9.8. INCOMMENSURATE AND COMMENSURATE MODULATED STRUCTURES

Table 9.8.3.3. (3 + 1)-*Dimensional point groups and arithmetic crystal classes*

The four-dimensional point group K_s has external part K_E, which belongs to a three-dimensional system. Depending on the Bravais class of the four-dimensional lattice left invariant by K_s, this point group gives rise to an integral 4×4 matrix group $\Gamma(K)$ which belongs to one of the arithmetic crystal classes given in the last column.

System	Point group		External Bravais class	Arithmetic crystal class(es)
	K_E	K_s		
Triclinic	1	$(1, 1)$	$\bar{1}P$	$1P(\alpha\beta\gamma)$
	$\bar{1}$	$(\bar{1}, \bar{1})$	$\bar{1}P$	$\bar{1}P(\alpha\beta\gamma)$
Monoclinic	2	$(2, \bar{1})$	$2/mP$	$2P(\alpha\beta0), 2P(\alpha\beta\frac{1}{2})$
			$2/mB$	$2B(\alpha\beta0)$
		$(2, 1)$	$2/mP$	$2P(00\gamma), 2P(\frac{1}{2}0\gamma)$
			$2/mB$	$2B(00\gamma), 2B(0\frac{1}{2}\gamma)$
	m	$(m, 1)$	$2/mP$	$mP(\alpha\beta0), mP(\alpha\beta\frac{1}{2})$
			$2/mB$	$mB(\alpha\beta0)$
		$(m, \bar{1})$	$2/mP$	$mP(00\gamma), mP(\frac{1}{2}0\gamma)$
			$2/mB$	$mB(00\gamma), mB(0\frac{1}{2}\gamma)$
	$2/m$	$(2/m, \bar{1}1)$	$2/mP$	$2/mP(\alpha\beta0), 2/mP(\alpha\beta\frac{1}{2})$
			$2/mB$	$2/mB(\alpha\beta0)$
		$(2/m, 1\bar{1})$	$2/mP$	$2/mP(00\gamma), 2/mP(\frac{1}{2}0\gamma)$
			$2/mB$	$2/mB(00\gamma), 2/mB(0\frac{1}{2}\gamma)$
Orthorhombic	222	$(222, \bar{1}\bar{1}1)$	$mmmP$	$222P(00\gamma), 222P(0\frac{1}{2}\gamma), 222P(\frac{1}{2}\frac{1}{2}\gamma)$
			$mmmI$	$222I(00\gamma)$
			$mmmF$	$222F(00\gamma), 222F(10\gamma)$
			$mmmC$	$222C(00\gamma), 222C(10\gamma)$
		$(222, 1\bar{1}\bar{1})$	$mmmC$	$222C(\alpha00), 222C(\alpha0\frac{1}{2})$
	$mm2$	$(mm2, 111)$	$mmmP$	$mm2P(00\gamma), mm2P(0\frac{1}{2}\gamma), mm2P(\frac{1}{2}\frac{1}{2}\gamma)$
			$mmmI$	$mm2I(00\gamma)$
			$mmmF$	$mm2F(00\gamma), mm2F(10\gamma)$
			$mmmC$	$mm2C(00\gamma), mm2C(10\gamma)$
		$(2mm, 111)$	$mmmC$	$2mmC(\alpha00), 2mmC(\alpha0\frac{1}{2})$
		$(2mm, \bar{1}1\bar{1})$	$mmmP$	$2mmP(00\gamma), 2mmP(0\frac{1}{2}\gamma), 2mmP(\frac{1}{2}\frac{1}{2}\gamma)$
			$mmmI$	$2mmI(00\gamma)$
			$mmmF$	$2mmF(00\gamma), 2mmF(10\gamma)$
			$mmmC$	$2mmC(00\gamma), 2mmC(10\gamma)$
		$(mm2, \bar{1}1\bar{1})$	$mmmC$	$mm2C(\alpha00), mm2C(\alpha0\frac{1}{2})$
		$(m2m, 1\bar{1}\bar{1})$	$mmmP$	$m2mP(0\frac{1}{2}\gamma)$
		$(m2m, \bar{1}\bar{1}1)$	$mmmC$	$m2mC(\alpha00), m2mC(\alpha0\frac{1}{2})$
	mmm	$(mmm, 11\bar{1})$	$mmmP$	$mmmP(00\gamma), mmmP(0\frac{1}{2}\gamma), mmmP(\frac{1}{2}\frac{1}{2}\gamma)$
			$mmmI$	$mmmI(00\gamma)$
			$mmmF$	$mmmF(00\gamma), mmmF(10\gamma)$
			$mmmC$	$mmmC(00\gamma), mmmC(10\gamma)$
		$(mmm, \bar{1}11)$	$mmmC$	$mmmC(\alpha00), mmmC(\alpha0\frac{1}{2})$
Tetragonal	4	$(4, 1)$	$4/mmmP$	$4P(00\gamma), 4P(\frac{1}{2}\frac{1}{2}\gamma)$
			$4/mmmI$	$4I(00\gamma)$
	$\bar{4}$	$(\bar{4}, \bar{1})$	$4/mmmP$	$\bar{4}P(00\gamma), \bar{4}P(\frac{1}{2}\frac{1}{2}\gamma)$
			$4/mmmI$	$\bar{4}I(00\gamma)$
	$4/m$	$(4/m, 1\bar{1})$	$4/mmmP$	$4/mP(00\gamma), 4/mP(\frac{1}{2}\frac{1}{2}\gamma)$
			$4/mmmI$	$4/mI(00\gamma)$
	422	$(422, 1\bar{1}\bar{1})$	$4/mmmP$	$422P(00\gamma), 422P(\frac{1}{2}\frac{1}{2}\gamma)$
			$4/mmmI$	$422I(00\gamma)$
	$4mm$	$(4mm, 111)$	$4/mmmP$	$4mmP(00\gamma), 4mmP(\frac{1}{2}\frac{1}{2}\gamma)$
			$4/mmmI$	$4mmI(00\gamma)$
	$\bar{4}2m$	$(\bar{4}2m, \bar{1}\bar{1}1)$	$4/mmmP$	$\bar{4}2mP(00\gamma), \bar{4}2mP(\frac{1}{2}\frac{1}{2}\gamma)$
			$4/mmmI$	$\bar{4}2mI(00\gamma)$
	$\bar{4}m2$	$(\bar{4}m2, \bar{1}1\bar{1})$	$4/mmmP$	$\bar{4}m2P(00\gamma), \bar{4}m2P(\frac{1}{2}\frac{1}{2}\gamma)$
			$4/mmmI$	$\bar{4}m2I(00\gamma)$
	$4/mmm$	$(4/mmm, 1\bar{1}11)$	$4/mmmP$	$4/mmmP(00\gamma), 4/mmmP(\frac{1}{2}\frac{1}{2}\gamma)$
			$4/mmmI$	$4/mmmI(00\gamma)$
Trigonal	3	$(3, 1)$	$\bar{3}mR$	$3R(00\gamma)$
			$6/mmmP$	$3P(00\gamma), 3P(\frac{1}{3}\frac{1}{3}\gamma)$
	$\bar{3}$	$(\bar{3}, \bar{1})$	$\bar{3}mR$	$\bar{3}R(00\gamma)$
			$6/mmmP$	$\bar{3}P(00\gamma), \bar{3}P(\frac{1}{3}\frac{1}{3}\gamma)$
	32	$(32, 1\bar{1})$	$\bar{3}mR$	$32R(00\gamma)$
			$6/mmmP$	$312P(00\gamma), 312P(\frac{1}{3}\frac{1}{3}\gamma), 321P(00\gamma)$

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Table 9.8.3.3. $(3+1)$-*Dimensional point groups and arithmetic crystal classes (cont.)*

System	Point group K_E	Point group K_s	External Bravais class	Arithmetic crystal class(es)
Trigonal (*cont.*)	$3m$	$(3m, 11)$	$\bar{3}mR$	$3mR(00\gamma)$
			$6/mmmP$	$3m1P(00\gamma)$, $31mP(00\gamma)$, $31mP(\frac{1}{3}\frac{1}{3}\gamma)$
	$\bar{3}m$	$(\bar{3}m, \bar{1}1)$	$\bar{3}mR$	$\bar{3}mR(00\gamma)$
			$6/mmmP$	$\bar{3}1mP(00\gamma)$, $\bar{3}1mP(\frac{1}{3}\frac{1}{3}\gamma)$, $\bar{3}m1P(00\gamma)$
Hexagonal	6	$(6, 1)$	$6/mmmP$	$6P(00\gamma)$
	$\bar{6}$	$(\bar{6}, \bar{1})$	$6/mmmP$	$\bar{6}P(00\gamma)$
	$6/m$	$(6/m, 1\bar{1})$	$6/mmmP$	$6/mP(00\gamma)$
	622	$(622, 1\bar{1}\bar{1})$	$6/mmmP$	$622P(00\gamma)$
	$6mm$	$(6mm, 111)$	$6/mmmP$	$6mmP(00\gamma)$
	$\bar{6}m2$	$(\bar{6}m2, \bar{1}1\bar{1})$	$6/mmmP$	$\bar{6}m2P(00\gamma)$
	$\bar{6}2m$	$(\bar{6}2m, \bar{1}\bar{1}1)$	$6/mmmP$	$\bar{6}2mP(00\gamma)$
	$6/mmm$	$(6/mmm, 1\bar{1}11)$	$6/mmmP$	$6/mmmP(00\gamma)$

Written in components, the non-primitive translation υ_s associated with the point-group element (R, R_I) is $(\mathbf{v}, \upsilon_I)$, where υ_I can be written as $\delta - \mathbf{q}\cdot\mathbf{v}$. In accordance with (9.8.1.12), δ is defined as υ_4. The origin-invariant part υ_s^o of υ_s is

$$\upsilon_s^o = (\mathbf{v}^o, \upsilon_I^o) = \frac{1}{n}\sum_{m=1}^{n}(R^m\mathbf{v}, R_I^m\upsilon_I) = (\mathbf{v}^o, \tau - \mathbf{q}\cdot\mathbf{v}^o), \quad (9.8.3.6)$$

where

$$\tau = \upsilon_4^o = \upsilon_I^o + \mathbf{q}\cdot\mathbf{v}^o.$$

The internal transformation $R_I(R) = \varepsilon(R) = \varepsilon$ is either $+1$ or -1. When $\varepsilon = -1$ it follows from (9.8.3.6) that $\upsilon_I^o = 0$. For $\varepsilon = +1$, one has $\upsilon_I^o = \upsilon_I$. Because in that case

$$\mathbf{q}\cdot\mathbf{v}^o = \frac{1}{n}\sum_{m=1}^{n}\mathbf{q}\cdot R^m\mathbf{v} = \mathbf{q}^i\cdot\mathbf{v}, \quad (9.8.3.7)$$

it follows that

$$\tau = \upsilon_I + \mathbf{q}\cdot\mathbf{v}^o = \delta - \mathbf{q}\cdot\mathbf{v} + \mathbf{q}\cdot\mathbf{v}^o = \delta - \mathbf{q}^r\cdot\mathbf{v}. \quad (9.8.3.8)$$

For R_s of order n, R_s^n is the identity and the associated translation is a lattice translation. The ensuing values for τ are $0, \frac{1}{2}, \pm\frac{1}{3}, \pm\frac{1}{4}$ or $\pm\frac{1}{6}$ (modulo integers). This remains true also in the case of a centred basis. The symbol of the $(3+1)$-dimensional space-group element is determined by the invariant part of its three-dimensional translation and τ. Again, that information can be given in terms of either a one-line or a two-line symbol.

In the one-line symbol, one finds: the symbol according to *International Tables for Crystallography*, Volume A, for the space group generated by the elements $\{R|\mathbf{v}\}$, in parentheses the components of the modulation vector $\mathbf{q}$ followed by the values of τ, one for each generator appearing in the three-dimensional space-group symbol. A letter symbolizes the value of τ according to

τ	0	$\frac{1}{2}$	$\pm\frac{1}{3}$	$\pm\frac{1}{4}$	$\pm\frac{1}{6}$
symbol	0	s	t	q	h

(9.8.3.9)

As an example, consider the superspace group

$$P2_1/m(\alpha\beta0)0s.$$

The external components $\{R|\mathbf{v}\}$ of the elements of this group form the three-dimensional space group $P2_1/m$. The modulation wavevector is $\alpha\mathbf{a}^* + \beta\mathbf{b}^*$ with respect to a conventional basis of the monoclinic lattice with unique axis $\mathbf{c}$. Therefore, the point group is $(2/m, \bar{1}1)$. The point-group element $(2, \bar{1})$ has associated a non-primitive translation with invariant part $(\frac{1}{2}\mathbf{c}, 0) = (00\frac{1}{2}0)$ and the point-group generator $(m, 1)$ one with $(\mathbf{0}, \frac{1}{2}) = (000\frac{1}{2})$.

Table 9.8.3.4(a). $(2+1)$-*Dimensional superspace groups*

The number labelling the superspace group is denoted by $n.m$, where n is the number attached to the two-dimensional basic space group and m numbers the various superspace groups having the same basic space group. The symbol of the basic space group, the symbol for the three-dimensional point group, the number of the three-dimensional Bravais class to which the superspace group belongs (Table 9.8.3.1a) and the superspace-group symbol are also given.

No.	Basic space group	Point group K_s	Bravais class No.	Group symbol
Oblique				
1.1	$p1$	$(1, \underline{1})$	1	$p1(\alpha\beta)$
2.1	$p2$	$(2, \bar{1})$	1	$p2(\alpha\beta)$
Rectangular				
3.1	pm	$(m, 1)$	2	$pm1(0\beta)$
3.2			2	$pm1(0\beta)s0$
3.3			3	$pm1(\frac{1}{2}\beta)$
3.4		$(m, \bar{1})$	2	$p1m(0\beta)$
3.5			3	$p1m(\frac{1}{2}\beta)$
4.1	pg	$(m, 1)$	2	$pg1(0\beta)$
4.2			3	$pg1(\frac{1}{2}\beta)$
4.3		$(m, \bar{1})$	2	$p1g(0\beta)$
5.1	cm	$(m, 1)$	4	$cm1(0\beta)$
5.2			4	$cm1(0\beta)s0$
5.3		$(m, \bar{1})$	4	$c1m(0\beta)$
6.1	pmm	$(mm, 1\bar{1})$	2	$pmm(0\beta)$
6.2			2	$pmm(0\beta)s0$
6.3			3	$pmm(\frac{1}{2}\beta)$
7.1	pmg	$(mm, 1\bar{1})$	2	$pmg(0\beta)$
7.2			2	$pgm(0\beta)$
7.3			3	$pgm(\frac{1}{2}\beta)$
8.1	pgg	$(mm, 1\bar{1})$	2	$pgg(0\beta)$
9.1	cmm	$(mm, 1\bar{1})$	4	$cmm(0\beta)$
9.2			4	$cmm(0\beta)s0$

references