

3.13: F(000)

The expression for a structure factor evaluated in the zeroth-order case $h = k = l = 0$ yields the result

$$|F(000)| = \left[\left(\sum f_r \right)^2 + \left(\sum f_i \right)^2 \right]^{1/2}$$

where f_r is the real part of the scattering factors at $\theta = 0^\circ$, f_i is the imaginary part of the scattering factors at $\theta = 0^\circ$, θ is the Bragg angle, and the sum is taken over each atom in the unit cell.

$F(000)$ is computed without dispersion effects in electron-density calculation by Fourier inversion. In all cases, non-dispersive $F(000)$ is a structure factor and not a structure amplitude: it has both magnitude and a sign.

For X-rays non-dispersive $F(000)$ is positive definite and in many cases an integer (but it is not an integer for non-stoichiometric compounds). It counts the number of electrons in the cell.

For neutrons non-dispersive $F(000)$ is either positive or negative and counts the total nuclear scattering power in the cell.

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