiency of the method, a broad selection of successful structure solution examples will be presented, often working with 5-10 times less data than the standard requirement of *Acta Cryst. C*.

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