

C_{4h}^6
 $I4_1/a$

No. 88

 $I4_1/a$

 ORIGIN CHOICE 1, Origin at $\bar{4}$, 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)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
	(0, 0, 0)+	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$		
16 <i>f</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) $\bar{x}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{4}$	(6) $x + \frac{1}{2}, y, \bar{z} + \frac{3}{4}$	(7) y, \bar{x}, \bar{z}	(8) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$

I Maximal translationengleiche subgroups

[2] $I\bar{4}$ (82)	(1; 2; 7; 8)+		
[2] $I4_1$ (80)	(1; 2; 3; 4)+		
[2] $I2/a$ (15, $A112/a$)	(1; 2; 5; 6)+	b, -a - b, c	0, 1/4, 1/8

II Maximal klassengleiche subgroups

• Loss of centring translations		none	
• Enlarged unit cell			
[3] $\mathbf{c}' = 3\mathbf{c}$			
$I4_1/a$ (88)	$\langle (2; 5) + (1, 0, 1); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}) \rangle$	a, b, 3c	1/2, 0, 1/4
$I4_1/a$ (88)	$\langle 2 + (1, 0, 1); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}); 5 + (1, 0, 3) \rangle$	a, b, 3c	1/2, 0, 5/4
$I4_1/a$ (88)	$\langle 2 + (1, 0, 1); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}); 5 + (1, 0, 5) \rangle$	a, b, 3c	1/2, 0, 9/4
• Series of maximal isomorphic subgroups			
[<i>p</i>] $\mathbf{c}' = p\mathbf{c}$			
$I4_1/a$ (88)	$\langle 2 + (0, 0, \frac{p}{2} - \frac{1}{2}); 3 + (0, 0, \frac{p}{4} - \frac{1}{4}); 5 + (0, 0, \frac{p}{4} - \frac{1}{4} + 2u) \rangle$ $p > 4; 0 \leq u < p$ <i>p</i> conjugate subgroups for prime $p \equiv 1 \pmod{4}$	a, b, pc	0, 0, <i>u</i>
$I4_1/a$ (88)	$\langle 2 + (1, 0, \frac{p}{2} - \frac{1}{2}); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{p}{4} - \frac{1}{4}); 5 + (1, 0, \frac{p}{4} + \frac{1}{4} + 2u) \rangle$ $p > 2; 0 \leq u < p$ <i>p</i> conjugate subgroups for prime $p \equiv 3 \pmod{4}$	a, b, pc	1/2, 0, 1/4 + <i>u</i>
[p^2] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$			
$I4_1/a$ (88)	$\langle 2 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2v, 0); 3 + (u + v, \frac{p}{2} - \frac{1}{2} - u + v, 0); 5 + (2u, \frac{p}{2} - \frac{1}{2} + 2v, 0) \rangle$ $p > 2; 0 \leq u < p; 0 \leq v < p$ p^2 conjugate subgroups for prime $p \equiv 3 \pmod{4}$	pa, pb, c	<i>u, v, 0</i>
[$p = q^2 + r^2$] $\mathbf{a}' = q\mathbf{a} - r\mathbf{b}, \mathbf{b}' = r\mathbf{a} + q\mathbf{b}$			
$I4_1/a$ (88)	$\langle 2 + (\frac{q}{2} + \frac{r}{2} - \frac{1}{2} + 2u, \frac{q}{2} - \frac{r}{2} - \frac{1}{2}, 0); 3 + (\frac{r}{2} + u, \frac{q}{2} - \frac{1}{2} - u, 0); 5 + (\frac{q}{2} + 2u, \frac{q}{2} - \frac{1}{2}, 0) \rangle$ $q > 0; r > 1; p > 4; 0 \leq u < p$ <i>p</i> conjugate subgroups for odd <i>q</i> and prime $p \equiv 1 \pmod{4}$	qa - rb, ra + qb, c	<i>u, 0, 0</i>
$I4_1/a$ (88)	$\langle 2 + (\frac{q}{2} + \frac{r}{2} + \frac{1}{2} + 2u, \frac{q}{2} - \frac{r}{2} - \frac{1}{2}, 0); 3 + (\frac{r}{2} + \frac{1}{2} + u, \frac{q}{2} - 1 - u, 0); 5 + (\frac{r}{2} + 1 + 2u, \frac{q}{2} - \frac{1}{2}, \frac{1}{2}) \rangle$ $q > 1; r > 0; p > 4; 0 \leq u < p$ <i>p</i> conjugate subgroups for even <i>q</i> and prime $p \equiv 1 \pmod{4}$	qa - rb, ra + qb, c	1/2 + <i>u, 0, 1/4</i>

I Minimal translationengleiche supergroups

 [2] $I4_1/amd$ (141); [2] $I4_1/acd$ (142)

II Minimal non-isomorphic klassengleiche supergroups

• Additional centring translations	none
• Decreased unit cell	
[2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $C4_2/e$ (86, $P4_2/n$)	

ORIGIN CHOICE 2, Origin at $\bar{1}$ on glide plane b , 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)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

16 f 1

- (0,0,0)+ $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$
 (1) x, y, z (2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (3) $\bar{y} + \frac{3}{4}, x + \frac{1}{4}, z + \frac{1}{4}$ (4) $y + \frac{3}{4}, \bar{x} + \frac{3}{4}, z + \frac{3}{4}$
 (5) $\bar{x}, \bar{y}, \bar{z}$ (6) $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ (7) $y + \frac{1}{4}, \bar{x} + \frac{3}{4}, \bar{z} + \frac{3}{4}$ (8) $\bar{y} + \frac{1}{4}, x + \frac{1}{4}, \bar{z} + \frac{1}{4}$

I Maximal translationengleiche subgroups

[2] $I\bar{4}$ (82)	(1; 2; 7; 8)+		0, 1/4, 5/8
[2] $I4_1$ (80)	(1; 2; 3; 4)+		1/2, 1/4, 0
[2] $I2/a$ (15, $A112/a$)	(1; 2; 5; 6)+	b, -a - b, c	

II Maximal klassengleiche subgroups

- Loss of centring translations none

- Enlarged unit cell

[3] $c' = 3c$

$I4_1/a$ (88)	$\langle 2 + (1, 0, 1); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}); 5 + (1, 0, 0) \rangle$	a, b, 3c	1/2, 0, 0
$I4_1/a$ (88)	$\langle 2 + (1, 0, 1); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}); 5 + (1, 0, 2) \rangle$	a, b, 3c	1/2, 0, 1
$I4_1/a$ (88)	$\langle 2 + (1, 0, 1); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}); 5 + (1, 0, 4) \rangle$	a, b, 3c	1/2, 0, 2

- Series of maximal isomorphic subgroups

[p] $c' = pc$

$I4_1/a$ (88)	$\langle 2 + (0, 0, \frac{p}{2} - \frac{1}{2}); 3 + (0, 0, \frac{p}{4} - \frac{1}{4}); 5 + (0, 0, 2u) \rangle$ $p > 4; 0 \leq u < p$ p conjugate subgroups for prime $p \equiv 1 \pmod{4}$	a, b, pc	0, 0, u
$I4_1/a$ (88)	$\langle 2 + (1, 0, \frac{p}{2} - \frac{1}{2}); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{p}{4} - \frac{1}{4}); 5 + (1, 0, 2u) \rangle$ $p > 2; 0 \leq u < p$ p conjugate subgroups for prime $p \equiv 3 \pmod{4}$	a, b, pc	1/2, 0, u

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

$I4_1/a$ (88)	$\langle 2 + (\frac{p}{2} + \frac{1}{2} + 2u, 2v, 0); 3 + (\frac{3p}{4} - \frac{1}{4} + u + v, \frac{p}{4} - \frac{3}{4} - u + v, 0); 5 + (1 + 2u, 2v, 0) \rangle$ $p > 2; 0 \leq u < p; 0 \leq v < p$ p^2 conjugate subgroups for prime $p \equiv 3 \pmod{4}$	pa, pb, c	1/2 + $u, v, 0$
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[$p = q^2 + r^2$] $a' = qa - rb, b' = ra + qb$

$I4_1/a$ (88)	$\langle 2 + (\frac{q}{2} + \frac{1}{2} + 2u, -\frac{r}{2}, 0); 3 + (\frac{3q}{4} + \frac{r}{4} - \frac{1}{4} + u, \frac{q}{4} - \frac{3r}{4} - \frac{3}{4} - u, 0); 5 + (1 + 2u, 0, 0) \rangle$ $q > 0; r > 1; p > 4; 0 \leq u < p; q$ odd; $q + r = 3 \pmod{4}$ p conjugate subgroups for each pair of q and r	qa - rb, ra + qb, c	1/2 + $u, 0, 0$
$I4_1/a$ (88)	$\langle 2 + (\frac{q}{2} - \frac{1}{2} + 2u, -\frac{r}{2}, 0); 3 + (\frac{3q}{4} + \frac{r}{4} - \frac{3}{4} + u, \frac{q}{4} - \frac{3r}{4} - \frac{1}{4} - u, 0); 5 + (2u, 0, 0) \rangle$ $q > 0; r > 1; p > 12; 0 \leq u < p; q$ odd; $q + r = 1 \pmod{4}$ p conjugate subgroups for each pair of q and r	qa - rb, ra + qb, c	$u, 0, 0$
$I4_1/a$ (88)	$\langle 2 + (\frac{q}{2} + 1 + 2u, -\frac{r}{2} + \frac{1}{2}, 0); 3 + (\frac{3q}{4} + \frac{r}{4} + \frac{1}{4} + u, \frac{q}{4} - \frac{3r}{4} - \frac{3}{4} - u, 0); 5 + (\frac{3}{2} + 2u, \frac{1}{2}, \frac{1}{2}) \rangle$ $q > 1; r > 0; p > 4; 0 \leq u < p; q$ even; $q + r = 3 \pmod{4}$ p conjugate subgroups for each pair of q and r	qa - rb, ra + qb, c	3/4 + $u, 1/4, 1/4$
$I4_1/a$ (88)	$\langle 2 + (\frac{q}{2} + 2u, -\frac{r}{2} + \frac{1}{2}, 0); 3 + (\frac{3q}{4} + \frac{r}{4} - \frac{1}{4} + u, \frac{q}{4} - \frac{3r}{4} - \frac{1}{4} - u, 0); 5 + (\frac{1}{2} + 2u, \frac{1}{2}, \frac{1}{2}) \rangle$ $q > 1; r > 0; p > 12; 0 \leq u < p; q$ even; $q + r = 1 \pmod{4}$ p conjugate subgroups for each pair of q and r	qa - rb, ra + qb, c	1/4 + $u, 1/4, 1/4$

I Minimal translationengleiche supergroups

[2] $I4_1/amd$ (141); [2] $I4_1/acd$ (142)

II Minimal non-isomorphic klassengleiche supergroups

- Additional centring translations none

- Decreased unit cell

[2] $c' = \frac{1}{2}c$ $C4_2/e$ (86, $P4_2/n$)