

$I4/m$

No. 87

$I4/m$

$C_{4h}^5$

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 *i* 1

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

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

I Maximal translationengleiche subgroups

[2]  $I\bar{4}$  (82) (1; 2; 7; 8)+  
[2]  $I4$  (79) (1; 2; 3; 4)+  
[2]  $I2/m$  (12,  $A112/m$ ) (1; 2; 5; 6)+ **b, -a - b, c**

II Maximal klassengleiche subgroups

• Loss of centring translations

[2]  $P4_2/n$  (86) 1; 2; 7; 8; (3; 4; 5; 6) +  $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$  1/4, 1/4, 1/4  
[2]  $P4/n$  (85) 1; 2; 3; 4; (5; 6; 7; 8) +  $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$  1/4, 1/4, 1/4  
[2]  $P4_2/m$  (84) 1; 2; 5; 6; (3; 4; 7; 8) +  $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$  0, 1/2, 0  
[2]  $P4/m$  (83) 1; 2; 3; 4; 5; 6; 7; 8

• Enlarged unit cell

[3]  $c' = 3c$   
 $\begin{cases} I4/m (87) & \langle 2; 3; 5 \rangle & \mathbf{a, b, 3c} \\ I4/m (87) & \langle 2; 3; 5 + (0,0,2) \rangle & \mathbf{a, b, 3c} & 0, 0, 1 \\ I4/m (87) & \langle 2; 3; 5 + (0,0,4) \rangle & \mathbf{a, b, 3c} & 0, 0, 2 \end{cases}$

• Series of maximal isomorphic subgroups

[*p*]  $c' = pc$   
 $I4/m (87) \quad \langle 2; 3; 5 + (0,0,2u) \rangle \quad \mathbf{a, b, pc} \quad 0, 0, u$   
 $p > 2; 0 \leq u < p$   
*p* conjugate subgroups for the prime *p*

[ $p^2$ ]  $a' = pa, b' = pb$   
 $I4/m (87) \quad \langle (2; 5) + (2u, 2v, 0); 3 + (u + v, -u + v, 0) \rangle \quad \mathbf{pa, pb, c} \quad u, v, 0$   
 $p > 2; 0 \leq u < p; 0 \leq v < p$   
 $p^2$  conjugate subgroups for prime  $p \equiv 3 \pmod{4}$

[ $p = q^2 + r^2$ ]  $a' = qa - rb, b' = ra + qb$   
 $I4/m (87) \quad \langle (2; 5) + (2u, 0, 0); 3 + (u, -u, 0) \rangle \quad \mathbf{qa - rb, ra + qb, c} \quad u, 0, 0$   
 $q > 0; r > 0; p > 4; 0 \leq u < p$   
 $p$  conjugate subgroups for prime  $p \equiv 1 \pmod{4}$

I Minimal translationengleiche supergroups

[2]  $I4/mmm$  (139); [2]  $I4/mcm$  (140)

II Minimal non-isomorphic klassengleiche supergroups

• Additional centring translations none

• Decreased unit cell

[2]  $c' = \frac{1}{2}c$   $C4/m$  (83),  $P4/m$