For the special case of $h = k = 0$ this reduces to

$$I = 2\Sigma + 4 \sum_{i \neq j}^{\frac{1}{2}N} \mathbf{f}_i \mathbf{f}_j^* \cos 2\pi l(z_i - z_j), \quad (2)$$

and for $l = 0$ to

$$I = \Sigma + 2 \sum_{i}^{\frac{1}{2}N} f_i^2 \cos 4\pi(hx_i + ky_i) + 4 \sum_{i \neq j}^{\frac{1}{2}N} \mathbf{f}_i \mathbf{f}_j^* \cos 2\pi(hx_i + ky_i) \cos 2\pi(hx_j + ky_j). \quad (3)$$

The average value of the first (constant) term in these equations is, of course, always Σ or 2Σ, however the averaging is done. The values of the trigonometric terms require detailed consideration. In the general case of h, k, l non-zero, the integral of the trigonometric terms over the entire unit cell is zero, and the z integral in the final term is zero even in the interior of the excluded cylinders. The middle term, however, is finite within the cylinders, and it has in fact the same value for each, since $\cos 4\pi(hx + ky)$ is unaffected by the translations $\frac{1}{2}0$ *etc.* Changing to cylindrical polar coordinates gives

$$\int_0^a \int_0^{2\pi} \cos(4\pi sr \cos\varphi) r \, dr \, d\varphi = (a/2s) J_1(4\pi sa), \quad (4)$$

where J_1s is the ordinary first-order Bessel function. Equation (1) then gives for the expected value of the intensity

$$E(I) = \Sigma[1 - 2aJ_1(4\pi as)/(C - 4\pi a^2)s], \quad (5)$$

the integral having the same value for every atom. This corresponds to the first and third terms of Nigam's equation (7), the middle one having been introduced by his method of approximation.

In the special case of l equal to zero there are additional terms arising from the double sum. Both the ith and the jth atom produce a factor like equation (4) but with $2\pi sa$ instead of $4\pi sa$. Also, the translations $0\frac{1}{2}$ *etc.* produce a change of sign unless h and k are even, so the contributions from the four cylinders cancel out for h or k or both odd.
For $l = 0$, h and k even, therefore,

$$E(I) = \Sigma[1 - 2aJ_1(4\pi as)/(C - 4\pi a^2)s] - 16[(\Phi - 2\Sigma)a^2 J_1^2(2\pi as)/(C - 4\pi a^2)^2 s^2], \quad (6)$$

where

$$\Phi = \left| \sum_i \mathbf{f}_i \right|^2. \quad (7)$$

For h or k or both odd, equation (5) holds even for $l = 0$. For $h = k = 0$

$$E(I) = 2\Sigma \quad (8)$$

for all values of l.

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Über den Zusammenhang zwischen der mittleren quadratischen Auslenkung $\langle u^2 \rangle$ der Atome im Kristallgitter und der spezifischen Wärme c_v für Zink. Erratum.

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Abstract

Four errors should be corrected in Rossmanith (*Acta Cryst.* (1980). A**36**, 416–420). In Fig. 1 the lowest curve (of the curves labelled 3) should be labelled $T = 100$ K (not 300 K). In the penultimate line of the caption to Fig. 2 the reference should be to equation (6), rather than to equation (5), while in the caption to Fig. 4 the calculations for line 5 and points ● should refer to equation (5), rather than to equation (6). In equation (5) the solidus and the letter m should be transposed:

$$\langle u^2(T) \rangle = \sum_{n=0}^{800} W(u)_{\omega_n} g(\omega_n)/m \sum_{n=0}^{800} g(\omega_n). \quad (5)$$

Die gesamte Information ist im *Abstract* enthalten.

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