

$I4_1/acd$

D_{4h}^{20}

$4/mmm$

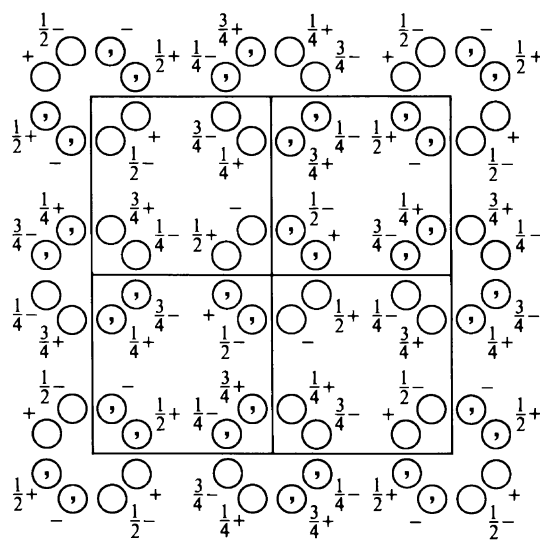
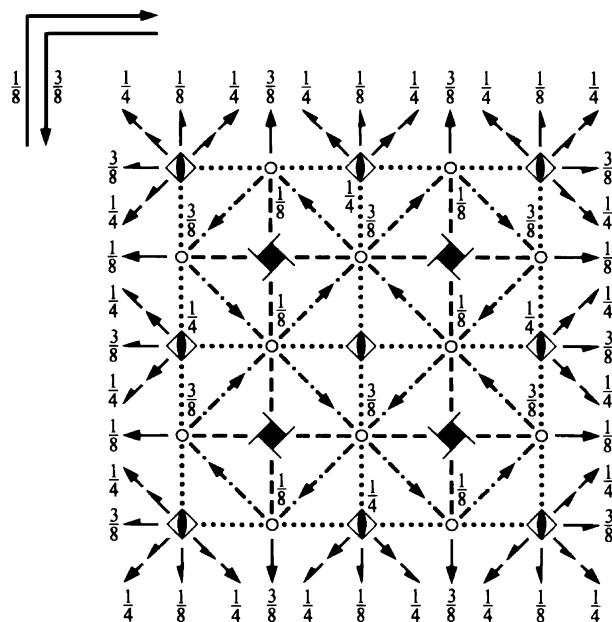
Tetragonal

No. 142

$I 4_1/a 2/c 2/d$

Patterson symmetry $I4/mmm$

ORIGIN CHOICE 1



Origin at $\bar{4}c2_1$, at $0, \frac{1}{4}, -\frac{1}{8}$ from $\bar{1}$

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

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) 2 $\frac{1}{4}, y, \frac{1}{8}$ | (6) 2 $x, \frac{1}{4}, \frac{3}{8}$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0)$ $x, x, 0$ | (8) 2 $x, \bar{x}, \frac{1}{4}$ |
| (9) $\bar{1}$ $0, \frac{1}{4}, \frac{1}{8}$ | (10) a $x, y, \frac{3}{8}$ | (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) a $x, \frac{1}{4}, z$ | (14) c $0, y, z$ | (15) $d(\frac{1}{4}, -\frac{1}{4}, \frac{1}{4})$ $x + \frac{1}{4}, \bar{x}, z$ | (16) $d(\frac{1}{4}, \frac{1}{4}, \frac{3}{4})$ $x - \frac{1}{4}, x, z$ |

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

- | | | | |
|--|--|--|---|
| (1) $i(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | (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) $2(0, \frac{1}{2}, 0)$ $0, y, \frac{3}{8}$ | (6) $2(\frac{1}{2}, 0, 0)$ $x, 0, \frac{1}{8}$ | (7) 2 $x, x, \frac{1}{4}$ | (8) 2 $x, \bar{x} + \frac{1}{2}, 0$ |
| (9) $\bar{1}$ $\frac{1}{4}, 0, \frac{3}{8}$ | (10) b $x, y, \frac{1}{8}$ | (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) c $x, 0, z$ | (14) b $\frac{1}{4}, y, z$ | (15) $d(-\frac{1}{4}, \frac{1}{4}, \frac{3}{4})$ $x + \frac{1}{4}, \bar{x}, z$ | (16) $d(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ $x + \frac{1}{4}, x, z$ |

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); (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>g</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) $y + \frac{1}{2}, \bar{x}, z + \frac{3}{4}$
			(5) $\bar{x} + \frac{1}{2}, y, \bar{z} + \frac{1}{4}$	(6) $x, \bar{y} + \frac{1}{2}, \bar{z} + \frac{3}{4}$	(7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$	(8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$
			(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) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$
			(13) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(14) $\bar{x}, y, z + \frac{1}{2}$	(15) $\bar{y} + \frac{1}{2}, \bar{x}, z + \frac{1}{4}$	(16) $y, x + \frac{1}{2}, z + \frac{3}{4}$

hkl : $h + k + l = 2n$
 $hk0$: $h, k = 2n$
 $0kl$: $k, l = 2n$
 hhl : $2h + l = 4n$
 $00l$: $l = 4n$
 $h00$: $h = 2n$
 $h\bar{h}0$: $h = 2n$

Special: as above, plus

16	<i>f</i>	. . 2	$x, x, \frac{1}{4}$ $\bar{x}, \bar{x} + \frac{1}{2}, 0$	$\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{3}{4}$ $x + \frac{1}{2}, x, \frac{1}{2}$	$\bar{x}, x + \frac{1}{2}, \frac{1}{2}$ $x, \bar{x}, \frac{3}{4}$	$x + \frac{1}{2}, \bar{x}, 0$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}$
----	----------	-------	--	--	--	--

hkl : $l = 2n + 1$
or $2h + l = 4n$

16	<i>e</i>	. 2 .	$\frac{1}{4}, y, \frac{1}{8}$ $\frac{3}{4}, \bar{y} + \frac{1}{2}, \frac{1}{8}$	$\frac{1}{4}, \bar{y} + \frac{1}{2}, \frac{5}{8}$ $\frac{3}{4}, y, \frac{5}{8}$	$\bar{y}, \frac{3}{4}, \frac{3}{8}$ $y, \frac{3}{4}, \frac{7}{8}$	$y + \frac{1}{2}, \frac{3}{4}, \frac{7}{8}$ $\bar{y} + \frac{1}{2}, \frac{3}{4}, \frac{3}{8}$
----	----------	-------	--	--	--	--

hkl : $l = 2n + 1$
or $h = 2n$

16	<i>d</i>	2 . .	$0, 0, z$ $0, \frac{1}{2}, \bar{z} + \frac{1}{4}$	$0, \frac{1}{2}, z + \frac{1}{4}$ $0, 0, \bar{z}$	$\frac{1}{2}, 0, \bar{z} + \frac{1}{4}$ $\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$ $\frac{1}{2}, 0, z + \frac{1}{4}$
----	----------	-------	--	--	--	--

hkl : $2h + l = 4n$

16	<i>c</i>	$\bar{1}$	$0, \frac{1}{4}, \frac{1}{8}$	$\frac{1}{2}, \frac{1}{4}, \frac{5}{8}$	$\frac{3}{4}, \frac{1}{2}, \frac{3}{8}$	$\frac{3}{4}, 0, \frac{7}{8}$	$\frac{1}{2}, \frac{1}{4}, \frac{1}{8}$	$0, \frac{1}{4}, \frac{5}{8}$	$\frac{3}{4}, \frac{1}{2}, \frac{7}{8}$	$\frac{3}{4}, 0, \frac{3}{8}$
----	----------	-----------	-------------------------------	---	---	-------------------------------	---	-------------------------------	---	-------------------------------

hkl : $h, k = 2n, h + k + l = 4n$

8	<i>b</i>	2 . 22	$0, 0, \frac{1}{4}$	$0, \frac{1}{2}, \frac{1}{2}$	$0, \frac{1}{2}, 0$	$0, 0, \frac{3}{4}$
---	----------	--------	---------------------	-------------------------------	---------------------	---------------------

hkl : $2h + l = 4n$

8	<i>a</i>	$\bar{4}$. .	$0, 0, 0$	$0, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, 0, \frac{1}{4}$	$\frac{1}{2}, \frac{1}{2}, 0$
---	----------	---------------	-----------	-------------------------------	-------------------------------	-------------------------------

hkl : $2h + l = 4n$

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 $[100]$ $p2mm$

$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at $x, 0, \frac{1}{8}$

Along $[110]$ $c2mm$

$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at $x, x, 0$

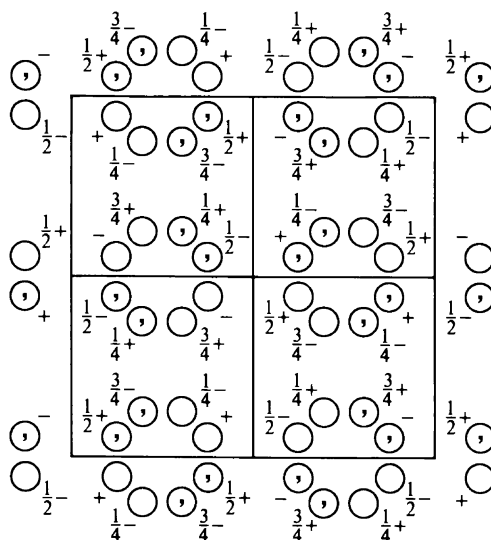
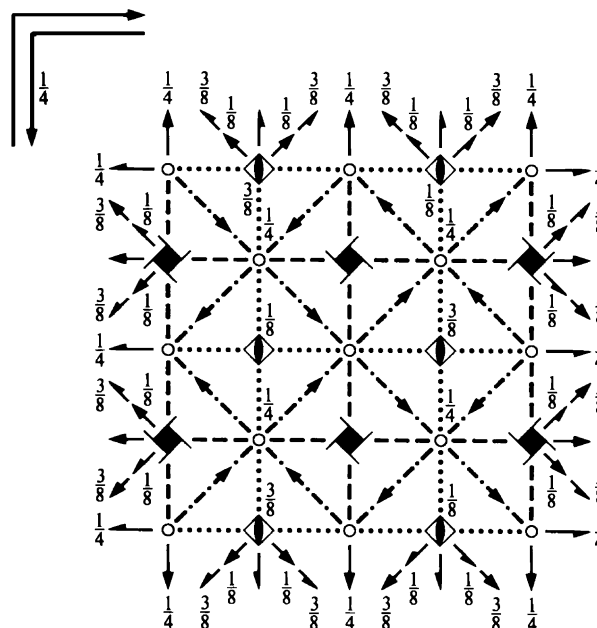
$I4_1/acd$ D_{4h}^{20} $4/mmm$

Tetragonal

No. 142

 $I 4_1/a 2/c 2/d$ Patterson symmetry $I4/mmm$

ORIGIN CHOICE 2

Origin at $\bar{1}$ at $b(c,a)d$, at $0, -\frac{1}{4}, \frac{1}{8}$ from $\bar{4}$ Asymmetric unit $0 \leq x \leq \frac{1}{2}; -\frac{1}{4} \leq y \leq \frac{1}{4}; 0 \leq z \leq \frac{1}{8}$

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) $4^-(0,0,\frac{3}{4})$ $\frac{1}{4}, 0, z$ |
| (5) 2 $\frac{1}{4}, y, 0$ | (6) 2 $x, 0, \frac{1}{4}$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0)$ $x, x + \frac{1}{4}, \frac{3}{8}$ | (8) 2 $x, \bar{x} + \frac{1}{4}, \frac{1}{8}$ |
| (9) $\bar{1}$ $0, 0, 0$ | (10) a $x, y, \frac{1}{4}$ | (11) 4^+ $\frac{1}{2}, -\frac{1}{4}, z$; $\frac{1}{2}, -\frac{1}{4}, \frac{3}{8}$ | (12) 4^- $0, \frac{3}{4}, z$; $0, \frac{3}{4}, \frac{1}{8}$ |
| (13) a $x, 0, z$ | (14) c $0, y, z$ | (15) $d(\frac{1}{4}, -\frac{1}{4}, \frac{1}{4})$ $x + \frac{1}{2}, \bar{x}, z$ | (16) $d(\frac{3}{4}, \frac{3}{4}, \frac{3}{4})$ 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 $0, \frac{1}{4}, z$ | (3) $4^+(0,0,\frac{3}{4})$ $\frac{1}{4}, \frac{1}{2}, z$ | (4) $4^-(0,0,\frac{1}{4})$ $\frac{3}{4}, 0, z$ |
| (5) $2(0, \frac{1}{2}, 0)$ $0, y, \frac{1}{4}$ | (6) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{4}, 0$ | (7) $2(\frac{1}{2}, \frac{1}{2}, 0)$ $x, x - \frac{1}{4}, \frac{1}{8}$ | (8) 2 $x, \bar{x} + \frac{3}{4}, \frac{3}{8}$ |
| (9) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | (10) b $x, y, 0$ | (11) 4^+ $\frac{1}{2}, \frac{1}{4}, z$; $\frac{1}{2}, \frac{1}{4}, \frac{1}{8}$ | (12) 4^- $0, \frac{1}{4}, z$; $0, \frac{1}{4}, \frac{3}{8}$ |
| (13) c $x, \frac{1}{4}, z$ | (14) b $\frac{1}{4}, y, z$ | (15) $d(-\frac{1}{4}, \frac{1}{4}, \frac{3}{4})$ $x + \frac{1}{2}, \bar{x}, z$ | (16) $d(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ 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); (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>g</i>	1	(1) x, y, z (5) $\bar{x} + \frac{1}{2}, y, \bar{z}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (13) $x + \frac{1}{2}, \bar{y}, z$	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (6) $x, \bar{y}, \bar{z} + \frac{1}{2}$ (10) $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ (14) $\bar{x}, y, z + \frac{1}{2}$	(3) $\bar{y} + \frac{1}{4}, x + \frac{3}{4}, z + \frac{1}{4}$ (7) $y + \frac{1}{4}, x + \frac{3}{4}, \bar{z} + \frac{3}{4}$ (11) $y + \frac{3}{4}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{3}{4}$ (15) $\bar{y} + \frac{3}{4}, \bar{x} + \frac{1}{4}, z + \frac{1}{4}$	(4) $y + \frac{1}{4}, \bar{x} + \frac{1}{4}, z + \frac{3}{4}$ (8) $\bar{y} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}$ (12) $\bar{y} + \frac{3}{4}, x + \frac{3}{4}, \bar{z} + \frac{1}{4}$ (16) $y + \frac{3}{4}, x + \frac{3}{4}, z + \frac{3}{4}$	$hkl: h + k + l = 2n$ $hk0: h, k = 2n$ $0kl: k, l = 2n$ $hhl: 2h + l = 4n$ $00l: l = 4n$ $h00: h = 2n$ $h\bar{h}0: h = 2n$	
16	<i>f</i>	..2	$x, x + \frac{1}{4}, \frac{1}{8}$ $\bar{x}, \bar{x} + \frac{3}{4}, \frac{7}{8}$	$\bar{x} + \frac{1}{2}, \bar{x} + \frac{3}{4}, \frac{5}{8}$ $x + \frac{1}{2}, x + \frac{1}{4}, \frac{3}{8}$	$\bar{x}, x + \frac{3}{4}, \frac{3}{8}$ $x, \bar{x} + \frac{1}{4}, \frac{5}{8}$	$x + \frac{1}{2}, \bar{x} + \frac{1}{4}, \frac{7}{8}$ $\bar{x} + \frac{1}{2}, x + \frac{3}{4}, \frac{1}{8}$	$hkl: l = 2n + 1$ or $2h + l = 4n$	
16	<i>e</i>	.2.	$x, 0, \frac{1}{4}$ $\bar{x}, 0, \frac{3}{4}$	$\bar{x} + \frac{1}{2}, 0, \frac{3}{4}$ $x + \frac{1}{2}, 0, \frac{1}{4}$	$\frac{1}{4}, x + \frac{3}{4}, \frac{1}{2}$ $\frac{3}{4}, \bar{x} + \frac{1}{4}, \frac{1}{2}$	$\frac{1}{4}, \bar{x} + \frac{1}{4}, 0$ $\frac{3}{4}, x + \frac{3}{4}, 0$	$hkl: l = 2n + 1$ or $h = 2n$	
16	<i>d</i>	2..	$0, \frac{1}{4}, z$ $0, \frac{3}{4}, \bar{z}$	$0, \frac{3}{4}, z + \frac{1}{4}$ $0, \frac{1}{4}, \bar{z} + \frac{3}{4}$	$\frac{1}{2}, \frac{1}{4}, \bar{z}$ $\frac{1}{2}, \frac{3}{4}, z$	$\frac{1}{2}, \frac{3}{4}, \bar{z} + \frac{3}{4}$ $\frac{1}{2}, \frac{1}{4}, z + \frac{1}{4}$	$hkl: 2h + l = 4n$	
16	<i>c</i>	$\bar{1}$	$0, 0, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{2}, 0, 0$ $0, 0, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$hkl: h, k = 2n, h + k + l = 4n$
8	<i>b</i>	2.22	$0, \frac{1}{4}, \frac{1}{8}$	$0, \frac{3}{4}, \frac{3}{8}$	$0, \frac{3}{4}, \frac{7}{8}$	$0, \frac{1}{4}, \frac{5}{8}$		$hkl: 2h + l = 4n$
8	<i>a</i>	$\bar{4}$..	$0, \frac{1}{4}, \frac{3}{8}$	$0, \frac{3}{4}, \frac{5}{8}$	$\frac{1}{2}, \frac{1}{4}, \frac{5}{8}$	$\frac{1}{2}, \frac{3}{4}, \frac{3}{8}$		$hkl: 2h + l = 4n$

Symmetry of special projections

Along [001] $p4mm$

$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$

Origin at $\frac{1}{4}, 0, z$

Along [100] $p2mm$

$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at $x, 0, 0$

Along [110] $c2mm$

$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$

Origin at $x, x + \frac{1}{4}, \frac{1}{8}$