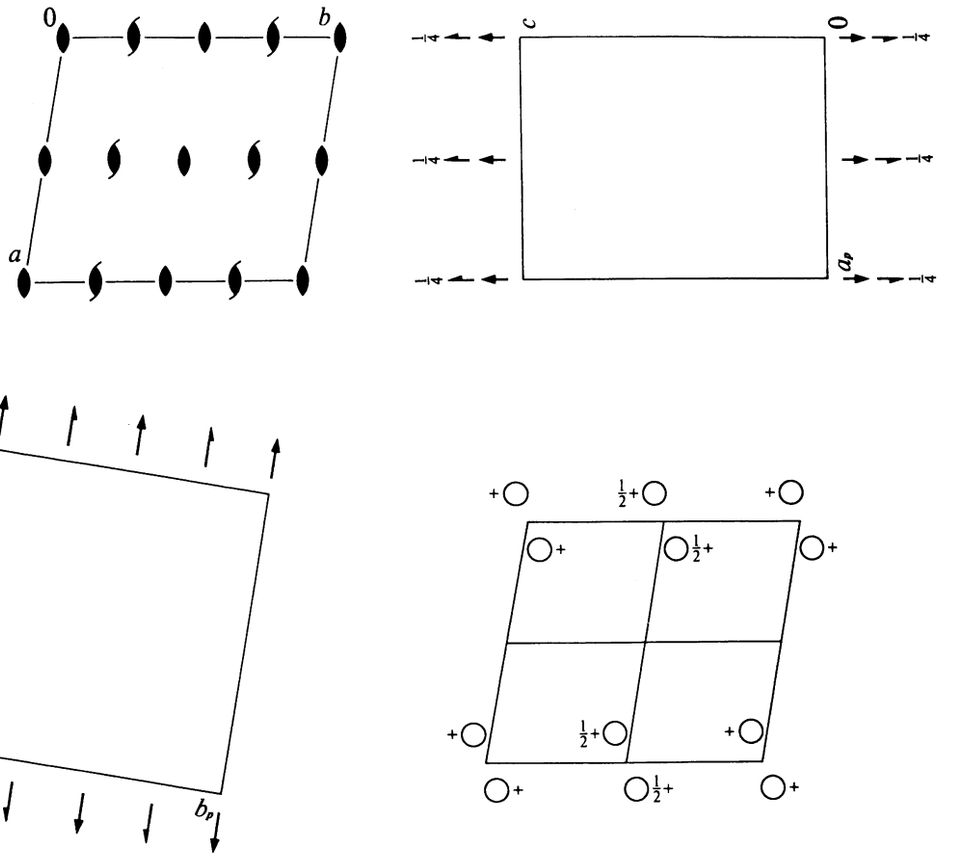
$C2$ C_2^3 2 Monoclinic

No. 5 $A112$ Patterson symmetry $A112/m$

UNIQUE AXIS c, CELL CHOICE 1



Origin on 2

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

Symmetry operations

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

(1) 1 (2) 2 $0,0,z$

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

(1) $t(0,\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
			$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	General:
4	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	hkl : $k+l=2n$ $hk0$: $k=2n$ $0kl$: $k+l=2n$ $h0l$: $l=2n$ $00l$: $l=2n$ $0k0$: $k=2n$
					Special: no extra conditions
2	b	2	$\frac{1}{2},0,z$		
2	a	2	$0,0,z$		

Symmetry of special projections

Along [001] $p2$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $c1m1$
$\mathbf{a}'=\mathbf{b}_p$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}_p$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $A1$ ($P1$, 1) 1+

IIa [2] $P112_1$ ($P2_1$, 4) 1; $2+(0,\frac{1}{2},\frac{1}{2})$
[2] $P112$ ($P2$, 3) 1; 2

IIb none

Maximal isomorphic subgroups of lowest index

IIc [2] $A112$ ($\mathbf{a}'=2\mathbf{a}$ or $\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{a}+\mathbf{b}$) ($C2$, 5); [3] $A112$ ($\mathbf{c}'=3\mathbf{c}$) ($C2$, 5)

Minimal non-isomorphic supergroups

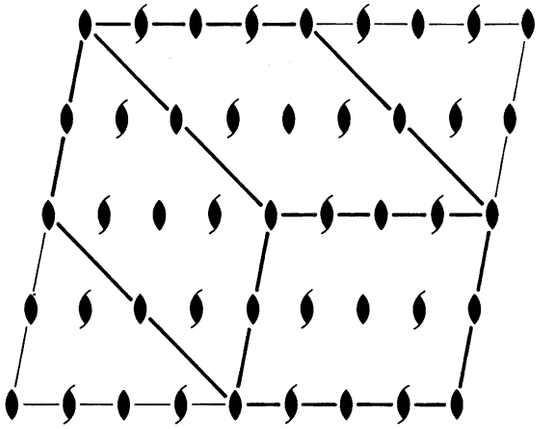
I [2] $C2/m$ (12); [2] $C2/c$ (15); [2] $C222_1$ (20); [2] $C222$ (21); [2] $F222$ (22); [2] $I222$ (23); [2] $I2_12_12_1$ (24); [2] $Amm2$ (38); [2] $Aem2$ (39); [2] $Ama2$ (40); [2] $Aea2$ (41); [2] $Fmm2$ (42); [2] $Fdd2$ (43); [2] $Imm2$ (44); [2] $Iba2$ (45); [2] $Ima2$ (46); [2] $I4$ (79); [2] $I4_1$ (80); [2] $I\bar{4}$ (82); [3] $P312$ (149); [3] $P321$ (150); [3] $P3_112$ (151); [3] $P3_121$ (152); [3] $P3_212$ (153); [3] $P3_221$ (154); [3] $R32$ (155)

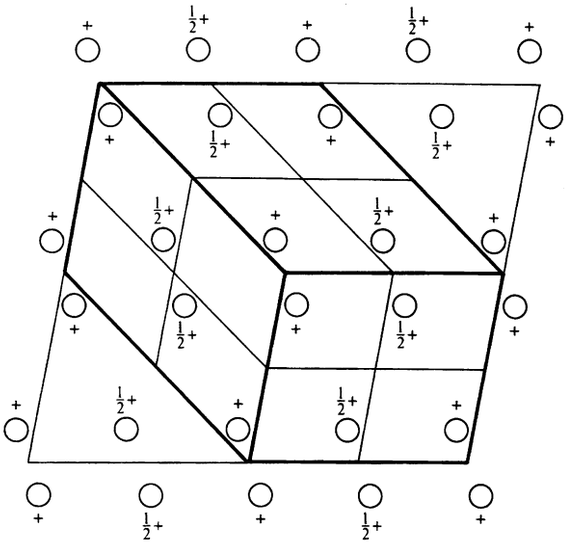
II [2] $P112$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b},\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P2$, 3)

$C2$ C_2^3 2 Monoclinic

No. 5

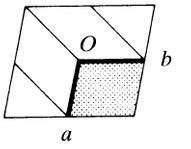
UNIQUE AXIS c, DIFFERENT CELL CHOICES





$A112$

UNIQUE AXIS c, CELL CHOICE 1



Origin on 2

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

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates	
			$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$
4	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$
2	b	2	$\frac{1}{2},0,z$	
2	a	2	$0,0,z$	

Reflection conditions

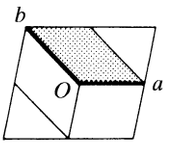
General:

hkl : $k+l=2n$
$hk0$: $k=2n$
$0kl$: $k+l=2n$
$h0l$: $l=2n$
$00l$: $l=2n$
$0k0$: $k=2n$

Special: no extra conditions

*B*112

UNIQUE AXIS *c*, CELL CHOICE 2



Origin on 2

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

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	Coordinates $(\frac{1}{2},0,\frac{1}{2})+$
4	*c*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$
2	*b*	2	$\frac{1}{2},\frac{1}{2},z$	
2	*a*	2	$0,0,z$	

Reflection conditions

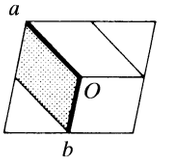
General:

hkl : $h+l=2n$
$hk0$: $h=2n$
$0kl$: $l=2n$
$h0l$: $h+l=2n$
$00l$: $l=2n$
$h00$: $h=2n$

Special: no extra conditions

*I*112

UNIQUE AXIS *c*, CELL CHOICE 3



Origin on 2

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

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	Coordinates $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$
4	*c*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$
2	*b*	2	$0,\frac{1}{2},z$	
2	*a*	2	$0,0,z$	

Reflection conditions

General:

hkl : $h+k+l=2n$
$hk0$: $h+k=2n$
$0kl$: $k+l=2n$
$h0l$: $h+l=2n$
$00l$: $l=2n$
$h00$: $h=2n$
$0k0$: $k=2n$

Special: no extra conditions