line is 2·11 eV (Krause & Oliver, 1979). It is apparent from the widths of the Renninger peaks that the monochromator has reduced this spectral width, with an opportunity to introduce asymmetry.

Juretschke (1986) provided another possible explanation of this experiment in advance of its publication: asymmetry of peak profiles can come from changes of absorption which are correlated with whether the third reciprocal-lattice point is inside or outside the Ewald sphere, regardless of the phase of the structure-factor triplet. For both explanations the predicted pattern of asymmetry is that reported by PL, and not that which corresponds to the rules for phases of equivalent reflections. Neither explanation involves any distinction between the very weak and the strictly absent reflections. Perhaps both effects occur in the experiment.

I thank Professor Juretschke for helpful discussions.

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Reply to *Comments on The phases of forbidden reflections, by B. Post & J. Ladell* (1987), by David H. Templeton.

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Abstract

Some general remarks regarding the experimental determination of X-ray reflection phases may help the reader assess the validity of Templeton's [*Acta Cryst.* (1988). A44, 394-395] comments on a paper by Post & Ladell [*Acta Cryst.* (1987). A43, 173-179].

The reality of the intensities of 'forbidden' reflections, such as {222} and {442} of germanium, is no longer in question. Nevertheless, substitution of the positions of the germanium atoms in the expressions cited by Templeton (1988) yields structure factors equal to zero. It is evident that the use of those expressions for the calculation of the phases of forbidden reflections may yield incorrect results.

The experimental phases listed by Post & Ladell (1987) are based on data which necessarily include effects due to anharmonic thermal vibrations, static distortions of electron density distributions and anomalous scattering of the incident X-ray beam. Those are not taken into account in the *International Tables for X-ray Crystallography* (1952) expressions. They play minor roles in the determination of the phases of moderately strong reflections but can be of decisive importance when ultra-weak forbidden reflections are considered. It would therefore have been surprising if the phases reported by Post & Ladell were in perfect agreement with those listed in *International Tables for X-ray Crystallography* (1952).

Willis & Pryor (1975) have drawn attention to the fact that the *International Tables* rules for special positions, such as those of germanium atoms in the diamond structure, are valid only for spherically symmetric atoms. Atoms in crystals are not spherically symmetric and may generate effects which differ from those calculated for spherical atoms.

Simple procedures were used by Post & Ladell (1987) for the determination of the phases of individual reflections. Invariant triplet phases are displayed in n-beam patterns in the form of asymmetric intensity profiles. The phases of two of the reflections in each triplet are well known; the third is the unknown phase of the forbidden reflection. Subtraction of the sum of the two known phases from the invariant experimental triplet phase yields the phase of the forbidden reflection.

Our replies to specific comments by Templeton (1988) are listed below.

(1) Templeton notes that relations among the phases of reflections of the forms {222} and {442}, listed in Post & Ladell (1987), do not correspond to those calculated on the basis of expressions given in *International Tables.* The experimentally determined phases of {222} were found to alternate in sign for the sequence $222, 22\bar{2}, 2\bar{2}\bar{2}, \bar{2}\bar{2}\bar{2}$. Templeton's calculations indicate that all four reflections have identical signs. Possible causes of the differences between the two sets of results have been outlined above. In addition, it is not clear whether Templeton's calculations, presumably based on expressions given in *International Tables*, are applicable to forbidden reflections. On p. 341 of *International Tables*, we are informed that only those reflections whose indices sum to $4n$ or $2n+1$ satisfy the conditions for possible reflection for eightfold positions in space group $Fd3m$. It is therefore difficult to understand why the Editors of *International Tables* would wish to list relations among the phases of structure factors to which they have assigned zero values. More likely, those expressions were intended to apply only to structure factors calculated for atoms in positions other than those of eightfold multiplicity in space group $Fd3m$.

(2) Templeton states that the *International Tables* rules 'are incompatible with the conclusion that the phase is correlated with the parity of n' in $4n-2$ (the sums of the indices of forbidden reflections equal $4n-2$). Templeton's

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equations, however, provide good examples of such correlations; in those expressions, a change of indices from, say, 222 to $22\bar{2}$ changes the value of n by unity, and can lead to reversal of the signs of structure factors.

(3) To illustrate a case in which the structure factor vanishes, Templeton postulates a situation in which there is no anharmonic motion. Unfortunately, the anharmonic vibrations of atoms cannot be wished away. Some implications of such postulates are outlined in Willis & Pryor (1975) as follows: 'A crystal with harmonic forces would have no thermal expansion, no temperature dependence of the elastic constants and many other properties not possessed by real crystals.'

(4) The derivation of equation (4) of Templeton (1988) appears to involve a significant error. Our calculations indicate that the equation should be written as

$$F = 8(-1)^n (f_1^{\rm real} T_1'' + T_1^{\rm real} f_1'').$$

The modified form of the equation is incompatible with the conclusions drawn by Templeton from his version of equation (4); it also indicates that the intensities of 'forbidden' and 'strictly forbiddden' reflections vanish only in the rare instances when the two products of real and imaginary quantities cancel exactly.

(5) All 24 forbidden triplet interactions described in Post & Ladell (1987) display identical asymmetries for reciprocal-lattice points entering the Ewald sphere, and the opposite asymmetries when they leave; the authors provide a simple explanation of the above in the Appendix to their publication. Nevertheless, Templeton has proposed an alternative explanation which is apparently considered to be compatible with the experimental evidence, but which rules out any relation between phases and the intensity asymmetries. His explanation is ingenious; it is also incorrect. It implies that all n-beam interactions involving forbidden reflections will show identical asymmetric intensity sequences corresponding to the asymmetry of the incident-beam intensity; all would, therefore, display identical sign indications. Post, Nicolosi & Ladell (1984) have, however, shown that both positive and negative signs are observed in $22\bar{2}$ n-beam patterns of germanium; in those patterns the forbidden 222 reflection participates in all the interactions.

Recently, Templeton modified some aspects of his critique to take into account results of calculations of the ratios of three-beam to two-beam (background) intensities for interactions of the types discussed above (Juretschke, 1986). Substitution of constants listed by the author into his final equation yields a remarkably simple expression for the ratios, for wide angular ranges about the exact three-beam setting, *i.e.* C/φ; C is a constant and φ is the variable angular distance from the three-beam point. A plot of the results is shown in Juretschke's (1986) Fig. 1. That simplified representation of the many complicated interactions that occur in three-beam dffraction would be acceptable, provided that it could be shown to represent a reasonable facsimile of the corresponding physical reality. As the reader can readily determine, the calculated curves bear no resemblance to any of the 24 experimental curves in Post & Ladell (1987) and, in particular, to the four experimental curves which deal with the cases discussed by Juretschke. We therefore see no need for additional discussions of either the Fig. 1 curves or of the calculations on which they were based.

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Compilation of temperature factors of cubic elements.

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Abstract

A compilation is presented of the temperature factors of 22 cubic elements. This represents the first stage of a Temperature Factor project initiated by the Neutron Diffraction Commission of the International Union of Crystallography [*Acta Cryst.* (1985), **B41**, 374].

Introduction

Several experimental methods have been used in the measurement of B factors, which are related to the mean square amplitudes of atomic vibrations, but there has been no systematic compilation of these thermal parameters in recent years. In this paper we present a list of recommended values at 293 K for the temperature factors, B, of 22 cubic elements.

Results

B is defined by the relation

$$F_{\rm obs} = F_c \exp[-B(\sin^2\theta)/\lambda^2],$$

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