Table 2.2.3.1. *Glossary of symbols used to specify quantities on diffraction patterns and in reciprocal space*

θ	Bragg angle
2θ	Angle of deviation of the reflected beam with respect to the incident beam
$\hat{\mathbf{S}}_o$	Unit vector lying along the direction of the incident beam
$\hat{\mathbf{S}}$	Unit vector lying along the direction of the reflected beam
$\mathbf{s} = (\hat{\mathbf{S}} - \hat{\mathbf{S}}_o)$	The scattering vector of magnitude $2\sin\theta$. $\mathbf{s}$ is perpendicular to the bisector of the angle between $\hat{\mathbf{S}}_o$ and $\hat{\mathbf{S}}$. $\mathbf{s}$ is identical to the reciprocal-lattice vector $\mathbf{d}^*$ of magnitude λ/d, where d is the interplanar spacing, when $\mathbf{d}^*$ is in the diffraction condition. In this notation, the radius of the Ewald sphere is unity. This convention is adopted because it follows that in Volume II of *International Tables* (p. 175). Note that in Section 2.2.1 *Laue geometry* the alternative convention ($\lvert\mathbf{d}^*\rvert = 1/d$) is adopted whereby the radius of each Ewald sphere is $1/\lambda$. This allows a nest of Ewald spheres between $1/\lambda_{\max}$ and $1/\lambda_{\min}$ to be drawn
ζ	Coordinate of a point P in reciprocal space parallel to a rotation axis as the axis of cylindrical coordinates relative to the origin of reciprocal space
ξ	Radial coordinate of a point P in reciprocal space; that is, the radius of a cylinder having the rotation axis as axis
τ	The angular coordinate of P, measured as the angle between ξ and $\hat{\mathbf{S}}_o$ [see Fig. 2.2.3.1(*b*)]
φ	The angle of rotation from a defined datum orientation to bring a relp onto the Ewald sphere in the rotation method (see Fig. 2.2.3.3)
μ	The angle of inclination of $\hat{\mathbf{S}}_o$ to the equatorial plane
Υ	The angle between the projections of $\hat{\mathbf{S}}_o$ and $\hat{\mathbf{S}}$ onto the equatorial plane
ν	The angle of inclination of $\hat{\mathbf{S}}$ to the equatorial plane
ω, χ, φ	The crystal setting angles on the four-circle diffractometer (see Fig. 2.2.6.1). The φ used here is not the same as that in the rotation method (Fig. 2.2.3.3). This clash in using the same symbol twice is inevitable because of the widespread use of the rotation camera and four-circle diffractometer.

The equatorial plane is the plane normal to the rotation axis.

The notation now follows that of Arndt & Wonacott (1977) for the coordinates of a spot on the film or detector. Z_F is parallel to the rotation axis and ζ. Y_F is perpendicular to the rotation axis and the beam. *IT* II (1959, p. 177) follows the convention of y being parallel and x perpendicular to the rotation-axis direction, *i.e.* $(Y_F, Z_F) \equiv (x, y)$. The advantage of the (Y_F, Z_F) notation is that the x-axis direction is then the same as the X-ray beam direction.

The coordinates of a reflection on a flat film (Y_F, Z_F) are related to the cylindrical coordinates of a relp (ξ, ζ) [Fig. 2.2.3.2(*a*)] by

$$Y_F = D\tan\Upsilon \qquad (2.2.3.13)$$

$$Z_F = D\sec\Upsilon\tan\nu, \qquad (2.2.3.14)$$

which becomes

$$Z_F = 2D\zeta/(2 - \xi^2 - \zeta^2), \qquad (2.2.3.15)$$

where D is the crystal-to-film distance.

For the case of a V-shaped cassette with the V axis parallel to the rotation axis and the film making an angle α to the beam direction [Fig. 2.2.3.2(*b*)], then

$$Y_F = D\tan\Upsilon/(\sin\alpha + \cos\alpha\tan\Upsilon) \qquad (2.2.3.16)$$

$$Z_F = (D - Y_F\cos\alpha)\zeta/(1 - d^{*2}/2). \qquad (2.2.3.17)$$

This situation also corresponds to the case of flat electronic area detector inclined to the incident beam in a similar way.

Note that Arndt & Wonacott (1977) use ν instead of α here. We use α and so follow *IT* II (1959). This avoids confusion with the ν of Table 2.2.3.1. D is the crystal to V distance. In the case of the V cassettes of Enraf–Nonius, α is 60°.

For the case of a cylindrical film or image plate where the axis of the cylinder is coincident with the rotation axis [Fig. 2.2.3.2(*c*)] then, for Υ in degrees,

$$Y_F = \frac{2\pi}{360}D\Upsilon \qquad (2.2.3.18)$$

$$Z_F = D\tan\nu, \qquad (2.2.3.19)$$

which becomes

$$Z_F = \frac{D\zeta}{\sqrt{(1 - \zeta^2)}}. \qquad (2.2.3.20)$$

Here, D is the radius of curvature of the cylinder assuming that the crystal is at the centre of curvature.

In the three geometries mentioned here, detector-misalignment errors have to be considered. These are three orthogonal angular errors, translation of the origin, and error in the crystal-to-film distance.

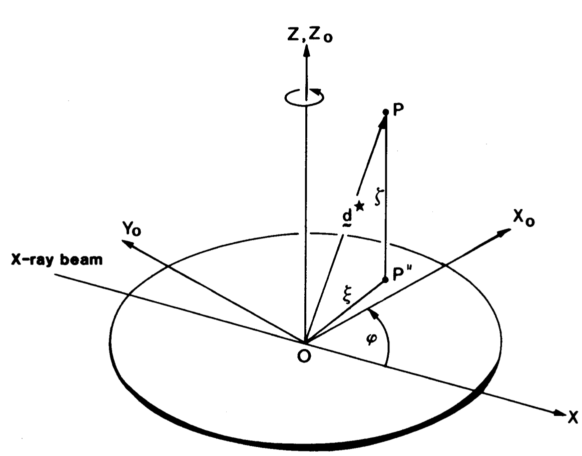

Fig. 2.2.3.3. The rotation method. Definition of coordinate systems. [Cylindrical coordinates of a relp P (ξ, ζ, φ) are defined relative to the axial system $X_0Y_0Z_0$ which rotates with the crystal.] The axial system XYZ is defined such that X is parallel to the incident beam and Z is coincident with the rotation axis. From Arndt & Wonacott (1977).