

$Fddd$ 

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)+ | <b>c, a, b</b>  |   |
| [2] $F2dd$ (43, $Fdd2$ )     | (1; 4; 6; 7)+ | <b>b, c, a</b>  |   |
| [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] $\mathbf{a}' = 3\mathbf{a}$  |  |                 |   |
| $\left\{ \begin{array}{l} Fddd (70) \\ Fddd (70) \\ Fddd (70) \end{array} \right.$ | $\langle 2 + (\frac{1}{2}, \frac{1}{2}, 0); 3 + (\frac{1}{2}, 0, \frac{1}{2}); 5 + (1, \frac{1}{2}, \frac{1}{2}) \rangle$  | <b>3a, b, c</b> | $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$     |
|  | $\langle 2 + (\frac{5}{2}, \frac{1}{2}, 0); 3 + (\frac{5}{2}, 0, \frac{1}{2}); 5 + (3, \frac{1}{2}, \frac{1}{2}) \rangle$  | <b>3a, b, c</b> | $\frac{5}{4}, \frac{1}{4}, \frac{1}{4}$     |
|  | $\langle 2 + (\frac{9}{2}, \frac{1}{2}, 0); 3 + (\frac{9}{2}, 0, \frac{1}{2}); 5 + (5, \frac{1}{2}, \frac{1}{2}) \rangle$  | <b>3a, b, c</b> | $\frac{9}{4}, \frac{1}{4}, \frac{1}{4}$     |
| [3] $\mathbf{b}' = 3\mathbf{b}$  |  |                 |   |
| $\left\{ \begin{array}{l} Fddd (70) \\ Fddd (70) \\ Fddd (70) \end{array} \right.$ | $\langle 2 + (\frac{1}{2}, \frac{1}{2}, 0); 3 + (\frac{1}{2}, 0, \frac{1}{2}); 5 + (\frac{1}{2}, 1, \frac{1}{2}) \rangle$  | <b>a, 3b, c</b> | $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$     |
|  | $\langle 2 + (\frac{1}{2}, \frac{5}{2}, 0); 3 + (\frac{1}{2}, 0, \frac{1}{2}); 5 + (\frac{1}{2}, 3, \frac{1}{2}) \rangle$  | <b>a, 3b, c</b> | $\frac{1}{4}, \frac{5}{4}, \frac{1}{4}$     |
|  | $\langle 2 + (\frac{1}{2}, \frac{9}{2}, 0); 3 + (\frac{1}{2}, 0, \frac{1}{2}); 5 + (\frac{1}{2}, 5, \frac{1}{2}) \rangle$  | <b>a, 3b, c</b> | $\frac{1}{4}, \frac{9}{4}, \frac{1}{4}$     |
| [3] $\mathbf{c}' = 3\mathbf{c}$  |  |                 |   |
| $\left\{ \begin{array}{l} Fddd (70) \\ Fddd (70) \\ Fddd (70) \end{array} \right.$ | $\langle 2 + (\frac{1}{2}, \frac{1}{2}, 0); 3 + (\frac{1}{2}, 0, \frac{1}{2}); 5 + (\frac{1}{2}, \frac{1}{2}, 1) \rangle$  | <b>a, b, 3c</b> | $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$     |
|  | $\langle 2 + (\frac{1}{2}, \frac{1}{2}, 0); 3 + (\frac{1}{2}, 0, \frac{5}{2}); 5 + (\frac{1}{2}, \frac{1}{2}, 3) \rangle$  | <b>a, b, 3c</b> | $\frac{1}{4}, \frac{1}{4}, \frac{5}{4}$     |
|  | $\langle 2 + (\frac{1}{2}, \frac{1}{2}, 0); 3 + (\frac{1}{2}, 0, \frac{9}{2}); 5 + (\frac{1}{2}, \frac{1}{2}, 5) \rangle$  | <b>a, b, 3c</b> | $\frac{1}{4}, \frac{1}{4}, \frac{9}{4}$     |
| • Series of maximal isomorphic subgroups   |  |                 |   |
| [p] $\mathbf{a}' = p\mathbf{a}$  |  |                 |   |
| $Fddd (70)$  | $\langle 2 + (\frac{1}{2} + 2u, \frac{1}{2}, 0); 3 + (\frac{1}{2} + 2u, 0, \frac{1}{2}); 5 + (\frac{p}{4} + \frac{1}{4} + 2u, \frac{1}{2}, \frac{1}{2}) \rangle$<br>$p > 2; 0 \leq u < p$<br>$p$ conjugate subgroups for prime $p \equiv 3 \pmod{4}$ | <b>pa, b, c</b> | $\frac{1}{4} + u, \frac{1}{4}, \frac{1}{4}$ |
| $Fddd (70)$  | $\langle (2; 3) + (2u, 0, 0); 5 + (\frac{p}{4} - \frac{1}{4} + 2u, 0, 0) \rangle$<br>$p > 4; 0 \leq u < p$<br>$p$ conjugate subgroups for prime $p \equiv 1 \pmod{4}$  | <b>pa, b, c</b> | $u, 0, 0$                                   |
| [p] $\mathbf{b}' = p\mathbf{b}$  |  |                 |   |
| $Fddd (70)$  | $\langle 2 + (\frac{1}{2}, \frac{1}{2} + 2u, 0); 3 + (\frac{1}{2}, 0, \frac{1}{2}); 5 + (\frac{1}{2}, \frac{p}{4} + \frac{1}{4} + 2u, \frac{1}{2}) \rangle$<br>$p > 2; 0 \leq u < p$<br>$p$ conjugate subgroups for prime $p \equiv 3 \pmod{4}$      | <b>a, pb, c</b> | $\frac{1}{4}, \frac{1}{4} + u, \frac{1}{4}$ |
| $Fddd (70)$  | $\langle (3; 2 + (0, 2u, 0)); 5 + (0, \frac{p}{4} - \frac{1}{4} + 2u, 0) \rangle$<br>$p > 4; 0 \leq u < p$<br>$p$ conjugate subgroups for prime $p \equiv 1 \pmod{4}$  | <b>a, pb, c</b> | $0, u, 0$                                   |
| [p] $\mathbf{c}' = p\mathbf{c}$  |  |                 |   |
| $Fddd (70)$  | $\langle 2 + (\frac{1}{2}, \frac{1}{2}, 0); 3 + (\frac{1}{2}, 0, \frac{1}{2} + 2u); 5 + (\frac{1}{2}, \frac{1}{2}, \frac{p}{4} + \frac{1}{4} + 2u) \rangle$<br>$p > 2; 0 \leq u < p$<br>$p$ conjugate subgroups for prime $p \equiv 3 \pmod{4}$      | <b>a, b, pc</b> | $\frac{1}{4}, \frac{1}{4}, \frac{1}{4} + u$ |
| $Fddd (70)$  | $\langle (2; 3 + (0, 0, 2u)); 5 + (0, 0, \frac{p}{4} - \frac{1}{4} + 2u) \rangle$<br>$p > 4; 0 \leq u < p$<br>$p$ conjugate subgroups for prime $p \equiv 1 \pmod{4}$  | <b>a, b, pc</b> | $0, 0, u$                                   |

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

II Maximal *klassengleiche* subgroups

• Loss of centring translations

none

• Enlarged unit cell

|  |   |                 |             |
|--|---|-----------------|-------------|
| [3] $\mathbf{a}' = 3\mathbf{a}$  |   |                 |             |
| $\left\{ \begin{array}{l} Fddd (70) \\ Fddd (70) \\ Fddd (70) \end{array} \right.$ | $\langle 2 + (\frac{3}{2}, \frac{1}{2}, 0); 3 + (\frac{3}{2}, 0, \frac{1}{2}); 5 + (0, \frac{1}{2}, \frac{1}{2}) \rangle$   | <b>3a, b, c</b> | 0, 1/4, 1/4 |
|  | $\langle 2 + (\frac{7}{2}, \frac{1}{2}, 0); 3 + (\frac{7}{2}, 0, \frac{1}{2}); 5 + (2, \frac{1}{2}, \frac{1}{2}) \rangle$   | <b>3a, b, c</b> | 1, 1/4, 1/4 |
|  | $\langle 2 + (\frac{11}{2}, \frac{1}{2}, 0); 3 + (\frac{11}{2}, 0, \frac{1}{2}); 5 + (4, \frac{1}{2}, \frac{1}{2}) \rangle$ | <b>3a, b, c</b> | 2, 1/4, 1/4 |
| [3] $\mathbf{b}' = 3\mathbf{b}$  |   |                 |             |
| $\left\{ \begin{array}{l} Fddd (70) \\ Fddd (70) \\ Fddd (70) \end{array} \right.$ | $\langle 2 + (\frac{1}{2}, \frac{3}{2}, 0); (3; 5) + (\frac{1}{2}, 0, \frac{1}{2}) \rangle$                                 | <b>a, 3b, c</b> | 1/4, 0, 1/4 |
|  | $\langle 2 + (\frac{1}{2}, \frac{7}{2}, 0); 3 + (\frac{1}{2}, 0, \frac{1}{2}); 5 + (\frac{1}{2}, 2, \frac{1}{2}) \rangle$   | <b>a, 3b, c</b> | 1/4, 1, 1/4 |
|  | $\langle 2 + (\frac{1}{2}, \frac{11}{2}, 0); 3 + (\frac{1}{2}, 0, \frac{1}{2}); 5 + (\frac{1}{2}, 4, \frac{1}{2}) \rangle$  | <b>a, 3b, c</b> | 1/4, 2, 1/4 |
| [3] $\mathbf{c}' = 3\mathbf{c}$  |   |                 |             |
| $\left\{ \begin{array}{l} Fddd (70) \\ Fddd (70) \\ Fddd (70) \end{array} \right.$ | $\langle (2; 5) + (\frac{1}{2}, \frac{1}{2}, 0); 3 + (\frac{1}{2}, 0, \frac{3}{2}) \rangle$                                 | <b>a, b, 3c</b> | 1/4, 1/4, 0 |
|  | $\langle 2 + (\frac{1}{2}, \frac{1}{2}, 0); 3 + (\frac{1}{2}, 0, \frac{7}{2}); 5 + (\frac{1}{2}, \frac{1}{2}, 2) \rangle$   | <b>a, b, 3c</b> | 1/4, 1/4, 1 |
|  | $\langle 2 + (\frac{1}{2}, \frac{1}{2}, 0); 3 + (\frac{1}{2}, 0, \frac{11}{2}); 5 + (\frac{1}{2}, \frac{1}{2}, 4) \rangle$  | <b>a, b, 3c</b> | 1/4, 1/4, 2 |

• Series of maximal isomorphic subgroups

|  |  |                 |               |
|--|--|-----------------|---------------|
| [ <i>p</i> ] $\mathbf{a}' = p\mathbf{a}$ |  |                 |               |
| <i>Fddd</i> (70)                         | $\langle 2 + (\frac{3p}{4} - \frac{3}{4} + 2u, \frac{1}{2}, 0); 3 + (\frac{3p}{4} - \frac{3}{4} + 2u, 0, \frac{1}{2}); 5 + (2u, \frac{1}{2}, \frac{1}{2}) \rangle$ | <b>pa, b, c</b> | $u, 1/4, 1/4$ |
|  | $p > 2; 0 \leq u < p$  |                 |               |
|  | $p$ conjugate subgroups for prime $p \equiv 3 \pmod{4}$  |                 |               |
| <i>Fddd</i> (70)                         | $\langle (2; 3) + (\frac{3p}{4} - \frac{3}{4} + 2u, 0, 0); 5 + (2u, 0, 0) \rangle$   | <b>pa, b, c</b> | $u, 0, 0$     |
|  | $p > 4; 0 \leq u < p$  |                 |               |
|  | $p$ conjugate subgroups for prime $p \equiv 1 \pmod{4}$  |                 |               |
| [ <i>p</i> ] $\mathbf{b}' = p\mathbf{b}$ |  |                 |               |
| <i>Fddd</i> (70)                         | $\langle 2 + (\frac{1}{2}, \frac{3p}{4} - \frac{3}{4} + 2u, 0); 3 + (\frac{1}{2}, 0, \frac{1}{2}); 5 + (\frac{1}{2}, 2u, \frac{1}{2}) \rangle$                     | <b>a, pb, c</b> | $1/4, u, 1/4$ |
|  | $p > 2; 0 \leq u < p$  |                 |               |
|  | $p$ conjugate subgroups for prime $p \equiv 3 \pmod{4}$  |                 |               |
| <i>Fddd</i> (70)                         | $\langle 3; 2 + (0, \frac{3p}{4} - \frac{3}{4} + 2u, 0); 5 + (0, 2u, 0) \rangle$   | <b>a, pb, c</b> | $0, u, 0$     |
|  | $p > 4; 0 \leq u < p$  |                 |               |
|  | $p$ conjugate subgroups for prime $p \equiv 1 \pmod{4}$  |                 |               |
| [ <i>p</i> ] $\mathbf{c}' = p\mathbf{c}$ |  |                 |               |
| <i>Fddd</i> (70)                         | $\langle 2 + (\frac{1}{2}, \frac{1}{2}, 0); 3 + (\frac{1}{2}, 0, \frac{3p}{4} - \frac{3}{4} + 2u); 5 + (\frac{1}{2}, \frac{1}{2}, 2u) \rangle$                     | <b>a, b, pc</b> | $1/4, 1/4, u$ |
|  | $p > 2; 0 \leq u < p$  |                 |               |
|  | $p$ conjugate subgroups for prime $p \equiv 3 \pmod{4}$  |                 |               |
| <i>Fddd</i> (70)                         | $\langle 2; 3 + (0, 0, \frac{3p}{4} - \frac{3}{4} + 2u); 5 + (0, 0, 2u) \rangle$   | <b>a, b, pc</b> | $0, 0, u$     |
|  | $p > 4; 0 \leq u < p$  |                 |               |
|  | $p$ conjugate subgroups for prime $p \equiv 1 \pmod{4}$  |                 |               |

(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)