as given by Pike (1959), eq. (16). If the absorption is included, the angular factor is given by

$$1/J(\theta) = (1+\cos^2 2\theta)/(\sin^2\theta\cos\theta) \qquad (3)$$

as in Ladell (1961), eq. (43), and Ladell, Parrish & Taylor (1957, 1959).

The methods of Pike (1959) can be easily extended to take into account the effect of absorption (in addition to the Lorentz, polarization and other factors) by substituting (3) for $B(2\theta)$ in his eq. (38). One obtains

$$(\psi-\psi_0)_U = -\frac{V}{\tilde{\lambda}^2}\tan^3\tilde{\theta}\left\{3-4\cot^2\tilde{\theta}-\frac{16\cos 2\tilde{\theta}\cos^2\tilde{\theta}}{1+\cos^2 2\tilde{\theta}}\right\}. \qquad (4)$$

(where the subscript 'U' has been used to indicate that the angular correction term now also accounts for absorption).

The correction term given by (4) can be compared with that reported by Ladell, Mack, Parrish & Taylor (1959) by calculating the spectral variance, $\tilde{V}$, and mean wavelength, $\tilde{\lambda}$, on their spectral model and substituting these quantities in (4).

Table 1. *Comparison of correction terms*

$\Delta_D+\Delta_{LPU}$ and $(\psi-\psi_0)_U$ for Cu $K\alpha$ radiation: $\tilde{\lambda}=1538{\cdot}745$ X.U., $\tilde{V}=3{\cdot}84957$

2θ	$(\psi-\psi_0)_U$	$(\Delta_D+\Delta_{LPU})$
120	−0·0016°	−0·0015°
130	−0·0032	−0·0033
140	−0·0065	−0·0066
150	−0·0157	−0·0164
155	−0·0272	−0·0279
160	−0·0530	−0·0554
162·5	−0·0789	−0·0821
165	−0·1252	−0·1336

Table 2. *Comparison of correction terms*

$\Delta_D+\Delta_{LPU}$ and $(\psi-\psi_0)_U$ for Cr $K\alpha$ radiation: $\tilde{\lambda}=2286{\cdot}450$ X.U., $\tilde{V}=4{\cdot}55732$

2θ	$(\psi-\psi_0)_U$	$(\Delta_D+\Delta_{LPU})$
120°	−0·0008°	−0·0008°
130	−0·0017	−0·0019
140	−0·0035	−0·0033
150	−0·0084	−0·0088
155	−0·0146	−0·0150
160	−0·0284	−0·0289
162·5	−0·0423	−0·0433
165	−0·0671	−0·0704

The correction term given by (4) was calculated for Cu and Cr $K\alpha$ radiation and is compared with the equivalent correction term $\Delta_D+\Delta_{LP}$ (Ladell, Mack, Parrish & Taylor, 1959, Figs. 1, 2). The results are given in Tables 1 and 2. These results indicate that the approximations which lead to the characterization of the correction in terms of the variance and mean wavelength are reasonable and that there is no significant difference between the numerical approach of Ladell, Mack, Parrish & Taylor (1959) and that of Pike.

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The choice of axes in the amphiboles.

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One of us (Zussman, 1959) has previously pointed out some of the confusion which has arisen in the literature of the amphiboles as a result of the possibility of describing the Bravais lattice by two different cells which have closely similar axial parameters. As a result of this some earlier comparisons of the unit-cell parameters of different amphiboles are invalidated by the fact that the parameters in question refer to different unit cells. It has since come to our notice that there are other sources of confusion in the literature which are related to this matter, and it is the purpose of the present note to discuss these for the benefit of future work.

1. Space group

The two conventional choices of axes correspond to descriptions of the space group in the settings $C2/m$ and $I2/m$, and the most convenient way of specifying which choice of unit cell is being used on any occasion is to denote it as either the C-cell or the I-cell. Although $C2/m$ is the standard setting for this space group, most papers on amphibole structure have used the I-cell because it best illustrates the relationship to the pyroxene structure when the latter is referred (as it usually is) to a C-cell. The first published structure of an amphibole, that of tremolite (Warren, 1930), was referred to the I-cell, but was published before the introduction of the Hermann–Mauguin symbols, and the space group was therefore given in the Wyckoff notation 2Ci-3, and later commentators translated this into the standard form $C2/m$ without noticing that this would involve a change in the unit-cell parameters (e.g. Bragg, 1937). Thus the parameters of the I-cell have appeared in the literature in conjunction with a statement that the space group is $C2/m$.

2. The angle β and the sense of the z-axis

Early morphological workers used the mineralogical convention with an acute angle $\beta = (100) \wedge (001)$. Warren (1930) kept β acute but defined it as $X\hat{O}Z$, and this contravention of currently accepted crystallographic usage was perpetuated by Whittaker (1949), describing crocidolite, and by Heritsch, Paulitsch & Walitzi (1957), describing hornblendes, in order to facilitate direct comparison with Warren's work. In *Structure Reports* (1949) the β angle for crocidolite was converted to the conventional obtuse value, but no allowance was made for the fact that this involved a change in the sense of the z-axis, so that the atomic z-coordinates should have been appropriately modified. Similarly, Zussman (1955), Heritsch, Bertoldi & Walitzi (1959), Heritsch & Kahler (1959) and Heritsch & Reichert (1959) all use the I-cell with β obtuse, and therefore should have reversed the signs of their z-coordinates, which were measured in the same sense as those given by Warren and by Whittaker.

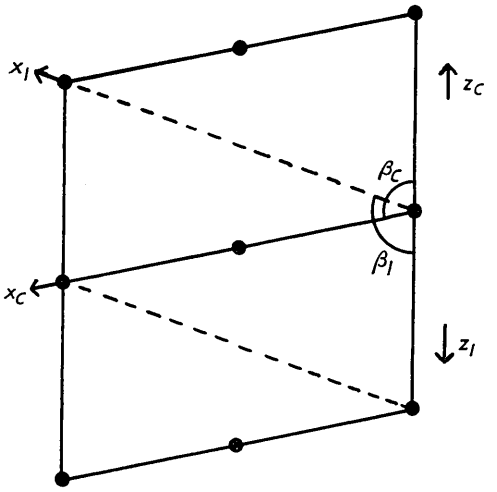

Fig. 1. Projection on (010) of clino-amphibole lattice showing the alternative C- and I-centred unit cells.

It is to be noted that this internal inconsistency occurs only in work which has been done or reported hitherto using the conventional I-cell with β obtuse. The C-cell with β obtuse has its z-axis in the same direction as the I-cell with β acute, so that there is no discrepancy from this source in the work of Heritsch, Paulitsch & Walitzi (1957) who used both of these directly comparable conventions. Nevertheless we consider that the continued use of an acute β-angle is likely to lead to increasing misunderstanding and confusion for future workers. For the future, therefore, it is recommended that $\beta (= X\hat{O}Z)$ shall always be made obtuse. This means:

(1) That the transformation relating the I-cell and the C-cell is as shown in Fig. 1, and is given by the matrix

I in terms of C

	C
I	1 0 1
	0 1 0
	0 0 $\bar{1}$

Thus the z parameters of all atoms must have opposite signs in the I-description and in the C-description.*

(2) That in comparing two structures where no change of cell is involved, but where the older description has β acute, the signs of z parameters should be reversed.*

As between the C-cell and the I-cell, however, no very definite grounds for choice exist. The C-setting was used earlier (e.g. Nordenskiold, 1855), and the I-setting was introduced by Tschermak (1884). The existence of alternative settings, and their inter-relationship, has been noted in many mineralogical texts, e.g. Hintze, 1897. The C-cell usually has the smaller a-axis and smaller obtuse β, and thus satisfies Donnay's rule 4 (Donnay & Nowacki, 1954), but in rare cases the converse may be true, and the differences are small. On the other hand the I-cell brings out the morphological and structural relationships to the pyroxenes when these are described in the conventional C-setting, and it also leads to much less variable values of a (Whittaker, 1960). The choice adopted is less important than ensuring that it is quite clear which convention is being used, or has been used in any quoted data.

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* In order to maintain a right-handed set of axes, the signs of y parameters should also be reversed; since (010) is a plane of symmetry this change is purely formal, and does not make any real difference to the description of the structure.