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

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

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 222 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

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

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where F_{obs} is the observed structure factor and F_c is the structure factor calculated in the absence of thermal motion. For most of the 22 elements the temperature factor has been measured by several methods, including neutron diffraction, X-ray diffraction, gamma-ray diffraction and high-voltage electron diffraction. The independent measurements given by these different techniques are listed in a separate table.* Table 1 in this paper contains the average values (with standard deviations in brackets) deduced from the set of independent estimates for each element. The sources of the data for each element are given in Table 2. With rare exceptions, the B factors were corrected for the influence of TDS. Failure to make a TDS correction leads to a serious underestimate of B (Willis & Pryor, 1975).

Table 1. *Recommended values of* B, $(\overline{u^2})^{1/2}$ *and* Θ

Element	B (Å^2)	$(\overline{u^2})^{1/2}$ (Å)	Θ (K)
Aluminium	0·86 (1)	0·181 (1)	394 (2)
Chromium	0·26 (1)	0·099 (1)	524 (10)
Copper	0·57 (1)	0·147 (1)	313 (3)
Germanium	0·57 (1)	0·147 (1)	293 (3)
Gold	0·57 (4)	0·147 (5)	174 (6)
Iridium	0·39 (4)	0·122 (6)	216 (11)
Iron	0·35 (1)	0·115 (2)	431 (6)
Lead	2·42 (7)	0·303 (5)	84 (1)
Lithium	4·1 (6)	0·395 (28)	352 (25)
Molybdenum	0·25 (2)	0·098 (4)	388 (15)
Nickel	0·37 (1)	0·119 (4)	408 (6)
Niobium	0·49 (2)	0·136 (2)	285 (3)
Palladium	0·45 (6)	0·131 (9)	272 (18)
Platinum	0·32 (2)	0·110 (3)	237 (7)
Potassium	12 (2)	0·675 (56)	86 (7)
Rhodium	0·26 (7)	0·099 (1)	362 (48)
Silicon	0·45 (1)	0·131 (2)	544 (6)
Silver	0·79 (2)	0·173 (2)	202 (3)
Sodium	7·9 (2)	0·548 (4)	139 (1)
Tantalum	0·32 (1)	0·110 (1)	245 (3)
Tungsten	0·18 (1)	0·083 (2)	320 (1)
Vanadium	0·55 (3)	0·145 (4)	358 (10)

Table 2. *Sources of temperature-factor data*

Aluminium	Chipman (1960) Pathak & Shah (1979) DeMarco (1967) Dingle & Medlin (1972) McDonald (1967) Butt & O'Connor (1967) Martin & O'Connor (1978) Watanabe & Uyeda (1968) Lally, Humphreys, Metherell & Fisher (1972)
Chromium	Paakkari (1974) Peljo (1982) Wilson, Skelton & Katz (1966) Shirley, Lally, Thomas & Fisher (1975) Feldman (1970)
Copper	Chipman & Paskin (1959) Webb (1962) Hosoya & Yamagishi (1966) Linkoaho (1971) Baldwin, Young & Merlini (1967) Baldwin (1968) Ghezzi, Merlini & Pace (1971) Martin & O'Connor (1978) Schneider, Hansen & Kretschmer (1981) Svensson, Brockhouse & Rowe (1967) Nicklow, Gilat, Smith, Raubenheimer & Wilkinson (1967) Nilsson & Rolandson (1973)
Germanium	Batterman & Chipman (1962) Ludewig (1973) Ghezzi, Merlini & Pace (1967)
Gold	Alexopoulos, Boskouits, Mourikis & Roilos (1965) Synecek, Chessin & Simerska (1970) Lynn, Smith & Nicklow (1973)
Iridium	Sedivy (1970)
Iron	Gazzara & Middleton (1961) Paakkari (1974) Watanabe & Uyeda (1968) Shirley, Lally, Thomas & Fisher (1975)
Lead	Chipman & Paskin (1959) Chipman (1960) Alexopoulos, Boskouits, Mourikis & Roilos (1965) Lisher (1978)
Lithium	Bednarz & Field (1982) Beg & Nielsen (1976)
Molybdenum	Paakkari (1974) Powell, Martel & Woods (1977)
Nickel	Linkoaho (1971) Paakkari (1974) Tarna & Laine (1981) Cole & Windsor (1980) Von Dreele, Jorgensen & Windsor (1982) Wilson, Skelton & Katz (1966) Dina, Mazzone & DeMarco (1969) Watanabe & Uyeda (1968) Barron & Smith (1966) Feldman (1969)
Niobium	Linkoaho (1971) Sharp (1969) Grimvall & Grimvall (1968)
Palladium	Korunskii, Genkin & Vigdorchik (1977) Miiller & Brockhouse (1971)
Platinum	Alexopoulos, Boskouits, Mourikis & Roilos (1965) Yokokawa & Takahashi (1979)
Potassium	Kumar & Viswamitra (1971) Bednarz & Field (1982)
Rhodium	Korunskii, Genkin & Vigdorchik (1977)
Silicon	Batterman & Chipman (1962) Fehlman (1979) Batterman (1962) Hattori, Kuriyama & Katagawa (1965) Aldred & Hart (1973) Graf, Schneider, Freund & Lehmann (1981)
Silver	Alexopoulos, Boskouits, Mourikis & Roilos (1965) Linkoaho (1971) Kashiwase (1979) Pathak & Shah (1979) Vega, Forsterling & Kleinstuck (1980)
Sodium	Kumar, Valvoda & Viswamitra (1971) Field & Medlin (1974)
Tantalum	Behr, Keppler, Steyrer, Metzger & Peisl (1983)
Tungsten	Paakkari (1974) Chen & Brockhouse (1964) Merisalo & Paakkari (1973)
Vanadium	Linkoaho (1971) Kamal, Malik & Rorer (1978) Ohba, Sato & Saito (1981)

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* The individual B factors of the twenty-two elements have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP44559 (26 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

We also list in Table 1 the quantities $(\overline{u^2})^{1/2}$ and Θ, where $(\overline{u^2})^{1/2}$ is the r.m.s. thermal displacement of an atom from its equilibrium position at 293 K and Θ is the Debye temperature. They are derived from the B factor using the formulae

$$B = 8\pi^2\overline{u^2}/3$$

and

$$B = (6h^2/mk_B)(T/\Theta^2)[\varphi(x) + x/4]$$

with $\varphi(x)$ the Debye integral and $x = \Theta/T$.

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Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (R. O. Gould, Department of Chemistry, University of Edinburgh, West Mains Road, Edinburgh EH9 3JJ, Scotland). As far as practicable books will be reviewed in a country different from that of publication.

Acta Cryst. (1988). A**44**, 399

Solid state science: past, present and predicted. Edited by D. L. Weaire & C. G. Windsor. Pp. xviii + 308. Bristol: Hilger, 1987. Price £35.00 (hardback), £15.00 (paperback).

This is an unusual and attractive book. It gives a readable and informative picture of ten distinct areas of present-day solid state physics, showing how these sciences got to where they are now. The selected areas are: diffraction; metallurgy; the Fermi surface; semiconductors; magnetism; superconductivity; critical phenomena; solid state optics; microelectronics; and solid state instruments. The chapter on diffraction is by Michael Woolfson. There is also a particularly interesting essay on the 'pre-history' of solid state physics. In a sense this is a book on the history of science; but it is written by physicists within these fields and its primary concern is the science itself. After outlining the technical and circumstantial details, it describes especially the drama and the human aspects of the development, as seen by the scientists who know the subject.

What is unusual is the division of the subject matter into these distinct subject areas, each of which is treated separately. Each of these chapters is thus a sort of cameo. Each starts with the state of knowledge in the early days of that subject, the theories at that time, and the personalities; then the advances, the crucial experiments, and the new theories are outlined, ending finally with the present-day outlook. The scientific coverage is necessarily somewhat sparse, but one learns a good deal and certainly finds a lot of interest in the essays in which one is not oneself a specialist. The book is very definitely recommended reading.

What is ironic is the manner in which the advances of science are so unpredictable, even by the best scientists. A book of this kind, venturing to point towards the future in each area, is almost inevitably going to miss something important happening directly after it comes into print. So, the essay on diffraction has missed 'maximum entropy', the latest development in direct methods; and, much more dramatic, the chapter on superconductivity has missed out on the recent explosive discovery of the 'high-temperature' superconducting ceramics. Embarrassing? Not really. This just illustrates, superbly, what an exciting thing science is.

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Quantum aspects of molecular motions in solids. Springer proceedings in physics, Vol. 17. **Proceedings of an ILL-IFF workshop, September 24–26, 1986.** Edited by A. Heidemann, A. Magerl, M. Prager, D. Richter and T. Springer. Pp. xii + 221. Berlin: Springer-Verlag, 1987. Price DM 85.00.

This volume is a collection of papers on quantum motions in molecular crystals, metals and glasses. It has been divided into five sections, *viz Rotational tunneling* I - *Potentials and phonon interactions*; *Rotational tunneling* II - *Coupled systems*; *Rotational tunneling* III - *Surfaces*; *Isotope effect and matrix isolation*; *Translational tunneling and disordered systems.*

The first three sections largely comprise experimental papers. These papers show how inelastic neutron and Raman scattering, nuclear magnetic resonance, heat capacity and dielectric loss measurements can be used to deduce the potential experienced by the tunneling groups, their mutual coupling, and influence of phonons on their behaviour. They are intended to stimulate further theoretical and experimental work as they are generally open ended.

There are two reviews in the sections on rotational tunneling. The first covers the theory of rotational tunneling and