

$I4_1/acd$ 

No. 142

 $I4_1/a2/c2/d$ 
 $D_{4h}^{20}$ 

 ORIGIN CHOICE 1, Origin at  $\bar{4}c2_1$ , at  $0, \frac{1}{4}, -\frac{1}{8}$  from  $\bar{1}$ 
**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ ; (2); (3); (5); (9)

**General position**

 Multiplicity,  
Wyckoff letter,  
Site symmetry

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

32	g	1	(1) $x, y, z$	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(3) $\bar{y}, x + \frac{1}{2}, z + \frac{1}{4}$	(4) $y + \frac{1}{2}, \bar{x}, z + \frac{3}{4}$
			(5) $\bar{x} + \frac{1}{2}, y, \bar{z} + \frac{1}{4}$	(6) $x, \bar{y} + \frac{1}{2}, \bar{z} + \frac{3}{4}$	(7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$	(8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$
			(9) $\bar{x}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{4}$	(10) $x + \frac{1}{2}, y, \bar{z} + \frac{3}{4}$	(11) $y, \bar{x}, \bar{z}$	(12) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$
			(13) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(14) $\bar{x}, y, z + \frac{1}{2}$	(15) $\bar{y} + \frac{1}{2}, \bar{x}, z + \frac{1}{4}$	(16) $y, x + \frac{1}{2}, z + \frac{3}{4}$

**I Maximal translationengleiche subgroups**

[2] $I\bar{4}2d$ (122)	(1; 2; 5; 6; 11; 12; 15; 16)+	0, 1/2, 1/4
[2] $I\bar{4}c2$ (120)	(1; 2; 7; 8; 11; 12; 13; 14)+	
[2] $I4_1cd$ (110)	(1; 2; 3; 4; 13; 14; 15; 16)+	
[2] $I4_122$ (98)	(1; 2; 3; 4; 5; 6; 7; 8)+	0, 0, 1/4
[2] $I4_1/a11$ (88, $I4_1/a$ )	(1; 2; 3; 4; 9; 10; 11; 12)+	
[2] $I2/a2/c1$ (73, $Ibca$ )	(1; 2; 5; 6; 9; 10; 13; 14)+	0, 1/4, 1/8
[2] $I2/a12/d$ (70, $Fddd$ )	(1; 2; 7; 8; 9; 10; 15; 16)+	0, 0, 1/4

 $\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, \mathbf{c}$ 
**II Maximal klassengleiche subgroups**

• <b>Loss of centring translations</b>		none
• <b>Enlarged unit cell</b>		
[3] $\mathbf{c}' = 3\mathbf{c}$		
$\left\{ \begin{array}{l} I4_1/acd \text{ (142)} \\ I4_1/acd \text{ (142)} \\ I4_1/acd \text{ (142)} \end{array} \right.$	$\langle (2; 5; 9) + (1,0,1); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}) \rangle$ $\langle 2 + (1,0,1); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}); (5; 9) + (1,0,3) \rangle$ $\langle 2 + (1,0,1); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}); (5; 9) + (1,0,5) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$ $\mathbf{a}, \mathbf{b}, 3\mathbf{c}$ $\mathbf{a}, \mathbf{b}, 3\mathbf{c}$
		1/2, 0, 1/4 1/2, 0, 5/4 1/2, 0, 9/4
• <b>Series of maximal isomorphic subgroups</b>		
[p] $\mathbf{c}' = p\mathbf{c}$		
$I4_1/acd$ (142)	$\langle 2 + (0,0, \frac{p}{2} - \frac{1}{2}); 3 + (0,0, \frac{p}{4} - \frac{1}{4}); (5; 9) + (0,0, \frac{p}{4} - \frac{1}{4} + 2u) \rangle$ prime $p > 4$ ; $0 \leq u < p$ $p$ conjugate subgroups for $p = 4n + 1$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
		0, 0, $u$
$I4_1/acd$ (142)	$\langle 2 + (1,0, \frac{p}{2} - \frac{1}{2}); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{p}{4} - \frac{1}{4}); (5; 9) + (1,0, \frac{p}{4} + \frac{1}{4} + 2u) \rangle$ prime $p > 2$ ; $0 \leq u < p$ $p$ conjugate subgroups for $p = 4n - 1$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
		1/2, 0, 1/4 + $u$
[p <sup>2</sup> ] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$		
$I4_1/acd$ (142)	$\langle 2 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2v, 0); 3 + (u + v, \frac{p}{2} - \frac{1}{2} - u + v, 0); 5 + (\frac{p}{2} - \frac{1}{2} + 2u, 0, 0); 9 + (2u, \frac{p}{2} - \frac{1}{2} + 2v, 0) \rangle$ prime $p > 2$ ; $0 \leq u < p$ ; $0 \leq v < p$ $p^2$ conjugate subgroups	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$
		$u, v, 0$

**I Minimal translationengleiche supergroups**

 [3]  $Fd\bar{3}c$  (228); [3]  $Ia\bar{3}d$  (230)

**II Minimal non-isomorphic klassengleiche supergroups**

• <b>Additional centring translations</b>	none
• <b>Decreased unit cell</b>	
[2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $C4_2/emd$ (134, $P4_2/nm$ )	

ORIGIN CHOICE 2, Origin at  $\bar{1}$  at  $b(c,a)d$ , at  $0, -\frac{1}{4}, \frac{1}{8}$  from  $\bar{4}$

Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ ; (2); (3); (5); (9)

General position

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

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

32	g	1	(1) $x, y, z$	(2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$	(3) $\bar{y} + \frac{1}{4}, x + \frac{3}{4}, z + \frac{1}{4}$	(4) $y + \frac{1}{4}, \bar{x} + \frac{1}{4}, z + \frac{3}{4}$
			(5) $\bar{x} + \frac{1}{2}, y, \bar{z}$	(6) $x, \bar{y}, \bar{z} + \frac{1}{2}$	(7) $y + \frac{1}{4}, x + \frac{3}{4}, \bar{z} + \frac{3}{4}$	(8) $\bar{y} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}$
			(9) $\bar{x}, \bar{y}, \bar{z}$	(10) $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$	(11) $y + \frac{3}{4}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{3}{4}$	(12) $\bar{y} + \frac{3}{4}, x + \frac{3}{4}, \bar{z} + \frac{1}{4}$
			(13) $x + \frac{1}{2}, \bar{y}, z$	(14) $\bar{x}, y, z + \frac{1}{2}$	(15) $\bar{y} + \frac{3}{4}, \bar{x} + \frac{1}{4}, z + \frac{1}{4}$	(16) $y + \frac{3}{4}, x + \frac{3}{4}, z + \frac{3}{4}$

I Maximal translationengleiche subgroups

[2] $I\bar{4}2d$ (122)	(1; 2; 5; 6; 11; 12; 15; 16)+	0, 3/4, 1/8
[2] $I\bar{4}c2$ (120)	(1; 2; 7; 8; 11; 12; 13; 14)+	0, 1/4, 3/8
[2] $I4_1cd$ (110)	(1; 2; 3; 4; 13; 14; 15; 16)+	0, 1/4, 0
[2] $I4_122$ (98)	(1; 2; 3; 4; 5; 6; 7; 8)+	0, 1/4, 1/8
[2] $I4_1/a11$ (88, $I4_1/a$ )	(1; 2; 3; 4; 9; 10; 11; 12)+	0, 1/2, 0
[2] $I2/a2/c1$ (73, $Ibca$ )	(1; 2; 5; 6; 9; 10; 13; 14)+	
[2] $I2/a12/d$ (70, $Fddd$ )	(1; 2; 7; 8; 9; 10; 15; 16)+	$a - b, a + b, c$ 1/4, 1/4, 1/4

II Maximal klassengleiche subgroups

- Loss of centring translations

none

- Enlarged unit cell

[3]  $c' = 3c$

$I4_1/acd$ (142)	$\langle 5; 9; 2 + (1,0,1); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}) \rangle$	$a, b, 3c$	1/2, 0, 0
$I4_1/acd$ (142)	$\langle 2 + (1,0,1); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}); (5; 9) + (0,0,2) \rangle$	$a, b, 3c$	1/2, 0, 1
$I4_1/acd$ (142)	$\langle 2 + (1,0,1); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}); (5; 9) + (0,0,4) \rangle$	$a, b, 3c$	1/2, 0, 2

- Series of maximal isomorphic subgroups

[p]  $c' = pc$

$I4_1/acd$ (142)	$\langle 2 + (0,0, \frac{p}{2} - \frac{1}{2}); 3 + (0,0, \frac{p}{4} - \frac{1}{4}); (5; 9) + (0,0,2u) \rangle$ prime $p > 4; 0 \leq u < p$ $p$ conjugate subgroups for $p = 4n + 1$	$a, b, pc$	0, 0, $u$
$I4_1/acd$ (142)	$\langle 2 + (1,0, \frac{p}{2} - \frac{1}{2}); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{p}{4} - \frac{1}{4}); (5; 9) + (1,0,2u) \rangle$ prime $p > 2; 0 \leq u < p$ $p$ conjugate subgroups for $p = 4n - 1$	$a, b, pc$	1/2, 0, $u$

[p<sup>2</sup>]  $a' = pa, b' = pb$

$I4_1/acd$ (142)	$\langle 2 + (\frac{p}{2} - \frac{1}{2} + 2u, 2v, 0); 3 + (\frac{p}{4} - \frac{1}{4} + u + v, \frac{3p}{4} - \frac{3}{4} - u + v, 0); 5 + (\frac{p}{2} - \frac{1}{2} + 2u, 0, 0); 9 + (2u, 2v, 0) \rangle$ prime $p > 4; 0 \leq u < p; 0 \leq v < p$ $p^2$ conjugate subgroups for $p = 4n + 1$	$pa, pb, c$	$u, v, 0$
$I4_1/acd$ (142)	$\langle 2 + (\frac{p}{2} + \frac{1}{2} + 2u, 2v, 0); 3 + (\frac{p}{4} + \frac{1}{4} + u + v, \frac{3p}{4} + \frac{5}{4} - u + v, 0); 5 + (\frac{p}{2} + \frac{1}{2} + 2u, 0, 0); 9 + (1 + 2u, 2v, 0) \rangle$ prime $p > 2; 0 \leq u < p; 0 \leq v < p$ $p^2$ conjugate subgroups for $p = 4n - 1$	$pa, pb, c$	1/2 + $u, v, 0$

I Minimal translationengleiche supergroups

[3]  $Fd\bar{3}c$  (228); [3]  $Ia\bar{3}d$  (230)

II Minimal non-isomorphic klassengleiche supergroups

- Additional centring translations

none

- Decreased unit cell

[2]  $c' = \frac{1}{2}c$   $C4_2/emd$  (134,  $P4_2/nm$ )