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

CUBIC, Laue classes $m\bar{3}$ and $m\bar{3}m$

Reflection conditions (Indices are permutable, apart from space group No. 205) ††				Extinction symbol	Laue class: $m\bar{3}$ $(2/m\,\bar{3})$		Laue class: $m\bar{3}m$ $(4/m\,\bar{3}\,2/m)$		
					Point group				
hkl	$0kl$	hhl	$00l$		23	$m\bar{3}$	432	$\bar{4}3m$	$m\bar{3}m$
				$P---$	$P23$ (195)	$Pm\bar{3}$ (200)	$P432$ (207)	$P\bar{4}3m$ (215)	$Pm\bar{3}m$ (221)
			l	$\{P2_1--$ $P4_2--$	$P2_13$ (198)		$P4_232$ (208)		
			$l=4n$	$P4_1--$			$\{P4_132$ (213) $P4_332$ (212)$\}$ ‡‡		
		l	l	$P--n$				$P\bar{4}3n$ (218)	$Pm\bar{3}n$ (223)
	k††		l	$Pa--$		$Pa\bar{3}$ (205)			
	$k+l$		l	$Pn--$		$Pn\bar{3}$ (201)			$Pn\bar{3}m$ (224)
	$k+l$	l	l	$Pn-n$					$Pn\bar{3}n$ (222)
$h+k+l$	$k+l$	l	l	$I---$	[$I23$ (197) $I2_13$ (199)] §§	$Im\bar{3}$ (204)	$I432$ (211)	$I\bar{4}3m$ (217)	$Im\bar{3}m$ (229)
$h+k+l$	$k+l$	l	$l=4n$	$I4_1--$			$I4_132$ (214)		
$h+k+l$	$k+l$	$2h+l=4n, l$	$l=4n$	$I--d$				$I\bar{4}3d$ (220)	
$h+k+l$	k, l	l	l	$Ia--$		$Ia\bar{3}$ (206)			
$h+k+l$	k, l	$2h+l=4n, l$	$l=4n$	$Ia-d$					$Ia\bar{3}d$ (230)
$h+k, h+l, k+l$	k, l	$h+l$	l	$F---$	$F23$ (196)	$Fm\bar{3}$ (202)	$F432$ (209)	$F\bar{4}3m$ (216)	$Fm\bar{3}m$ (225)
$h+k, h+l, k+l$	k, l	$h+l$	$l=4n$	$F4_1--$			$F4_132$ (210)		
$h+k, h+l, k+l$	k, l	h, l	l	$F--c$				$F\bar{4}3c$ (219)	$Fm\bar{3}c$ (226)
$h+k, h+l, k+l$	$k+l=4n, k, l$	$h+l$	$l=4n$	$Fd--$		$Fd\bar{3}$ (203)			$Fd\bar{3}m$ (227)
$h+k, h+l, k+l$	$k+l=4n, k, l$	h, l	$l=4n$	$Fd-c$					$Fd\bar{3}c$ (228)

†† For No. 205, only cyclic permutations are permitted. Conditions are $0kl$: $k=2n$; $h0l$: $l=2n$; $hk0$: $h=2n$.

‡‡ Pair of enantiomorphic space groups, *cf.* Section 3.1.5.

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

3.1.6.2. *Point-group determination by methods other than the use of X-ray diffraction*

This is discussed in Chapter 10.2. In favourable cases, suitably chosen methods can prove the absence of an inversion centre or a mirror plane.

3.1.6.3. *Study of X-ray intensity distributions*

X-ray data can give a strong clue to the presence or absence of an inversion centre if not only the symmetry of the diffraction pattern but also the distribution of the intensities of the reflection spots is taken into account. Methods have been developed by Wilson and others that involve a statistical examination of certain groups of reflections. For a textbook description, see Lipson & Cochran (1966) and Wilson (1970). In this way, the presence of an inversion centre in a three-dimensional structure or in certain projections can be tested. Usually it is difficult, however, to obtain reliable conclusions from projection data. The same applies to crystals possessing pseudo-symmetry, such as a centrosymmetric arrangement of heavy atoms in a noncentrosymmetric structure. Several computer programs performing the statistical analysis of the diffraction intensities are available.

3.1.6.4. *Consideration of maxima in Patterson syntheses*

The application of Patterson syntheses for space-group determination is described by Buerger (1950, 1959).

3.1.6.5. *Anomalous dispersion*

Friedel's rule, $|F(hkl)|^2 = |F(\bar{h}\bar{k}\bar{l})|^2$, does not hold for noncentrosymmetric crystals containing atoms showing anomalous dispersion. The difference between these intensities becomes particularly strong when use is made of a wavelength near the resonance level (absorption edge) of a particular atom in the crystal. Synchrotron radiation, from which a wide variety of wavelengths can be chosen, may be used for this purpose. In such cases, the diffraction pattern reveals the symmetry of the actual point group of the crystal (including the orientation of the point group with respect to the lattice).

3.1.6.6. *Summary*

One or more of the methods discussed above may reveal whether or not the point group of the crystal has an inversion centre. With this information, in addition to the diffraction symbol, 192 space groups can be uniquely identified. The rest consist of the eleven pairs of enantiomorphic space groups, the two 'special pairs' and six further ambiguities: 3 in the orthorhombic system (Nos. 26 & 28, 35 & 38, 36 & 40), 2 in the tetragonal system (Nos. 111 & 115, 119 & 121), and 1 in the hexagonal system (Nos. 187 & 189). If not only the point group but also its orientation with respect to the lattice can be determined, the six ambiguities can be resolved. This implies that 204 space groups can be uniquely identified, the only exceptions being the eleven pairs of enantiomorphic space groups and the two 'special pairs'.

references