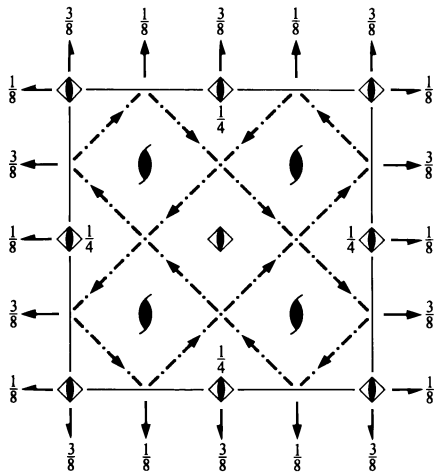
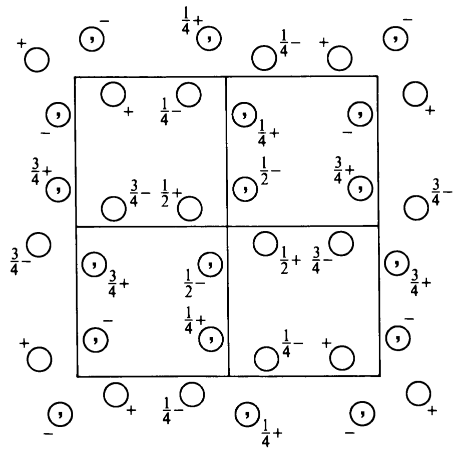
International Tables for Crystallography (2006). Vol. A, Space group 122, pp. 428–429.

$I\bar{4}2d$ D_{2d}^{12} $\bar{4}2m$ Tetragonal

No. 122 $I\bar{4}2d$ Patterson symmetry $I4/mmm$





Origin at $\bar{4}$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le 1$; $0 \le z \le \frac{1}{8}$

Symmetry operations

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

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

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

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

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

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

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,\frac{3}{8}$

Along [110] $c1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $I\bar{4}11$ ($I\bar{4}$, 82) (1; 2; 3; 4)+
[2] $I121d$ ($Fdd2$, 43) (1; 2; 7; 8)+
[2] $I221$ ($I2_12_12_1$, 24) (1; 2; 5; 6)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $I\bar{4}2d$ ($\mathbf{c}'=3\mathbf{c}$) (122); [9] $I\bar{4}2d$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (122)

Minimal non-isomorphic supergroups

I [2] $I4_1/amd$ (141); [2] $I4_1/acd$ (142); [3] $I\bar{4}3d$ (220)

II [2] $C\bar{4}2d$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P\bar{4}n2$, 118)