Table 2. *Coefficients* K_1, K_2, K_3 *for the formula*: $A=(1/\mu^2)\{K_1L+K_2+K_3L'\}$ (valid for L and $L'\gtrsim 4$)

Group	K_1	K_2	K_3
1–2	$\frac{1}{m'+q'}$	$\frac{1}{(m'+q')^2}\left[\frac{m'}{nq'}+\frac{q'}{rm'}\right]$ when $\psi=0°$	0
	$\frac{1}{2q'}$	$\frac{1}{2qq'}$	0
3	0	$\frac{1}{qm'}+\frac{1}{mq'}=\sin 2\psi$ when $\psi=45°$	0
	0	1	0
4–5	$\frac{1}{m'+q'}$	$\frac{(n-r)}{r(m+q)(m'+q')}-\frac{1}{r(m'+q')^2}-\frac{n}{(m+q)^2}$ when $\psi=45°$	$\frac{1}{m+q}$
	$\frac{1}{m+q}$	$\frac{n-1}{q(m+q)}-\frac{2n}{(m+q)^2}$	$\frac{1}{m+q}$
6–7	0	$\frac{1}{(m+q)^2}\left[\frac{nm}{q}+\frac{rq}{m}\right]$ when $\psi=90°$	$\frac{1}{m+q}$
	0	$\frac{1}{2qq'}$	$\frac{1}{2q}$

$L=\mu\mathscr{L}$ $n=|\tan(\theta+\psi)|$ $m=|\sec(\theta+\psi)|$ $m'=|\mathrm{cosec}(\theta+\psi)|$
$L'=\mu\mathscr{L}'$ $r=|\tan(\theta-\psi)|$ $q=|\sec(\theta-\psi)|$ $q'=|\mathrm{cosec}(\theta-\psi)|$

evaluated graphically by the method of Henshaw (1958). The method has been successfully applied to the study of the crystal structure of aluminium periodate dodecahydrate, $Al(IO_4)_3.12\,H_2O$.

The agreement between our formulae and those proposed by Grdenić (1952, 1956) is exact for groups 1–2 and 6–7 of Table 2 (Reflections of the face-type). The discrepancies for the group 3 and 4–5 seem due to incompleteness of the Grdenić formulae.

References

Hendershot, O. P. (1937). *Rev. Sci. Instrum.* **8**, 324
Howells, R. G. (1950). *Acta Cryst.* **3**, 366.
Grdenić, D. (1949). *Glasn. mat. fiz. astr.* (II), **4**, 149.
Grdenić, D. (1952). *Acta Cryst.* **5**, 283.
Grdenić, D. (1956). *Acta Cryst.* **9**, 540.
Evans, H. T. (1952). *J. Appl. Phys.* **23**, 663.
Henshaw, D. E. (1958). *Acta Cryst.* **11**, 302.

Acta Cryst. (1961). **14**, 1090

An explicit expression for the lattice parameters of cubic crystals for the ratio method.

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In the ratio method of determining lattice parameters only the ratio of diameters of two back reflection lines is necessary to determine a cell dimension, assuming of course that the lines have been indexed and the wavelength of the radiation is known (Rovinskij & Kostjukova, 1958; M. Černohorský, 1960). In this paper the camera geometry is introduced into the simultaneous Bragg equations in order to obtain an explicit expression for the lattice parameter, a, of a cubic crystal. An extension to crystals of lower symmetry can be made.

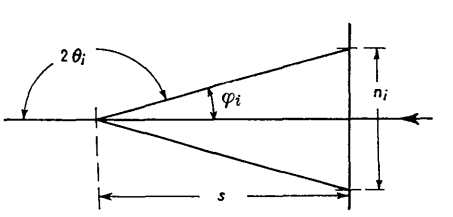

Fig. 1. Camera geometry of flat back reflection camera.

We consider the flat back reflection camera in Fig. 1 and find,

$$\cos\varphi_i = -\cos 2\theta_i = 2\sin^2\theta_i - 1 = s/[s^2 + (\tfrac{1}{2}n_i)^2]^{\frac{1}{2}}. \quad (1)$$

For two different lines we have

$$(h_i^2 + k_i^2 + l_i^2)\lambda_i^2 = (2a)^2 \sin^2\theta_i \quad (i = 1, 2) \quad (2)$$

which together yield

$$R \equiv (n_1/n_2)^2 = \frac{[((h_1^2 + k_1^2 + l_1^2)\lambda_1^2/2a^2) - 1]^{-2} - 1}{[((h_2^2 + k_2^2 + l_2^2)\lambda_2^2/2a^2) - 1]^{-2} - 1} .$$

If we now let $m_i = (h_i^2 + k_i^2 + l_i^2)\lambda_i^2/2$ and $x = 1/a^2$ we obtain

$$x^3 + px^2 + qx + r = 0 , \quad (4)$$

where

$$p = -2\frac{(m_1 + m_2)}{m_1 m_2} \quad (5)$$

$$q = \frac{(m_1 + m_2)^2}{(m_1 m_2)^2} + \frac{2}{m_1 m_2} + \frac{m_2^2 - Rm_1^2}{m_1^2 m_2^2 (R - 1)} \quad (6)$$

and

$$r = -2\left[\frac{(m_1 + m_2)}{(m_1 m_2)^2} + \frac{(m_2 - Rm_1)}{m_1^2 m_2^2 (R - 1)}\right] . \quad (7)$$

This cubic equation can readily be solved for a.

We can now investigate the error in $x = 1/a^2$ introduced by an error in $R = (n_1/n_2)^2$.

$$\Delta x = \Delta R(\partial x/\partial R) \equiv \Delta R . Z' \quad (8)$$

$$Z' = (\partial x/\partial q)(dq/dR) + (\partial x/dr)(dr/dR)$$
$$= \frac{2(m_1 - m_2) - x(m_1^2 - m_2^2)}{(R - 1)^2 m_1 m_2 [3x^2 m_1 m_2 - 4x(m_1 + m_2) + 4 + (Rm_2^2 - m_1^2)/m_1 m_2 (R - 1)]} . \quad (9)$$

More conventionally, we can introduce Z by

$$\Delta x/x = Z(\Delta R/R) = Z'(R/x) . (\Delta R/R)$$
$$\text{or} \quad \Delta a/a = Z . \frac{\Delta(n_1/n_2)}{(n_1/n_2)} . \quad (10)$$

As a specific example of this result, let us consider the α_1, α_2 doublet of the (7, 5, 2) line produced by Mo radiation incident on tungsten. Here

$$h_1^2 + k_1^2 + l_1^2 = h_2^2 + k_2^2 + l_2^2 = 78, \ \lambda_1 = 0{\cdot}70926 \text{ Å} ,$$
$$\lambda_2 = 0{\cdot}71354 \text{ Å}, \ a \simeq 3{\cdot}165 \text{ Å}, \text{ and } R \simeq 2{\cdot}39 .$$

This implies if n_1/n_2 is known to one part in 10^2, a would be known to 1·6 parts in 10^4.

Of course, in an attempt to determine the accuracy of a particular measurement of a, we must include all systematic and random errors in our estimate of

$$\Delta(n_1/n_2)/(n_1/n_2) .$$

Fortunately, the two lines are fairly close together, hence their spectral profiles are similar. Thus, most of the systematic errors in measuring the two lines are in the same direction and of nearly the same magnitude. From this it can easily be shown that taking the ratio cancels the individual errors in n_1 and n_2 to first order.

I would like to thank Dr J. Karle and Dr H. Hauptman for continued interest and helpful discussions.

References

ČERNOHORSKÝ, M. (1960). *Acta Cryst.* **13**, 822.
ROVINSKIJ, B. M. & KOSTJUKOVA, E. P. (1958). *Kristallografija*, **3**, 383.

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The compound Li_2MgPb.*

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We have prepared the compound Li_2MgPb, determined its structure and melting point. Samples were prepared by melting together metallic elements of greater than 99·5% purity. Melting and thermal analysis were done on samples in a pure iron crucible in an argon atmosphere. Crystals, a centimeter on an edge, grew easily in a 300 g. sample which required about thirty minutes to freeze. The compound is brittle, has a metallic blue color, and tarnishes in a matter of minutes in laboratory air.

The measured and calculated weight percentages of the elements are, respectively: Li, 5·71 ± 0·06, 5·66; Mg, 9·99 ± 0·02, 9·91; Pb, 84·1 ± 0·3, 84·43. A congruent melting point of 859 °C. was measured for the compound. The true melting point of the pure compound is probably within 10 °C. of this value.

X-ray diffraction powder patterns showed this compound to have a face-centered cubic structure. We compare our proposed structure for this compound with Li_3Pb (Zalkin & Ramsey, 1956) and Mg_2Pb (Brauer & Tiesler, 1950*a*):

	Li_3Pb	Mg_2Pb	Li_2MgPb
a_0 (Å)	6·687	6·813	6·781
Positions*			
0, 0, 0,	Pb	Pb	Pb
½, ½, ½,	Li	Vacant	Mg
¼, ¼, ¼; ¾, ¾, ¾	2 Li	2 Mg	2 Li

* To all positions is added face-centering.

Since X-ray diffraction does not readily reveal light atom positions in this structure, we propose soon to carry out neutron diffraction. If the structure is as ordered as we suppose, we may look for disordering among the light element positions by electrical resistivity measurements. (The nuclear magnetic resonance adsorption line of the Li in the compound is sharp as it is in semiconducting Li_3Bi, whereas the line is broad in conducting lithium intermetallic compounds (Holder, 1960).)

The compound satisfies the criteria of Mooser & Pear-

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