

$C_{2v}^{21}$  $Iba2$ 

No. 45

 $Iba2$ 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 c 1

(1)  $x,y,z$  (2)  $\bar{x},\bar{y},z$  (3)  $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$  (4)  $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$ 

## I Maximal translationengleiche subgroups

[2] $I1a1$ (9, $C1c1$ )	(1; 3)+	$\mathbf{a}-\mathbf{c}, \mathbf{b}, \mathbf{c}$
[2] $Ib11$ (9, $C1c1$ )	(1; 4)+	$-\mathbf{b}-\mathbf{c}, \mathbf{a}, \mathbf{c}$
[2] $I112$ (5, $A112$ )	(1; 2)+	$\mathbf{b}, -\mathbf{a}-\mathbf{b}, \mathbf{c}$

## II Maximal klassengleiche subgroups

## • Loss of centring translations

[2] $Pba2$ (32)	1; 2; 3; 4		
[2] $Pca2_1$ (29)	1; 3; (2; 4) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$		1/4, 1/4, 0
[2] $Pbc2_1$ (29, $Pca2_1$ )	1; 4; (2; 3) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$-\mathbf{b}, \mathbf{a}, \mathbf{c}$	1/4, 1/4, 0
[2] $Pcc2$ (27)	1; 2; (3; 4) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$		

## • Enlarged unit cell

[3] $\mathbf{a}' = 3\mathbf{a}$			
$\left\{ \begin{array}{l} Iba2 \text{ (45)} \\ Iba2 \text{ (45)} \\ Iba2 \text{ (45)} \end{array} \right.$	$\langle 2; 3 + (1, 0, 0) \rangle$ $\langle 2 + (2, 0, 0); 3 + (1, 0, 0) \rangle$ $\langle 2 + (4, 0, 0); 3 + (1, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$ $3\mathbf{a}, \mathbf{b}, \mathbf{c}$ $3\mathbf{a}, \mathbf{b}, \mathbf{c}$	 1, 0, 0 2, 0, 0
[3] $\mathbf{b}' = 3\mathbf{b}$			
$\left\{ \begin{array}{l} Iba2 \text{ (45)} \\ Iba2 \text{ (45)} \\ Iba2 \text{ (45)} \end{array} \right.$	$\langle 2; 3 + (0, 1, 0) \rangle$ $\langle 2 + (0, 2, 0); 3 + (0, 3, 0) \rangle$ $\langle 2 + (0, 4, 0); 3 + (0, 5, 0) \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$ $\mathbf{a}, 3\mathbf{b}, \mathbf{c}$ $\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	 0, 1, 0 0, 2, 0
[3] $\mathbf{c}' = 3\mathbf{c}$			
$Iba2$ (45)	$\langle 2; 3 \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	

## • Series of maximal isomorphic subgroups

[p] $\mathbf{a}' = p\mathbf{a}$			
$Iba2$ (45)	$\langle 2 + (2u, 0, 0); 3 + (\frac{p}{2} - \frac{1}{2}, 0, 0) \rangle$ prime $p > 2$ ; $0 \leq u < p$ $p$ conjugate subgroups	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$u, 0, 0$
[p] $\mathbf{b}' = p\mathbf{b}$			
$Iba2$ (45)	$\langle 2 + (0, 2u, 0); 3 + (0, \frac{p}{2} - \frac{1}{2} + 2u, 0) \rangle$ prime $p > 2$ ; $0 \leq u < p$ $p$ conjugate subgroups	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$0, u, 0$
[p] $\mathbf{c}' = p\mathbf{c}$			
$Iba2$ (45)	$\langle 2; 3 \rangle$ prime $p > 2$ no conjugate subgroups	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	

## I Minimal translationengleiche supergroups

[2]  $Ibam$  (72); [2]  $Ibca$  (73); [2]  $I4cm$  (108); [2]  $I4_1cd$  (110); [2]  $I\bar{4}c2$  (120)

## II Minimal non-isomorphic klassengleiche supergroups

## • Additional centring translations

none

## • Decreased unit cell

[2]  $\mathbf{c}' = \frac{1}{2}\mathbf{c}$   $Cmm2$  (35); [2]  $\mathbf{a}' = \frac{1}{2}\mathbf{a}$   $Aem2$  (39); [2]  $\mathbf{b}' = \frac{1}{2}\mathbf{b}$   $Bme2$  (39,  $Aem2$ )