(*b*) $T[I_p]=C_p\pi K_p^{-1}\exp\{-2\pi|u|/K_p\}$

$T[I_s]=\sqrt{\pi}C_sK_s^{-1}\exp\{-\pi^2u^2/K_s^2\}$

$B_p=\pi/K_p=\lambda/L\cos\theta,\ B_s=\sqrt{\pi}/K_s=e\tan\theta\ .$

Using these relations in (1) gives

(*a*) $B_{\rm obs}=(2B_s+B_p)^2(4B_s+B_p)^{-1}$

(*b*) $B_{\rm obs}=\frac{1}{2}B_s\exp\{-(B_p/B_s)^2/\pi\}(\frac{1}{2}-{\rm erf}\{\sqrt{2/\pi}B_p/B_s\})^{-1}$ (2)

where ${\rm erf}\{x\}=\sqrt{1/2\pi}\int_0^x\exp\{-t^2/2\}dt$ as tabulated (*Handbook of Chemistry and Physics*, 1963).

An easy separation of strain broadening from particle size is possible if two orders of reflexions from the same plane are used. The method is demonstrated and numerical data are given for the most frequently occurring case of the *n*th and 2*n*th order (*e.g.* 111 and 222, 200 and 400). In general any two reflexions at θ_1 and θ_2 can be used, but a graph, different from that given in Fig. 1, has to be plotted if $(\sin\theta_1)/\sin\theta_2\neq\frac{1}{2}$.

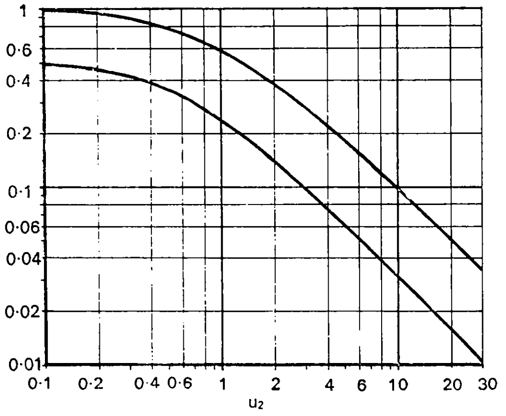

Fig. 1. Top curve: $1/LB_2$. Bottom curve: $B_1B_2-\frac{1}{2}$, plotted *versus* u_2.

The following abbreviations are introduced:

$$\left.\begin{array}{l}B_i=B_{i{\rm obs}}(\cos\theta_i)/\lambda\\ u_i=Le(\sin\theta_i)/\lambda\end{array}\right\}i=1,2$$

$$a=(\sin\theta_1)/\sin\theta_2\ ,$$

1 and 2 referring to the two orders of the reflexion. Therewith, and using (2),

$$(a)\left\{\begin{array}{l}B_1/B_2=(au_2+\frac{1}{2})^2(2u_2+\frac{1}{2})(2au_2+\frac{1}{2})^{-1}(u_2+\frac{1}{2})^{-2}\\ 1/LB_2=\frac{1}{2}(2u_2+\frac{1}{2})(u_2+\frac{1}{2})^{-2}\end{array}\right.$$

$$(b)\left\{\begin{array}{l}B_1/B_2=a\exp\{(1-1/a^2)/\pi u_2^2\}(\frac{1}{2}-{\rm erf}\{\sqrt{2/\pi}/u_2\})\\ \quad\times(\frac{1}{2}-{\rm erf}\{\sqrt{2/\pi}/u_2a\})^{-1}\\ 1/LB_2=(2/u_2)\exp\{1/\pi u_2^2\}(\frac{1}{2}-{\rm erf}\{\sqrt{2/\pi}/u_2\})\end{array}\right.$$

The results of the calculations of B_1/B_2 and $1/LB_2$ as functions of u_2 and for $a=\frac{1}{2}$ are given in Table 1 and are shown in Fig. 1 for case (*b*).

Table 1. *Values of* B_1/B_2 *and* $1/LB_2$ *calculated as functions of* u_2

	(*a*)		(*b*)	
u_2	B_1/B_2	$1/LB_2$	B_1/B_2	$1/LB_2$
0·1	0·9803	0·9722	0·9888	0·9849
0·2	0·9446	0·9184	0·9620	0·9464
0·3	0·9077	0·8594	0·9270	0·8955
0·4	0·8738	0·8025	0·8898	0·8421
0·6	0·8174	0·7025	0·8257	0·7409
0·8	0·7742	0·6213	0·7775	0·6549
1·0	0·7407	0·5556	0·7397	0·5843
1·5	0·6836	0·4375	0·6769	0·4568
2·0	0·6480	0·3600	0·6394	0·3736
3·0	0·6064	0·2653	0·5974	0·2729
4·0	0·5830	0·2099	0·5747	0·2147
6·0	0·5576	0·1479	0·5510	0·1504
8·0	0·5441	0·1142	0·5387	0·1157
10·0	0·5357	0·0930	0·5311	0·0939
15·0	0·5242	0·0635	0·5210	0·0639
20·0	0·5183	0·0482	0·5157	0·0484
30·0	0·5123	0·0325	0·5105	0·0326
40·0	0·5093	0·0245	0·5080	0·0246
60·0	0·5062	0·0165	0·5053	0·0165
80·0	0·5047	0·0124	0·5040	0·0124
100·0	0·5037	0·0099	0·5021	0·0099

The use of Fig. 1 may be illustrated by taking the broadening of the 200 and 400 reflexions which were observed with Cu radiation from a film of gold deposited in vacuum on sodium chloride. The integral breadths are $B_{1{\rm obs}}(2\theta_{200}=44{\cdot}4^\circ)=0{\cdot}0037$ rad 2θ and $B_{2{\rm obs}}(2\theta_{400}=98{\cdot}2^\circ)=0{\cdot}0070$ rad 2θ after correction for $\alpha_1-\alpha_2$ overlap and instrumental broadening. These breadths give $B_1=0{\cdot}00224$ Å^{-1}, $B_2=0{\cdot}00298$ Å^{-1} and $B_1/B_2=0{\cdot}753$. The $(B_1/B_2)-\frac{1}{2}$ and $1/LB_2$ curves in Fig. 1 give, respectively, $u_2=0{\cdot}92$ and $1/LB_2=0{\cdot}61$ from which $L=550$ Å and $e=u_2\lambda/L\sin\theta_2=0{\cdot}0034$ is obtained as final result.

The assistance of Mr T. Turton is gratefully acknowledged.

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A further development of the crystal setter.

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Some of the well known graphical, analytical methods which are used to find the arc corrections of a goniometer head with crossed arcs from oscillation photographs require the use of the following convention: the crossed arcs of the goniometer head have a special position relative to the primary beam (one arc parallel or both arcs at 45° to the beam) (Kratky & Krebs, 1936; Hendershot, 1937; Weisz & Cole, 1948; Jeffrey, 1949*a*, *b*; Bunn, 1949; Davies, 1950, 1961). In our method (Kulpe, 1963; Kulpe & Dornberger-Schiff, 1965) a similar convention is given. To

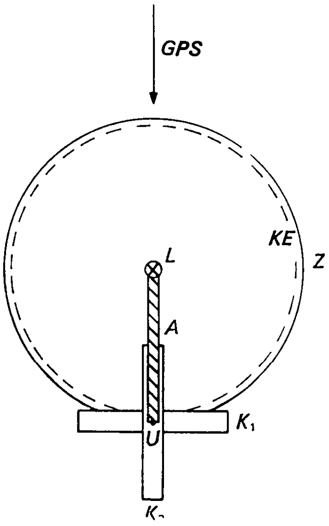

Fig. 1

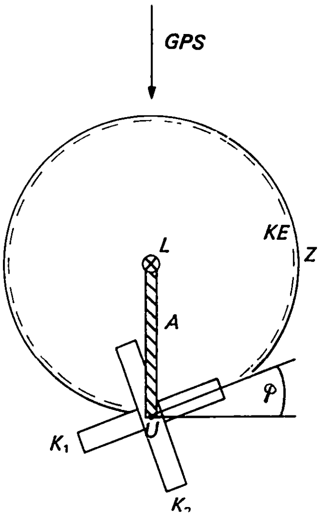

Fig. 2

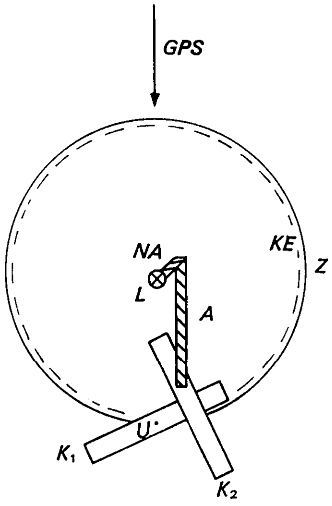

Fig. 3

Fig. 1. Normal position of the measuring device of the crystal setter (arcs K_1, K_2 and the special device *A*, *NA*, *KE*, *L* inside the transparent cylinder *Z*). Plane of paper is perpendicular to the axis of the cylinder. The axes of the two arcs K_1 and K_2 intersect at point *U* on the surface of the cylinder. *GPS* denotes the imagined X-ray beam.

Fig. 2. Crossed arcs turned by an angle φ from the normal position. Setting angles on crossed arcs equal zero.

Fig. 3. Crossed arcs as in Fig. 2 (turned by angle φ from normal position). Setting angles on crossed arcs different from zero.

obtain the arc corrections from an oscillation photograph with the crystal setter as described earlier (Kulpe, 1963) the lower arc of the goniometer has to be perpendicular to the X-ray beam.

However, this limitation is unnecessary. In a new instrument the two crossed arcs of the measuring device of the crystal setter may be turned around a vertical axis going through point *U* (Figs. 1,2 and Fig. 2 of Kulpe, 1963). Before turning, the arm *A* (carrying *NA*, *KE* and *L*) has to be disconnected from the crossed arcs K_1 and K_2 and held in its original position (Fig. 1). After turning the arcs (Fig. 2), arm *A* is again connected to them. With this device the setting angles for both arcs may be obtained for a goniometer head in any position relative to the X-ray beam during exposure. This is shown schematically in Figs. 1,2 and 3.

However, if by chance no attention was paid to the position of the crossed arcs in taking the oscillation photograph or if the particular shape of the crystal and its mounting makes it difficult or impossible to take the oscillation photograph in the normal position the modified crystal setter described here may be of real value.

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X-ray determination of the thermal expansion of potassium dihydrogen arsenate.

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Introduction

Potassium dihydrogen arsenate (KDA) crystallizes, at room temperature, in the space group $I\bar{4}2d$ of the tetragonal system and is isomorphous with the room-temperature form of potassium dihydrogen phosphate (KDP). The temperature variation of the lattice parameters and of the coefficients of thermal expansion of KDP at elevated temperatures has recently been studied in this laboratory (Sirdeshmukh, 1963). However, the lattice parameters of KDA have been determined only at room temperature (Helmholtz & Levine, 1942; Dickson & Ubbelohde, 1950) and no data are available on the temperature variation of these parameters either at low or at high temperatures. This paper gives the results of a systematic measurement in the high-temperature region.