

$I4_1/acd$

$D_{4h}^{20}$

$4/mmm$

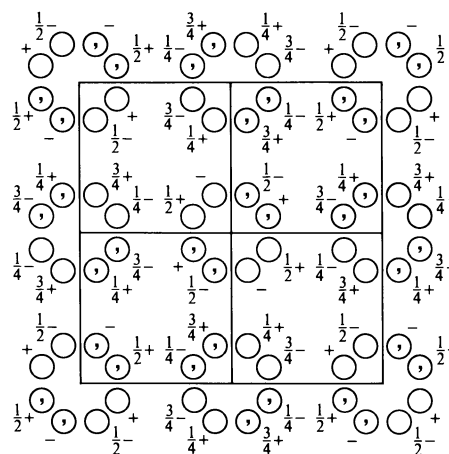
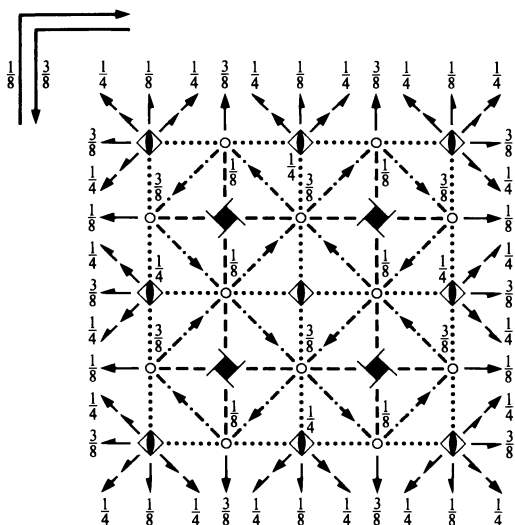
Tetragonal

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  $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{8}$

**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) $4^+$ $0, 0, z; 0, 0, 0$                                                  | (12) $4^-$ $0, \frac{1}{2}, z; 0, \frac{1}{2}, \frac{1}{4}$             |
| (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) $4^+$ $\frac{1}{2}, 0, z; \frac{1}{2}, 0, \frac{1}{4}$                    | (12) $4^-$ $0, 0, z; 0, 0, 0$                                           |
| (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				Reflection conditions				
	$(0,0,0)+ (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$				General:				
32 <i>g</i> 1	(1) $x, y, z$ (5) $\bar{x} + \frac{1}{2}, y, \bar{z} + \frac{1}{4}$ (9) $\bar{x}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{4}$ (13) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ (6) $x, \bar{y} + \frac{1}{2}, \bar{z} + \frac{3}{4}$ (10) $x + \frac{1}{2}, y, \bar{z} + \frac{3}{4}$ (14) $\bar{x}, y, z + \frac{1}{2}$	(3) $\bar{y}, x + \frac{1}{2}, z + \frac{1}{4}$ (7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$ (11) $y, \bar{x}, \bar{z}$ (15) $\bar{y} + \frac{1}{2}, \bar{x}, z + \frac{1}{4}$	(4) $y + \frac{1}{2}, \bar{x}, z + \frac{3}{4}$ (8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$ (12) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (16) $y, x + \frac{1}{2}, z + \frac{3}{4}$	$hkl : h + k + l = 2n$ $hk0 : h, k = 2n$ $0kl : k, l = 2n$ $hhl : 2h + l = 4n$ $00l : l = 4n$ $h00 : h = 2n$ $h\bar{h}0 : h = 2n$				
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  $x, x, 0$

**Maximal non-isomorphic subgroups**

<b>I</b>	[2] $I\bar{4}2d$ (122)	(1; 2; 5; 6; 11; 12; 15; 16)+
	[2] $I\bar{4}c2$ (120)	(1; 2; 7; 8; 11; 12; 13; 14)+
	[2] $I4, cd$ (110)	(1; 2; 3; 4; 13; 14; 15; 16)+
	[2] $I4, 22$ (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] $I2/a2/c1$ ( $Ibca$ , 73)	(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]  $I4_1/acd$  ( $\mathbf{c}' = 3\mathbf{c}$ ) (142); [9]  $I4_1/acd$  ( $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$ ) (142)**Minimal non-isomorphic supergroups****I** [3]  $Fd\bar{3}c$  (228); [3]  $Ia\bar{3}d$  (230)**II** [2]  $C4_2/amd$  ( $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ ) ( $P4_2/nm$ , 134)

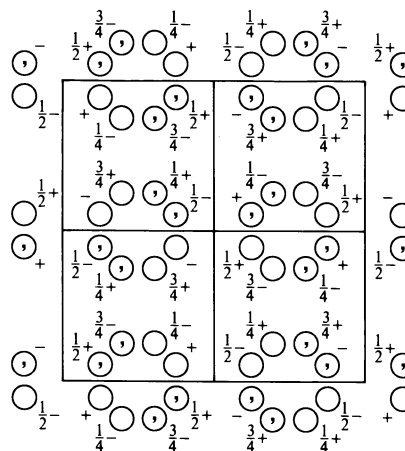
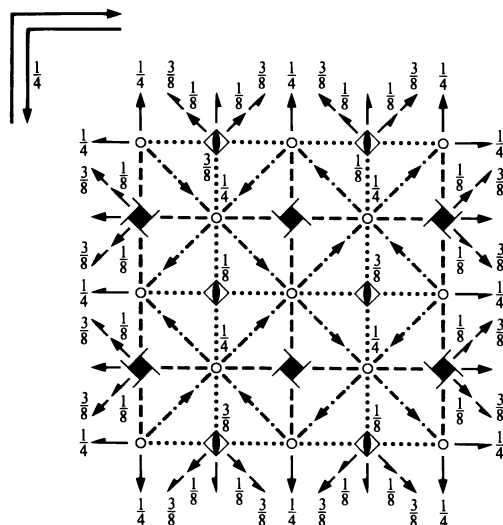
$I4_1/acd$  $D_{4h}^{20}$  $4/mmm$ 

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) $i(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$        | (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		Reflection conditions			
	$(0,0,0) + (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) +$		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  $x, x + \frac{1}{4}, \frac{1}{8}$ **Maximal non-isomorphic subgroups**

<b>I</b>	[2] $I\bar{4}2d$ (122)	(1; 2; 5; 6; 11; 12; 15; 16)+
	[2] $I\bar{4}c2$ (120)	(1; 2; 7; 8; 11; 12; 13; 14)+
	[2] $I4, cd$ (110)	(1; 2; 3; 4; 13; 14; 15; 16)+
	[2] $I4, 22$ (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] $I2/a2/c1$ ( $Ibca, 73$ )	(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]  $I4_1/acd$  ( $\mathbf{c}' = 3\mathbf{c}$ ) (142); [9]  $I4_1/acd$  ( $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$ ) (142)**Minimal non-isomorphic supergroups****I** [3]  $Fd\bar{3}c$  (228); [3]  $Ia\bar{3}d$  (230)**II** [2]  $C4_2/amd$  ( $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ ) ( $P4_2/nm, 134$ )