

$I4_1/amd$

No. 141

 $I4_1/a2/m2/d$
 D_{4h}^{19}

 ORIGIN CHOICE 1, Origin at $\bar{4}m2$, at $0, \frac{1}{4}, -\frac{1}{8}$ from centre ($2/m$)

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	<i>i</i>	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) $\bar{x} + \frac{1}{2}, y, \bar{z} + \frac{3}{4}$	(6) $x, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{4}$	(7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(8) $\bar{y}, \bar{x}, \bar{z}$
			(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) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(14) \bar{x}, y, z	(15) $\bar{y} + \frac{1}{2}, \bar{x}, z + \frac{3}{4}$	(16) $y, x + \frac{1}{2}, z + \frac{1}{4}$

I Maximal translationengleiche subgroups

[2] $I\bar{4}2d$ (122)	(1; 2; 5; 6; 11; 12; 15; 16)+		
[2] $I\bar{4}m2$ (119)	(1; 2; 7; 8; 11; 12; 13; 14)+		
[2] $I4_1md$ (109)	(1; 2; 3; 4; 13; 14; 15; 16)+		
[2] $I4_122$ (98)	(1; 2; 3; 4; 5; 6; 7; 8)+		
[2] $I4_1/a11$ (88, $I4_1/a$)	(1; 2; 3; 4; 9; 10; 11; 12)+		
[2] $I2/a2/m1$ (74, $Imma$)	(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	$0, 1/2, 1/4$

II Maximal klassengleiche subgroups

• Loss of centring translations		none	
• Enlarged unit cell			
[3] $\mathbf{c}' = 3\mathbf{c}$			
$\left\{ \begin{array}{l} I4_1/amd \text{ (141)} \\ I4_1/amd \text{ (141)} \\ I4_1/amd \text{ (141)} \end{array} \right.$	$\langle (2; 9) + (1, 0, 1); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}); 5 + (1, 0, 2) \rangle$ $\langle 2 + (1, 0, 1); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}); 5 + (1, 0, 4); 9 + (1, 0, 3) \rangle$ $\langle 2 + (1, 0, 1); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}); 5 + (1, 0, 6); 9 + (1, 0, 5) \rangle$	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			
[<i>p</i>] $\mathbf{c}' = p\mathbf{c}$			
$I4_1/amd$ (141)	$\langle 2 + (0, 0, \frac{p}{2} - \frac{1}{2}); 3 + (0, 0, \frac{p}{4} - \frac{1}{4}); 5 + (0, 0, \frac{3p}{4} - \frac{3}{4} + 2u); 9 + (0, 0, \frac{p}{4} - \frac{1}{4} + 2u) \rangle$ prime $p > 4$; $0 \leq u < p$ p conjugate subgroups for $p = 4n + 1$	a, b, pc	$0, 0, u$
$I4_1/amd$ (141)	$\langle 2 + (1, 0, \frac{p}{2} - \frac{1}{2}); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{p}{4} - \frac{1}{4}); 5 + (1, 0, \frac{3p}{4} - \frac{1}{4} + 2u); 9 + (1, 0, \frac{p}{4} + \frac{1}{4} + 2u) \rangle$ prime $p > 2$; $0 \leq u < p$ p conjugate subgroups for $p = 4n - 1$	a, b, pc	$1/2, 0, 1/4 + u$
[p^2] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$			
$I4_1/amd$ (141)	$\langle 2 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2v, 0); 3 + (u + v, \frac{p}{2} - \frac{1}{2} - u + v, 0); 5 + (\frac{p}{2} - \frac{1}{2} + 2u, 0, 0); 9 + (2u, \frac{p}{2} - \frac{1}{2} + 2v, 0) \rangle$ prime $p > 2$; $0 \leq u < p$; $0 \leq v < p$ p^2 conjugate subgroups	pa, pb, c	$u, v, 0$

I Minimal translationengleiche supergroups

 [3] $Fd\bar{3}m$ (227)

II Minimal non-isomorphic klassengleiche supergroups

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

ORIGIN CHOICE 2, Origin at centre $(2/m)$ at $b(2/m, 2_1/n)d$, at $0, -\frac{1}{4}, \frac{1}{8}$ from $\bar{4}m2$

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 <i>i</i> 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) $\bar{x} + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$	(6) x, \bar{y}, \bar{z}	(7) $y + \frac{1}{4}, x + \frac{3}{4}, \bar{z} + \frac{1}{4}$	(8) $\bar{y} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{3}{4}$
	(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) $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$	(14) \bar{x}, y, z	(15) $\bar{y} + \frac{3}{4}, \bar{x} + \frac{1}{4}, z + \frac{3}{4}$	(16) $y + \frac{3}{4}, x + \frac{3}{4}, z + \frac{1}{4}$

I Maximal translationengleiche subgroups

[2] $I\bar{4}2d$ (122)	(1; 2; 5; 6; 11; 12; 15; 16)+		0, 1/4, 3/8
[2] $I\bar{4}m2$ (119)	(1; 2; 7; 8; 11; 12; 13; 14)+		0, 1/4, 3/8
[2] $I4_1md$ (109)	(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, 3/8
[2] $I4_1/a11$ (88, $I4_1/a$)	(1; 2; 3; 4; 9; 10; 11; 12)+		0, 1/2, 0
[2] $I2/a2/m1$ (74, $Imma$)	(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, 3/4, 1/4

II Maximal klassengleiche subgroups

• **Loss of centring translations**

none

• **Enlarged unit cell**

[3] $c' = 3c$			
$I4_1/amd$ (141)	$\langle (2; 5) + (1, 0, 1); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}); 9 + (1, 0, 0) \rangle$	a, b, 3c	1/2, 0, 0
$I4_1/amd$ (141)	$\langle 2 + (1, 0, 1); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}); 5 + (1, 0, 3); 9 + (1, 0, 2) \rangle$	a, b, 3c	1/2, 0, 1
$I4_1/amd$ (141)	$\langle 2 + (1, 0, 1); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}); 5 + (1, 0, 5); 9 + (1, 0, 4) \rangle$	a, b, 3c	1/2, 0, 2

• **Series of maximal isomorphic subgroups**

[p] $c' = pc$			
$I4_1/amd$ (141)	$\langle 2 + (0, 0, \frac{p}{2} - \frac{1}{2}); 3 + (0, 0, \frac{p}{4} - \frac{1}{4}); 5 + (0, 0, \frac{p}{2} - \frac{1}{2} + 2u); 9 + (0, 0, 2u) \rangle$ prime $p > 4; 0 \leq u < p$ p conjugate subgroups for $p = 4n + 1$	a, b, pc	0, 0, u
$I4_1/amd$ (141)	$\langle 2 + (1, 0, \frac{p}{2} - \frac{1}{2}); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{p}{4} - \frac{1}{4}); 5 + (1, 0, \frac{p}{2} - \frac{1}{2} + 2u); 9 + (1, 0, 2u) \rangle$ prime $p > 2; 0 \leq u < p$ p conjugate subgroups for $p = 4n - 1$	a, b, pc	1/2, 0, u
[p ²] $a' = pa, b' = pb$			
$I4_1/amd$ (141)	$\langle 2 + (\frac{p}{2} - \frac{1}{2} + 2u, 2v, 0); 3 + (\frac{p}{4} - \frac{1}{4} + u + v, \frac{3p}{4} - \frac{3}{4} - u + v, 0); 5 + (\frac{p}{2} - \frac{1}{2} + 2u, 0, 0); 9 + (2u, 2v, 0) \rangle$ prime $p > 4; 0 \leq u < p; 0 \leq v < p$ p^2 conjugate subgroups for $p = 4n + 1$	pa, pb, c	$u, v, 0$
$I4_1/amd$ (141)	$\langle 2 + (\frac{p}{2} + \frac{1}{2} + 2u, 2v, 0); 3 + (\frac{p}{4} + \frac{1}{4} + u + v, \frac{3p}{4} - \frac{5}{4} - u + v, 0); 5 + (\frac{p}{2} + \frac{1}{2} + 2u, 0, 0); 9 + (1 + 2u, 2v, 0) \rangle$ 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] $Fd\bar{3}m$ (227)

II Minimal non-isomorphic klassengleiche supergroups

• **Additional centring translations**

none

• **Decreased unit cell**

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