

$C_4^2$ 
 $P4_1$ 

No. 76

 $P4_1$ 
**Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ; (2); (3)

**General position**

 Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

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

 [2]  $P2_1$  (4,  $P112_1$ ) 1; 2

**II Maximal klassengleiche subgroups**

## • Enlarged unit cell

 [2]  $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$ 
 $C4_1$  (76,  $P4_1$ )

 $\langle 2; 3 \rangle$ 
 $\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, \mathbf{c}$ 
 $C4_1$  (76,  $P4_1$ )

 $\langle 2 + (1, 1, 0); 3 + (1, 0, 0) \rangle$ 
 $\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, \mathbf{c}$ 
 $1/2, 1/2, 0$ 

 [3]  $\mathbf{c}' = 3\mathbf{c}$ 
 $P4_3$  (78)

 $\langle 2 + (0, 0, 1); 3 + (0, 0, 2) \rangle$ 
 $\mathbf{a}, \mathbf{b}, 3\mathbf{c}$ 

## • Series of maximal isomorphic subgroups

 [p]  $\mathbf{c}' = p\mathbf{c}$ 
 $P4_3$  (78)

 $\langle 2 + (0, 0, \frac{p}{2} - \frac{1}{2}); 3 + (0, 0, \frac{3p}{4} - \frac{1}{4}) \rangle$   
 prime  $p > 2$ ;  $p = 4n - 1$ 
 $\mathbf{a}, \mathbf{b}, p\mathbf{c}$ 
 $P4_1$  (76)

 $\langle 2 + (0, 0, \frac{p}{2} - \frac{1}{2}); 3 + (0, 0, \frac{p}{4} - \frac{1}{4}) \rangle$   
 prime  $p > 4$ ;  $p = 4n + 1$   
 no conjugate subgroups

 $\mathbf{a}, \mathbf{b}, p\mathbf{c}$ 

 [ $p^2$ ]  $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$ 
 $P4_1$  (76)

 $\langle 2 + (2u, 2v, 0); 3 + (u + v, -u + v, 0) \rangle$   
 prime  $p > 2$ ;  $0 \leq u < p$ ;  $0 \leq v < p$   
 $p^2$  conjugate subgroups for  $p = 4n - 1$ 
 $p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ 
 $u, v, 0$ 

 [ $p = q^2 + r^2$ ]  $\mathbf{a}' = q\mathbf{a} - r\mathbf{b}, \mathbf{b}' = r\mathbf{a} + q\mathbf{b}$ 
 $P4_1$  (76)

 $\langle 2 + (2u, 0, 0); 3 + (u, -u, 0) \rangle$   
 prime  $p > 4$ ;  $q > 0$ ;  $r > 0$ ;  $0 \leq u < p$   
 $p$  conjugate subgroups for  $p = 4n + 1$ 
 $q\mathbf{a} - r\mathbf{b}, r\mathbf{a} + q\mathbf{b}, \mathbf{c}$ 
 $u, 0, 0$ 
**I Minimal translationengleiche supergroups**

 [2]  $P4_122$  (91); [2]  $P4_12_12$  (92)

**II Minimal non-isomorphic klassengleiche supergroups**

## • Additional centring translations

 [2]  $I4_1$  (80)

## • Decreased unit cell

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