

## 9. BASIC STRUCTURAL FEATURES

Table 9.7.1.1. Kitajgorodskij's categorization of the triclinic, monoclinic and orthorhombic space groups, as modified by Wilson (1993a)

Wilson's additions are enclosed in square brackets [...] and the original positions of space groups transferred by him by round brackets (· · ·). Space groups not listed belong to the 'impossible' category.

Molecular symmetry	1	$\bar{1}$	2	$m$	$2/m$	222	$mm$	$mmm$
Closest packed	$P\bar{1}$ $P2_1$ $P2_1/c$ [ $C2/c$ ] $P2_12_12_1$ $Pca2_1$ $Pna2_1$ [ $Pbca$ ]	$P\bar{1}$ $P2_1/c$ [ $C2/c$ ] $Pbca$						
Limitingly close packed	[ $P2_12_12$ ]  [ $Pbcn$ ]		( $C2/c$ ) $P2_12_12$  $Pbcn$	$Pmc2_1$ $Cmc2_1$ $Pnma$	$C2/m$  $Cmca$	$C222$ $F222$ $I222$  $Ccca$ *	$Fmm2$  $Pmma, Pmnn$	$Cmmm$ $Fmmm$ $Immm$
Permissible	$P1$ $C2$ [ $Pc$ ] $Cc$ [ $P2/c$ ] $(P2_12_12)$ [ $C222_1$ ]  ( $Pbca$ ) [ $Pccn$ ]		$C2$  $Pccn$	$Cm$ $P2_1/m$  $[P2/c]$ $[C222_1]$ $Aba2$ [ $Fdd2$ ]	$Pbam$			

\*Kitajgorodskij (1961) includes  $Pnnm$  at this position, but this is inconsistent with the text of either the Russian or the English version.  
†Kitajgorodskij (1961) correctly includes  $Pbcm$  at this position.

$2_1, 3_{1,2}, 4_{1,3}, 6_{1,5}$ ; any glide plane.

The remaining symmetry elements

$$1, \bar{1}; 4_2; \bar{4}; 6_{2,4} = 2 + 3_{1,2}; 6_3 = 2_1 + 3$$

are 'atropic'. The two triclinic space groups,  $P1$  and  $P\bar{1}$ , contain only 'atropic' elements, and are thus not classified by these criteria. The rest are divided into five groups, in accordance with the balance of symmetry elements within the unit cell. For the 71 non-triclinic space groups symmorphic in the strict sense (Wilson, 1993d; Subsection 1.4.2.1), the classification gives:

- (1) Fully symmorphic (only syntropic elements): 14.
- (2) Tending to symmorphism (mainly syntropic elements): 28.
- (3) Equally balanced (equal numbers of syntropic and antitropic elements): 20.
- (4) Tending to antimorphism (mainly antitropic elements): 9.
- (5) Fully antimorphic (only antitropic elements): 0.

The distribution of the 230 space groups (11 enantiomorphous couples merged) by arithmetic crystal class and degree of symmorphism is given in Table 9.7.1.2.

A few points about the symmorphic groups are worth noting. The 14 'fully symmorphic' space groups are those that (i) have primitive cells and (ii) have no secondary or tertiary axes (three each monoclinic, orthorhombic, tetragonal, hexagonal; two trigonal; no cubic). Secondary axes, even though syntropic in the conventional space-group notation, generate additional antitropic axes in accordance with the principles set out by Bertaut (1995, Chap. 4.1). These additional axes are not indicated in the 'full' Hermann–Mauguin space-group symbol, but should appear in the 'extended' symbol (Bertaut, 1995, Table 4.3.1‡). As a result of the additional axes, 21 symmorphic space groups with primitive cells are shifted to the 'tending to symmorphism' column (five tetragonal, six trigonal, five hexagonal, five cubic). Lattice centring has a similar or greater effect; the 36 centred symmorphic space groups are spread over the three columns 'tending to symmorphism' (seven), 'equally balanced' (20) and 'tending to antimorphism' (nine).

‡ Table 4.3.1 is not strictly consistent in its treatment of the 'extended' symbols. Tetragonal space groups are extended in full detail, but the extension of orthorhombic space groups is minimal.