5.7: Phase problem

Waves diffracted from a primitive lattice of simple scatterers obey Bragg's law, which allows ready determination of interplanar distances and thus the easy recovery of a description of the crystal lattice. Where the scattering objects are complex (*e.g.* in molecular crystals) the diffracted radiation suffers a phase shift arising from the spatial distribution of individual scatterers. The amplitudes of the resulting structure factors are directly derivable from the experimental measured intensities of the diffracted beams, but the phases are not. Without a knowledge of the phases, it is not possible to reconstruct the individual atomic positions. Estimating the phases is an essential step in successful structure determination.