The equations: (Good-Parts version: what you really need to remember, cont'd.)

A light wave ray diffracted from a molecule in a crystal:

A wave is defined by an Amplitude $|F_{hk\ell}|$ and a Phase: $e^{i\phi_{hk\ell}}$

Each diffracted "wave" is a sum of contributions from ALL atoms:

$\sum_{n}^{N}$ (Amplitude-factors) • (Phase-factor) ...the sum is over all atoms.

Amplitude-factors are a property of the atom, including uncertainty about its position.

(Uncertainties are put into the B-factor. Many people think they understand the B-factor because they remember hearing about the Temperature Factor from Physics, for macromolecules the temperature part of the B-factor is only a minor part, most of the effect comes from other kinds of disorder.)

Phase-factor is just dependent on the position of the atom.

And now the equation we will derive (and that crystallographers should be familiar with):

Remember this equation for your prelim!

Amplitude Phase = (Amplitude-factors) • (Phase-factor)

$$\vec{F} = |F_{hk\ell}| \cdot e^{i\phi_{hk\ell}} = \sum_{n}^{N} O_n \cdot f_{n,\theta_{hk\ell}} \cdot e^{-B_n (\sin\theta_{hk\ell}/\lambda)^2} \cdot e^{i\,2\pi(\,hx_n + ky_n + \ell z_n\,)}$$

h, k, ℓ	:	integer index numbers of a particular Bragg Plane, a diffracted ray, a "reflection".
$\theta_{hk\ell}$	:	angle of incident beam to the h, k, ℓ Bragg plane
$\|F_{hk\ell}\|$	:	amplitude of the $hk\ell^{th}$ diffracted ray
$\phi_{hk\ell}$	:	the phase of the $hk\ell^{th}$ diffracted ray
B	:	B-factor (historically the Temperature Factor, but dominated by other uncertainties)
$f_{n,\theta_{hk\ell}}$	:	individual atomic scattering factor of the n^{th} atom as a function of $\theta_{hk\ell}$
x_n, y_n, z_n	:	coordinates of the n^{th} atom
N	:	total number of atoms in the repeating unit of the crystal
O_n	:	occupancy of the n^{th} atom. (e.g. for a half-occupied ligand, sidechain alternate rotamer, etc.)