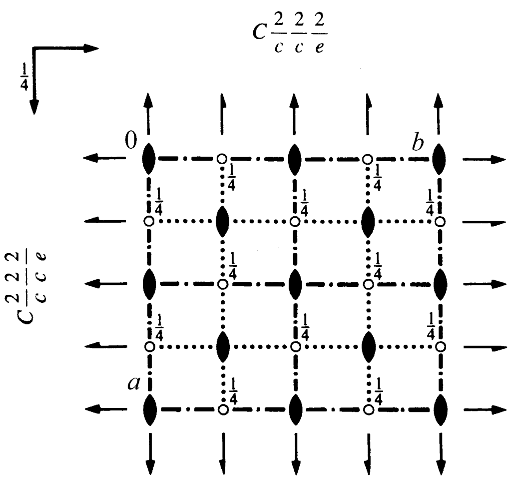
International Tables for Crystallography (2016). Vol. A, Space group 68, pp. 366–369.

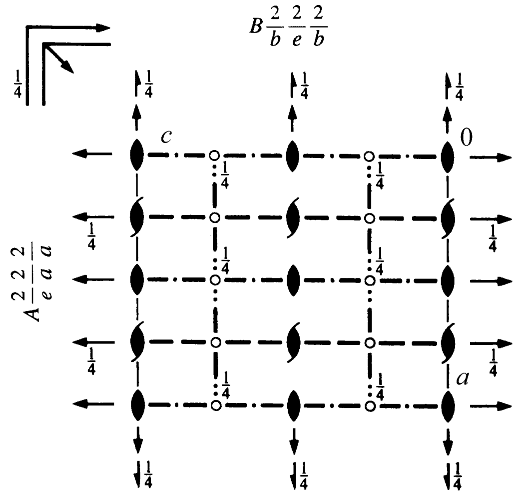
$Ccce$ D_{2h}^{22} mmm Orthorhombic

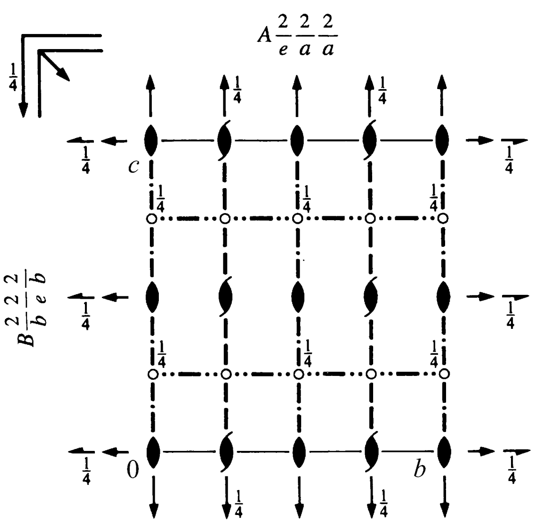
No. 68 $C\,2/c\,2/c\,2/e$ Patterson symmetry $Cmmm$

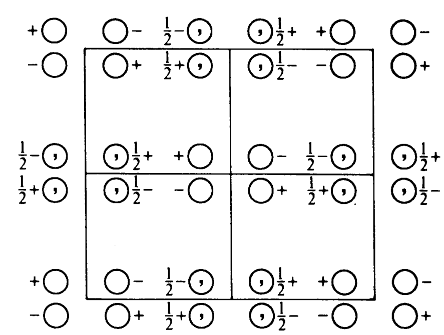
Former space-group symbol $Ccca$; *cf.* Section 2.1.2

ORIGIN CHOICE 1









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

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

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) $n(0,\frac{1}{2},\frac{1}{2})\ \ 0,y,z$

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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 $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$				Reflection conditions
							General:
16	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: $h+k=2n$ $0kl$: $k,l=2n$ $h0l$: $h,l=2n$ $hk0$: $h,k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
8	h	..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	g	..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	f	.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	e	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	d	$\bar{1}$	$0,\frac{1}{4},\frac{1}{4}$	$\frac{1}{2},\frac{1}{4},\frac{1}{4}$	$0,\frac{1}{4},\frac{3}{4}$	$\frac{1}{2},\frac{1}{4},\frac{3}{4}$	hkl: $k,l=2n$
8	c	$\bar{1}$	$\frac{1}{4},0,\frac{1}{4}$	$\frac{1}{4},\frac{1}{2},\frac{1}{4}$	$\frac{3}{4},0,\frac{3}{4}$	$\frac{3}{4},\frac{1}{2},\frac{3}{4}$	hkl: $k,l=2n$
4	b	222	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$			hkl: $k+l=2n$
4	a	222	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $k+l=2n$

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 $x,0,0$

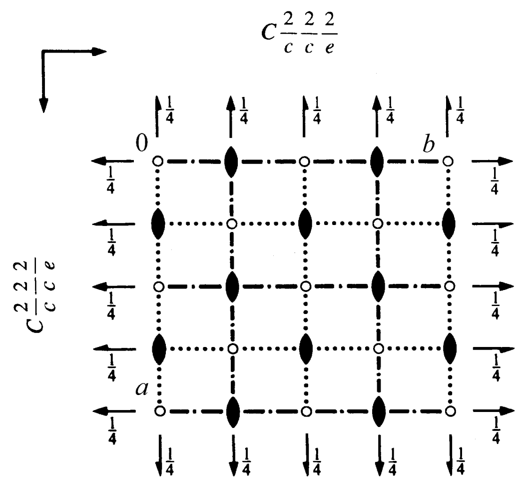
Along [010] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

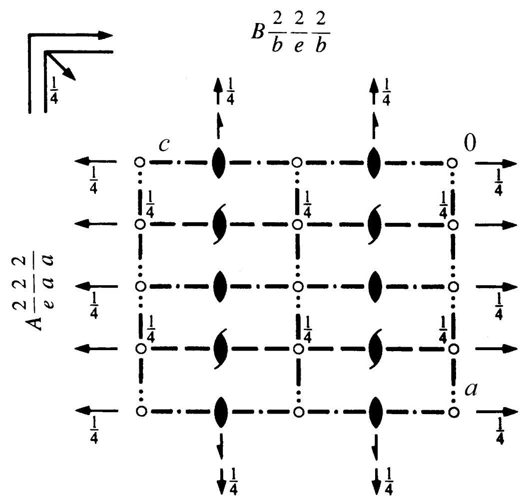
$Ccce$ D_{2h}^{22} mmm Orthorhombic

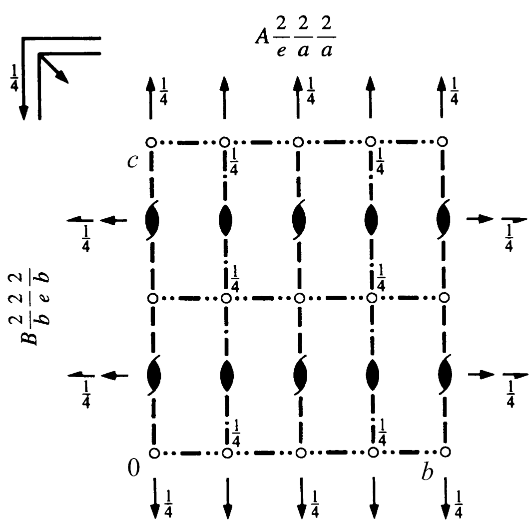
No. 68 $C\ 2/c\ 2/c\ 2/e$ Patterson symmetry $Cmmm$

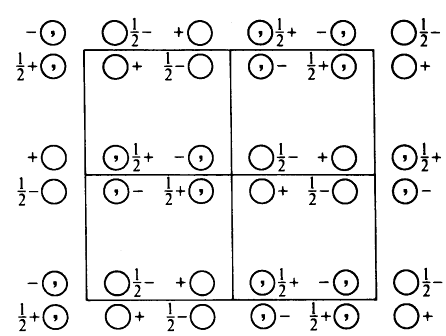
Former space-group symbol $Ccca$; *cf.* Section 2.1.2

ORIGIN CHOICE 2









Origin at $\bar{1}$ at nce, at $0,-\frac{1}{4},-\frac{1}{4}$ from 222

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

Symmetry operations

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

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

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

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

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

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 $0,y,0$