

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] $c' = 3c$

$\left\{ \begin{array}{l} I4_1/a \text{ (88)} \\ I4_1/a \text{ (88)} \\ I4_1/a \text{ (88)} \end{array} \right.$	$\langle (2; 5) + (1, 0, 1); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}) \rangle$ $\langle 2 + (1, 0, 1); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}); 5 + (1, 0, 3) \rangle$ $\langle 2 + (1, 0, 1); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}); 5 + (1, 0, 5) \rangle$	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] $c' = pc$

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

 [p²] $a' = pa, b' = pb$

$I4_1/a$ (88)	$\langle 2 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2v, 0); 3 + (u + v, \frac{p}{2} - \frac{1}{2} - u + v, 0); 5 + (2u, \frac{p}{2} - \frac{1}{2} + 2v, 0) \rangle$ prime $p > 2$; $0 \leq u < p$; $0 \leq v < p$ p^2 conjugate subgroups for $p = 4n - 1$	pa, pb, c	$u, v, 0$
---------------	--	------------------	-----------

 [p = q² + r²] $a' = qa - rb, b' = ra + qb$

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

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, $P4_2/n$)

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

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

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

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

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

[$p = q^2 + r^2$] $a' = qa - rb, b' = ra + qb$
 $I4_1/a$ (88) $\langle 2 + (\frac{q}{2} - \frac{1}{2} + 2u, -\frac{r}{2}, 0); 3 + (\frac{3q}{4} + \frac{r}{4} - \frac{3}{4} + u, \frac{q}{4} - \frac{3r}{4} - \frac{1}{4} - u, 0); 5 + (2u, 0, 0) \rangle$ $qa - rb, ra + qb, c$ $u, 0, 0$
prime $p = 4n + 1$; $0 \leq u < p$; $q > 0$; $r = 2n'$; $q + r = 4n'' + 1$
 $p > 12$; p conjugate subgroups for each triplet of q, r and p

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

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

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

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, $P4_2/n$)