Table 9.7.1.2. *Space groups arranged by arithmetic crystal class and degree of symmorphism (Wilson, 1993d), as frequented by homomolecular structures with one molecule in the general position (in superscript numerals; according to Belsky, Zorkaya & Zorky, 1995)*

(*a*) Triclinic, monoclinic and orthorhombic systems. The triclinic space groups are a special case, with 'degree of symmorphism' undefined, and they are not assigned to any particular column. For *, † see Subsection 9.7.4.1.

Arithmetic crystal class	Fully symmorphic	Tending to symmorphism	Equally balanced	Tending to antimorphism	Fully antimorphic
$1P$			$*P1\dagger^{(90)}$		
$\bar{1}P$			$*P\bar{1}\dagger^{(1796)}$		
$2P$	$*P2^{(0)}$	...	...	...	$P2_1\dagger^{(1327)}$
$2C$	...	...	$*C2\dagger^{(109)}$	...	...
mP	$*Pm^{(0)}$	...	...	...	$Pc\dagger^{(58)}$
mC	...	...	$*Cm^{(0)}$	...	$Cc\dagger^{(144)}$
$2/mP$	$*P2/m^{(0)}$	...	$P2_1/m^{(0)}$	...	$P2_1/c\dagger^{(5951)}$
			$P2/c^{(11)}$		
$2/mC$	...	...	$*C2/m^{(0)}$	$C2/c\dagger^{(587)}$	...
$222P$	$*P222^{(0)}$	$P222_1^{(0)}$	...	$P2_12_12^{(30)}$	$P2_12_12_1\dagger^{(2795)}$
$222C$	...	$*C222^{(0)}$	...	$C222_1\dagger^{(11)}$	...
$222F$	...	...	$*F222^{(0)}$	...	...
$222I$	...	...	$*I222^{(0)}$	...	...
			$I2_12_12_1\dagger^{(0)}$		
$mm2P$	$*Pmm2^{(0)}$	$Pma2^{(0)}$	...	$Pmc2_1^{(0)}$	$Pca2_1^{(153)}$
				$Pcc2^{(1)}$	$Pna2_1\dagger^{(367)}$
				$Pnc2^{(1)}$	
				$Pmn2_1^{(0)}$	
				$Pba2^{(1)}$	
				$Pnn2^{(1)}$	
$mm2C$	...	$*Cmm2^{(0)}$	...	$Cmc2_1\dagger^{(0)}$	...
				$Ccc2^{(0)}$	
$2mmC$	...	$*Amm2^{(0)}$	...	$Abm2^{(0)}$	...
				$Ama2^{(0)}$	
				$Aba2\dagger^{(11)}$	
$mm2F$			$*Fmm2^{(0)}$	$Fdd2\dagger^{(35)}$	
$mm2I$	...	...	$*Imm2^{(0)}$	$Iba2\dagger^{(14)}$	
				$Ima2^{(0)}$	
$mmmP$	$*Pmmm^{(0)}$	$Pccm^{(0)}$	$Pnnn^{(0)}$	$Pnna^{(1)}$	$Pbca\dagger^{(827)}$
		$Pmma^{(0)}$	$Pban^{(0)}$	$Pcca^{(3)}$	
			$Pmna^{(0)}$	$Pbam^{(0)}$	
			$Pmmn^{(0)}$	$Pccn^{(37)}$	
				$Pbcm^{(0)}$	
				$Pnnm^{(0)}$	
				$Pbcn^{(60)}$	
				$Pnma^{(0)}$	
$mmmC$	...	$*Cmmm^{(0)}$	$Cmma^{(0)}$	$Cmcm^{(0)}$	...
				$Cmca^{(0)}$	
				$Cccm^{(0)}$	
				$Ccca\dagger^{(0)}$	
$mmmF$	...	...	$*Fmmm^{(0)}$	$Fddd\dagger^{(2)}$	...
$mmmI$	...	...	$*Immm^{(0)}$	$Ibam^{(0)}$	
				$Ibca^{(0)}$	
				$Imma^{(0)}$	

From the nature of the definitions, no symmorphic space group can be 'fully antimorphic'. The 14 groups under the latter heading consist of (i) 12 space groups with no special positions (Subsection 9.7.4.1), and (ii) two space groups whose only special positions have symmetry $\bar{1}$ (Subsection 9.7.4.2). On these criteria, the two triclinic groups excluded from discussion would fall naturally into the column 'fully antimorphic'. The remaining space groups have no obvious outstanding characteristics. Most of them fall under the heading 'tending to antimorphism', though there are some in each of the columns 'tending to symmorphism' and 'equally balanced'.

9.7.1.3. *Comparison of Kitajgorodskij's and Wilson's classifications*

Since both Kitajgorodskij's and Wilson's classifications were made with a view to 'explaining' the empirically observed frequencies of space groups – though neither makes any use of

Table 9.7.1.2. *Space groups arranged by arithmetic crystal class and degree of symmorphism (cont.)*

(*b*) Tetragonal space groups. For *, † see Subsection 9.7.4.1.

Arithmetic crystal class	Fully symmorphic	Tending to symmorphism	Equally balanced	Tending to antimorphism	Fully antimorphic
$4P$	$*P4^{(0)}$	$P4_2^{(1)}$	...	...	$P4_{1,3}\dagger^{(40)}$
$4I$	...	...	$I4_1\dagger^{(3)}$	$*I4^{(3)}$	...
$\bar{4}P$	$*P\bar{4}\dagger^{(0)}$	...	...	...	...
$\bar{4}I$	...	...	$*I\bar{4}\dagger^{(7)}$	...	...
$4/mP$	$*P4/m^{(0)}$	$P4_2/m^{(0)}\ P4/n^{(1)}$	$P4_2/n\dagger^{(20)}$	...	...
$4/mI$	...	...	...	$*I4/m^{(0)}\ I4_1/a\dagger^{(29)}$	...
$422P$	...	$*P422^{(0)}$	$P42_12^{(0)}$	$P4_{1,3}2_12\dagger^{(49)}$	...
		$P4_222^{(0)}$	$P4_{1,3}22^{(1)}$	$P4_22_12^{(1)}$	
$422I$	...	...	$I4_122\dagger^{(0)}$	$*I422^{(0)}$	...
$4mmP$	...	$*P4mm^{(0)}$	$P4bm^{(0)}$	$P4_2cm^{(0)}$	...
				$P4_2nm^{(0)}$	
				$P4cc^{(0)}$	
				$P4nc^{(0)}$	
				$P4_2mc^{(0)}$	
				$P4_2bc\dagger^{(1)}$	
$4mmI$	...	...	...	$*I4mm^{(0)}$	...
				$I4cm^{(0)}$	
				$I4_1md^{(0)}$	
				$I4_1cd\dagger^{(5)}$	
$\bar{4}2mP$	...	$*P\bar{4}2m^{(0)}$	$P\bar{4}2c^{(0)}$	$P\bar{4}2_1c\dagger^{(12)}$	...
			$P\bar{4}2_1m^{(0)}$		
$\bar{4}m2P$	...	$*P\bar{4}m2^{(0)}$	$P\bar{4}c2^{(0)}$	...	...
			$P\bar{4}b2^{(0)}$		
			$P\bar{4}n2^{(0)}$		
$\bar{4}m2I$	...	...	$*I\bar{4}m2^{(0)}$	$I\bar{4}c2\dagger^{(0)}$	...
$\bar{4}2mI$	...	...	$*I\bar{4}2m^{(0)}$	$I\bar{4}2d\dagger^{(0)}$	...
$4/mmmP$	...	$*P4/mmm^{(0)}$	$P4/mcc^{(0)}$	$P4/nbm^{(0)}$	...
		$P4_2/mmc^{(0)}$	$P4/nmm^{(0)}$	$P4/nnc^{(0)}$	
		$P4_2/mcm^{(0)}$		$P4/mbm^{(0)}$	
				$P4/mnc^{(0)}$	
				$P4/ncc^{(0)}$	
				$P4_2/nbc^{(0)}$	
				$P4_2/nnm^{(0)}$	
				$P4_2/mbc^{(0)}$	
				$P4_2/mnm^{(0)}$	
				$P4_2/nmc^{(0)}$	
				$P4_2/ncm^{(0)}$	
$4/mmmI$	...	$*I4/mmm^{(0)}$	...	$I4/mcm^{(0)}$	
				$I4_1/amd^{(0)}$	
				$I4_1/acd\dagger^{(0)}$	

empirical frequencies – it would be expected that there should be considerable correlation between them. All 'closest-packed' space groups are also 'fully antimorphic', and most of the 'limitingly close packed' and 'permissible' are 'tending to antimorphism'; a few requiring high molecular symmetry (222, *mm*2, *mmm*) and a couple of others are 'equally balanced'. Two 'fully antimorphic' groups, *Pc* and *Cc*, are merely 'permissible'. All 'fully symmorphic' space groups are 'impossible'.

9.7.1.4. *Relation to structural classes*

Structural classes (Belsky & Zorky, 1977, and papers cited there and below) are not an *a priori* classification of space groups but are a classification of structures within a space-group type in accordance with the number and kind of Wyckoff positions occupied by the molecules. As a considerable knowledge of the structures is required before their structural classes can be assigned, they form an *a posteriori* classification, and will be described (Section 9.7.5 below) after the empirical frequencies of space groups have been discussed.

9.7.2. Special positions of given symmetry

As noted by Kitajgorodskij, in many crystal structures molecules with inherent symmetry may occupy Wyckoff special positions, so that molecular and crystallographic symmetry elements coincide, and this may affect the relative frequencies of occurrence of structures with particular space groups. Tables of the frequency of occurrence of space groups have been published by many authors, from Nowacki (1942) onwards. Some typical recent papers are Brock & Dunitz (1994), Donohue (1985), Mighell, Himes & Rodgers (1983), Padmaya, Ramakumar & Viswamitra (1990), Wilson (1988, 1990,

Table 9.7.1.2. *Space groups arranged by arithmetic crystal class and degree of symmorphism (cont.)*

(*c*) Trigonal space groups. For *, † see Subsection 9.7.4.1.

Arithmetic crystal class	Fully symmorphic	Tending to symmorphism	Equally balanced	Tending to antimorphism	Fully antimorphic
$3P$	$*P3^{(0)}$	...	...	...	$P3_{1,2}\dagger^{(33)}$
$3R$	...	...	...	$*R3\dagger^{(11)}$	...
$\bar{3}P$	$*P\bar{3}\dagger^{(1)}$	...	...	...	...
$\bar{3}R$	...	...	...	$*R\bar{3}\dagger^{(30)}$	...
$312P$ $321P$	...	$*P312^{(0)}$ $*P321^{(0)}$	...	$P3_{1,2}12\dagger^{(0)}$ $P3_{1,2}21\dagger^{(10)}$	...
$32R$	...	...	...	$*R32\dagger^{(0)}$	...
$3m1P$ $31mP$	...	$*P3m1^{(0)}$ $*P31m^{(0)}$	...	$P3c1\dagger^{(0)}$ $P31c\dagger^{(0)}$	...
$3mR$	...	...	...	$*R3m^{(0)}$ $R3c\dagger^{(7)}$	...
$\bar{3}m1P$ $\bar{3}1mP$	...	$*P\bar{3}m1^{(0)}$ $*P\bar{3}1m^{(0)}$	...	$P\bar{3}c1\dagger^{(0)}$ $P\bar{3}1c\dagger^{(0)}$	...
$\bar{3}mR$	...	...	...	$*R\bar{3}m^{(0)}$ $R\bar{3}c\dagger^{(0)}$	...

(*d*) Hexagonal space groups. For *, † see Subsection 9.7.4.1.

Arithmetic crystal class	Fully symmorphic	Tending to symmorphism	Equally balanced	Tending to antimorphism	Fully antimorphic
$6P$	$*P6^{(0)}$	...	$P6_{2,4}^{(1)}$ $P6_3^{(0)}$	...	$P6_{1,5}\dagger^{(22)}$
$\bar{6}P$	$*P\bar{6}\dagger^{(0)}$	...	...	...	...
$6/mP$	$*P6/m^{(0)}$	...	$P6_3/m\dagger^{(0)}$	...	...
$622P$	...	$*P622^{(0)}$ $P6_{2,4}22^{(0)}$	...	$P6_322^{(1)}$ $P6_{1,5}22\dagger^{(2)}$	...
$6mmP$	...	$*P6mm^{(0)}$	...	$P6cc^{(0)}$	...
				$P6_3cm^{(0)}$ $P6_3mc^{(0)}$	
$\bar{6}m2P$ $\bar{6}2mP$	...	$*P\bar{6}m2^{(0)}$ $*P\bar{6}2m^{(0)}$	...	$P\bar{6}c2\dagger^{(0)}$ $P\bar{6}2c\dagger^{(0)}$	
$6/mmmP$	...	$*P6/mmm^{(0)}$	...	$P6/mcc\dagger^{(0)}$	...
				$P6_3/mcm^{(0)}$ $P6_3/mmc^{(0)}$	

(*e*) Cubic space groups. For *, †, see Subsection 9.7.4.1. No examples with one molecule in general position were found, so the frequencies are omitted.

Arithmetic crystal class	Fully symmorphic	Tending to symmorphism	Equally balanced	Tending to antimorphism	Antimorphic except for 3
$23P$	...	$*P23$	...	...	$P2_13\dagger$
$23F$	...	...	$*F23\dagger$	...	...
$23I$	...	...	$*I23$ $I2_13\dagger$	...	...
$m\bar{3}P$	...	$*Pm\bar{3}$	$Pn\bar{3}$	...	$Pa\bar{3}\dagger$
$m\bar{3}F$	...	...	$*Fm\bar{3}$	$Fd\bar{3}\dagger$	...
$m\bar{3}I$	...	...	$*Im\bar{3}$	$Ia\bar{3}\dagger$	...
$432P$	...	$*P432$	...	$P4_232\dagger$ $P4_{1,3}32\dagger$	...
$432F$	...	...	$*F432$	$F4_132\dagger$	...
$432I$	...	...	$*I432$	$I4_132\dagger$	...
$\bar{4}3mP$	...	$*P\bar{4}3m$	...	$P\bar{4}3n\dagger$	...
$\bar{4}3mF$	...	...	$*F\bar{4}3m$	$F\bar{4}3c\dagger$	...
$\bar{4}3mI$	...	...	$*I\bar{4}3m$	$I\bar{4}3d\dagger$	...
$m\bar{3}mP$	...	$*Pm\bar{3}m$	$Pm\bar{3}n$ $Pn\bar{3}m$	$Pn\bar{3}\dagger$	...
$m\bar{3}mF$	...	$*Fm\bar{3}m$	...	$Fm\bar{3}c$ $Fd\bar{3}m$	$Fd\bar{3}c\dagger$
$m\bar{3}mI$	...	$*Im\bar{3}m$	...	$Ia\bar{3}d\dagger$	...

1993*b*,*c*), but many of them hardly go beyond recognizing the fact that structures frequently made use of molecular symmetry – Wilson (1988) explicitly chose to ignore it. The early work of Belsky, Zorky and their colleagues did not attract much attention outside Russian-speaking areas. Recently, however, there has been a spate of interest (Wilson, 1991, 1993*b*,*c*,*d*; Brock & Dunitz, 1994; Belsky, Zorkaya & Zorky, 1995). Earlier lack of results is partly due to the fact that the Cambridge Structural Database (Section 9.7.3) did not provide a search program that would distinguish between occupation of a general position and multiple occupation of special positions of the required symmetry (Wilson, 1993*d*, Section 3). Belsky, Zorkaya & Zorky (1995) were able to make this distinction, and their paper is the source of many of the statistics quoted without special citation here.

It would be interesting to know which space groups possess positions with the symmetry of each of the 32 point groups 1, $\bar{1}$, 2, m, $2/m$, ..., $m\bar{3}m$. Volume A of *International Tables for Crystallography* (Hahn, 1995) enumerates the symmetry of all the special positions of a given space group, but does not readily

references