described above and five, rather than four, reflexions whose signs will be varied. The h, k and l indices of these five reflexions should also include all possible combinations of + and − signs. Structures in space group $P2_12_12_1$ are routinely solved by using as origin definers reflexions $h0l$, $0kl$ and $hk0$; the need for orthogonality is automatically satisfied for this case. The problems involved in correct phasing of reflexions in structures containing fused six-membered rings have previously been discussed in detail and different approaches to their solution have been suggested (Thiessen & Busing, 1974; Hazell & Hazell, 1975).

The suggestions outlined above seem to offer a simpler and more direct approach because the maximum amount of structural and chemical information is used before the phase refinement is even begun. Most of these suggestions can be programmed into the automatic modes of the programs by requiring that the origin-defining reflexions should correspond to the appropriate d spacings and, as far as possible, be orthogonal; and that the reflexions whose phases will be varied should have d spacings between 3 and 4 Å.

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The Debye–Waller factor of KBr by powder elastic neutron diffraction.

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The Debye–Waller parameter B of KBr has been determined by triple-axis neutron diffraction with a powder sample. Calculations have also been made to find the contributions of TDS to the diffraction peaks obtained by this technique and they were found to be negligible as expected. The B value thus found is $2{\cdot}33 \pm 0{\cdot}09$ Å^2.

Introduction

The temperature factors of alkali halide crystals have been the subject of several X-ray and neutron investigations (Table 1). The Debye–Waller parameter B for KBr has been determined by Meisalo & Inkinen (1967) using X-ray powder diffraction and by Pryor (1966) and Atoji (1972) using the double-axis powder neutron-diffraction technique. The B value has also been determined by Bacon, Titterton & Walker (1973) using the single-crystal neutron-diffraction method. Pryor (1966) has calculated the B value from the phonon dispersion relations measured by Woods, Cochran & Brockhouse (1960) at 400 K. Reid & Smith (1970) have theoretically calculated the B values using the shell model. In two-axis diffraction the corrections due to thermal diffuse scattering (TDS) are quite large and are often corrected by the method of Chipman & Paskin (1959).

In the present work, B has been determined from a powder sample by observing the diffraction pattern in the triple-axis mode of a neutron spectrometer. By this method the TDS correction is essentially eliminated (Caglioti, 1964; Beg, Aslam, Butt, Khan & Rolandson, 1974). Further, the diffraction peaks can be well focused in this geometry.

Experimental procedure and data analysis

KBr powder was ground, dried at 100°C and sealed in a 2 cm diameter and 10 cm high cylindrical vanadium container. The triple-axis neutron spectrometer TKSN-400 installed at the PINSTECH 5 MW research reactor was used to measure the triple-axis powder diffraction pattern. Cu(220) single crystals were used as monochromator and analyser at a neutron wavelength of 1·07 Å. The horizontal collimations used before and after the sample were 30′ and 40′ respectively. Three odd-order and eight even-order reflexions up to the index 620 were measured. The structure factors were evaluated from the diffraction data in the usual manner (Bacon, 1975). The scattering lengths given by Bacon (1975) were used.

Calculations were performed to evaluate the percentage thermal diffuse scattering under the Bragg peaks according to Beg (1976). For the TDS calculations an isotropic value of the sound velocity on the model of Nilsson (1957) was used, employing the elastic constants given by Federov (1968). The TDS varied from 0·45% for the 111 peak to 4·8% for the 620 peak. The correction to the B value due to TDS was found to be small and was within the experimental errors.

Results and discussion

The Debye–Waller parameter B for KBr was evaluated from the data of 11 peaks by a least-squares fit. Sufficient data could not be obtained on the odd peaks due to the intensity and angular constraints; therefore separate values for B_{K} and B_{Br} could not be determined accurately and only the average value B_{KBr} was obtained. This was found to be $(2{\cdot}33 \pm 0{\cdot}09)$ Å^2 which corresponds to a Debye temperature

Table 1. *Room-temperature B values for* KBr

Reference	B_K (Å^2)	B_{Br} (Å^2)	Method
Pryor (1966)*	2·17 ± 0·3	2·67 ± 0·3	Neutron (*P*)
Pryor (1966)	2·21	2·49	Calculated from 400 K dispersion relations
Meisalo & Inkinen (1967)*	2·45 ± 0·15	2·23 ± 0·15	X-ray (*P*)
Atoji (1972)	2·6 ± 0·2	2·5 ± 0·2	Neutron (*P*)
Bacon *et al.* (1973)*	2·39 ± 0·05	2·36 ± 0·05	Neutron (*S*)
Reid & Smith (1973)	2·26	2·46	Calculated on shell model
Present work	B_{KBr} = 2·33 ± 0·09		Neutron (*P*)

P: Powder; *S*: Single-crystal.

* Corrected for TDS.

of (158 ± 4) K in the harmonic approximation. The observed and calculated structure factors corrected for TDS are compared in Table 2, which also shows the calculated TDS correction for each peak. The *R* value for the fit is 2·6%. The correction to the *B* value due to TDS is only 0·08 Å^2, which is within experimental error.

Table 2. *The observed and calculated structure factors and the TDS correction for* KBr *at room temperature*

λ = 1·07 Å, a = 6·578 Å.

hkl	F_o	F_c	TDS (%)
111	1·264	1·440	0·4
200	1·357	1·401	0·6
220	1·267	1·256	1·2
311	1·167	1·184	1·2
222	1·140	1·125	1·8
400	1·042	1·009	2·3
331	0·846	0·929	1·6
420	0·866	0·906	1·9
422	0·814	0·810	3·5
440	0·660	0·651	2·7
620	0·524	0·525	4·8

R = 0·026.

The *B* value is compared with the results of other authors in Table 1. The present value is in excellent agreement with the mass-weighted average B_{KBr} of value 2·33 Å^2 calculated from the values of Reid & Smith (1970) and with (2·37 ± 0·05) Å^2 obtained experimentally by Bacon *et al.* (1973) from a single crystal.

The present results also agree well with the recently determined *B* value of (2·32 ± 0·05) Å^2 (Butt, Thomas & Rouse, 1975) for KBr determined from two-axis powder neutron-diffraction data corrected for TDS by the method of Chipman & Paskin (1959).

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A Table of the colored crystallographic and icosahedral point groups, including their chirality and diamorphism: Errata.

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The following errors should be corrected in Harker's article [*Acta Cryst.* (1976). A**32**, 133–139]. In the author's address the number 14253 should be changed to 14263. In the Table, in section IV, under the heading *F*, the first entry should be C_1 not C_2; in section IX, under the heading *d*, the eighth entry should be 11! not 60, the fourteenth entry should be 120 not 20, and the fifteenth entry should be 60 not 160.

All the information is contained in the abstract.