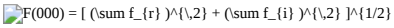
3.13: F(000)

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



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.