

9. BASIC STRUCTURAL FEATURES

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

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, $mm2$, 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,