O_h^7 $\qquad$ $F\,4_1/d\,\bar{3}\,2/m$ $\qquad$ No. 227 $\qquad$ $F\,d\,\bar{3}\,m$

ORIGIN CHOICE 1, Origin at $\bar{4}3m$, at $-\frac{1}{8}, -\frac{1}{8}, -\frac{1}{8}$ from centre $(\bar{3}m)$

Generators selected $\quad$ (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); (13); (25)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

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

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(1) x,y,z $\qquad$ (2) $\bar{x},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ $\qquad$ (3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$ $\qquad$ (4) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$

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

(9) y,z,x $\qquad$ (10) $\bar{y}+\frac{1}{2},z+\frac{1}{2},\bar{x}$ $\qquad$ (11) $y+\frac{1}{2},\bar{z},\bar{x}+\frac{1}{2}$ $\qquad$ (12) $\bar{y},\bar{z}+\frac{1}{2},x+\frac{1}{2}$

(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{3}{4}$ $\quad$ (14) $\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4}$ $\quad$ (15) $y+\frac{1}{4},\bar{x}+\frac{3}{4},z+\frac{3}{4}$ $\quad$ (16) $\bar{y}+\frac{3}{4},x+\frac{3}{4},z+\frac{1}{4}$

(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}+\frac{3}{4}$ $\quad$ (18) $\bar{x}+\frac{3}{4},z+\frac{3}{4},y+\frac{1}{4}$ $\quad$ (19) $\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4},\bar{y}+\frac{1}{4}$ $\quad$ (20) $x+\frac{1}{4},\bar{z}+\frac{3}{4},y+\frac{3}{4}$

(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}+\frac{3}{4}$ $\quad$ (22) $z+\frac{1}{4},\bar{y}+\frac{3}{4},x+\frac{3}{4}$ $\quad$ (23) $\bar{z}+\frac{3}{4},y+\frac{3}{4},x+\frac{1}{4}$ $\quad$ (24) $\bar{z}+\frac{1}{4},\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4}$

(25) $\bar{x}+\frac{1}{4},\bar{y}+\frac{1}{4},\bar{z}+\frac{1}{4}$ $\quad$ (26) $x+\frac{1}{4},y+\frac{3}{4},\bar{z}+\frac{3}{4}$ $\quad$ (27) $x+\frac{3}{4},\bar{y}+\frac{3}{4},z+\frac{1}{4}$ $\quad$ (28) $\bar{x}+\frac{3}{4},y+\frac{1}{4},z+\frac{3}{4}$

(29) $\bar{z}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{y}+\frac{1}{4}$ $\quad$ (30) $\bar{z}+\frac{3}{4},x+\frac{1}{4},y+\frac{3}{4}$ $\quad$ (31) $z+\frac{1}{4},x+\frac{3}{4},\bar{y}+\frac{3}{4}$ $\quad$ (32) $z+\frac{3}{4},\bar{x}+\frac{3}{4},y+\frac{1}{4}$

(33) $\bar{y}+\frac{1}{4},\bar{z}+\frac{1}{4},\bar{x}+\frac{1}{4}$ $\quad$ (34) $y+\frac{3}{4},\bar{z}+\frac{3}{4},x+\frac{1}{4}$ $\quad$ (35) $\bar{y}+\frac{3}{4},z+\frac{1}{4},x+\frac{3}{4}$ $\quad$ (36) $y+\frac{1}{4},z+\frac{3}{4},\bar{x}+\frac{3}{4}$

(37) $\bar{y}+\frac{1}{2},\bar{x},z+\frac{1}{2}$ $\qquad$ (38) y,x,z $\qquad$ (39) $\bar{y},x+\frac{1}{2},\bar{z}+\frac{1}{2}$ $\qquad$ (40) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$

(41) $\bar{x}+\frac{1}{2},\bar{z},y+\frac{1}{2}$ $\qquad$ (42) $x+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}$ $\qquad$ (43) x,z,y $\qquad$ (44) $\bar{x},z+\frac{1}{2},\bar{y}+\frac{1}{2}$

(45) $\bar{z}+\frac{1}{2},\bar{y},x+\frac{1}{2}$ $\qquad$ (46) $\bar{z},y+\frac{1}{2},\bar{x}+\frac{1}{2}$ $\qquad$ (47) $z+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}$ $\qquad$ (48) z,y,x

I Maximal *translationengleiche* subgroups

[2] $F\bar{4}3m$ (216) $\qquad$ (1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48)+

[2] $F4_132$ (210) $\qquad$ (1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24)+

[2] $Fd\bar{3}1$ (203, $Fd\bar{3}$) $\qquad$ (1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36)+

$\left\{\begin{array}{l}\end{array}\right.$ [3] $F4_1/d12/m$ (141, $I4_1/amd$) $\quad$ (1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40)+ $\qquad$ $1/2(\mathbf{a}-\mathbf{b}), 1/2(\mathbf{a}+\mathbf{b}), \mathbf{c}$

[3] $F4_1/d12/m$ (141, $I4_1/amd$) $\quad$ (1; 4; 2; 3; 18; 19; 17; 20; 25; 28; 26; 27; 42; 43; 41; 44)+ $\qquad$ $1/2(\mathbf{b}-\mathbf{c}), 1/2(\mathbf{b}+\mathbf{c}), \mathbf{a}$

[3] $F4_1/d12/m$ (141, $I4_1/amd$) $\quad$ (1; 3; 4; 2; 22; 24; 23; 21; 25; 27; 28; 26; 46; 48; 47; 45)+ $\qquad$ $1/2(-\mathbf{a}+\mathbf{c}), 1/2(\mathbf{a}+\mathbf{c}), \mathbf{b}$

$\left\{\begin{array}{l}\end{array}\right.$ [4] $F1\bar{3}2/m$ (166, $R\bar{3}m$) $\quad$ (1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48)+ $\qquad$ $1/2(-\mathbf{a}+\mathbf{b}), 1/2(-\mathbf{b}+\mathbf{c}), \mathbf{a}+\mathbf{b}+\mathbf{c}$
$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ $1/8,1/8,1/8$

[4] $F1\bar{3}2/m$ (166, $R\bar{3}m$) $\quad$ (1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48)+ $\qquad$ $1/2(\mathbf{a}+\mathbf{b}), 1/2(-\mathbf{b}-\mathbf{c}), -\mathbf{a}+\mathbf{b}-\mathbf{c}$
$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ $3/8,1/8,3/8$

[4] $F1\bar{3}2/m$ (166, $R\bar{3}m$) $\quad$ (1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46)+ $\qquad$ $1/2(-\mathbf{a}-\mathbf{b}), 1/2(\mathbf{b}-\mathbf{c}), \mathbf{a}-\mathbf{b}-\mathbf{c}$
$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ $1/8,3/8,3/8$

[4] $F1\bar{3}2/m$ (166, $R\bar{3}m$) $\quad$ (1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46)+ $\qquad$ $1/2(\mathbf{a}-\mathbf{b}), 1/2(\mathbf{b}+\mathbf{c}), -\mathbf{a}-\mathbf{b}+\mathbf{c}$
$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ $3/8,3/8,1/8$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** $\qquad\qquad\qquad\qquad\qquad\qquad$ none

- **Enlarged unit cell** $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ none

● **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}' = p\mathbf{a}$, $\mathbf{b}' = p\mathbf{b}$, $\mathbf{c}' = p\mathbf{c}$

$F d\bar{3} m$ (227)	$\langle 2 + (\frac{1}{2} + 2u, \frac{p}{2} + 2v, \frac{p}{2} - \frac{1}{2});$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$	u, v, w
	$3 + (\frac{p}{2} + 2u, \frac{p}{2} - \frac{1}{2}, \frac{1}{2} + 2w);$		
	$5 + (u - w, -u + v, -v + w);$		
	$13 + (\frac{3p}{4} - \frac{3}{4} + u - v, \frac{p}{4} - \frac{1}{4} - u + v, \frac{3p}{4} - \frac{1}{4} + 2w);$		
	$25 + (\frac{p}{4} + \frac{1}{4} + 2u, \frac{p}{4} + \frac{1}{4} + 2v, \frac{p}{4} + \frac{1}{4} + 2w)\rangle$		
	$p > 2$; $0 \leq u < p$; $0 \leq v < p$; $0 \leq w < p$		
	p^3 conjugate subgroups for prime $p \equiv 3 \pmod 4$		
$F d\bar{3} m$ (227)	$\langle 2 + (2u, \frac{p}{2} - \frac{1}{2} + 2v, \frac{p}{2} - \frac{1}{2});$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$	u, v, w
	$3 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2}, 2w);$		
	$5 + (u - w, -u + v, -v + w);$		
	$13 + (\frac{3p}{4} - \frac{3}{4} + u - v, \frac{p}{4} - \frac{1}{4} - u + v, \frac{3p}{4} - \frac{3}{4} + 2w);$		
	$25 + (\frac{p}{4} - \frac{1}{4} + 2u, \frac{p}{4} - \frac{1}{4} + 2v, \frac{p}{4} - \frac{1}{4} + 2w)\rangle$		
	$p > 4$; $0 \leq u < p$; $0 \leq v < p$; $0 \leq w < p$		
	p^3 conjugate subgroups for prime $p \equiv 1 \pmod 4$		

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

● **Additional centring translations** none

● **Decreased unit cell**

$[2]$ $\mathbf{a}' = \frac{1}{2}\mathbf{a}$, $\mathbf{b}' = \frac{1}{2}\mathbf{b}$, $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $Pn\bar{3}m$ (224)

● **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}' = p\mathbf{a}$, $\mathbf{b}' = p\mathbf{b}$, $\mathbf{c}' = p\mathbf{c}$

$F d\bar{3} m$ (227)	$\langle 2 + (\frac{3p}{4} - \frac{3}{4} + 2u, \frac{p}{4} - \frac{1}{4} + 2v, \frac{p}{2} - \frac{1}{2});$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$	u, v, w
	$3 + (\frac{p}{4} - \frac{1}{4} + 2u, \frac{p}{2} - \frac{1}{2}, \frac{3p}{4} - \frac{3}{4} + 2w);$		
	$5 + (u - w, -u + v, -v + w);$		
	$13 + (\frac{3p}{4} - \frac{3}{4} + u - v, \frac{p}{4} - \frac{1}{4} - u + v, \frac{p}{2} - \frac{1}{2} + 2w);$		
	$25 + (2u, 2v, 2w)\rangle$		
	$p > 2$; $0 \leq u < p$; $0 \leq v < p$; $0 \leq w < p$		
	p^3 conjugate subgroups for the prime p		

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

● **Additional centring translations** none

● **Decreased unit cell**

$[2]$ $\mathbf{a}' = \frac{1}{2}\mathbf{a}$, $\mathbf{b}' = \frac{1}{2}\mathbf{b}$, $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $Pn\bar{3}m$ (224)