

F222

No. 22

F222

 $D_2^7$ **Generators selected** (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(0,\frac{1}{2},\frac{1}{2})$ ;  $t(\frac{1}{2},0,\frac{1}{2})$ ; (2); (3)**General position**Multiplicity,  
Wyckoff letter,  
Site symmetryCoordinates  
 $(0,0,0) + (0,\frac{1}{2},\frac{1}{2}) + (\frac{1}{2},0,\frac{1}{2}) + (\frac{1}{2},\frac{1}{2},0) +$ 16       $k$       1(1)  $x,y,z$     (2)  $\bar{x},\bar{y},z$     (3)  $\bar{x},y,\bar{z}$     (4)  $x,\bar{y},\bar{z}$ **I Maximal translationengleiche subgroups**

[2] $F112$ (5, $A112$ )	(1; 2) +	$1/2(\mathbf{a} - \mathbf{b}), \mathbf{b}, \mathbf{c}$
[2] $F121$ (5, $C121$ )	(1; 3) +	$\mathbf{a}, \mathbf{b}, 1/2(-\mathbf{a} + \mathbf{c})$
[2] $F211$ (5, $C121$ )	(1; 4) +	$\mathbf{c}, \mathbf{a}, 1/2(\mathbf{b} - \mathbf{c})$

**II Maximal klassengleiche subgroups****• Loss of centring translations**

[2] $A222$ (21, $C222$ )	1; 2; 3; 4; (1; 2; 3; 4) + $(0, \frac{1}{2}, \frac{1}{2})$	$\mathbf{b}, \mathbf{c}, \mathbf{a}$	
[2] $A222$ (21, $C222$ )	1; 4; (1; 4) + $(0, \frac{1}{2}, \frac{1}{2})$ ; (2; 3) + $(\frac{1}{2}, 0, \frac{1}{2})$ ; (2; 3) + $(\frac{1}{2}, \frac{1}{2}, 0)$	$\mathbf{b}, \mathbf{c}, \mathbf{a}$	1/4, 1/4, 1/4
[2] $B222$ (21, $C222$ )	1; 2; 3; 4; (1; 2; 3; 4) + $(\frac{1}{2}, 0, \frac{1}{2})$	$\mathbf{c}, \mathbf{a}, \mathbf{b}$	
[2] $B222$ (21, $C222$ )	1; 3; (1; 3) + $(\frac{1}{2}, 0, \frac{1}{2})$ ; (2; 4) + $(\frac{1}{2}, \frac{1}{2}, 0)$ ; (2; 4) + $(0, \frac{1}{2}, \frac{1}{2})$	$\mathbf{c}, \mathbf{a}, \mathbf{b}$	1/4, 1/4, 1/4
[2] $C222$ (21)	1; 2; 3; 4; (1; 2; 3; 4) + $(\frac{1}{2}, \frac{1}{2}, 0)$		
[2] $C222$ (21)	1; 2; (1; 2) + $(\frac{1}{2}, \frac{1}{2}, 0)$ ; (3; 4) + $(0, \frac{1}{2}, \frac{1}{2})$ ; (3; 4) + $(\frac{1}{2}, 0, \frac{1}{2})$		1/4, 1/4, 1/4
[2] $A2_{1}22$ (20, $C222_1$ )	1; 2; (1; 2) + $(0, \frac{1}{2}, \frac{1}{2})$ ; (3; 4) + $(\frac{1}{2}, 0, \frac{1}{2})$ ; (3; 4) + $(\frac{1}{2}, \frac{1}{2}, 0)$	$\mathbf{b}, \mathbf{c}, \mathbf{a}$	1/4, 0, 1/4
[2] $A2_{1}22$ (20, $C222_1$ )	1; 3; (1; 3) + $(0, \frac{1}{2}, \frac{1}{2})$ ; (2; 4) + $(\frac{1}{2}, 0, \frac{1}{2})$ ; (2; 4) + $(\frac{1}{2}, \frac{1}{2}, 0)$	$\mathbf{b}, \mathbf{c}, \mathbf{a}$	0, 1/4, 0
[2] $B22_{1}2$ (20, $C222_1$ )	1; 2; (1; 2) + $(\frac{1}{2}, 0, \frac{1}{2})$ ; (3; 4) + $(\frac{1}{2}, \frac{1}{2}, 0)$ ; (3; 4) + $(0, \frac{1}{2}, \frac{1}{2})$	$\mathbf{c}, \mathbf{a}, \mathbf{b}$	0, 0, 1/4
[2] $B22_{1}2$ (20, $C222_1$ )	1; 4; (1; 4) + $(\frac{1}{2}, 0, \frac{1}{2})$ ; (2; 3) + $(\frac{1}{2}, \frac{1}{2}, 0)$ ; (2; 3) + $(0, \frac{1}{2}, \frac{1}{2})$	$\mathbf{c}, \mathbf{a}, \mathbf{b}$	1/4, 1/4, 0
[2] $C222_{1}$ (20)	1; 3; (1; 3) + $(\frac{1}{2}, \frac{1}{2}, 0)$ ; (2; 4) + $(0, \frac{1}{2}, \frac{1}{2})$ ; (2; 4) + $(\frac{1}{2}, 0, \frac{1}{2})$		0, 1/4, 1/4
[2] $C222_{1}$ (20)	1; 4; (1; 4) + $(\frac{1}{2}, \frac{1}{2}, 0)$ ; (2; 3) + $(0, \frac{1}{2}, \frac{1}{2})$ ; (2; 3) + $(\frac{1}{2}, 0, \frac{1}{2})$		1/4, 0, 0

**• Enlarged unit cell**

[3] $\mathbf{a}' = 3\mathbf{a}$			
$\left\{ \begin{array}{l} F222 \text{ (22)} \\ F222 \text{ (22)} \\ F222 \text{ (22)} \end{array} \right.$	$\langle 2; 3 \rangle$ $\langle (2; 3) + (2, 0, 0) \rangle$ $\langle (2; 3) + (4, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$ $3\mathbf{a}, \mathbf{b}, \mathbf{c}$ $3\mathbf{a}, \mathbf{b}, \mathbf{c}$	1, 0, 0 2, 0, 0
[3] $\mathbf{b}' = 3\mathbf{b}$			
$\left\{ \begin{array}{l} F222 \text{ (22)} \\ F222 \text{ (22)} \\ F222 \text{ (22)} \end{array} \right.$	$\langle 2; 3 \rangle$ $\langle 3; 2 + (0, 2, 0) \rangle$ $\langle 3; 2 + (0, 4, 0) \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$ $\mathbf{a}, 3\mathbf{b}, \mathbf{c}$ $\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	0, 1, 0 0, 2, 0
[3] $\mathbf{c}' = 3\mathbf{c}$			
$\left\{ \begin{array}{l} F222 \text{ (22)} \\ F222 \text{ (22)} \\ F222 \text{ (22)} \end{array} \right.$	$\langle 2; 3 \rangle$ $\langle 2; 3 + (0, 0, 2) \rangle$ $\langle 2; 3 + (0, 0, 4) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$ $\mathbf{a}, \mathbf{b}, 3\mathbf{c}$ $\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	0, 0, 1 0, 0, 2

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**I Minimal *translationengleiche* supergroups**

[2] *Cmmm* (65); [2] *Cccm* (66); [2] *Cmme* (67); [2] *Ccce* (68); [2] *P422* (89); [2] *P4<sub>2</sub>12* (90); [2] *P4<sub>2</sub>22* (93); [2] *P4<sub>2</sub>12* (94); [2] *P4̄m2* (115); [2] *P4̄c2* (116); [2] *P4̄b2* (117); [2] *P4̄n2* (118); [3] *P622* (177); [3] *P6<sub>2</sub>22* (180); [3] *P6<sub>4</sub>22* (181)

**II Minimal non-isomorphic *klassengleiche* supergroups**

- Additional centring translations

[2] *F222* (22)

- Decreased unit cell

[2]  $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ ,  $\mathbf{b}' = \frac{1}{2}\mathbf{b}$  *P222* (16)

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- Series of maximal isomorphic subgroups

[ <i>p</i> ] $\mathbf{a}' = p\mathbf{a}$ <i>F222</i> (22)	$\langle(2; 3) + (2u, 0, 0)\rangle$ $p > 2; 0 \leq u < p$ <i>p</i> conjugate subgroups for the prime <i>p</i>	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	<i>u, 0, 0</i>
[ <i>p</i> ] $\mathbf{b}' = p\mathbf{b}$ <i>F222</i> (22)	$\langle(3; 2 + (0, 2u, 0))\rangle$ $p > 2; 0 \leq u < p$ <i>p</i> conjugate subgroups for the prime <i>p</i>	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	<i>0, u, 0</i>
[ <i>p</i> ] $\mathbf{c}' = p\mathbf{c}$ <i>F222</i> (22)	$\langle(2; 3 + (0, 0, 2u))\rangle$ $p > 2; 0 \leq u < p$ <i>p</i> conjugate subgroups for the prime <i>p</i>	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	<i>0, 0, u</i>

**I Minimal *translationengleiche* supergroups**

[2] *Fmmm* (69); [2] *Fddd* (70); [2] *I422* (97); [2] *I4<sub>1</sub>22* (98); [2] *I4̄m2* (119); [2] *I4̄c2* (120); [3] *F23* (196)

**II Minimal non-isomorphic *klassengleiche* supergroups**

- Additional centring translations

none

- Decreased unit cell

[2]  $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ ,  $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ ,  $\mathbf{c}' = \frac{1}{2}\mathbf{c}$  *P222* (16)