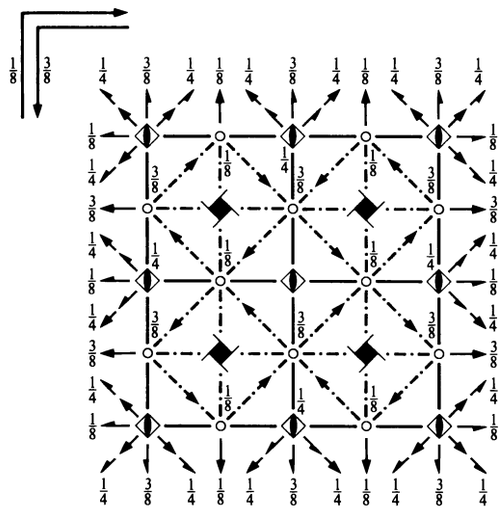
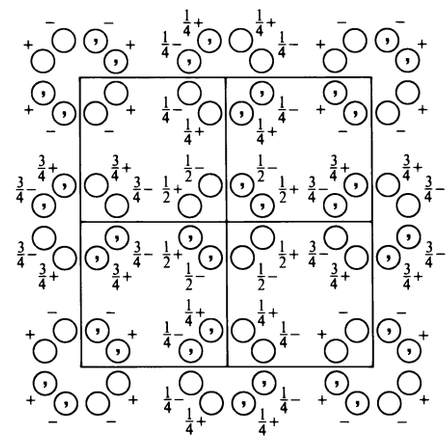
International Tables for Crystallography (2006). Vol. A, Space group 141, pp. 482–483.

$I4_1/amd$ $\quad D_{4h}^{19}$ $\quad 4/mmm$ $\quad$ Tetragonal

No. 141 $\quad I\ 4_1/a\ 2/m\ 2/d$ $\quad$ Patterson symmetry $I4/mmm$

ORIGIN CHOICE 1





Origin at $\bar{4}m2$, at $0,\frac{1}{4},-\frac{1}{8}$ from centre $(2/m)$

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

Symmetry operations

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

(1) 1	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},\frac{1}{4},z$	(3) $4^{+}(0,0,\frac{1}{4})\quad -\frac{1}{4},\frac{1}{4},z$	(4) $4^{-}(0,0,\frac{3}{4})\quad \frac{1}{4},-\frac{1}{4},z$
(5) $2\quad \frac{1}{4},y,\frac{3}{8}$	(6) $2\quad x,\frac{1}{4},\frac{1}{8}$	(7) $2(\frac{1}{2},\frac{1}{2},0)\quad x,x,\frac{1}{4}$	(8) $2\quad x,\bar{x},0$
(9) $\bar{1}\quad 0,\frac{1}{4},\frac{1}{8}$	(10) $a\quad x,y,\frac{3}{8}$	(11) $\bar{4}^{+}\ 0,0,z;\ 0,0,0$	(12) $\bar{4}^{-}\ 0,\frac{1}{2},z;\ 0,\frac{1}{2},\frac{1}{4}$
(13) $n(\frac{1}{2},0,\frac{1}{2})\quad x,\frac{1}{4},z$	(14) $m\quad 0,y,z$	(15) $d(\frac{1}{4},-\frac{1}{4},\frac{3}{4})\quad x+\frac{1}{4},\bar{x},z$	(16) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})\quad x-\frac{1}{4},x,z$

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

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2\quad 0,0,z$	(3) $4^{+}(0,0,\frac{3}{4})\quad \frac{1}{4},\frac{1}{4},z$	(4) $4^{-}(0,0,\frac{1}{4})\quad \frac{1}{4},\frac{1}{4},z$
(5) $2(0,\frac{1}{2},0)\quad 0,y,\frac{1}{8}$	(6) $2(\frac{1}{2},0,0)\quad x,0,\frac{3}{8}$	(7) $2\quad x,x,0$	(8) $2\quad x,\bar{x}+\frac{1}{2},\frac{1}{4}$
(9) $\bar{1}\quad \frac{1}{4},0,\frac{3}{8}$	(10) $b\quad x,y,\frac{1}{8}$	(11) $\bar{4}^{+}\ \frac{1}{2},0,z;\ \frac{1}{2},0,\frac{1}{4}$	(12) $\bar{4}^{-}\ 0,0,z;\ 0,0,0$
(13) $m\quad x,0,z$	(14) $n(0,\frac{1}{2},\frac{1}{2})\quad \frac{1}{4},y,z$	(15) $d(-\frac{1}{4},\frac{1}{4},\frac{1}{4})\quad x+\frac{1}{4},\bar{x},z$	(16) $d(\frac{1}{4},\frac{1}{4},\frac{3}{4})\quad x+\frac{1}{4},x,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
32	i	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$	hkl : $h+k+l=2n$
			(5) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{3}{4}$	(6) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}$	$hk0$: $h,k=2n$
			(9) $\bar{x},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$	(10) $x+\frac{1}{2},y,\bar{z}+\frac{3}{4}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	$0kl$: $k+l=2n$
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{x},y,z$	(15) $\bar{y}+\frac{1}{2},\bar{x},z+\frac{3}{4}$	(16) $y,x+\frac{1}{2},z+\frac{1}{4}$	hhl : $2h+l=4n$
							$00l$: $l=4n$
							$h00$: $h=2n$
							$h\bar{h}0$: $h=2n$
							Special: as above, plus
16	h	$.\,m\,.$	$0,y,z$	$\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$\bar{y},\frac{1}{2},z+\frac{1}{4}$	$y+\frac{1}{2},0,z+\frac{3}{4}$	no extra conditions
			$\frac{1}{2},y,\bar{z}+\frac{3}{4}$	$0,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$	$y+\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$\bar{y},0,\bar{z}$	
16	g	$..\,2$	$x,x,0$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\frac{1}{4}$	$x+\frac{1}{2},\bar{x},\frac{3}{4}$	hkl : $l=2n+1$
			$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$	$x+\frac{1}{2},x,\frac{3}{4}$	$x,\bar{x},0$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	or $2h+l=4n$
16	f	$.\,2\,.$	$x,\frac{1}{4},\frac{1}{8}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{5}{8}$	$\frac{3}{4},x+\frac{1}{2},\frac{3}{8}$	$\frac{3}{4},\bar{x},\frac{7}{8}$	hkl : $l=2n+1$
			$\bar{x},\frac{1}{4},\frac{1}{8}$	$x+\frac{1}{2},\frac{1}{4},\frac{5}{8}$	$\frac{1}{4},\bar{x},\frac{7}{8}$	$\frac{1}{4},x+\frac{1}{2},\frac{3}{8}$	or $h=2n$
8	e	$2\,m\,m\,.$	$0,0,z$	$0,\frac{1}{2},z+\frac{1}{4}$	$\frac{1}{2},0,\bar{z}+\frac{3}{4}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	hkl : $l=2n+1$
							or $2h+l=4n$
8	d	$.\,2/m\,.$	$0,\frac{1}{4},\frac{5}{8}$	$\frac{1}{2},\frac{1}{4},\frac{1}{8}$	$\frac{3}{4},\frac{1}{2},\frac{7}{8}$	$\frac{3}{4},0,\frac{3}{8}$	hkl : $l=2n+1$
8	c	$.\,2/m\,.$	$0,\frac{1}{4},\frac{1}{8}$	$\frac{1}{2},\frac{1}{4},\frac{5}{8}$	$\frac{3}{4},\frac{1}{2},\frac{3}{8}$	$\frac{3}{4},0,\frac{7}{8}$	or $h,k=2n,\ h+k+l=4n$
4	b	$\bar{4}\,m\,2$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},\frac{3}{4}$			hkl : $l=2n+1$
4	a	$\bar{4}\,m\,2$	$0,0,0$	$0,\frac{1}{2},\frac{1}{4}$			or $2h+l=4n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
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] $c2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $I\bar{4}2d$ (122) (1; 2; 5; 6; 11; 12; 15; 16)+
[2] $I\bar{4}m2$ (119) (1; 2; 7; 8; 11; 12; 13; 14)+
[2] $I4_1md$ (109) (1; 2; 3; 4; 13; 14; 15; 16)+
[2] $I4_122$ (98) (1; 2; 3; 4; 5; 6; 7; 8)+
[2] $I4_1/a11$ ($I4_1/a$, 88) (1; 2; 3; 4; 9; 10; 11; 12)+
[2] $I2/a2/m1$ ($Imma$, 74) (1; 2; 5; 6; 9; 10; 13; 14)+
[2] $I2/a12/d$ ($Fddd$, 70) (1; 2; 7; 8; 9; 10; 15; 16)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $I4_1/amd$ ($\mathbf{c}'=3\mathbf{c}$) (141); [9] $I4_1/amd$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) (141)

Minimal non-isomorphic supergroups

I [3] $Fd\bar{3}m$ (227)

II [2] $C4_2/amd$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P4_2/nnm$, 134)