

$I4_1/acd$

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)+	a – b, a + b, c 0, 0, 1/4

II Maximal klassengleiche subgroups

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

• Additional centring translations	none
• Decreased unit cell	
[2] $c' = \frac{1}{2}c$ $C4_2/emd$ (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)	$\langle 2 + (1, 0, \frac{p}{2} - \frac{1}{2}); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{p}{4} - \frac{1}{4}); (5; 9) + (1, 0, 2u) \rangle$ $p > 2; 0 \leq u < p$	a, b, pc	1/2, 0, u
$I4_1/acd$ (142)	$\langle 2 + (0, 0, \frac{p}{2} - \frac{1}{2}); 3 + (0, 0, \frac{p}{4} - \frac{1}{4}); (5; 9) + (0, 0, 2u) \rangle$ $p > 4; 0 \leq u < p$ p conjugate subgroups for prime $p \equiv 3 \pmod{4}$	a, b, pc	0, 0, u
	p conjugate subgroups for prime $p \equiv 1 \pmod{4}$		

[p^2] $a' = pa, b' = pb$

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

• **Additional centring translations**

none

• **Decreased unit cell**

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