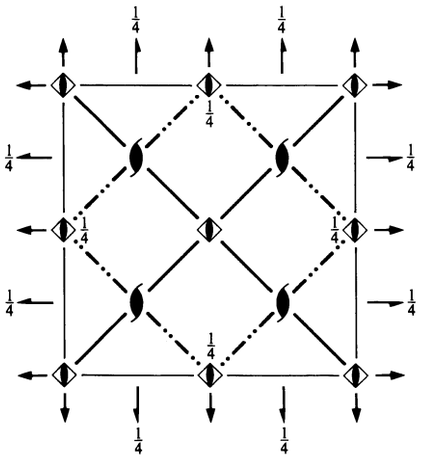
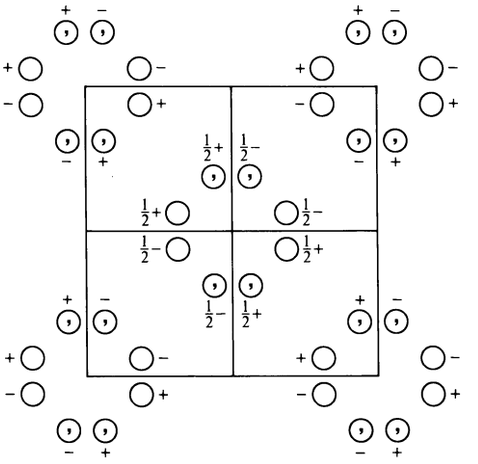
$I\bar{4}2m$ D_{2d}^{11} $\bar{4}2m$ Tetragonal

No. 121 $I\bar{4}2m$ Patterson symmetry $I4/mmm$





Origin at $\bar{4}2m$

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

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 $0,y,0$
(6) 2 $x,0,0$
(7) m $x,\bar{x},z$
(8) m x,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) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$
(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(7) c $x+\frac{1}{2},\bar{x},z$
(8) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,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
							General:
16	j	1	(1) x,y,z (5) $\bar{x},y,\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,\bar{y},\bar{z}$	(3) $y,\bar{x},\bar{z}$ (7) $\bar{y},\bar{x},z$	(4) $\bar{y},x,\bar{z}$ (8) y,x,z	hkl : $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ hhl : $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
							Special: as above, plus
8	i	. . m	x,x,z	$\bar{x},\bar{x},z$	$x,\bar{x},\bar{z}$	$\bar{x},x,\bar{z}$	no extra conditions
8	h	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,z$	hkl : $l=2n$
8	g	. 2 .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$0,x,\frac{1}{2}$	no extra conditions
8	f	. 2 .	$x,0,0$	$\bar{x},0,0$	$0,\bar{x},0$	$0,x,0$	no extra conditions
4	e	2 . mm	$0,0,z$	$0,0,\bar{z}$			no extra conditions
4	d	$\bar{4}$ . .	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$			hkl : $l=2n$
4	c	2 2 2 .	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl : $l=2n$
2	b	$\bar{4}$ 2 m	$0,0,\frac{1}{2}$				no extra conditions
2	a	$\bar{4}$ 2 m	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

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

Along [110] $p1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $I\bar{4}11$ $(I\bar{4}, 82)$ (1; 2; 3; 4)+
[2] $I21m$ $(Fmm2, 42)$ (1; 2; 7; 8)+
[2] $I221$ $(I222, 23)$ (1; 2; 5; 6)+

IIa [2] $P\bar{4}2_1c$ (114) 1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] $P\bar{4}2_1m$ (113) 1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] $P\bar{4}2c$ (112) 1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] $P\bar{4}2m$ (111) 1; 2; 3; 4; 5; 6; 7; 8

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $I\bar{4}2m$ $(\mathbf{c}' = 3\mathbf{c})$ (121); [9] $I\bar{4}2m$ $(\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b})$ (121)

Minimal non-isomorphic supergroups

I [2] $I4/mmm$ (139); [2] $I4/mcm$ (140); [3] $I\bar{4}3m$ (217)

II [2] $C\bar{4}2m$ $(\mathbf{c}' = \frac{1}{2}\mathbf{c})$ $(P\bar{4}m2, 115)$