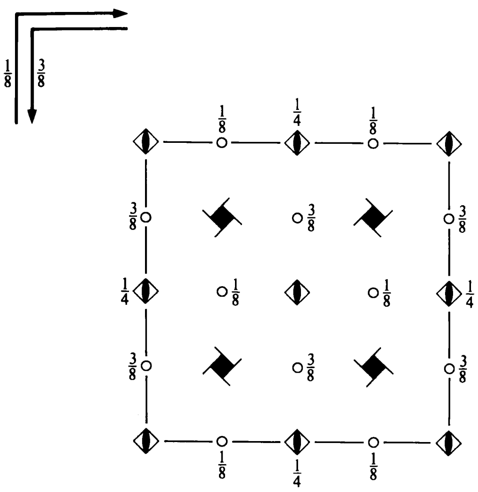
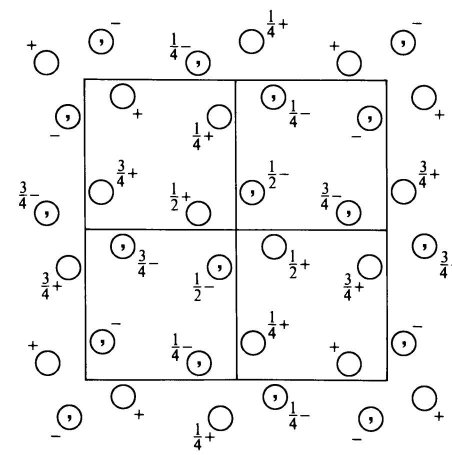
International Tables for Crystallography (2016). Vol. A, Space group 88, pp. 400–401.

$I4_1/a$ C_{4h}^6 $4/m$ Tetragonal

No. 88 $I4_1/a$ Patterson symmetry $I4/m$

ORIGIN CHOICE 1





Origin at $\bar{4}$, at $0,-\frac{1}{4},-\frac{1}{8}$ from $\bar{1}$

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

Symmetry operations

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

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

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

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

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); (3); (5)

Positions

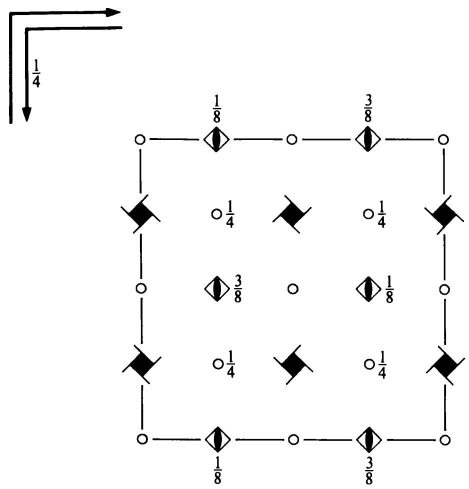
Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
16	f	1	(1) x,y,z (5) $\bar{x},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (6) $x+\frac{1}{2},y,\bar{z}+\frac{3}{4}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$ (7) $y,\bar{x},\bar{z}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$ (8) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	hkl: $h+k+l=2n$ $hk0$: $h,k=2n$ $0kl$: $k+l=2n$ hhl: $l=2n$ $00l$: $l=4n$ $h00$: $h=2n$ $h\bar{h}0$: $h=2n$
							Special: as above, plus
8	e	$2..$	$0,0,z$	$0,\frac{1}{2},z+\frac{1}{4}$	$0,\frac{1}{2},\bar{z}+\frac{1}{4}$	$0,0,\bar{z}$	hkl: $l=2n+1$ or $2h+l=4n$
8	d	$\bar{1}$	$0,\frac{1}{4},\frac{5}{8}$	$\frac{1}{2},\frac{1}{4},\frac{1}{8}$	$\frac{3}{4},\frac{1}{2},\frac{7}{8}$	$\frac{3}{4},0,\frac{3}{8}$	hkl: $l=2n+1$ or $h,k=2n$, $h+k+l=4n$
8	c	$\bar{1}$	$0,\frac{1}{4},\frac{1}{8}$	$\frac{1}{2},\frac{1}{4},\frac{5}{8}$	$\frac{3}{4},\frac{1}{2},\frac{3}{8}$	$\frac{3}{4},0,\frac{7}{8}$	
4	b	$\bar{4}..$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},\frac{3}{4}$			hkl: $l=2n+1$ or $2h+l=4n$
4	a	$\bar{4}..$	$0,0,0$	$0,\frac{1}{2},\frac{1}{4}$			

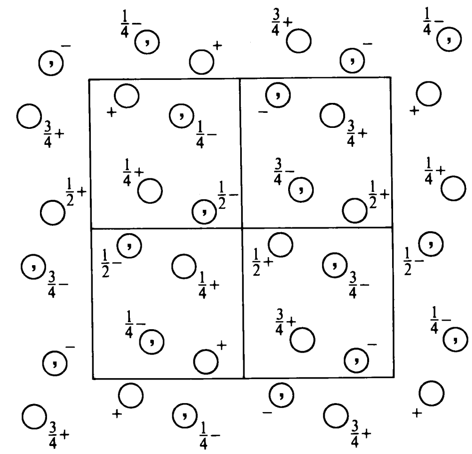
Symmetry of special projections

Along [001] $p4$	Along [100] $c2mm$	Along [110] $p2mg$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$	$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$	$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,\frac{3}{8}$	Origin at $x,x+\frac{1}{4},\frac{1}{8}$

Patterson symmetry $I4/m$ $I4_1/a$ No. 88

ORIGIN CHOICE 2





Origin at $\bar{1}$ on glide plane b, at $0,\frac{1}{4},\frac{1}{8}$ from $\bar{4}$

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

Symmetry operations

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

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

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

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

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); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
					General:
16 f 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{y}+\frac{3}{4},x+\frac{1}{4},z+\frac{1}{4}$	(4) $y+\frac{3}{4},\bar{x}+\frac{3}{4},z+\frac{3}{4}$	hkl: $h+k+l=2n$
	(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(7) $y+\frac{1}{4},\bar{x}+\frac{3}{4},\bar{z}+\frac{3}{4}$	(8) $\bar{y}+\frac{1}{4},x+\frac{1}{4},\bar{z}+\frac{1}{4}$	$hk0$: $h,k=2n$
					$0kl$: $k+l=2n$
					hhl: $l=2n$
					$00l$: $l=4n$
					$h00$: $h=2n$
					$h\bar{h}0$: $h=2n$
					Special: as above, plus
8 e $2\,.\,.$	$0,\frac{1}{4},z$	$\frac{1}{2},\frac{1}{4},z+\frac{1}{4}$	$0,\frac{3}{4},\bar{z}$	$\frac{1}{2},\frac{3}{4},\bar{z}+\frac{3}{4}$	hkl: $l=2n+1$ or $2h+l=4n$
8 d $\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	hkl: $l=2n+1$ or $h,k=2n$, $h+k+l=4n$ (for d and c)
8 c $\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	
4 b $\bar{4}\,.\,.$	$0,\frac{1}{4},\frac{5}{8}$	$\frac{1}{2},\frac{1}{4},\frac{7}{8}$			hkl: $l=2n+1$ or $2h+l=4n$ (for b and a)
4 a $\bar{4}\,.\,.$	$0,\frac{1}{4},\frac{1}{8}$	$\frac{1}{2},\frac{1}{4},\frac{3}{8}$			

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $\frac{1}{4},0,z$

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

Along [110] $p2mg$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$