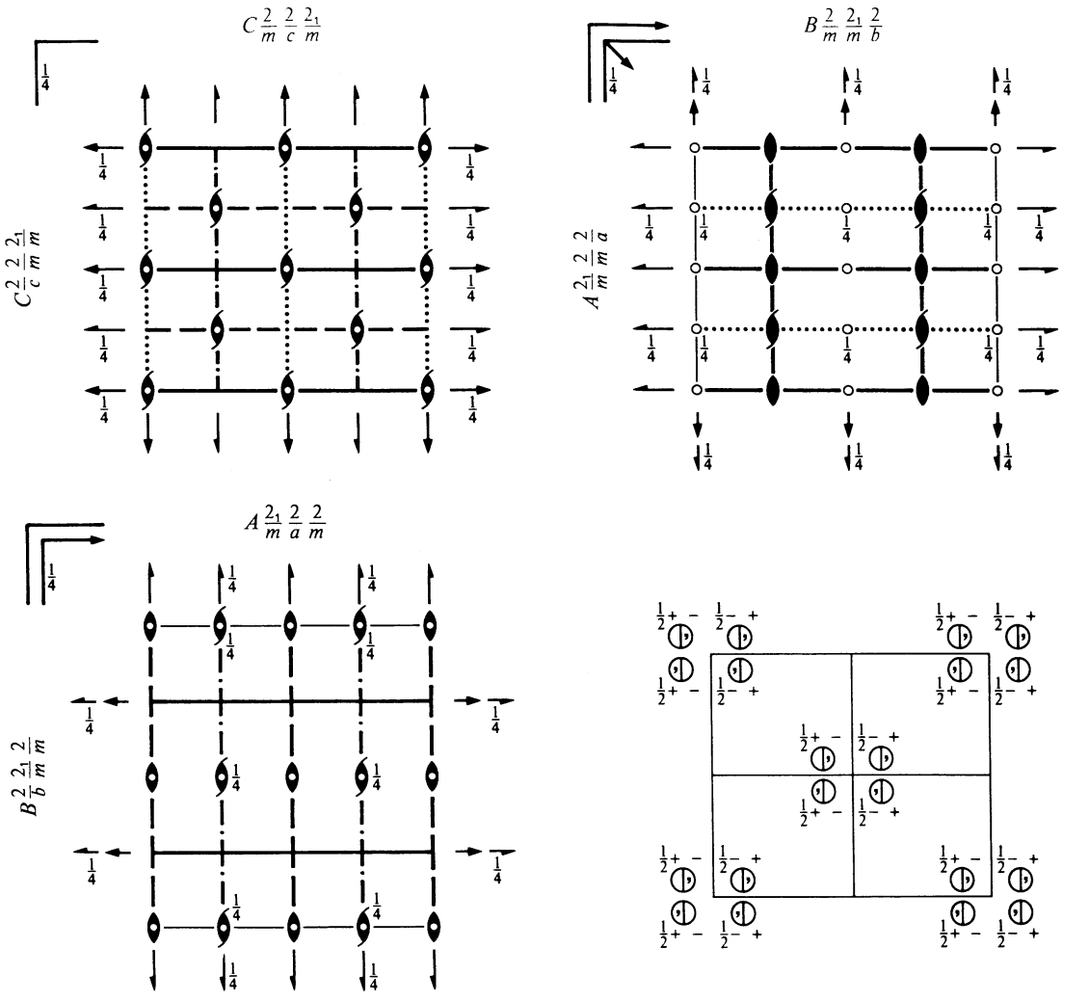
# $Cmcm$ $D_{2h}^{17}$ $mmm$ Orthorhombic

No. 63 $C\ 2/m\ 2/c\ 2_1/m$ Patterson symmetry $Cmmm$




**Origin** at centre $(2/m)$ at $2/mc2_1$

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

**Symmetry operations**

For $(0,0,0)+$ set

| | | | |
|---|---|---|---|
| (1) 1 | (2) $2(0,0,\frac{1}{2})$ $0,0,z$ | (3) $2$ $0,y,\frac{1}{4}$ | (4) $2$ $x,0,0$ |
| (5) $\bar{1}$ $0,0,0$ | (6) $m$ $x,y,\frac{1}{4}$ | (7) $c$ $x,0,z$ | (8) $m$ $0,y,z$ |

For $(\frac{1}{2},\frac{1}{2},0)+$ set

| | | | |
|---|---|---|---|
| (1) $t(\frac{1}{2},\frac{1}{2},0)$ | (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$ | (3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$ | (4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$ |
| (5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$ | (6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,\frac{1}{4}$ | (7) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$ | (8) $b$ $\frac{1}{4},y,z$ |

**Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

**Positions**

| Multiplicity, Wyckoff letter, Site symmetry | | | Coordinates | | | | Reflection conditions |
|---|---|---|---|---|---|---|---|
| | | | $(0,0,0)+$ | $(\frac{1}{2},\frac{1}{2},0)+$ | | | General: |
| 16 | $h$ | 1 | (1) $x,y,z$<br>(5) $\bar{x},\bar{y},\bar{z}$ | (2) $\bar{x},\bar{y},z+\frac{1}{2}$<br>(6) $x,y,\bar{z}+\frac{1}{2}$ | (3) $\bar{x},y,\bar{z}+\frac{1}{2}$<br>(7) $x,\bar{y},z+\frac{1}{2}$ | (4) $x,\bar{y},\bar{z}$<br>(8) $\bar{x},y,z$ | $hkl$ : $h+k=2n$<br>$0kl$ : $k=2n$<br>$h0l$ : $h,l=2n$<br>$hk0$ : $h+k=2n$<br>$h00$ : $h=2n$<br>$0k0$ : $k=2n$<br>$00l$ : $l=2n$ |
| | | | | | | | Special: as above, plus |
| 8 | $g$ | $..m$ | $x,y,\frac{1}{4}$ | $\bar{x},\bar{y},\frac{3}{4}$ | $\bar{x},y,\frac{1}{4}$ | $x,\bar{y},\frac{3}{4}$ | no extra conditions |
| 8 | $f$ | $m..$ | $0,y,z$ | $0,\bar{y},z+\frac{1}{2}$ | $0,y,\bar{z}+\frac{1}{2}$ | $0,\bar{y},\bar{z}$ | no extra conditions |
| 8 | $e$ | $2..$ | $x,0,0$ | $\bar{x},0,\frac{1}{2}$ | $\bar{x},0,0$ | $x,0,\frac{1}{2}$ | $hkl$ : $l=2n$ |
| 8 | $d$ | $\bar{1}$ | $\frac{1}{4},\frac{1}{4},0$ | $\frac{3}{4},\frac{3}{4},\frac{1}{2}$ | $\frac{3}{4},\frac{1}{4},\frac{1}{2}$ | $\frac{1}{4},\frac{3}{4},0$ | $hkl$ : $k,l=2n$ |
| 4 | $c$ | $m\,2\,m$ | $0,y,\frac{1}{4}$ | $0,\bar{y},\frac{3}{4}$ | | | no extra conditions |
| 4 | $b$ | $2/m..$ | $0,\frac{1}{2},0$ | $0,\frac{1}{2},\frac{1}{2}$ | | | $hkl$ : $l=2n$ |
| 4 | $a$ | $2/m..$ | $0,0,0$ | $0,0,\frac{1}{2}$ | | | $hkl$ : $l=2n$ |

**Symmetry of special projections**

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

**Maximal non-isomorphic subgroups**

**I**
[2] $C2cm$ ($Ama2$, 40) (1; 4; 6; 7)+
[2] $Cm2m$ ($Amm2$, 38) (1; 3; 6; 8)+
[2] $Cmc2_1$ (36) (1; 2; 7; 8)+
[2] $C222_1$ (20) (1; 2; 3; 4)+
[2] $C12/c1$ ($C2/c$, 15) (1; 3; 5; 7)+
[2] $C2/m11$ ($C2/m$, 12) (1; 4; 5; 8)+
[2] $C112_1/m$ ($P2_1/m$, 11) (1; 2; 5; 6)+

**IIa**
[2] $Pbnm$ ($Pnma$, 62) 1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
[2] $Pmcn$ ($Pnma$, 62) 1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},0)$
[2] $Pbcn$ (60) 1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},0)$
[2] $Pmnm$ ($Pmmn$, 59) 1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},0)$
[2] $Pmnn$ ($Pnnm$, 58) 1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},0)$
[2] $Pbcm$ (57) 1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},0)$
[2] $Pbnn$ ($Pnna$, 52) 1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
[2] $Pmcm$ ($Pmma$, 51) 1; 2; 3; 4; 5; 6; 7; 8

**IIb** none

**Maximal isomorphic subgroups of lowest index**

**IIc** [3] $Cmcm$ ($\mathbf{a}'=3\mathbf{a}$) (63); [3] $Cmcm$ ($\mathbf{b}'=3\mathbf{b}$) (63); [3] $Cmcm$ ($\mathbf{c}'=3\mathbf{c}$) (63)

**Minimal non-isomorphic supergroups**

**I** [3] $P6_3/mcm$ (193); [3] $P6_3/mmc$ (194)

**II** [2] $Fmmm$ (69); [2] $Pmcm$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($Pmma$, 51); [2] $Cmmm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (65)