

C_4^6
 $I4_1$

No. 80

 $I4_1$
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)

General position

 Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

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

 8 b 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) $y + \frac{1}{2}, \bar{x}, z + \frac{3}{4}$
I Maximal translationengleiche subgroups

 [2] $I2$ (5, A112) (1; 2)+ **b, -a - b, c**
II Maximal klassengleiche subgroups

• Loss of centring translations

| | | | |
|-----------------|--|--|---------------|
| [2] $P4_3$ (78) | 1; 2; (3; 4) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ | | $3/4, 3/4, 0$ |
| [2] $P4_1$ (76) | 1; 2; 3; 4 | | $3/4, 1/4, 0$ |

• Enlarged unit cell

| | | | |
|---------------|---|-----------------|-------------|
| [3] $c' = 3c$ | | | |
| $I4_1$ (80) | $\langle 2 + (1,0,1); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}) \rangle$ | a, b, 3c | $1/2, 0, 0$ |

• Series of maximal isomorphic subgroups

| | | | |
|--|---|----------------------------|-----------------|
| [p] $c' = pc$ | | | |
| $I4_1$ (80) | $\langle 2 + (0,0,\frac{p}{2} - \frac{1}{2}); 3 + (0,0,\frac{p}{4} - \frac{1}{4}) \rangle$ prime $p > 4$; $p = 4n + 1$ no conjugate subgroups | a, b, pc | |
| $I4_1$ (80) | $\langle 2 + (1,0,\frac{p}{2} - \frac{1}{2}); 3 + (\frac{1}{2}, -\frac{1}{2}, \frac{p}{4} - \frac{1}{4}) \rangle$ prime $p > 2$; $p = 4n - 1$ no conjugate subgroups | a, b, pc | $1/2, 0, 0$ |
| [p^2] $a' = pa, b' = pb$ | | | |
| $I4_1$ (80) | $\langle 2 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2v, 0); 3 + (u+v, \frac{p}{2} - \frac{1}{2} - u + v, 0) \rangle$ prime $p > 2$; $0 \leq u < p$; $0 \leq v < p$ p^2 conjugate subgroups for $p = 4n - 1$ | pa, pb, c | $u, v, 0$ |
| [$p = q^2 + r^2$] $a' = qa - rb, b' = ra + qb$ | | | |
| $I4_1$ (80) | $\langle 2 + (\frac{q}{2} + \frac{r}{2} - \frac{1}{2} + 2u, -\frac{r}{2} + \frac{q}{2} - \frac{1}{2}, 0); 3 + (\frac{r}{2} + u, \frac{q}{2} - u - \frac{1}{2}, 0) \rangle$ prime $p > 4$; $q > 0$; $r > 1$; q odd; r even; $0 \leq u < p$ p conjugate subgroups for $p = 4n + 1$ | qa - rb, ra + qb, c | $u, 0, 0$ |
| $I4_1$ (80) | $\langle 2 + (\frac{q}{2} + \frac{r}{2} + \frac{1}{2} + 2u, -\frac{r}{2} + \frac{q}{2} - \frac{1}{2}, 0); 3 + (\frac{r}{2} + \frac{1}{2} + u, \frac{q}{2} - 1 - u, 0) \rangle$ prime $p > 4$; $q > 1$; $r > 0$; q even; r odd; $0 \leq u < p$ p conjugate subgroups for $p = 4n + 1$ | qa - rb, ra + qb, c | $1/2 + u, 0, 0$ |

I Minimal translationengleiche supergroups

 [2] $I4_1/a$ (88); [2] $I4_1/22$ (98); [2] $I4_1/md$ (109); [2] $I4_1/cd$ (110)

II Minimal non-isomorphic klassengleiche supergroups

• Additional centring translations

none

• Decreased unit cell

 [2] $c' = \frac{1}{2}c$ $C4_2$ (77, $P4_2$)