

$F d d d$

D_{2h}^{24}

$m m m$

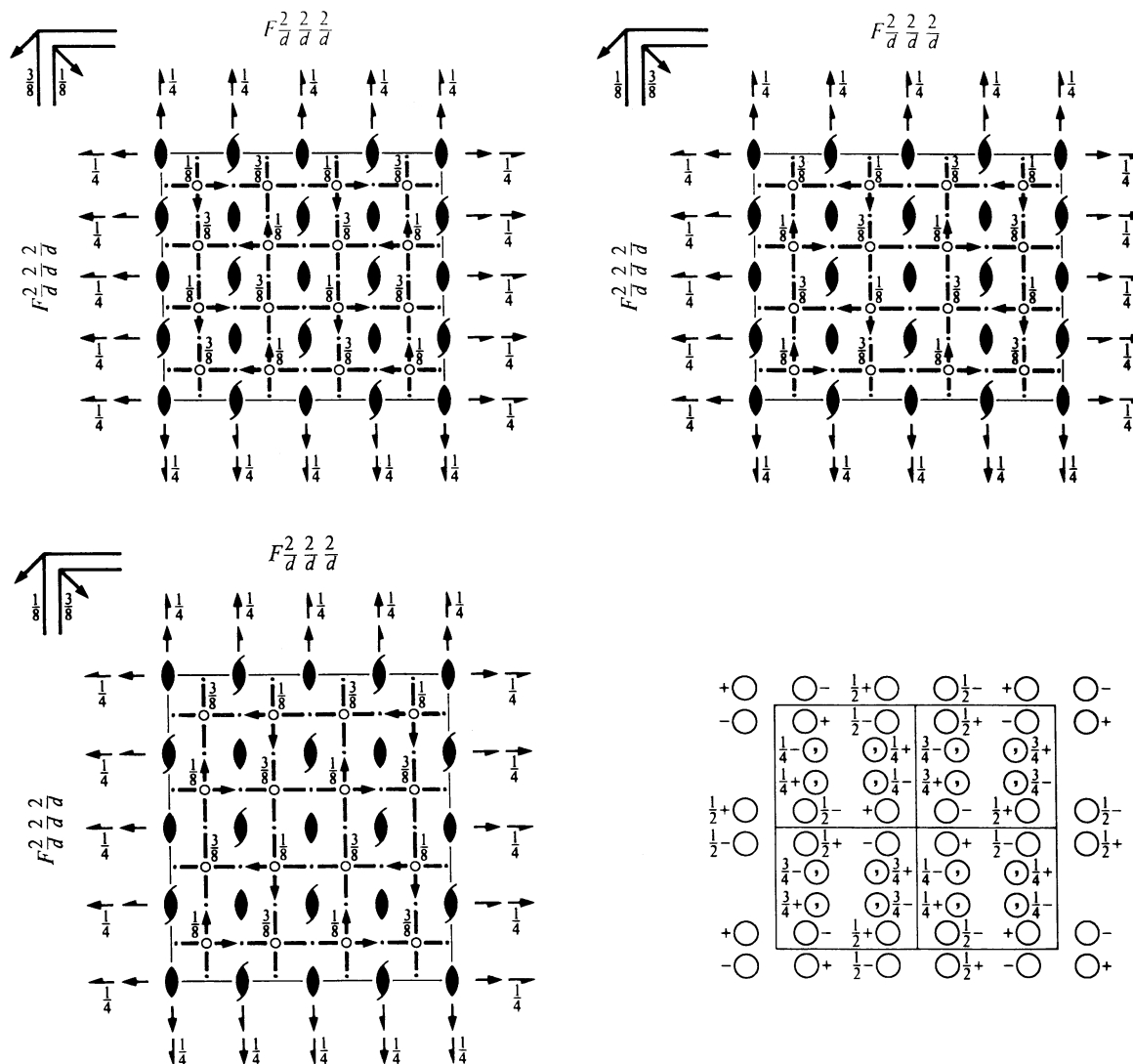
Orthorhombic

No. 70

$F 2/d 2/d 2/d$

Patterson symmetry $F m m m$

ORIGIN CHOICE 1



Origin at 222, at $-\frac{1}{8}, -\frac{1}{8}, -\frac{1}{8}$ from $\bar{1}$

Asymmetric unit $0 \leq x \leq \frac{1}{8}; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$

Symmetry operations

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

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

For $(0, \frac{1}{2}, \frac{1}{2})+$ set

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

For $(\frac{1}{2}, 0, \frac{1}{2})+$ set

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

For $(\frac{1}{2}, \frac{1}{2}, 0)+$ set

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

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

Positions

		Coordinates				Reflection conditions
Multiplicity,						
Wyckoff letter,						
Site symmetry		$(0,0,0)+$	$(0, \frac{1}{2}, \frac{1}{2})+$	$(\frac{1}{2}, 0, \frac{1}{2})+$	$(\frac{1}{2}, \frac{1}{2}, 0)+$	
32	<i>h</i> 1	(1) x, y, z (5) $\bar{x} + \frac{1}{4}, \bar{y} + \frac{1}{4}, \bar{z} + \frac{1}{4}$	(2) \bar{x}, \bar{y}, z (6) $x + \frac{1}{4}, y + \frac{1}{4}, \bar{z} + \frac{1}{4}$	(3) \bar{x}, y, \bar{z} (7) $x + \frac{1}{4}, \bar{y} + \frac{1}{4}, z + \frac{1}{4}$	(4) x, \bar{y}, \bar{z} (8) $\bar{x} + \frac{1}{4}, y + \frac{1}{4}, z + \frac{1}{4}$	General: hkl : $h+k=2n$ and $h+l, k+l=2n$ $0kl$: $k+l=4n$ and $k, l=2n$ $h0l$: $h+l=4n$ and $h, l=2n$ $hk0$: $h+k=4n$ and $h, k=2n$ $h00$: $h=4n$ $0k0$: $k=4n$ $00l$: $l=4n$ Special: as above, plus
16	<i>g</i> ..2	0,0, z	0,0, \bar{z}	$\frac{1}{4}, \frac{1}{4}, \bar{z} + \frac{1}{4}$	$\frac{1}{4}, \frac{1}{4}, z + \frac{1}{4}$	hkl : $h=2n+1$ or $h+k+l=4n$
16	<i>f</i> .2.	0, y ,0	0, \bar{y} ,0	$\frac{1}{4}, \bar{y} + \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, y + \frac{1}{4}, \frac{1}{4}$	
16	<i>e</i> 2..	x ,0,0	\bar{x} ,0,0	$\bar{x} + \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$x + \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	
16	<i>d</i> $\bar{1}$	$\frac{5}{8}, \frac{5}{8}, \frac{5}{8}$	$\frac{3}{8}, \frac{3}{8}, \frac{5}{8}$	$\frac{3}{8}, \frac{5}{8}, \frac{3}{8}$	$\frac{5}{8}, \frac{3}{8}, \frac{3}{8}$	hkl : $h=2n+1$ or $h, k, l=4n+2$ or $h, k, l=4n$
16	<i>c</i> $\bar{1}$	$\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$	$\frac{7}{8}, \frac{7}{8}, \frac{1}{8}$	$\frac{7}{8}, \frac{1}{8}, \frac{7}{8}$	$\frac{1}{8}, \frac{7}{8}, \frac{7}{8}$	
8	<i>b</i> 222	0,0, $\frac{1}{2}$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\left. \begin{array}{l} \\ \\ \end{array} \right\}$		hkl : $h=2n+1$ or $h+k+l=4n$
8	<i>a</i> 222	0,0,0	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$			

Symmetry of special projections

Along [001] $c2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
 Origin at 0,0, z

Along [100] $c2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
 Origin at $x, 0, 0$

Along [010] $c2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
 Origin at 0, $y, 0$

Maximal non-isomorphic subgroups

I	[2] $Fdd2$ (43)	(1; 2; 7; 8)+
	[2] $Fd2d$ ($Fdd2$, 43)	(1; 3; 6; 8)+
	[2] $F2dd$ ($Fdd2$, 43)	(1; 4; 6; 7)+
	[2] $F222$ (22)	(1; 2; 3; 4)+
	[2] $F112/d$ ($C2/c$, 15)	(1; 2; 5; 6)+
	[2] $F12/d1$ ($C2/c$, 15)	(1; 3; 5; 7)+
	[2] $F2/d11$ ($C2/c$, 15)	(1; 4; 5; 8)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $Fddd$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$ or $\mathbf{c}' = 3\mathbf{c}$) (70)

Minimal non-isomorphic supergroups

I [2] $I4_1/amd$ (141); [2] $I4_1/acd$ (142); [3] $Fd\bar{3}$ (203)

II [2] $Pnnn$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (48)

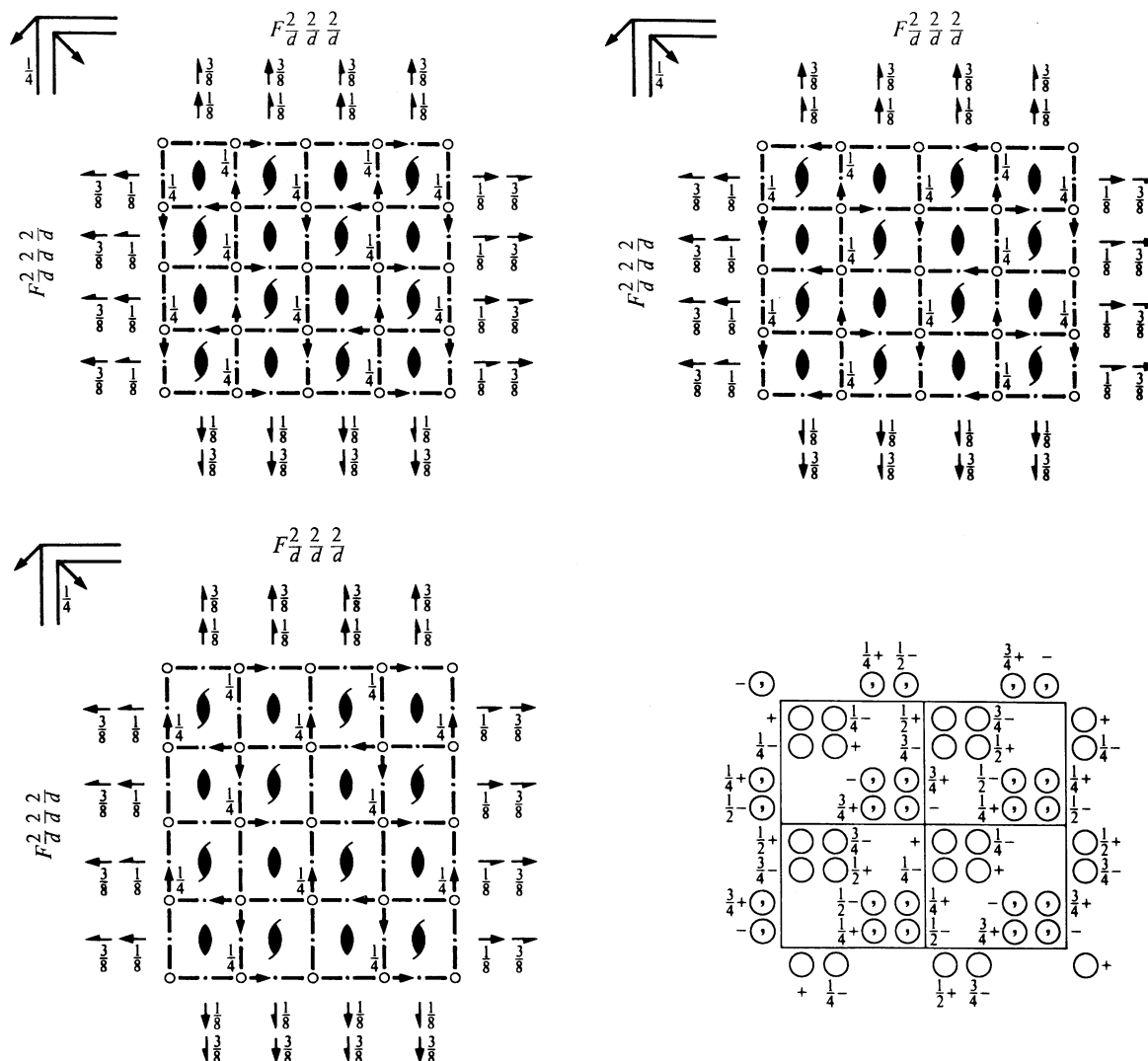
$F d d d$ D_{2h}^{24} $m m m$

Orthorhombic

No. 70

 $F 2/d 2/d 2/d$ Patterson symmetry $F m m m$

ORIGIN CHOICE 2

Origin at $\bar{1}$ at $d d d$, at $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ from 222 Asymmetric unit $0 \leq x \leq \frac{1}{8}; -\frac{1}{8} \leq y \leq \frac{1}{8}; 0 \leq z \leq 1$ **Symmetry operations**For $(0, 0, 0)+$ set

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

For $(0, \frac{1}{2}, \frac{1}{2})+$ set

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

For $(\frac{1}{2}, 0, \frac{1}{2})+$ set

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

For $(\frac{1}{2}, \frac{1}{2}, 0)+$ set

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

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

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

		(0,0,0)+	(0, $\frac{1}{2}$, $\frac{1}{2}$)+	($\frac{1}{2}$, 0, $\frac{1}{2}$)+	($\frac{1}{2}$, $\frac{1}{2}$, 0)+	
32	<i>h</i> 1	(1) x, y, z (5) $\bar{x}, \bar{y}, \bar{z}$	(2) $\bar{x} + \frac{3}{4}, \bar{y} + \frac{3}{4}, z$ (6) $x + \frac{1}{4}, y + \frac{1}{4}, \bar{z}$	(3) $\bar{x} + \frac{3}{4}, y, \bar{z} + \frac{3}{4}$ (7) $x + \frac{1}{4}, \bar{y}, z + \frac{1}{4}$	(4) $x, \bar{y} + \frac{3}{4}, \bar{z} + \frac{3}{4}$ (8) $\bar{x}, y + \frac{1}{4}, z + \frac{1}{4}$	<p>General:</p> <p>$hkl : h+k, h+l, k+l = 2n$ $Ok_l : k+l = 4n, k, l = 2n$ $h0l : h+l = 4n, h, l = 2n$ $hk0 : h+k = 4n, h, k = 2n$ $h00 : h = 4n$ $0k0 : k = 4n$ $00l : l = 4n$</p> <p>Special: as above, plus</p> <p>$hkl : h = 2n + 1$ or $h+k+l = 4n$</p> <p>$hkl : h = 2n + 1$ or $h, k, l = 4n + 2$ or $h, k, l = 4n$</p> <p>$hkl : h = 2n + 1$ or $h+k+l = 4n$</p>
16	<i>g</i> ..2	$\frac{1}{8}, \frac{1}{8}, z$	$\frac{5}{8}, \frac{1}{8}, \bar{z} + \frac{3}{4}$	$\frac{7}{8}, \frac{7}{8}, \bar{z}$	$\frac{3}{8}, \frac{7}{8}, z + \frac{1}{4}$	}
16	<i>f</i> .2.	$\frac{1}{8}, y, \frac{1}{8}$	$\frac{5}{8}, \bar{y} + \frac{3}{4}, \frac{1}{8}$	$\frac{7}{8}, \bar{y}, \frac{7}{8}$	$\frac{3}{8}, y + \frac{1}{4}, \frac{7}{8}$	
16	<i>e</i> 2..	$x, \frac{1}{8}, \frac{1}{8}$	$\bar{x} + \frac{3}{4}, \frac{5}{8}, \frac{1}{8}$	$\bar{x}, \frac{7}{8}, \frac{7}{8}$	$x + \frac{1}{4}, \frac{3}{8}, \frac{7}{8}$	
16	<i>d</i> $\bar{1}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$	$\frac{1}{4}, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{2}, \frac{1}{4}, \frac{1}{4}$	}
16	<i>c</i> $\bar{1}$	0,0,0	$\frac{3}{4}, \frac{3}{4}, 0$	$\frac{3}{4}, 0, \frac{3}{4}$	$0, \frac{3}{4}, \frac{3}{4}$	
8	<i>b</i> 222	$\frac{1}{8}, \frac{1}{8}, \frac{5}{8}$	$\frac{7}{8}, \frac{7}{8}, \frac{3}{8}$			}
8	<i>a</i> 222	$\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$	$\frac{7}{8}, \frac{7}{8}, \frac{7}{8}$			

Symmetry of special projections

Along [001] $c2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $\frac{1}{8}, \frac{1}{8}, z$

Along [100] $c2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x, \frac{1}{8}, \frac{1}{8}$

Along [010] $c2mm$
 $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $\frac{1}{8}, y, \frac{1}{8}$

Maximal non-isomorphic subgroups

I	[2] $Fddd(43)$	(1; 2; 7; 8)+
	[2] $Fd2d(Fdd2, 43)$	(1; 3; 6; 8)+
	[2] $F2dd(Fdd2, 43)$	(1; 4; 6; 7)+
	[2] $F222(22)$	(1; 2; 3; 4)+
	[2] $F112/d(C2/c, 15)$	(1; 2; 5; 6)+
	[2] $F12/d1(C2/c, 15)$	(1; 3; 5; 7)+
	[2] $F2/d11(C2/c, 15)$	(1; 4; 5; 8)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3] $Fddd(\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$ or $\mathbf{c}' = 3\mathbf{c})(70)$

Minimal non-isomorphic supergroups

I [2] $I4_1/amd(141)$; [2] $I4_1/acd(142)$; [3] $Fd\bar{3}(203)$

II [2] $Pnnn(\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c})(48)$