Table 9.7.4.1. *Occurrence of molecules with specified point group in centred symmorphic and other space groups, based on the statistics by Belsky, Zorkaya & Zorky (1995)*

There is no entry in the 'other space group' column if examples are found in the centred symmorphic group.

Point group	Symmorphic space group	Other space group	Frequency
2	$C2$	...	18
m	Cm	...	6
$2/m$	$C2/m$	...	20
222	None	$Ccca$	4
	...	$Fddd$	2
	...	$P\bar{4}n2$	2
	...	$P4/ncc$	1
	...	$I4_1/acd$	3
$mm2$	$Fmm2$	...	2
mmm	None	$P4_2/mnm$	6
	...	$Im\bar{3}$	1
4	$I4$	...	1
$\bar{4}$	None	$P4/n$	1
	...	$P4_2/n$	3
	...	$I4_1/a$	12
	...	$P\bar{4}2_1c$	17
	...	$I\bar{4}2d$	1
	...	$I4_1/acd$	1
$4/m$	$I4/m$	...	1
422	None	$P4/nnc$	1
$4mm$	None	None	None
$\bar{4}2m$	$I\bar{4}2m$	...	3
$4/mmm$	$I4/mmm$	...	1
3	$R3$	...	8
$\bar{3}$	$R\bar{3}$	...	6
32	None	$R\bar{3}c$	5
$3m$	$R3m$	...	10
$\bar{3}m$	$R\bar{3}m$	...	2
6	None	None	None
$\bar{6}$	None	$P6_3/m$	12
$6/m$	None	None	None
622	None	None	None
$6mm$	None	None	None
$\bar{6}m2$	None	$P6_3/mmc$	1
$6/mmm$	None	None	None
23	None	$F\bar{4}3c$	1
$m\bar{3}$	$Fm\bar{3}$	...	2
432	None	None	None
$\bar{4}3m$	$I\bar{4}3m$	...	4
$m\bar{3}m$	$Fm\bar{3}m$	...	9
	$Im\bar{3}m$	...	2

in the packing. In about 90% of crystalline compounds, the molecules crystallize in low-symmetry space groups, so that a given molecule has a 12-point contact with neighbouring molecules. As 12 corresponds to the number of nearest neighbours in cubic and hexagonal closest packing of spheres, the periodic assembly of most molecular structures can be regarded as the closest packing of distorted spheres, where symmetry ensures the interlocking of complex shapes (Gavezzotti, 1994).

For the relatively infrequent cases where high molecular symmetry is reflected in high crystal symmetry, the packing of molecules can be derived from the appropriate, though not necessarily the densest, packing of spheres. For example, ten-point, eight-point and six-point molecular contacts can be achieved, respectively, by tetragonal close packing ($I4/mmm$), by I-centred cubic packing ($Im\bar{3}m$), and by primitive cubic packing ($Pm\bar{3}m$). For a review and some derivations of the densest packing of equal spheres, see Chapter 9.1 and Patterson & Kasper (1959), Coutanceau Clarke (1972), and Smith (1973); and for packing of clusters of unequal spheres, see Williams (1987).

With spheres having infinite point symmetry $\mathcal{K}_{\infty h}$, every sphere can be located on syntropic symmetry elements at special positions with high symmetry up to the symmetry of the lattice. The lattice translations, pertinent to the fully symmorphic space group, are then able to generate the entire crystal structure. When spheres are deformed, symmetry is removed and the non-lattice translations involved with antimorphic space groups

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