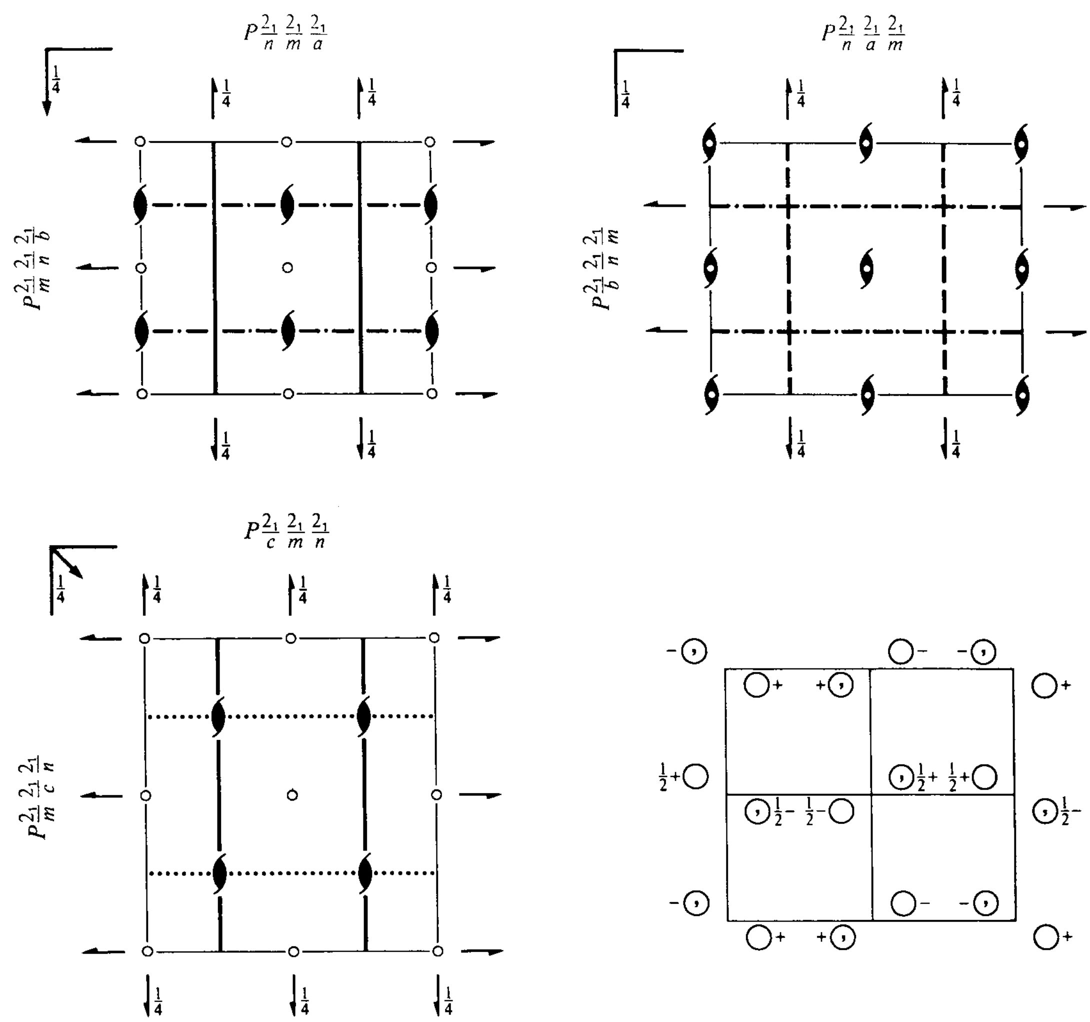
Pnma D_{2h}^{16} *mmm* Orthorhombic

No. 62 $P\ 2_1/n\ 2_1/m\ 2_1/a$ Patterson symmetry *Pmmm*



Origin at $\bar{1}$ on $1\,2_1\,1$

Asymmetric unit $0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{4};\quad 0 \le z \le 1$

Symmetry operations

(1) 1	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)\quad 0,y,0$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}\quad 0,0,0$	(6) $a\quad x,y,\frac{1}{4}$	(7) $m\quad x,\frac{1}{4},z$	(8) $n(0,\frac{1}{2},\frac{1}{2})\quad \frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	d	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	$0kl$: $k+l=2n$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(7) $x,\bar{y}+\frac{1}{2},z$	(8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	$hk0$: $h=2n$
							$h00$: $h=2n$
							$0k0$: $k=2n$
							$00l$: $l=2n$
							Special: as above, plus
4	c	$.m.$	$x,\frac{1}{4},z$	$\bar{x}+\frac{1}{2},\frac{3}{4},z+\frac{1}{2}$	$\bar{x},\frac{3}{4},\bar{z}$	$x+\frac{1}{2},\frac{1}{4},\bar{z}+\frac{1}{2}$	no extra conditions
4	b	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	hkl : $h+l,k=2n$
4	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl : $h+l,k=2n$

Symmetry of special projections

Along [001] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},\frac{1}{4}$

Along [010] $p2gg$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I
- [2] $Pn2_1a$ ($Pna2_1$, 33) 1; 3; 6; 8
- [2] $Pnm2_1$ ($Pmn2_1$, 31) 1; 2; 7; 8
- [2] $P2_1ma$ ($Pmc2_1$, 26) 1; 4; 6; 7
- [2] $P2_12_12_1$ (19) 1; 2; 3; 4
- [2] $P112_1/a$ ($P2_1/c$, 14) 1; 2; 5; 6
- [2] $P2_1/n11$ ($P2_1/c$, 14) 1; 4; 5; 8
- [2] $P12_1/m1$ ($P2_1/m$, 11) 1; 3; 5; 7

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $Pnma$ ($\mathbf{a}'=3\mathbf{a}$) (62); [3] $Pnma$ ($\mathbf{b}'=3\mathbf{b}$) (62); [3] $Pnma$ ($\mathbf{c}'=3\mathbf{c}$) (62)

Minimal non-isomorphic supergroups

I none

II [2] $Amma$ ($Cmcm$, 63); [2] $Bbmm$ ($Cmcm$, 63); [2] $Ccme$ ($Cmce$, 64); [2] $Imma$ (74); [2] $Pcma$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($Pbam$, 55); [2] $Pbma$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($Pbcm$, 57); [2] $Pnmm$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a}$) ($Pmmn$, 59)