

mation, were performed by Hahn & Ludwig (1961), Hahn (1961) and Ludwig (1967). In these papers, (12a) was not explicitly established, but it appears that anharmonicity changes the intensity distribution of TDS, but neither its location between the reciprocal lattice points nor its inelastic nature.

In a recent paper, Stewart (1977) posed the question whether, for the Bragg intensities, the Boltzmann factor of a thermal state has to be applied as a factor to the amplitude or to the intensity. For the harmonic approximation and the convolution approximation (rigid pseudo-atoms), Stewart has shown that the Boltzmann factor is a factor of the amplitude, in agreement with earlier work of Born (1942–1943), but he could not prove this generally. With our results above, a general proof can be given.

We insert (1) into (11b) and obtain

$$F(\mathbf{K})_{\text{av}} = \iint \rho(\mathbf{x}, \mathbf{Q}) f(\mathbf{Q}) d\mathbf{Q} \exp(i\mathbf{K} \cdot \mathbf{x}) d\mathbf{x}. \quad (13)$$

Performing the Fourier transformation in (13) we obtain

$$F(\mathbf{K})_{\text{av}} = \int F(\mathbf{K}, \mathbf{Q}) f(\mathbf{Q}) d\mathbf{Q}. \quad (14)$$

To introduce the Boltzmann weight factor, we write with Stewart (1977)

$$f(\mathbf{Q}) = \sum_n W_n |\chi_n(\mathbf{Q})|^2, \quad (15)$$

$$W_n = \exp(-E_n/kT) / \sum_n \exp(-E_n/kT). \quad (16)$$

Note that our $f(\mathbf{Q})$ is identical with Stewart's $t(\mathbf{Q})/\int t(\mathbf{Q}) d\mathbf{Q}$. $\chi_n(\mathbf{Q})$ are the normalized vibrational eigenfunctions, and E_n the eigenvalues of the Hamiltonian of the nuclear motions. We insert (15) into (14) and obtain

$$F(\mathbf{K})_{\text{av}} = \sum_n W_n \int \chi_n^*(\mathbf{Q}) F(\mathbf{K}, \mathbf{Q}) \chi_n(\mathbf{Q}) d\mathbf{Q}. \quad (17)$$

Inserting (17) into (11a) we obtain Stewart's equation (17). Thus, with (17) and (11a) we have shown that, for the Bragg intensities, the Boltzmann factor W_n is a factor of $F(\mathbf{K}, \mathbf{Q})$,

but not a factor of $|\int \chi_n^* F \chi_n d\mathbf{Q}|^2$. Hence, Stewart's alternative equation (21) is not valid for the Bragg intensities, and, since it is incompatible with Stewart's equation (17), it is generally not correct. In the general formula (3) for the average intensity, the weighting is transferred from $\rho(\mathbf{x}, \mathbf{Q})$ to the intensities; whereas, for the Bragg intensities, the Fourier transform relations (11b) and (13) cause the weighting to be transferred from $\rho(\mathbf{x}, \mathbf{Q})$ to the amplitudes.

In our derivation of (10), (11) and (17) no model of the thermal motions of the nuclei has been assumed. Rather, the physical basis is that a crystal must have a mean periodic density distribution. A general derivation of (12a) by means of lattice dynamics appears to be a difficult project, although it seems that the only essential requirement is also the periodicity of the average crystal.

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Crystallographic pedigree of organic compounds: erratum. By MASAO HAISA, *Faculty of Science, Okayama University, Tsushima, Okayama 700, Japan*

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Abstract

In Haisa [*Acta Cryst.* (1978), **A34**, 753–759], to correct a printer's error, the first ten lines in the left-hand column on page 758 should be moved to the bottom of that column.

All information is given in the Abstract.