

1. GENERAL RELATIONSHIPS AND TECHNIQUES

relatively small effort required to derive the list. A disadvantage may be that there are protruding flagpoles or wings. Points of these lines or planes are no longer neighbours of inner points (an inner point has a full three-dimensional sphere of neighbours which belong to the asymmetric unit).

(2) In the *compact description* one lists each \mathbf{k} vector exactly once such that each point of the asymmetric unit is either an inner point itself or has inner points as neighbours. Such a description may not be uni-arm for some Wintgen positions, and the determination of the parameter ranges may become less straightforward. Under this approach, all points fulfil the conditions for the asymmetric units of *IT A*, which are always closed. The boundary conditions of *IT A* have to be modified: in reality the boundary is not closed everywhere; there are frequently open parts (see Section 1.5.5.3).

(3) In the *non-unique description* one gives up the condition that each \mathbf{k} vector is listed exactly once. The uni-arm and the compact descriptions are combined but the equivalence relations (\sim) are stated explicitly for those \mathbf{k} vectors which occur in more than one entry. Such tables are most informative and not too complicated for practical applications.

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Appendix 1.5.1.

Reciprocal-space groups \mathcal{G}^*

This table is based on Table 1 of Wintgen (1941).

In order to obtain the Hermann–Mauguin symbol of \mathcal{G}^* from that of \mathcal{G} , one replaces any screw rotations by rotations and any glide reflections by reflections. The result is the symmorphous space group \mathcal{G}_0 assigned to \mathcal{G} . For most space groups \mathcal{G} , the reciprocal-space group \mathcal{G}^* is isomorphic to \mathcal{G}_0 , *i.e.* \mathcal{G}^* and \mathcal{G} belong to the same arithmetic crystal class. In the following cases the arithmetic crystal classes of \mathcal{G} and \mathcal{G}^* are different, *i.e.* \mathcal{G}^* can not be obtained in this simple way:

(1) If the lattice symbol of \mathcal{G} is F or I , it has to be replaced by I or F . The tetragonal space groups form an exception to this rule; for these the symbol I persists.

(2) The other exceptions are listed in the following table (for the symbols of the arithmetic crystal classes see *IT A*, Section 8.2.2):

Arithmetic crystal class of \mathcal{G}	Reciprocal-space group \mathcal{G}^*
$\bar{4}m2I$	$I\bar{4}2m$
$\bar{4}2mI$	$I\bar{4}m2$
$321P$	$P312$
$312P$	$P321$
$3m1P$	$P31m$
$31mP$	$P3m1$
$\bar{3}1mP$	$P\bar{3}m1$
$\bar{3}m1P$	$P\bar{3}1m$
$\bar{6}m2P$	$P\bar{6}2m$
$\bar{6}2mP$	$P\bar{6}m2$