

$I4/mmm$ 

No. 139

 $I4/m2/m2/m$ 
 $D_{4h}^{17}$ 
**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); (9)

**General position**

 Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

	(0,0,0)+	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				
32	<i>o</i>	1	(1) $x,y,z$	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
			(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$
			(13) $x,\bar{y},z$	(14) $\bar{x},y,z$	(15) $\bar{y},\bar{x},z$	(16) $y,x,z$

**I Maximal translationengleiche subgroups**

[2] $I\bar{4}2m$ (121)	(1; 2; 5; 6; 11; 12; 15; 16)+	
[2] $I\bar{4}m2$ (119)	(1; 2; 7; 8; 11; 12; 13; 14)+	
[2] $I4mm$ (107)	(1; 2; 3; 4; 13; 14; 15; 16)+	
[2] $I422$ (97)	(1; 2; 3; 4; 5; 6; 7; 8)+	
[2] $I4/m11$ (87, $I4/m$ )	(1; 2; 3; 4; 9; 10; 11; 12)+	
[2] $I2/m2/m1$ (71, $Immm$ )	(1; 2; 5; 6; 9; 10; 13; 14)+	
[2] $I2/m12/m$ (69, $Fmmm$ )	(1; 2; 7; 8; 9; 10; 15; 16)+	<b>a – b, a + b, c</b>

**II Maximal klassengleiche subgroups**

## • Loss of centring translations

[2] $P4_2/nmc$ (137)	1; 2; 7; 8; 11; 12; 13; 14; (3; 4; 5; 6; 9; 10; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	1/4, 3/4, 1/4
[2] $P4_2/nmm$ (136)	1; 2; 7; 8; 9; 10; 15; 16; (3; 4; 5; 6; 11; 12; 13; 14) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	
[2] $P4_2/nm$ (134)	1; 2; 5; 6; 11; 12; 15; 16; (3; 4; 7; 8; 9; 10; 13; 14) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	1/4, 3/4, 1/4
[2] $P4_2/mmc$ (131)	1; 2; 5; 6; 9; 10; 13; 14; (3; 4; 7; 8; 11; 12; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	0, 1/2, 0
[2] $P4/nmm$ (129)	1; 2; 3; 4; 13; 14; 15; 16; (5; 6; 7; 8; 9; 10; 11; 12) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	1/4, 1/4, 1/4
[2] $P4/mnc$ (128)	1; 2; 3; 4; 9; 10; 11; 12; (5; 6; 7; 8; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	
[2] $P4/nnc$ (126)	1; 2; 3; 4; 5; 6; 7; 8; (9; 10; 11; 12; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	1/4, 1/4, 1/4
[2] $P4/mmm$ (123)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16	

## • Enlarged unit cell

[3] $\mathbf{c}' = 3\mathbf{c}$			
$\left\{ \begin{array}{l} I4/mmm \text{ (139)} \\ I4/mmm \text{ (139)} \\ I4/mmm \text{ (139)} \end{array} \right.$	$\langle 2; 3; 5; 9 \rangle$ $\langle 2; 3; (5; 9) + (0,0,2) \rangle$ $\langle 2; 3; (5; 9) + (0,0,4) \rangle$	<b>a, b, 3c</b> <b>a, b, 3c</b> <b>a, b, 3c</b>	0, 0, 1 0, 0, 2

## • Series of maximal isomorphic subgroups

[ $p$ ] $\mathbf{c}' = p\mathbf{c}$			
$I4/mmm$ (139)	$\langle 2; 3; (5; 9) + (0,0,2u) \rangle$ $p > 2; 0 \leq u < p$ $p$ conjugate subgroups for the prime $p$	<b>a, b, pc</b>	0, 0, $u$
[ $p^2$ ] $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$			
$I4/mmm$ (139)	$\langle (2; 9) + (2u, 2v, 0); 3 + (u + v, -u + v, 0); 5 + (2u, 0, 0) \rangle$ $p > 2; 0 \leq u < p; 0 \leq v < p$ $p^2$ conjugate subgroups for the prime $p$	<b>pa, pb, c</b>	$u, v, 0$

**I Minimal translationengleiche supergroups**

 [3]  $Fm\bar{3}m$  (225); [3]  $Im\bar{3}m$  (229)

**II Minimal non-isomorphic klassengleiche supergroups**

## • Additional centring translations

none

## • Decreased unit cell

 [2]  $\mathbf{c}' = \frac{1}{2}\mathbf{c}$   $C4/mmm$  (123,  $P4/mmm$ )