

Problem statement

Only amplitude information is directly available from a single-crystal X-ray diffraction experiment. Several techniques exist for determining a phase set from measurements of diffraction amplitude alone. With both phase and amplitude information in-hand, for a sufficient number of reflections, a map can be constructed, which presents a picture of electron density in 3-D. Unfortunately, errors in measurements combined with the inability of many phasing techniques to provide accurate phases often results in inaccurate density maps. Given the potential locations of atoms, which are represented by maxima of the density map as well as other suitably obtained points, one would like to assign atoms to these positions in a way that minimizes the error between calculated and experimental diffraction amplitudes. This is possible as, for any given assignment of atoms to positions in 3-D, a Fourier transform can be used to calculate the diffraction amplitudes that would result from a diffraction experiment.

The set K will denote the constituent atoms of the molecular structure, indexed by k . Let M denote the set of data reflections, indexed by m , with corresponding Miller indices \mathbf{h}_m . To resolve the phase ambiguity, we will use a set J of grid points in 3-D, indexed by j , each at position \mathbf{x}_j in 3-D. This set of points can be obtained using Patterson techniques, or more generally, by lightly transforming any experimental density map. The details of the generation of the set of grid points go beyond the level of detail that can be provided in this document and can be found in Chapter 4 of [4]. For our purposes, we will assume that this grid has been developed.

The following are given parameters:

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| s_m | Observed normalized structure factor amplitude from experimental data ($m \in M$) |
| g_{jm} | Coefficient for real portion of Fourier transform $g_{jm} = \cos(2\pi\mathbf{h}_m \cdot \mathbf{x}_j), (j \in J, m \in M)$ |
| z_k | Atomic number of element in chemical formula ($k \in K$) |
| μ | Normalization applied to Fourier transform $\mu = (\sum_k z_k^2)^{-1/2}$ |

Given \mathbf{h}_m and s_m , $m \in M$, and z_k , $k \in K$, as well as a specification of the grid as defined by \mathbf{x}_k , $k \in K$, one can then calculate the parameters g_{jm} , $j \in J, m \in M$, and μ . The problem then is to assign atoms to points on the grid so that the resulting structure factors are as close as possible to the experimentally measured ones.