the distances from hydrogen to nitrogen and to oxygen, but is the distance from nitrogen to oxygen. (The hydrogen is not on the line joining these two atoms.) The N–O distance in the table refers to the set of four oxygens that are not hydrogen-bonded with the ammonium group. (Each oxygen atom *is* hydrogen-bonded to *some* ammonium group, but a particular ammonium group is surrounded by eight oxygen neighbors, four of which are linked to the group by hydrogen bonds.)

Table 7 also gives a comparison (where possible) between the ADP results and those obtained by Bacon & Pease in their room-temperature neutron study of KDP. One finds a remarkable similarity in the H_2PO_4 systems in the two crystals. The only significant difference occurs in the angle between the P–O bond and O–H $\cdots$ O bond. This one might expect from differences in c-direction packing (compare cell dimensions: $a = 7 \cdot 502$ Å, $c = 7 \cdot 546$ Å for ADP, and $a = 7 \cdot 434$ Å, $c = 6 \cdot 945$ Å for KDP). However, it would seem from the difference in ADP between this bond angle and the angle between P–O and O–H that the structure 'wants' to assume an angle more nearly equal to that observed in KDP, but is prevented from doing so by the size and shape of the ammonium ion.

The tetrahedral ammonium ion is found to be slightly distorted, presumably as a result of hydrogen bonding with neighboring PO_4-groups. The distortion is not so great, however, as to result in linear N–H $\cdots$ O bonds. The N–H bond is about 14° off the line joining nitrogen and oxygen centers.

The temperature parameters were excluded from the comparison in Table 7, since these quantities would not be expected to compare closely in the three studies. If one analyses the temperature parameters given in Table 4, it appears that the oxygens and the ammonium hydrogens both have their major vibration axes in planes $x = k_j y$, where the constant k_j equals x_j/y_j (the ratio of the coordinates of the jth atom).

In the case of H_N the major vibration axis is approximately perpendicular to the N–H bond. In the case of oxygen the major vibration axis is tilted from the vertical (c direction) by about 30°, the tilt being such as to approach being transverse to the P–O bond.

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Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 500 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible; and proofs will not generally be submitted to authors. Publication will be quicker if the contributions are without illustrations.

On the adoption of standard symbols for the settings of single-crystal diffractometers. By

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The settings of three-circle single-crystal diffractometers when used as 'cone diffractometers' (Furnas & Harker, 1955) are simply the spherical polar co-ordinates of the reciprocal lattice points with θ, the Bragg angle, given by the radial co-ordinate $2 \sin \theta$. It seems desirable,

therefore, that the symbols used to identify the diffractometer circles should be those used for reciprocal-lattice co-ordinates. For this reason the notation adopted in our paper on the determination of diffractometer settings (Arndt & Phillips, 1957) was based on Bernal's

(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

	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

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.

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. By I. D. BROWN,
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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
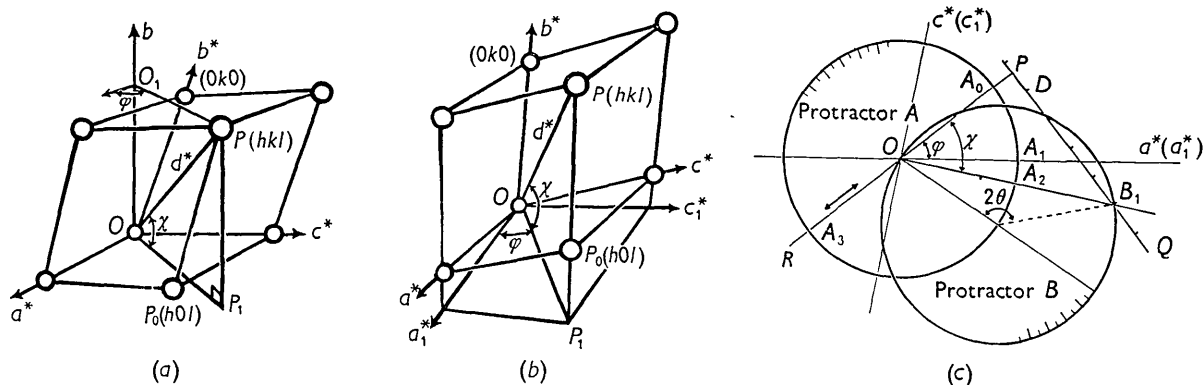

Fig. 1. (a) Position of reciprocal lattice in the real-axis setting. (b) Position of reciprocal lattice in reciprocal-axis setting. (c) Analogue computer for determination of crystal and counter settings.