

$Fddd$

No. 70

 $F2/d2/d2/d$ D_{2h}^{24} ORIGIN CHOICE 1, Origin at 222, at $-\frac{1}{8}, -\frac{1}{8}, -\frac{1}{8}$ from $\bar{1}$ 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)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

	(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	h	1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) \bar{x}, y, \bar{z}	(4) x, \bar{y}, \bar{z}
			(5) $\bar{x} + \frac{1}{4}, \bar{y} + \frac{1}{4}, \bar{z} + \frac{1}{4}$	(6) $x + \frac{1}{4}, y + \frac{1}{4}, \bar{z} + \frac{1}{4}$	(7) $x + \frac{1}{4}, \bar{y} + \frac{1}{4}, z + \frac{1}{4}$	(8) $\bar{x} + \frac{1}{4}, y + \frac{1}{4}, z + \frac{1}{4}$

I Maximal *translationengleiche* subgroups

[2] $Fdd2$ (43)	(1; 2; 7; 8)+		
[2] $Fd2d$ (43, $Fdd2$)	(1; 3; 6; 8)+	c, a, b	
[2] $F2dd$ (43, $Fdd2$)	(1; 4; 6; 7)+	b, c, a	
[2] $F222$ (22)	(1; 2; 3; 4)+		
[2] $F112/d$ (15, $A112/a$)	(1; 2; 5; 6)+	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \mathbf{b}, \mathbf{c}$	$\frac{1}{8}, \frac{3}{8}, \frac{3}{8}$
[2] $F12/d1$ (15, $C12/c1$)	(1; 3; 5; 7)+	$-\mathbf{c}, \mathbf{b}, \frac{1}{2}(\mathbf{a}+\mathbf{c})$	$\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$
[2] $F2/d11$ (15, $C12/c1$)	(1; 4; 5; 8)+	$-\mathbf{b}, \mathbf{a}, \frac{1}{2}(\mathbf{b}+\mathbf{c})$	$\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$

II Maximal *klassengleiche* subgroups

• Loss of centring translations		none	
• Enlarged unit cell			
[3] $\mathbf{a}' = 3\mathbf{a}$			
$\left\{ \begin{array}{l} Fddd (70) \\ Fddd (70) \\ Fddd (70) \end{array} \right.$	$\langle 2 + (\frac{1}{2}, \frac{1}{2}, 0); 3 + (\frac{1}{2}, 0, \frac{1}{2}); 5 + (1, \frac{1}{2}, \frac{1}{2}) \rangle$	3a, b, c	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$
	$\langle 2 + (\frac{5}{2}, \frac{1}{2}, 0); 3 + (\frac{5}{2}, 0, \frac{1}{2}); 5 + (3, \frac{1}{2}, \frac{1}{2}) \rangle$	3a, b, c	$\frac{5}{4}, \frac{1}{4}, \frac{1}{4}$
	$\langle 2 + (\frac{9}{2}, \frac{1}{2}, 0); 3 + (\frac{9}{2}, 0, \frac{1}{2}); 5 + (5, \frac{1}{2}, \frac{1}{2}) \rangle$	3a, b, c	$\frac{9}{4}, \frac{1}{4}, \frac{1}{4}$
[3] $\mathbf{b}' = 3\mathbf{b}$			
$\left\{ \begin{array}{l} Fddd (70) \\ Fddd (70) \\ Fddd (70) \end{array} \right.$	$\langle 2 + (\frac{1}{2}, \frac{1}{2}, 0); 3 + (\frac{1}{2}, 0, \frac{1}{2}); 5 + (\frac{1}{2}, 1, \frac{1}{2}) \rangle$	a, 3b, c	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$
	$\langle 2 + (\frac{1}{2}, \frac{5}{2}, 0); 3 + (\frac{1}{2}, 0, \frac{1}{2}); 5 + (\frac{1}{2}, 3, \frac{1}{2}) \rangle$	a, 3b, c	$\frac{1}{4}, \frac{5}{4}, \frac{1}{4}$
	$\langle 2 + (\frac{1}{2}, \frac{9}{2}, 0); 3 + (\frac{1}{2}, 0, \frac{1}{2}); 5 + (\frac{1}{2}, 5, \frac{1}{2}) \rangle$	a, 3b, c	$\frac{1}{4}, \frac{9}{4}, \frac{1}{4}$
[3] $\mathbf{c}' = 3\mathbf{c}$			
$\left\{ \begin{array}{l} Fddd (70) \\ Fddd (70) \\ Fddd (70) \end{array} \right.$	$\langle 2 + (\frac{1}{2}, \frac{1}{2}, 0); 3 + (\frac{1}{2}, 0, \frac{1}{2}); 5 + (\frac{1}{2}, \frac{1}{2}, 1) \rangle$	a, b, 3c	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$
	$\langle 2 + (\frac{1}{2}, \frac{5}{2}, 0); 3 + (\frac{1}{2}, 0, \frac{5}{2}); 5 + (\frac{1}{2}, \frac{1}{2}, 3) \rangle$	a, b, 3c	$\frac{1}{4}, \frac{1}{4}, \frac{5}{4}$
	$\langle 2 + (\frac{1}{2}, \frac{9}{2}, 0); 3 + (\frac{1}{2}, 0, \frac{9}{2}); 5 + (\frac{1}{2}, \frac{1}{2}, 5) \rangle$	a, b, 3c	$\frac{1}{4}, \frac{1}{4}, \frac{9}{4}$
• Series of maximal isomorphic subgroups			
[p] $\mathbf{a}' = p\mathbf{a}$			
$Fddd (70)$	$\langle (2; 3) + (2u, 0, 0); 5 + (\frac{p}{4} - \frac{1}{4} + 2u, 0, 0) \rangle$	pa, b, c	$u, 0, 0$
	prime $p > 4$; $0 \leq u < p$		
	p conjugate subgroups for $p = 4n + 1$		
$Fddd (70)$	$\langle 2 + (\frac{1}{2} + 2u, \frac{1}{2}, 0); 3 + (\frac{1}{2} + 2u, 0, \frac{1}{2}); 5 + (\frac{p}{4} + \frac{1}{4} + 2u, \frac{1}{2}, \frac{1}{2}) \rangle$	pa, b, c	$\frac{1}{4} + u, \frac{1}{4}, \frac{1}{4}$
	prime $p > 2$; $0 \leq u < p$		
	p conjugate subgroups for $p = 4n - 1$		
[p] $\mathbf{b}' = p\mathbf{b}$			
$Fddd (70)$	$\langle 3; 2 + (0, 2u, 0); 5 + (0, \frac{p}{4} - \frac{1}{4} + 2u, 0) \rangle$	a, pb, c	$0, u, 0$
	prime $p > 4$; $0 \leq u < p$		
	p conjugate subgroups for $p = 4n + 1$		
$Fddd (70)$	$\langle 2 + (\frac{1}{2}, \frac{1}{2} + 2u, 0); 3 + (\frac{1}{2}, 0, \frac{1}{2}); 5 + (\frac{1}{2}, \frac{p}{4} + \frac{1}{4} + 2u, \frac{1}{2}) \rangle$	a, pb, c	$\frac{1}{4}, \frac{1}{4} + u, \frac{1}{4}$
	prime $p > 2$; $0 \leq u < p$		
	p conjugate subgroups for $p = 4n - 1$		
[p] $\mathbf{c}' = p\mathbf{c}$			
$Fddd (70)$	$\langle 2; 3 + (0, 0, 2u); 5 + (0, 0, \frac{p}{4} - \frac{1}{4} + 2u) \rangle$	a, b, pc	$0, 0, u$
	prime $p > 4$; $0 \leq u < p$		
	p conjugate subgroups for $p = 4n + 1$		
$Fddd (70)$	$\langle 2 + (\frac{1}{2}, \frac{1}{2}, 0); 3 + (\frac{1}{2}, 0, \frac{1}{2} + 2u); 5 + (\frac{1}{2}, \frac{1}{2}, \frac{p}{4} + \frac{1}{4} + 2u) \rangle$	a, b, pc	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4} + u$
	prime $p > 2$; $0 \leq u < p$		
	p conjugate subgroups for $p = 4n - 1$		

I Minimal *translationengleiche* supergroups[2] $I4_1/amd$ (141); [2] $I4_1/acd$ (142); [3] $Fd\bar{3}$ (203)**II Minimal non-isomorphic *klassengleiche* supergroups**

- Additional centring translations

none

- Decreased unit cell

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$, $\mathbf{b}' = \frac{1}{2}\mathbf{b}$, $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $Pnnn$ (48)*(Continued from the following page)***I Minimal *translationengleiche* supergroups**[2] $I4_1/amd$ (141); [2] $I4_1/acd$ (142); [3] $Fd\bar{3}$ (203)**II Minimal non-isomorphic *klassengleiche* supergroups**

- Additional centring translations

none

- Decreased unit cell

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

ORIGIN CHOICE 2, Origin at $\bar{1}$ at *ddd*, at $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ from 222

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)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

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

I Maximal translationengleiche subgroups

[2] <i>Fdd2</i> (43)	(1; 2; 7; 8)+		3/8, 3/8, 0
[2] <i>Fd2d</i> (43, <i>Fdd2</i>)	(1; 3; 6; 8)+	c, a, b	3/8, 0, 3/8
[2] <i>F2dd</i> (43, <i>Fdd2</i>)	(1; 4; 6; 7)+	b, c, a	0, 3/8, 3/8
[2] <i>F222</i> (22)	(1; 2; 3; 4)+		1/8, 1/8, 1/8
[2] <i>F112/d</i> (15, <i>A112/a</i>)	(1; 2; 5; 6)+	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \mathbf{b}, \mathbf{c}$	0, 1/4, 1/4
[2] <i>F12/d1</i> (15, <i>C12/c1</i>)	(1; 3; 5; 7)+	$-\mathbf{c}, \mathbf{b}, \frac{1}{2}(\mathbf{a}+\mathbf{c})$	
[2] <i>F2/d11</i> (15, <i>C12/c1</i>)	(1; 4; 5; 8)+	$-\mathbf{b}, \mathbf{a}, \frac{1}{2}(\mathbf{b}+\mathbf{c})$	

II Maximal klassengleiche subgroups

• **Loss of centring translations**

none

• **Enlarged unit cell**

[3] $\mathbf{a}' = 3\mathbf{a}$

$\left\{ \begin{array}{l} Fddd (70) \\ Fddd (70) \\ Fddd (70) \end{array} \right.$	$\langle 2 + (\frac{3}{2}, \frac{1}{2}, 0); 3 + (\frac{3}{2}, 0, \frac{1}{2}); 5 + (0, \frac{1}{2}, \frac{1}{2}) \rangle$	3a, b, c	0, 1/4, 1/4
	$\langle 2 + (\frac{7}{2}, \frac{1}{2}, 0); 3 + (\frac{7}{2}, 0, \frac{1}{2}); 5 + (2, \frac{1}{2}, \frac{1}{2}) \rangle$	3a, b, c	1, 1/4, 1/4
	$\langle 2 + (\frac{11}{2}, \frac{1}{2}, 0); 3 + (\frac{11}{2}, 0, \frac{1}{2}); 5 + (4, \frac{1}{2}, \frac{1}{2}) \rangle$	3a, b, c	2, 1/4, 1/4

[3] $\mathbf{b}' = 3\mathbf{b}$

$\left\{ \begin{array}{l} Fddd (70) \\ Fddd (70) \\ Fddd (70) \end{array} \right.$	$\langle 2 + (\frac{1}{2}, \frac{3}{2}, 0); (3; 5) + (\frac{1}{2}, 0, \frac{1}{2}) \rangle$	a, 3b, c	1/4, 0, 1/4
	$\langle 2 + (\frac{1}{2}, \frac{7}{2}, 0); 3 + (\frac{1}{2}, 0, \frac{1}{2}); 5 + (\frac{1}{2}, 2, \frac{1}{2}) \rangle$	a, 3b, c	1/4, 1, 1/4
	$\langle 2 + (\frac{1}{2}, \frac{11}{2}, 0); 3 + (\frac{1}{2}, 0, \frac{1}{2}); 5 + (\frac{1}{2}, 4, \frac{1}{2}) \rangle$	a, 3b, c	1/4, 2, 1/4

[3] $\mathbf{c}' = 3\mathbf{c}$

$\left\{ \begin{array}{l} Fddd (70) \\ Fddd (70) \\ Fddd (70) \end{array} \right.$	$\langle (2; 5) + (\frac{1}{2}, \frac{1}{2}, 0); 3 + (\frac{1}{2}, 0, \frac{3}{2}) \rangle$	a, b, 3c	1/4, 1/4, 0
	$\langle 2 + (\frac{1}{2}, \frac{1}{2}, 0); 3 + (\frac{1}{2}, 0, \frac{7}{2}); 5 + (\frac{1}{2}, \frac{1}{2}, 2) \rangle$	a, b, 3c	1/4, 1/4, 1
	$\langle 2 + (\frac{1}{2}, \frac{1}{2}, 0); 3 + (\frac{1}{2}, 0, \frac{11}{2}); 5 + (\frac{1}{2}, \frac{1}{2}, 4) \rangle$	a, b, 3c	1/4, 1/4, 2

• **Series of maximal isomorphic subgroups**

[*p*] $\mathbf{a}' = p\mathbf{a}$

<i>Fddd</i> (70)	$\langle (2; 3) + (\frac{3p}{4} - \frac{3}{4} + 2u, 0, 0); 5 + (2u, 0, 0) \rangle$ prime $p > 4$; $0 \leq u < p$ <i>p</i> conjugate subgroups for $p = 4n + 1$	pa, b, c	$u, 0, 0$
<i>Fddd</i> (70)	$\langle 2 + (\frac{3p}{4} - \frac{3}{4} + 2u, \frac{1}{2}, 0); 3 + (\frac{3p}{4} - \frac{3}{4} + 2u, 0, \frac{1}{2}); 5 + (2u, \frac{1}{2}, \frac{1}{2}) \rangle$ prime $p > 2$; $0 \leq u < p$ <i>p</i> conjugate subgroups for $p = 4n - 1$	pa, b, c	$u, 1/4, 1/4$

[*p*] $\mathbf{b}' = p\mathbf{b}$

<i>Fddd</i> (70)	$\langle 3; 2 + (0, \frac{3p}{4} - \frac{3}{4} + 2u, 0); 5 + (0, 2u, 0) \rangle$ prime $p > 4$; $0 \leq u < p$ <i>p</i> conjugate subgroups for $p = 4n + 1$	a, pb, c	$0, u, 0$
<i>Fddd</i> (70)	$\langle 2 + (\frac{1}{2}, \frac{3p}{4} - \frac{3}{4} + 2u, 0); 3 + (\frac{1}{2}, 0, \frac{1}{2}); 5 + (\frac{1}{2}, 2u, \frac{1}{2}) \rangle$ prime $p > 2$; $0 \leq u < p$ <i>p</i> conjugate subgroups for $p = 4n - 1$	a, pb, c	$1/4, u, 1/4$

[*p*] $\mathbf{c}' = p\mathbf{c}$

<i>Fddd</i> (70)	$\langle 2; 3 + (0, 0, \frac{3p}{4} - \frac{3}{4} + 2u); 5 + (0, 0, 2u) \rangle$ prime $p > 4$; $0 \leq u < p$ <i>p</i> conjugate subgroups for $p = 4n + 1$	a, b, pc	$0, 0, u$
<i>Fddd</i> (70)	$\langle 2 + (\frac{1}{2}, \frac{1}{2}, 0); 3 + (\frac{1}{2}, 0, \frac{3p}{4} - \frac{3}{4} + 2u); 5 + (\frac{1}{2}, \frac{1}{2}, 2u) \rangle$ prime $p > 2$; $0 \leq u < p$ <i>p</i> conjugate subgroups for $p = 4n - 1$	a, b, pc	$1/4, 1/4, u$

(Continued on the preceding page)

I Minimal *translationengleiche* supergroups[2] $I4_1/amd$ (141); [2] $I4_1/acd$ (142); [3] $Fd\bar{3}$ (203)**II Minimal non-isomorphic *klassengleiche* supergroups**

- Additional centring translations

none

- Decreased unit cell

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$, $\mathbf{b}' = \frac{1}{2}\mathbf{b}$, $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $Pnnn$ (48)*(Continued from the following page)***I Minimal *translationengleiche* supergroups**[2] $I4_1/amd$ (141); [2] $I4_1/acd$ (142); [3] $Fd\bar{3}$ (203)**II Minimal non-isomorphic *klassengleiche* supergroups**

- Additional centring translations

none

- Decreased unit cell

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