

$S_4^2$ 
 $I\bar{4}$ 

No. 82

 $I\bar{4}$ 
**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)

**General position**

 Multiplicity,  
Wyckoff letter,  
Site symmetry

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

 8  $g$  1

 (1)  $x, y, z$  (2)  $\bar{x}, \bar{y}, z$  (3)  $y, \bar{x}, \bar{z}$  (4)  $\bar{y}, x, \bar{z}$ 
**I Maximal translationengleiche subgroups**

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

## • Loss of centring translations

 [2]  $P\bar{4}$  (81) 1; 2; 3; 4

 [2]  $P\bar{4}$  (81) 1; 2; (3; 4) +  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$  1/2, 0, 1/4

## • Enlarged unit cell

 [3]  $\mathbf{c}' = 3\mathbf{c}$ 

$I\bar{4}$ (82)	$\langle 2; 3 \rangle$	<b>a, b, 3c</b>	
$I\bar{4}$ (82)	$\langle 2; 3 + (0, 0, 2) \rangle$	<b>a, b, 3c</b>	0, 0, 1
$I\bar{4}$ (82)	$\langle 2; 3 + (0, 0, 4) \rangle$	<b>a, b, 3c</b>	0, 0, 2

## • Series of maximal isomorphic subgroups

 [p]  $\mathbf{c}' = p\mathbf{c}$ 

$I\bar{4}$ (82)	$\langle 2; 3 + (0, 0, 2u) \rangle$ $p > 2; 0 \leq u < p$ $p$ conjugate subgroups for the prime $p$	<b>a, b, pc</b>	0, 0, $u$
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 [ $p^2$ ]  $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$ 

$I\bar{4}$ (82)	$\langle 2 + (2u, 2v, 0); 3 + (u - v, u + v, 0) \rangle$ $p > 2; 0 \leq u < p; 0 \leq v < p$ $p^2$ conjugate subgroups for prime $p \equiv 3 \pmod{4}$	<b>pa, pb, c</b>	$u, v, 0$
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 [ $p = q^2 + r^2$ ]  $\mathbf{a}' = q\mathbf{a} - r\mathbf{b}, \mathbf{b}' = r\mathbf{a} + q\mathbf{b}$ 

$I\bar{4}$ (82)	$\langle 2 + (2u, 0, 0); 3 + (u, u, 0) \rangle$ $q > 0; r > 0; p > 4; 0 \leq u < p$ $p$ conjugate subgroups for prime $p \equiv 1 \pmod{4}$	<b>qa - rb, ra + qb, c</b>	$u, 0, 0$
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**I Minimal translationengleiche supergroups**

 [2]  $I4/m$  (87); [2]  $I4_1/a$  (88); [2]  $I\bar{4}m2$  (119); [2]  $I\bar{4}c2$  (120); [2]  $I\bar{4}2m$  (121); [2]  $I\bar{4}2d$  (122)

**II Minimal non-isomorphic klassengleiche supergroups**

## • Additional centring translations

none

## • Decreased unit cell

 [2]  $\mathbf{c}' = \frac{1}{2}\mathbf{c}$   $C\bar{4}$  (81,  $P\bar{4}$ )