

$Fd\bar{3}$

No. 203

$F2/d\bar{3}$

T_h^4

ORIGIN CHOICE 1, Origin at 23, at $-\frac{1}{8}, -\frac{1}{8}, -\frac{1}{8}$ from centre ($\bar{3}$)

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); (13)

General position

Multiplicity,	Coordinates			
Wyckoff letter,				
Site symmetry	(0, 0, 0)+	(0, $\frac{1}{2}, \frac{1}{2}$)+	($\frac{1}{2}, 0, \frac{1}{2}$)+	($\frac{1}{2}, \frac{1}{2}, 0$)+
96 g 1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) \bar{x}, y, \bar{z}	(4) x, \bar{y}, \bar{z}
	(5) z, x, y	(6) z, \bar{x}, \bar{y}	(7) \bar{z}, \bar{x}, y	(8) \bar{z}, x, \bar{y}
	(9) y, z, x	(10) \bar{y}, z, \bar{x}	(11) y, \bar{z}, \bar{x}	(12) \bar{y}, \bar{z}, x
	(13) $\bar{x} + \frac{1}{4}, \bar{y} + \frac{1}{4}, \bar{z} + \frac{1}{4}$	(14) $x + \frac{1}{4}, y + \frac{1}{4}, \bar{z} + \frac{1}{4}$	(15) $x + \frac{1}{4}, \bar{y} + \frac{1}{4}, z + \frac{1}{4}$	(16) $\bar{x} + \frac{1}{4}, y + \frac{1}{4}, z + \frac{1}{4}$
	(17) $\bar{z} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{y} + \frac{1}{4}$	(18) $\bar{z} + \frac{1}{4}, x + \frac{1}{4}, y + \frac{1}{4}$	(19) $z + \frac{1}{4}, x + \frac{1}{4}, \bar{y} + \frac{1}{4}$	(20) $z + \frac{1}{4}, \bar{x} + \frac{1}{4}, y + \frac{1}{4}$
	(21) $\bar{y} + \frac{1}{4}, \bar{z} + \frac{1}{4}, \bar{x} + \frac{1}{4}$	(22) $y + \frac{1}{4}, \bar{z} + \frac{1}{4}, x + \frac{1}{4}$	(23) $\bar{y} + \frac{1}{4}, z + \frac{1}{4}, x + \frac{1}{4}$	(24) $y + \frac{1}{4}, z + \frac{1}{4}, \bar{x} + \frac{1}{4}$

I Maximal translationengleiche subgroups

[2] $F2\bar{3}$ (196)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+		
[3] $Fd1$ (70, $Fddd$)	(1; 2; 3; 4; 13; 14; 15; 16)+		
{	[4] $F1\bar{3}$ (148, $R\bar{3}$)	(1; 5; 9; 13; 17; 21)+	$1/2(-\mathbf{a} + \mathbf{b}), 1/2(-\mathbf{b} + \mathbf{c}), \mathbf{a} + \mathbf{b} + \mathbf{c}$ 1/8, 1/8, 1/8
	[4] $F1\bar{3}$ (148, $R\bar{3}$)	(1; 6; 12; 13; 18; 24)+	$1/2(\mathbf{a} + \mathbf{b}), 1/2(-\mathbf{b} - \mathbf{c}), -\mathbf{a} + \mathbf{b} - \mathbf{c}$ 3/8, 1/8, 3/8
	[4] $F1\bar{3}$ (148, $R\bar{3}$)	(1; 7; 10; 13; 19; 22)+	$1/2(-\mathbf{a} - \mathbf{b}), 1/2(\mathbf{b} - \mathbf{c}), \mathbf{a} - \mathbf{b} - \mathbf{c}$ 1/8, 3/8, 3/8
	[4] $F1\bar{3}$ (148, $R\bar{3}$)	(1; 8; 11; 13; 20; 23)+	$1/2(\mathbf{a} - \mathbf{b}), 1/2(\mathbf{b} + \mathbf{c}), -\mathbf{a} - \mathbf{b} + \mathbf{c}$ 3/8, 3/8, 1/8

II Maximal klassengleiche subgroups

• Loss of centring translations	none	
• Enlarged unit cell	none	
• Series of maximal isomorphic subgroups		
$[p^3] \mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}, \mathbf{c}' = p\mathbf{c}$		
$Fd\bar{3}$ (203)	$\langle 2 + (\frac{1}{2} + 2u, \frac{1}{2} + 2v, 0); 3 + (\frac{1}{2} + 2u, 0, \frac{1}{2} + 2w); 5 + (u - w, -u + v, -v + w); 13 + (\frac{p}{4} + \frac{1}{4} + 2u, \frac{p}{4} + \frac{1}{4} + 2v, \frac{p}{4} + \frac{1}{4} + 2w) \rangle$ $p > 2; 0 \leq u < p; 0 \leq v < p; 0 \leq w < p$ p^3 conjugate subgroups for prime $p \equiv 3 \pmod{4}$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$ 1/4 + u, 1/4 + v, 1/4 + w
$Fd\bar{3}$ (203)	$\langle 2 + (2u, 2v, 0); 3 + (2u, 0, 2w); 5 + (u - w, -u + v, -v + w); 13 + (\frac{p}{4} - \frac{1}{4} + 2u, \frac{p}{4} - \frac{1}{4} + 2v, \frac{p}{4} - \frac{1}{4} + 2w) \rangle$ $p > 2; 0 \leq u < p; 0 \leq v < p; 0 \leq w < p$ p^3 conjugate subgroups for prime $p \equiv 1 \pmod{4}$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$ u, v, w

I Minimal translationengleiche supergroups

[2] $Fd\bar{3}m$ (227); [2] $Fd\bar{3}c$ (228)

II Minimal non-isomorphic klassengleiche supergroups

• Additional centring translations none

• Decreased unit cell

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c} Pn\bar{3}$ (201)

ORIGIN CHOICE 2, Origin at centre ($\bar{3}$), at $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ from 23

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); (13)

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)+	
96	g	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) z, x, y	(6) $z, \bar{x} + \frac{3}{4}, \bar{y} + \frac{3}{4}$	(7) $\bar{z} + \frac{3}{4}, \bar{x} + \frac{3}{4}, y$	(8) $\bar{z} + \frac{3}{4}, x, \bar{y} + \frac{3}{4}$
			(9) y, z, x	(10) $\bar{y} + \frac{3}{4}, z, \bar{x} + \frac{3}{4}$	(11) $y, \bar{z} + \frac{3}{4}, \bar{x} + \frac{3}{4}$	(12) $\bar{y} + \frac{3}{4}, \bar{z} + \frac{3}{4}, x$
			(13) $\bar{x}, \bar{y}, \bar{z}$	(14) $x + \frac{1}{4}, y + \frac{1}{4}, \bar{z}$	(15) $x + \frac{1}{4}, \bar{y}, z + \frac{1}{4}$	(16) $\bar{x}, y + \frac{1}{4}, z + \frac{1}{4}$
			(17) $\bar{z}, \bar{x}, \bar{y}$	(18) $\bar{z}, x + \frac{1}{4}, y + \frac{1}{4}$	(19) $z + \frac{1}{4}, x + \frac{1}{4}, \bar{y}$	(20) $z + \frac{1}{4}, \bar{x}, y + \frac{1}{4}$
			(21) $\bar{y}, \bar{z}, \bar{x}$	(22) $y + \frac{1}{4}, \bar{z}, x + \frac{1}{4}$	(23) $\bar{y}, z + \frac{1}{4}, x + \frac{1}{4}$	(24) $y + \frac{1}{4}, z + \frac{1}{4}, \bar{x}$

I Maximal translationengleiche subgroups

[2] $F23$ (196)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+		1/8, 1/8, 1/8
[3] $Fd1$ (70, $Fddd$)	(1; 2; 3; 4; 13; 14; 15; 16)+		
{	[4] $F1\bar{3}$ (148, $R\bar{3}$)	(1; 5; 9; 13; 17; 21)+	$1/2(-\mathbf{a} + \mathbf{b}), 1/2(-\mathbf{b} + \mathbf{c}), \mathbf{a} + \mathbf{b} + \mathbf{c}$
	[4] $F1\bar{3}$ (148, $R\bar{3}$)	(1; 6; 12; 13; 18; 24)+	$1/2(\mathbf{a} + \mathbf{b}), 1/2(-\mathbf{b} - \mathbf{c}), -\mathbf{a} + \mathbf{b} - \mathbf{c}$
	[4] $F1\bar{3}$ (148, $R\bar{3}$)	(1; 7; 10; 13; 19; 22)+	$1/2(-\mathbf{a} - \mathbf{b}), 1/2(\mathbf{b} - \mathbf{c}), \mathbf{a} - \mathbf{b} - \mathbf{c}$
	[4] $F1\bar{3}$ (148, $R\bar{3}$)	(1; 8; 11; 13; 20; 23)+	$1/2(\mathbf{a} - \mathbf{b}), 1/2(\mathbf{b} + \mathbf{c}), -\mathbf{a} - \mathbf{b} + \mathbf{c}$

II Maximal klassengleiche subgroups

- Loss of centring translations none
- Enlarged unit cell none
- Series of maximal isomorphic subgroups

$[p^3] \mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}, \mathbf{c}' = p\mathbf{c}$
 $Fd\bar{3}$ (203) $\langle 2 + (\frac{3p}{4} - \frac{3}{4} + 2u, \frac{3p}{4} - \frac{3}{4} + 2v, 0);$
 $3 + (\frac{3p}{4} - \frac{3}{4} + 2u, 0, \frac{3p}{4} - \frac{3}{4} + 2w);$
 $5 + (u - w, -u + v, -v + w); 13 + (2u, 2v, 2w) \rangle$
 $p > 2; 0 \leq u < p; 0 \leq v < p; 0 \leq w < p$
 p^3 conjugate subgroups for the prime p $p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$ u, v, w

I Minimal translationengleiche supergroups

[2] $Fd\bar{3}m$ (227); [2] $Fd\bar{3}c$ (228)

II Minimal non-isomorphic klassengleiche supergroups

- Additional centring translations none
- Decreased unit cell

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$ $Pn\bar{3}$ (201)