(1927) notation (ξ, ζ, ω) for cylindrical polar co-ordinates in reciprocal space, with the addition of the symbol φ for the elevation angle, $\tan^{-1} \zeta/\xi$, required for the conversion to spherical polar co-ordinates. A survey of the literature shows, however, that this notation is not in general use and that it is liable to lead to some confusion since many authors, e.g. Buerger (1942) and Henry, Lipson & Wooster (1951) have used the symbol φ in place of ω to denote the azimuth angle in cylindrical and spherical polar co-ordinates.

Furnas & Harker (1955) in their pioneering work on three-circle diffractometers were concerned with the general problem of orientating crystals in three dimensions; their nomenclature is based on that of Euler (1776). Furnas (1957) in his comprehensive handbook on the General Electric Single-Crystal Orienter has now changed one of the symbols in this notation. These two sets of symbols are compared with ours in the table.

	F. & H. (1955)	A. & P. (1957)	F. (1957)
Rotation about vertical axis of diffractometer	$\theta, 2\theta, \omega$	$\theta, 2\theta, \Theta$	$\theta, 2\theta, \omega$
Rotation about axis of goniometer head. (Azimuth angle)	R	ω	φ
Rotation of goniometer head about horizontal axis. (Elevation angle)	χ	φ	χ

Furnas's (1957) notation agrees as well as possible with the rather uncertain conventions and in the hope of minimizing confusion in the use of these instruments, it will be employed in any further publication on this subject from this laboratory, including the note by Brown (1958) which follows.

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Determination of triclinic crystal settings for a single-crystal diffractometer.

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A simple analogue computer has been described by Arndt & Phillips (1957) for calculating crystal settings on a single-crystal cone diffractometer, similar to the one described by Furnas & Harker (1955). The computer, as described, is suitable for use only with crystals of monoclinic or higher symmetry, but by a simple modification it can be used for calculating the settings of triclinic crystals. Two schemes of data collecting are possible, which will be referred to as the 'Real-Axis Setting' and the 'Reciprocal-Axis Setting'.

In the Real-Axis Setting (Fig. 1(*a*)), the *b* axis (say) is made to coincide with the goniometer axis, which is identical with the axis of the φ circle (see Arndt & Phillips (1958)). The reciprocal-lattice net ($h0l$) is then in the plane perpendicular to the axis of the φ circle and settings for reflexions in this layer are calculated in the same way as those for monoclinic crystals. For upper levels, rotation of the reciprocal-lattice net about the axis of the φ circle is no longer a rotation about the point ($0k0$) but about a point O_1 which is the projection of the origin on the kth layer. If then the centre of the protractor A of the computer (Fig. 1(*c*)) is superimposed over the point O_1 on the reciprocal-lattice net, settings for the reflexions on the kth layer can be determined as for

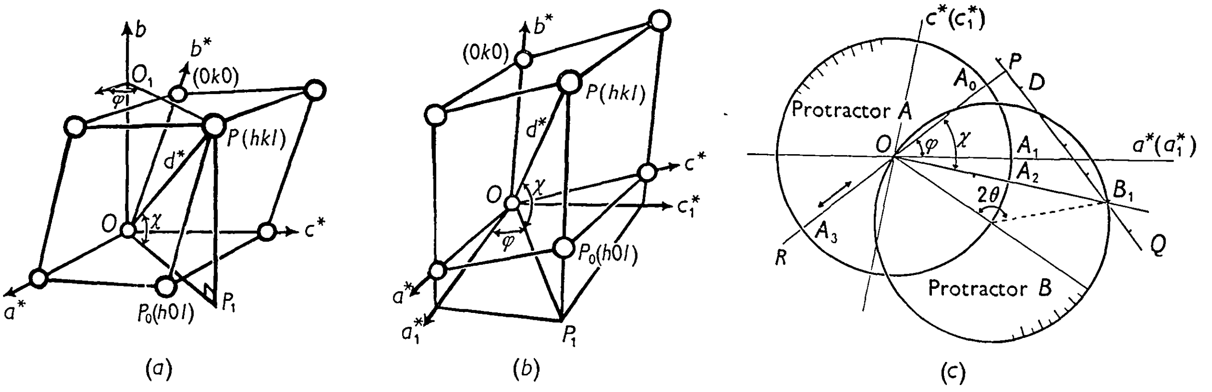

Fig. 1. (*a*) Position of reciprocal lattice in the real-axis setting. (*b*) Position of reciprocal lattice in reciprocal-axis setting. (*c*) Analogue computer for determination of crystal and counter settings.

monoclinic crystals, providing that the line PQ (Fig. 1(*c*)) is marked out in intervals of λ/b (corresponding to the distance OO_1 in Fig. 1(*a*)), rather than in intervals of b^*.

In the Reciprocal-Axis Setting, the b^* axis is chosen to coincide with the axis of the φ circle (Fig. 1(*b*)). The $(h0l)$ reflexions now no longer have a χ setting of zero. In this case it is convenient to construct the projection of the $(h0l)$ net on the plane perpendicular to b^*. This projection (a_1^*, c_1^*) is then used in place of the reciprocal-lattice net in the computer. The angle φ is given by the angle between P_1O and the a_1^* axis and is computed in the manner described by Arndt & Phillips (1957). The angle χ is measured if the distance PB_1 (Fig. 1(*c*)) is made to correspond to the distance PP_1 (Fig. 1(*b*)). This is done by providing a scale, free to move along PQ (Fig. 1(*c*)) and marked out in units of b^*, which is displaced by an amount PD corresponding to the distance (Fig. 1(*b*)) $P_1P_0 = ha^* \cos \gamma^* + lc^* \cos \alpha^*$. This displacement is found by means of a two-sided rule marked out on one side in units of $a^* \cos \gamma^*$ and on the other in units of $c^* \cos \alpha^*$, each measured from a common origin. It will be observed that all reflexions on a row parallel to b^* can then be found with one setting of the scale PQ, and that these will also all have the same φ setting.

The Real-Axis Setting is most suitable for the collection of data from the $(h0l)$ layer, since in this setting the angle χ is always zero, and only φ and θ need to be computed. In computing the settings for other levels, the reciprocal-lattice net has to be shifted for each level, and no other class of reflexions will, in general, have the same φ or χ setting. The Reciprocal-Axis Setting is more suitable for the collection of three-dimensional data, since reflexions on central zones will have the same φ setting (cf. Furnas & Harker's zone diffractometer) and all reflexions in rows of these zones parallel to b^* will have the same setting of the computer scale PQ. These two triclinic settings also, of course, allow monoclinic crystals to be mounted about axes other than their unique axis on occasions when it may be advantageous to do this.

I should like to thank Dr D. C. Phillips for his encouragement and assistance in this work, the Managers of the Royal Institution for permission to use the Davy Faraday Research Laboratory, and the Department of Scientific and Industrial Research for a maintainance grant.

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Note on the hydrogen bonding in the crystal structure of hydroxylamine.

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In the crystal structure of hydroxylamine (Meyers & Lipscomb, 1955) the molecules are associated by two different hydrogen bonds between oxygen and nitrogen in neighbouring molecules; the lengths of these hydrogen bonds are 2·74 and 3·07 Å respectively. Since the hydrogen atoms did not show up in the structure determination, the authors refrain from deciding between the three possible arrangements of the hydrogen atoms:

(*a*) the 2·74 Å bond is O–H ··· N, the 3·07 Å bond is O ··· H–N.
(*b*) the 3·07 Å bond is O–H ··· N, the 2·74 Å bond is O ··· H–N.
(*c*) both the 2·74 Å bond and the 3·07 Å bond are O ··· H–N.

From a consideration of the crystal structures of five different oximes published so far it has been inferred, that the hydrogen bonds between oxygen and nitrogen, by which the molecules in all the structures are associated, are of the type O–H ··· N (Jerslev, 1957). In two of the oxime structures, *anti-p*-chlorobenzaldoxime and formamidoxime, the hydrogen bonds result in the formation of chains $\cdots > \mathrm{N{-}O{-}H} \cdots > \mathrm{N{-}O{-}H} \cdots$, the geometry of which is very similar to one of two chains similarly formed by identical hydrogen bonds in the crystal structure of hydroxylamine.

	anti-p-chloro-benzald-oxime	Form-amid-oxime	Hydroxyl-amine	Hydroxyl-amine
∠ N–O ··· N′	109°	100°	101°	129°
∠ O–N ··· O′	112°	122°	111°	83°
O ··· N′ = N ··· O′	2·82 Å	2·81 Å	2·74 Å	3·07 Å

It would seem very likely that a hydrogen bond between oxygen and nitrogen in the hydroxylamine crystal structure is of the same type as that found with the oximes; and both the angles connected with the hydrogen bonds and the lengths of these favour among the systems of hydrogen bonding the one designated by (*a*).

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