


### 3.13: F(000)

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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  $\theta = 0^\circ$ ,  $\theta$  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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