Table 9.1.7.1. *Standard choice of asymmetric unit in reciprocal space for different point groups from the CCP4 program suite*

Point group	Index limits	
1	hkl:	$l \geq 0$
	$hk0$:	$h \geq 0$
	$0k0$:	$k \geq 0$
2	hkl:	$k \geq 0, l \geq 0$
	$hk0$:	$h \geq 0$
222	hkl:	$h \geq 0, k \geq 0, l \geq 0$
4	hkl:	$h \geq 0, k > 0, l \geq 0$
	$0kl$:	$k \geq 0$
422	hkl:	$h \geq k, k \geq 0, l \geq 0$
3	hkl:	$h \geq 0, k > 0$
	$00l$:	$l > 0$
321	hkl:	$h \geq k, k \geq 0$
	hhl:	$l \geq 0$
312	hkl:	$h \geq k, k \geq 0$
	$h0l$:	$l \geq 0$
6	hkl:	$h \geq 0, k > 0, l \geq 0$
	$0kl$:	$k \geq 0$
622	hkl:	$h \geq k, k \geq 0, l \geq 0$
23	hkl:	$h \geq 0, k > h, l > h$
	hkh:	$k \geq h$
432	hkl:	$h \geq 0, k \geq l, l \geq h$

$$\bar{h}_{\min} \leq h \leq h_{\max}, \qquad 0 \leq k \leq k_{\max}, \qquad \bar{l}_{\min} \leq l \leq l_{\max},$$

or

$$\bar{h}_{\min} \leq h \leq h_{\max}, \qquad \bar{k}_{\min} \leq k \leq k_{\max}, \qquad 0 \leq l \leq l_{\max}.$$

The standard choices of asymmetric unit taken from the *CCP*4 program suite (Collaborative Computational Project Number 4, 1994) are shown in Table 9.1.7.1.

The data are complete if the Ewald sphere has been crossed by all reflections in the asymmetric part of the reciprocal lattice. During data acquisition and reduction, all measured indices are conventionally transformed to this asymmetric unit of reciprocal space. Firstly, this allows merging of symmetry-equivalent measurements as appropriate. Secondly, it allows the completeness of the data to be assessed efficiently, using contributions from the whole sphere.

For all point groups, rotation of the crystal by 180° from any starting angle on the φ spindle axis is sufficient to provide a complete set of data (this is not sufficient if anomalous measurements are required; see Section 9.1.7.2). Given such a total rotation, the redundancy of the measurements will increase with higher crystal symmetry. Thus, for a triclinic space group, the unique data will be measured almost twice on average (see the blind region below); for orthorhombic, eight times; for hexagonal class 6, 12 times; and for 622, 24 times. Redundancy is, in principle, advantageous, giving improved data quality (again see below), but it is generally possible to record complete unique data with a minimal overall rotation and correctly chosen starting angle on the spindle. It is of course necessary to determine the crystal orientation matrix, and this remains a vital part of data-collection strategy. With the intense time pressure currently on both SR beamlines and home sources, it is often essential to collect complete data with the minimal rotation range. This may well change with the advent of extremely fast detectors on the brightest SR sources, when the decision-making process may take longer than data collection.

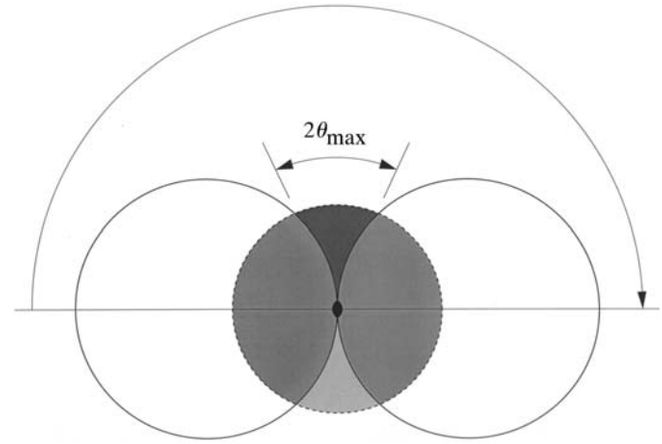

Fig. 9.1.7.1. Rotation of a triclinic crystal by 180° in the X-ray beam, represented as rotating the Ewald sphere with a stationary crystal, projected along the rotation axis. For the purpose of analysing the relation of data completeness to crystal symmetry and orientation both representations are equivalent.

Thus, the crystal point-group symmetry has a profound effect on the total rotation range and the optimal starting spindle and crystal orientation for the most efficient recording of complete unique data. The rest of this section suggests strategies for the collection of complete data with minimal total rotation when anomalous measurements are not required.

As stated above, for all crystals, rotation by 180° is fully sufficient to cover both sides of the Ewald sphere with intensity measurements. This is necessary for a triclinic crystal rotated around any arbitrary axis and also for a monoclinic crystal rotated around its unique b axis (Fig. 9.1.7.1). A twofold redundancy of unique data results; fourfold for the monoclinic case. Now consider a rotation of less than 180° (Fig. 9.1.7.2). Owing to the curvature of the Ewald sphere and the centre of symmetry arising from Friedel's law, the region of the sphere with reflections measured twice is diminished, and for part of the sphere there are no measurements. Most importantly, the proportions are resolution dependent. With a limited rotation, the high-resolution intensities reach a higher

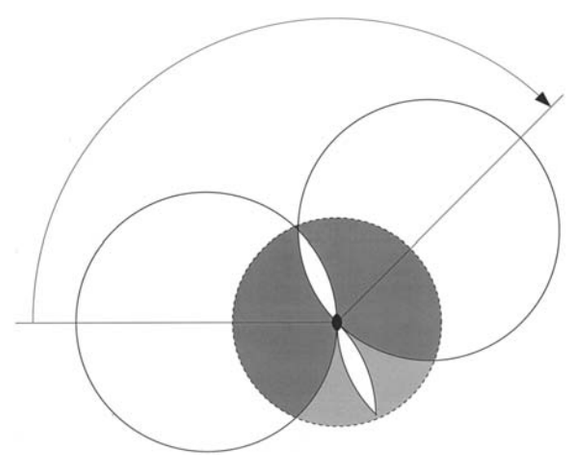

Fig. 9.1.7.2. Rotation of a triclinic crystal by 135° is not sufficient to obtain totally complete data. At high resolution the completeness is higher than at low resolution, where a full 180° rotation is required.

references