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Table 3.1.4.1. *Reflection conditions, diffraction symbols and possible space groups* (*cont.*)

ORTHORHOMBIC, Laue class *mmm* (2/*m* 2/*m* 2/*m*) (*cont.*)

Reflection conditions								Laue class *mmm* (2/*m* 2/*m* 2/*m*)		
								Point group		
hkl	0*kl*	*h*0*l*	*hk*0	*h*00	0*k*0	00*l*	Extinction symbol	222	*mm*2 *m*2*m* 2*mm*	*mmm*
									*I*2*mm* (44)	
$h+k+l$	$k+l$	$h+l$	h, k	h	k	l	*I* − −(*ab*)		*Im*2*a* (46)	***Imma*** (74)
									*I*2*mb* (46)	*Immb* (74)
$h+k+l$	$k+l$	h, l	$h+k$	h	k	l	*I* −(*ac*)−		***Ima*2** (46)	*Imam* (74)
									*I*2*cm* (46)	*lmcm* (74)
$h+k+l$	$k+l$	h, l	h, k	h	k	l	*I* − *cb*		*I*2*cb* (45)	*Imcb* (72)
$h+k+l$	k, l	$h+l$	$h+k$	h	k	l	*I*(*bc*)− −		*Iem*2 (46)	*Iemm* (74)
									*Ie*2*m* (46)	
$h+k+l$	k, l	$h+l$	h, k	h	k	l	*Ic* − *a*		*Ic*2*a* (45)	*Icma* (72)
$h+k+l$	k, l	h, l	$h+k$	h	k	l	*Iba* −		***Iba*2** (45)	***Ibam*** (72)
$h+k+l$	k, l	h, l	h, k	h	k	l	*Ibca*			***Ibca*** (73)
										Icab (73)
$h+k, h+l, k+l$	k, l	h, l	h, k	h	k	l	*F* − − −	***F*222** (22)	***Fmm*2** (42)	***Fmmm*** (69)
									*Fm*2*m* (42)	
									*F*2*mm* (42)	
$h+k, h+l, k+l$	k, l	$h+l=4n$; h, l	$h+k=4n$; h, k	$h=4n$	$k=4n$	$l=4n$	*F*−*dd*		*F*2*dd* (43)	
$h+k, h+l, k+l$	$k+l=4n$; k, l	h, l	$h+k=4n$; h, k	$h=4n$	$k=4n$	$l=4n$	*Fd*−*d*		*Fd*2*d* (43)	
$h+k, h+l, k+l$	$k+l=4n$; k, l	$h+l=4n$; h, l	h, k	$h=4n$	$k=4n$	$l=4n$	*Fdd*−		***Fdd*2** (43)	
$h+k, h+l, k+l$	$k+l=4n$; k, l	$h+l=4n$; h, l	$h+k=4n$; h, k	$h=4n$	$k=4n$	$l=4n$	*Fddd*			***Fddd*** (70)

* Pair of space groups with common point group and symmetry elements but differing in the relative location of these elements.

TETRAGONAL, Laue classes 4/*m* and 4/*mmm*

Reflection conditions							Extinction symbol	Laue class						
								4/*m*			4/*mmm* (4/*m* 2/*m* 2/*m*)			
								Point group						
hkl	*hk*0	0*kl*	*hhl*	00*l*	0*k*0	*hh*0		4	$\bar{4}$	4/*m*	422	4*mm*	$\bar{4}2m$ $\bar{4}m2$	4/*mmm*
							$P---$	*P*4 (75)	$P\bar{4}$ (81)	*P*4/*m* (83)	*P*422 (89)	*P*4*mm* (99)	$P\bar{4}2m$ (111)	*P*4/*mmm* (123)
													$P\bar{4}m2$ (115)	
					k		$P{-}2_1{-}$				$P42_12$ (90)		$P\bar{4}2_1m$ (113)	
				l			$P4_2--$	$P4_2$ (77)		$P4_2/m$ (84)	$P4_222$ (93)			
				l	k		$P4_22_1-$				$P4_22_12$ (94)			
				$l=4n$			$P4_1--$	$\left\{ \begin{matrix} P4_1\ (76) \\ P4_3\ (78) \end{matrix} \right\}\dagger$			$\left\{ \begin{matrix} P4_122\ (91) \\ P4_322\ (95) \end{matrix} \right\}\dagger$			
				$l=4n$	k		$P4_12_1-$				$\left\{ \begin{matrix} P4_12_12\ (92) \\ P4_32_12\ (96) \end{matrix} \right\}\dagger$			
			l	l			$P--c$					$P4_2mc$ (105)	$P\bar{4}2c$ (112)	$P4_2/mmc$ (131)
			l	l	k		$P{-}2_1c$						$P\bar{4}2_1c$ (114)	
		k			k		$P-b-$					*P*4*bm* (100)	$P\bar{4}b2$ (117)	*P*4/*mbm* (127)
		k	l	l	k		$P-bc$					$P4_2bc$ (106)		$P4_2/mbc$ (135)
		l		l			$P-c-$					$P4_2cm$ (101)	$P\bar{4}c2$ (116)	$P4_2/mcm$ (132)
		l	l	l			$P-cc$					*P*4*cc* (103)		*P*4/*mcc* (124)
		$k+l$		l	k		$P-n-$					$P4_2nm$ (102)	$P\bar{4}n2$ (118)	$P4_2/mnm$ (136)
		$k+l$	l	l	k		$P-nc$					*P*4*nc* (104)		*P*4/*mnc* (128)
	$h+k$				k		$Pn--$			*P*4/*n* (85)				*P*4/*nmm* (129)
	$h+k$			l	k		$P4_2/n--$			$P4_2/n$ (86)				
	$h+k$		l	l	k		$Pn-c$							$P4_2/nmc$ (137)

Table 3.1.4.1. *Reflection conditions, diffraction symbols and possible space groups* (*cont.*)

TETRAGONAL, Laue classes $4/m$ and $4/mmm$ (*cont.*)

Reflection conditions							Extinction symbol	Laue class						
								$4/m$			$4/mmm$ ($4/m\ 2/m\ 2/m$)			
								Point group						
hkl	$hk0$	$0kl$	hhl	$00l$	$0k0$	$hh0$		4	$\bar{4}$	$4/m$	422	$4mm$	$\bar{4}2m$ $\bar{4}m2$	$4/mmm$
	$h+k$	k			k		$Pnb-$							$P4/nbm$ (125)
	$h+k$	k	l	l	k		$Pnbc$							$P4_2/nbc$ (133)
	$h+k$	l		l	k		$Pnc-$							$P4_2/ncm$ (138)
	$h+k$	l	l	l	k		$Pncc$							$P4/ncc$ (130)
	$h+k$	$k+l$		l	k		$Pnn-$							$P4_2/nnm$ (134)
	$h+k$	$k+l$	l	l	k		$Pnnc$							$P4/nnc$ (126)
$h+k+l$	$h+k$	$k+l$	l	l	k		$I---$	$I4$ (79)	$I\bar{4}$ (82)	$I4/m$ (87)	$I422$ (97)	$I4mm$ (107)	$I\bar{4}2m$ (121) $I\bar{4}m2$ (119)	$I4/mmm$ (139)
$h+k+l$	$h+k$	$k+l$	l	$l=4n$	k		$I4_1--$	$I4_1$ (80)			$I4_122$ (98)			
$h+k+l$	$h+k$	$k+l$	‡	$l=4n$	k	h	$I--d$					$I4_1md$ (109)	$I\bar{4}2d$ (122)	
$h+k+l$	$h+k$	k, l	l	l	k		$I-c-$					$I4cm$ (108)	$I\bar{4}c2$ (120)	$I4/mcm$ (140)
$h+k+l$	$h+k$	k, l	‡	$l=4n$	k	h	$I-cd$					$I4_1cd$ (110)		
$h+k+l$	h, k	$k+l$	l	$l=4n$	k		$I4_1/a--$			$I4_1/a$ (88)				
$h+k+l$	h, k	$k+l$	‡	$l=4n$	k	h	$Ia-d$							$I4_1/amd$ (141)
$h+k+l$	h, k	k, l	‡	$l=4n$	k	h	$Iacd$							$I4_1/acd$ (142)

† Pair of enantiomorphic space groups, *cf.* Section 3.1.5.
‡ Condition: $2h+l=4n$; l.

(as well as for the R space groups of the trigonal system), the different cell choices and settings of one space group are disregarded, 101 extinction symbols* and 122 diffraction symbols for the 230 space-group types result.

Only in 50 cases does a diffraction symbol uniquely identify just one space group, thus leaving 72 diffraction symbols that correspond to more than one space group. The 50 unique cases can be easily recognized in Table 3.1.4.1 because the line for the possible space groups in the particular Laue class contains just one entry.

The non-uniqueness of the space-group determination has two reasons:

(i) Friedel's rule, *i.e.* the effect that, with neglect of anomalous dispersion, the diffraction pattern contains an inversion centre, even if such a centre is not present in the crystal.

Example

A monoclinic crystal (with unique axis b) has the diffraction symbol $1\,2/m\,1P1c1$. Possible space groups are $P1c1$ (7) without an inversion centre, and $P12/c1$ (13) with an inversion centre. In both cases, the diffraction pattern has the Laue symmetry $1\,2/m\,1$.

One aspect of Friedel's rule is that the diffraction patterns are the same for two enantiomorphic space groups. Eleven diffraction symbols each correspond to a pair of enantiomorphic space groups. In Table 3.1.4.1, such pairs are grouped between braces. Either of the two space groups may be chosen for structure solution. If due to anomalous scattering Friedel's rule does not hold, at the refinement stage of structure determination it may be possible to determine the absolute structure and consequently the correct space group from the enantiomorphic pair.

(ii) The occurrence of four space groups in two 'special' pairs, each pair belonging to the same point group: $I222$ (23) & $I2_12_12_1$ (24) and $I23$ (197) & $I2_13$ (199). The two space groups of each pair differ in the location of the symmetry elements with respect to each other. In Table 3.1.4.1, these two special pairs are given in square brackets.

3.1.6. Space-group determination by additional methods

3.1.6.1. *Chemical information*

In some cases, chemical information determines whether or not the space group is centrosymmetric. For instance, all proteins crystallize in noncentrosymmetric space groups as they are constituted of L-amino acids only. Less certain indications may be obtained by considering the number of molecules per cell and the possible space-group symmetry. For instance, if experiment shows that there are two molecules of formula $A_\alpha B_\beta$ per cell in either space group $P2_1$ or $P2_1/m$ and if the molecule $A_\alpha B_\beta$ cannot possibly have either a mirror plane or an inversion centre, then there is a strong indication that the correct space group is $P2_1$. Crystallization of $A_\alpha B_\beta$ in $P2_1/m$ with random disorder of the molecules cannot be excluded, however. In a similar way, multiplicities of Wyckoff positions and the number of formula units per cell may be used to distinguish between space groups.

* The increase from 97 (*IT*, 1952) to 101 extinction symbols is due to the separate treatment of the trigonal and hexagonal crystal systems in Table 3.1.4.1, in contradistinction to *IT* (1952), Table 4.4.3, where they were treated together. In *IT* (1969), diffraction symbols were listed by Laue classes and thus the number of extinction symbols is the same as that of diffraction symbols, namely 122.