

Ccce

D_{2h}^{22}

mmm

Orthorhombic

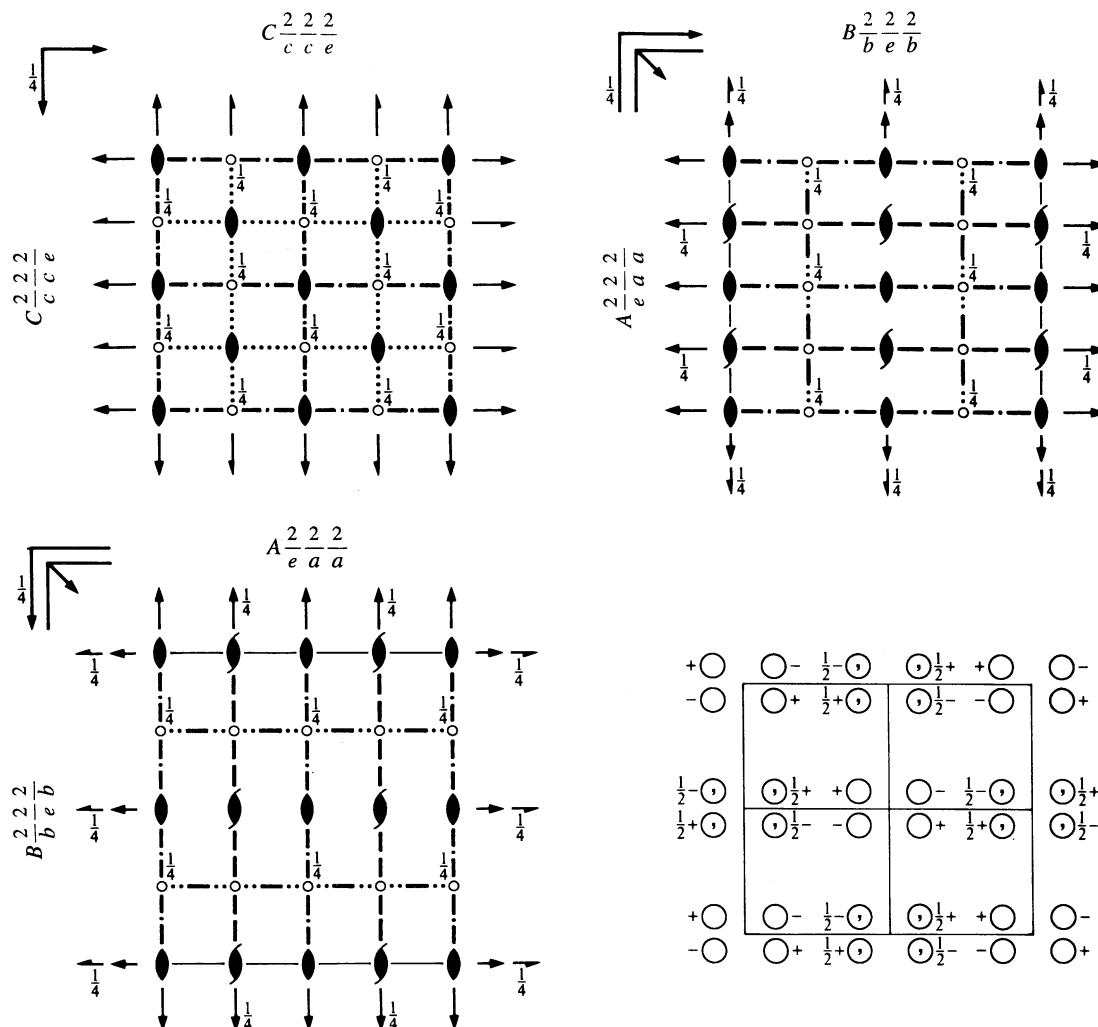
No. 68

$C 2/c 2/c 2/e$

Patterson symmetry $Cmmm$

Former space-group symbol $Ccca$; cf. Chapter 1.3

ORIGIN CHOICE 1



Origin at 222 at $2/n2/n2$, at $0, \frac{1}{4}, \frac{1}{4}$ from $\bar{1}$

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

Symmetry operations

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

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

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

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

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 <i>i</i> 1	(1) x,y,z (5) $\bar{x},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(3) \bar{x},y,\bar{z} (7) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ (8) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$	$hkl : h+k=2n$ $0kl : k,l=2n$ $h0l : h,l=2n$ $hk0 : h,k=2n$ $h00 : h=2n$ $0k0 : k=2n$ $00l : l=2n$
8 <i>h</i> ..2	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{1}{4},\frac{1}{4},z+\frac{1}{2}$	$hkl : l=2n$
8 <i>g</i> ..2	$0,0,z$	$0,0,\bar{z}$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},z+\frac{1}{2}$	$hkl : k+l=2n$
8 <i>f</i> .2.	$0,y,0$	$\frac{1}{2},\bar{y}+\frac{1}{2},0$	$0,\bar{y}+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},y,\frac{1}{2}$	$hkl : k+l=2n$
8 <i>e</i> 2..	$x,0,0$	$\bar{x}+\frac{1}{2},\frac{1}{2},0$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},0,\frac{1}{2}$	$hkl : k+l=2n$
8 <i>d</i> $\bar{1}$	$0,\frac{1}{4},\frac{1}{4}$	$\frac{1}{2},\frac{1}{4},\frac{1}{4}$	$0,\frac{1}{4},\frac{3}{4}$	$\frac{1}{2},\frac{1}{4},\frac{3}{4}$	$hkl : k,l=2n$
8 <i>c</i> $\bar{1}$	$\frac{1}{4},0,\frac{1}{4}$	$\frac{1}{4},\frac{1}{2},\frac{1}{4}$	$\frac{3}{4},0,\frac{3}{4}$	$\frac{3}{4},\frac{1}{2},\frac{3}{4}$	$hkl : k,l=2n$
4 <i>b</i> 222	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$			$hkl : k+l=2n$
4 <i>a</i> 222	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$			$hkl : k+l=2n$

Special: as above, plus

Symmetry of special projections

Along [001] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at 0,0,z

Along [100] $p2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
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] $Cc2e$ ($Aea2$, 41)	(1; 3; 6; 8)+
	[2] $C2ce$ ($Aea2$, 41)	(1; 4; 6; 7)+
	[2] $Ccc2$ (37)	(1; 2; 7; 8)+
	[2] $C222$ (21)	(1; 2; 3; 4)+
	[2] $C12/c1$ ($C2/c$, 15)	(1; 3; 5; 7)+
	[2] $C2/c11$ ($C2/c$, 15)	(1; 4; 5; 8)+
	[2] $C112/e$ ($P2/c$, 13)	(1; 2; 5; 6)+
IIa	[2] $Pcnb$ ($Pbcn$, 60)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pnca$ ($Pbcn$, 60)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pcca$ (54)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $Pccb$ ($Pcca$, 54)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pnnb$ ($Pnna$, 52)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pnna$ (52)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pncb$ ($Pban$, 50)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pcna$ ($Pban$, 50)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},0)$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $Ccce$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (68); [3] $Ccce$ ($\mathbf{c}' = 3\mathbf{c}$) (68)

Minimal non-isomorphic supergroups

I [2] $P4/nnc$ (126); [2] $P4/ncc$ (130); [2] $P4_2/nbc$ (133); [2] $P4_2/nmc$ (137)
II [2] $Fmmm$ (69); [2] $Pccm$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$, $\mathbf{b}' = \frac{1}{2}\mathbf{b}$) (49); [2] $Cmme$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (67)

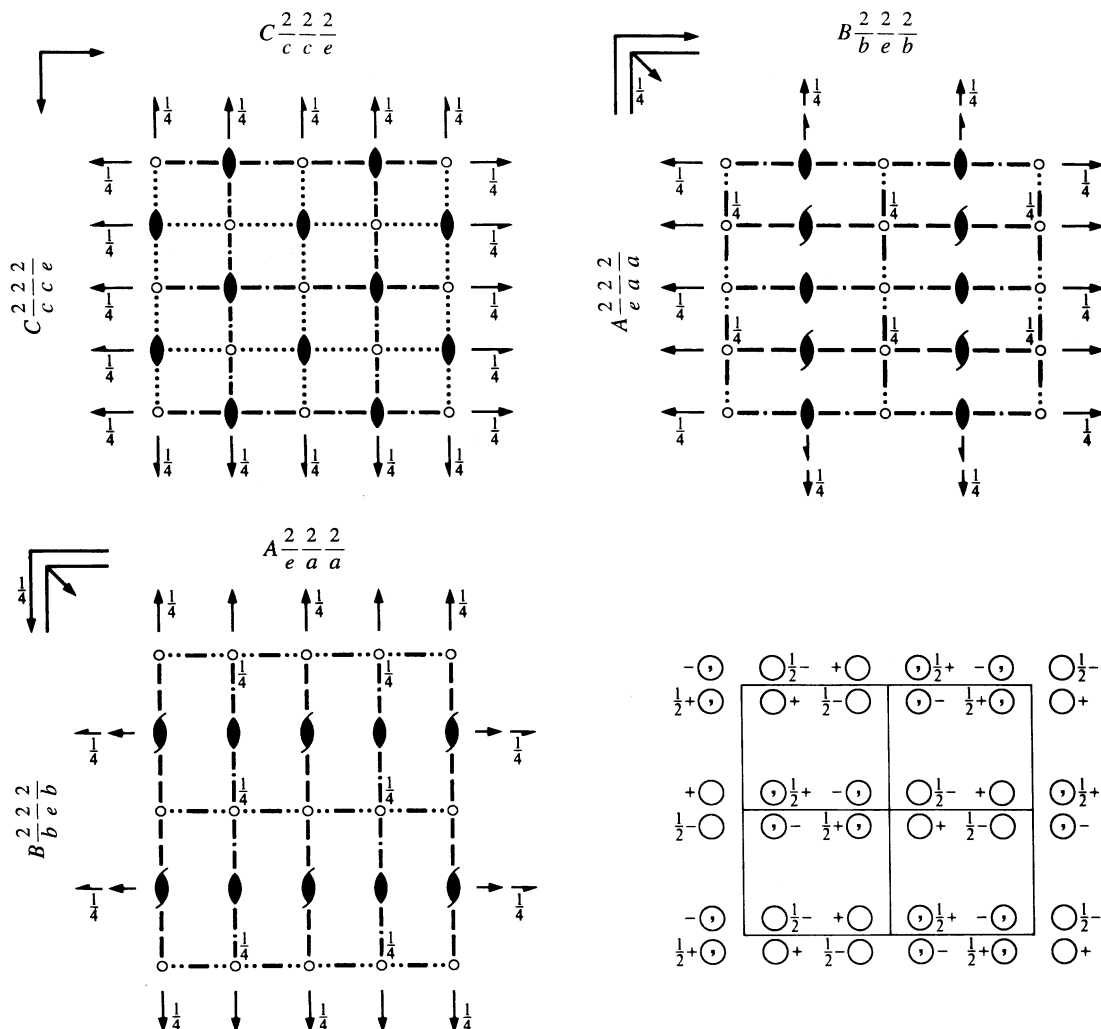
$Ccce$ D_{2h}^{22} mmm

Orthorhombic

No. 68

 $C 2/c 2/c 2/e$ Patterson symmetry $Cmmm$ Former space-group symbol $Ccca$; cf. Chapter 1.3

ORIGIN CHOICE 2

Origin at $\bar{1}$ at nce , at $0, -\frac{1}{4}, -\frac{1}{4}$ from 222Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq \frac{1}{2}$ **Symmetry operations**For $(0,0,0)+$ set

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

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

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

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
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16	<i>i</i> 1	(1) x,y,z (5) \bar{x},\bar{y},\bar{z}	(2) $\bar{x}+\frac{1}{2},\bar{y},z$ (6) $x+\frac{1}{2},y,\bar{z}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$ (7) $x,\bar{y},z+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$ (8) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$	$hkl : h+k=2n$ $Ok l : k,l=2n$ $h0l : h,l=2n$ $hk0 : h,k=2n$ $h00 : h=2n$ $0k0 : k=2n$ $00l : l=2n$
8	<i>h</i> ..2	$\frac{1}{4},0,z$	$\frac{3}{4},0,\bar{z}+\frac{1}{2}$	$\frac{3}{4},0,\bar{z}$	$\frac{1}{4},0,z+\frac{1}{2}$	$hkl : l=2n$
8	<i>g</i> ..2	$0,\frac{1}{4},z$	$0,\frac{1}{4},\bar{z}+\frac{1}{2}$	$0,\frac{3}{4},\bar{z}$	$0,\frac{3}{4},z+\frac{1}{2}$	$hkl : k+l=2n$
8	<i>f</i> .2.	$0,y,\frac{1}{4}$	$\frac{1}{2},\bar{y},\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$	$\frac{1}{2},y,\frac{3}{4}$	$hkl : k+l=2n$
8	<i>e</i> 2..	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{3}{4}$	$x+\frac{1}{2},\frac{1}{4},\frac{3}{4}$	$hkl : k+l=2n$
8	<i>d</i> $\bar{1}$	$0,0,0$	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$hkl : k,l=2n$
8	<i>c</i> $\bar{1}$	$\frac{1}{4},\frac{3}{4},0$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$hkl : k,l=2n$
4	<i>b</i> 222	$0,\frac{1}{4},\frac{3}{4}$	$0,\frac{3}{4},\frac{1}{4}$			$hkl : k+l=2n$
4	<i>a</i> 222	$0,\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{3}{4}$			$hkl : k+l=2n$

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