Short Communications

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Two papers on the calculation of ε for obtaining normalized structure factors.

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It is pointed out that ε_{II}, as defined by Iwasaki & Ito [*Acta Cryst.* (1977), A**33**, 227–229]is equal to ε_{SK}, as defined by Stewart & Karle [*Acta Cryst.* (1976), A**32**, 1005–1007], multiplied by L, the multiplicity of the chosen unit cell relative to a primitive one, *i.e.* $\varepsilon_{II}=\varepsilon_{SK}L$.

Two papers on the calculation of ε for obtaining normalized structure factors have recently appeared (Stewart & Karle, 1976; Iwasaki & Ito, 1977). Although it may not be immediately apparent, the ε's as defined in the two papers may be different. It is the purpose of this note to point out the relationship between the two.

We call ε_{SK} the ε of Stewart & Karle and ε_{II} the ε of Iwasaki & Ito. The key point is that ε_{SK} is defined for a primitive unit cell whether the space group of interest is conventionally centered or not. On this basis, we write

$$E(\mathbf{h})=F(\mathbf{h})/[\varepsilon_{SK}(\mathbf{h})\sum_{j=1}^{N_p}f_{j\mathbf{h}}^2]^{1/2}, \quad (1)$$

where the $F_{\mathbf{h}}$ are the crystal structure factors placed on an absolute scale and corrected for thermal motion. The vector $\mathbf{h}\equiv(h,k,l)$ labels the plane in the crystal associated with a particular reflection, $f_{j\mathbf{h}}$ is the atomic scattering factor of the jth atom in a crystal unit cell (primitive) containing N_p atoms and the quantity ε as a function of $\mathbf{h}$, $\varepsilon_{SK}(\mathbf{h})$, is an integer whose value depends upon the point-group symmetry and the reflection class. Equation (1) is the same as that of Stewart & Karle except that ε is now written as ε_{SK} and N is now written as N_p to emphasize that the latter refers to a primitive cell.

If $F(\mathbf{h}')$ were to represent the structure factor for a centered cell, (1) would become

$$E(\mathbf{h}')=F(\mathbf{h}')/L[\varepsilon_{SK}(\mathbf{h}')\sum_{j=1}^{N_p}f_{j\mathbf{h}'}^2]^{1/2} \quad (2)$$

or

$$E(\mathbf{h}')=F(\mathbf{h}')/[\varepsilon_{SK}(\mathbf{h}')L\sum_{j=1}^{N_pL}f_{j\mathbf{h}'}^2]^{1/2}, \quad (3)$$

where L is the multiplicity of the centered cell in the notation of Iwasaki & Ito, $\mathbf{h}'$ for the centered cell corresponds to $\mathbf{h}$ for the primitive cell, $\varepsilon_{SK}(\mathbf{h})=\varepsilon_{SK}(\mathbf{h}')$ and $f_{j\mathbf{h}}=f_{j\mathbf{h}'}$. Equation (3) may immediately be rewritten as the initial equation of Iwasaki & Ito,

$$E(\mathbf{h}')=F(\mathbf{h}')/[\varepsilon_{II}(\mathbf{h}')\sum_{j=1}^{N}f_{j\mathbf{h}'}^2]^{1/2}. \quad (4)$$

Here, clearly, N refers to the number of atoms in the centered cell and

$$\varepsilon_{II}=\varepsilon_{SK}L. \quad (5)$$

For a primitive cell, $\varepsilon_{II}=\varepsilon_{SK}$. In the case of a centered cell ε_{II} is some multiple of ε_{SK} as given by L, the multiplicity of the cell.

References

IWASAKI, H. & ITO, T. (1977). *Acta Cryst.* A**33**, 227–229.
STEWART, J. M. & KARLE, J. (1976). *Acta Cryst.* A**32**, 1005–1007.