photographs can be obtained, giving all three reciprocal-cell lengths and two of the three angles; the third angle is derived from these and from the corresponding direct cell angle, which is the difference in camera dial settings for the two photographs.

We have found it useful to develop a method for deriving precise parameters from precession photographs. This need arose from a set of circumstances including (i) the availability of a precession camera and an accurate device for measurement of (x,y) Cartesian coordinates from films; and (ii) the use of an older type of four-circle diffractometer (Hilger & Watts Y290), for which a previous knowledge of reasonably precise unit-cell dimensions can save considerable time and effort in setting up a crystal for data collection. Devices for accurate measurement of coordinates from films are commercially available from crystallographic suppliers, or a two-direction travelling microscope can be used.

A zero-layer of the reciprocal lattice is described by three parameters, which we can take to be a^*, b^* and γ^* without loss of generality. The photograph is laid on the measuring device with its centre in an arbitrary position (with coordinates X, Y), such that the $+a^*$ axis is rotated anticlockwise from the instrument x axis by an arbitrary angle φ and the $+b^*$ axis by the angle $\gamma^* + \varphi$. Pairs of (x,y) coordinates are measured for a number of reflexions (typically 10–20), preferably well distributed over the film. These are used for a non-linear least-squares refinement of the six parameters a^*, b^*, γ^*, X, Y and φ, in which the quantity $\sum [(x_0 - x_c)^2 + (y_o - y_c)^2]$ is minimized. The basic equations are

$$x = X + S\lambda[ha^* \cos \varphi + kb^* \cos (\varphi + \gamma^*)]$$

$$y = Y + S\lambda[ha^* \sin \varphi + kb^* \sin (\varphi + \gamma^*)],$$

where S is the crystal-to-film distance, λ is the X-ray wavelength in Å, and a^* and b^* have the units of Å^{-1}. Derivatives are obtained analytically and for photographs displaying crystallographic symmetry any of the constraints $a^* = b^*$, $\gamma^* = 60°$ or $\gamma^* = 90°$ can easily be applied. Approximate starting parameters are required, and convergence is reached in a few cycles.

We have found that the results obtained are usually not significantly different from the final values obtained by refinement from diffractometric measurements. A precision of *ca* 0·1% in a^* and b^*, and 0·05° in γ^* is easily attainable. As in all precession measurement methods, the value of S must be accurately known (Buerger, 1964).

A computer listing in Basic for the Hewlett–Packard 2000 series of computers is available from the author on request. Translation into other dialects of Basic or into Fortran would not be difficult.

Table 1. *Comparison of reciprocal-cell parameters calculated from precession photographs and diffractometer measurements*

	*hk*0	*h*0*l*	Diffractometer
a^* (Å^{-1})	0·1272 (1)	0·1273 (1)	0·12715 (3)
b^*	0·0810 (1)		0·08082 (2)
c^*		0·0542 (1)	0·05424 (1)
γ^* (°)		77·91 (6)	77·98 (2)
Number of reflexions	12	10	
R.m.s. deviation (mm)	0·018	0·036	

Example

*hk*0 and *h*0*l* photographs were measured for the monoclinic substance $Mo_2(O_2CCH_3)_2(CH_3COCHCOCH_3)_2$ (Garner, Parkes, Walton & Clegg, 1978). 12 and 10 reflexions respectively were measured, and the results are summarized in Table 1, and compared with the reciprocal-cell parameters derived from diffractometer measurements.

This work was carried out in the University of Newcastle upon Tyne, England. I thank the Crystallography Laboratory and the Computing Laboratory for the use of their equipment.

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Corrections to equations in § 3 of *International Tables for X-ray Crystallography*, Vol. IV.

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Abstract

Two misprinted equations in *International Tables for X-ray Crystallography*, Vol. IV [(1974). Birmingham: Kynoch Press], should be corrected.

Misprints have been found in § 3 (*Angle Settings for Four-Circle Diffractometers*) of *International Tables for X-ray Crystallography*, Vol. IV (1974).

1. P. 277, paragraph 3.2.2.4., equation (2):
   Replace $a^*c^* \cos\alpha^*$ by $b^*c^* \cos\alpha^*$.
2. P. 280, paragraph 3.4.3., equation (3):
   Replace $(a^*c^* \cos\beta^* - t_{12}t_{32})t_{11}$ by $(a^*c^* \cos\beta^* - t_{12}t_{32})/t_{11}$.

Reference

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press.

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