

$Pcca$

No. 54

 $P2_1/c2/c2/a$ D_{2h}^8 Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

| | | | | | | |
|---|-----|---|---------------------------------|---|---|---|
| 8 | f | 1 | (1) x, y, z | (2) $\bar{x} + \frac{1}{2}, \bar{y}, z$ | (3) $\bar{x}, y, \bar{z} + \frac{1}{2}$ | (4) $x + \frac{1}{2}, \bar{y}, \bar{z} + \frac{1}{2}$ |
| | | | (5) $\bar{x}, \bar{y}, \bar{z}$ | (6) $x + \frac{1}{2}, y, \bar{z}$ | (7) $x, \bar{y}, z + \frac{1}{2}$ | (8) $\bar{x} + \frac{1}{2}, y, z + \frac{1}{2}$ |

I Maximal translationengleiche subgroups

| | | | |
|----------------------------------|------------|---------------------------------------|-----------|
| [2] $Pc2a$ (32, $Pba2$) | 1; 3; 6; 8 | $\mathbf{a}, -\mathbf{c}, \mathbf{b}$ | 0, 0, 1/4 |
| [2] $P2_1ca$ (29, $Pca2_1$) | 1; 4; 6; 7 | $\mathbf{c}, \mathbf{b}, -\mathbf{a}$ | 0, 0, 1/4 |
| [2] $Pcc2$ (27) | 1; 2; 7; 8 | | 1/4, 0, 0 |
| [2] $P2_122$ (17, $P222_1$) | 1; 2; 3; 4 | $\mathbf{b}, \mathbf{c}, \mathbf{a}$ | 0, 0, 1/4 |
| [2] $P2_1/c11$ (14, $P12_1/c1$) | 1; 4; 5; 8 | $-\mathbf{b}, \mathbf{a}, \mathbf{c}$ | |
| [2] $P112/a$ (13) | 1; 2; 5; 6 | | |
| [2] $P12/c1$ (13) | 1; 3; 5; 7 | | |

II Maximal klassengleiche subgroups

• Enlarged unit cell

| | | | |
|---------------------------------|---|---------------------------------------|-----------|
| [2] $\mathbf{b}' = 2\mathbf{b}$ | | | |
| $Pnca$ (60, $Pbcn$) | $\langle 2; 5; 3 + (0, 1, 0) \rangle$ | $2\mathbf{b}, \mathbf{c}, \mathbf{a}$ | |
| $Pnca$ (60, $Pbcn$) | $\langle (2; 3; 5) + (0, 1, 0) \rangle$ | $2\mathbf{b}, \mathbf{c}, \mathbf{a}$ | 0, 1/2, 0 |
| $Pccn$ (56) | $\langle 5; (2; 3) + (0, 1, 0) \rangle$ | $\mathbf{a}, 2\mathbf{b}, \mathbf{c}$ | |
| $Pccn$ (56) | $\langle 2; (3; 5) + (0, 1, 0) \rangle$ | $\mathbf{a}, 2\mathbf{b}, \mathbf{c}$ | 0, 1/2, 0 |
| $Pcca$ (54) | $\langle 2; 3; 5 \rangle$ | $\mathbf{a}, 2\mathbf{b}, \mathbf{c}$ | |
| $Pcca$ (54) | $\langle 3; (2; 5) + (0, 1, 0) \rangle$ | $\mathbf{a}, 2\mathbf{b}, \mathbf{c}$ | 0, 1/2, 0 |
| $Pncn$ (52, $Pnna$) | $\langle 3; 5; 2 + (0, 1, 0) \rangle$ | $\mathbf{c}, \mathbf{a}, 2\mathbf{b}$ | |
| $Pncn$ (52, $Pnna$) | $\langle 2; 3; 5 + (0, 1, 0) \rangle$ | $\mathbf{c}, \mathbf{a}, 2\mathbf{b}$ | 0, 1/2, 0 |
| [3] $\mathbf{a}' = 3\mathbf{a}$ | | | |
| $Pcca$ (54) | $\langle 3; 5; 2 + (1, 0, 0) \rangle$ | $3\mathbf{a}, \mathbf{b}, \mathbf{c}$ | |
| $Pcca$ (54) | $\langle 2 + (3, 0, 0); (3; 5) + (2, 0, 0) \rangle$ | $3\mathbf{a}, \mathbf{b}, \mathbf{c}$ | 1, 0, 0 |
| $Pcca$ (54) | $\langle 2 + (5, 0, 0); (3; 5) + (4, 0, 0) \rangle$ | $3\mathbf{a}, \mathbf{b}, \mathbf{c}$ | 2, 0, 0 |
| [3] $\mathbf{b}' = 3\mathbf{b}$ | | | |
| $Pcca$ (54) | $\langle 2; 3; 5 \rangle$ | $\mathbf{a}, 3\mathbf{b}, \mathbf{c}$ | |
| $Pcca$ (54) | $\langle 3; (2; 5) + (0, 2, 0) \rangle$ | $\mathbf{a}, 3\mathbf{b}, \mathbf{c}$ | 0, 1, 0 |
| $Pcca$ (54) | $\langle 3; (2; 5) + (0, 4, 0) \rangle$ | $\mathbf{a}, 3\mathbf{b}, \mathbf{c}$ | 0, 2, 0 |
| [3] $\mathbf{c}' = 3\mathbf{c}$ | | | |
| $Pcca$ (54) | $\langle 2; 5; 3 + (0, 0, 1) \rangle$ | $\mathbf{a}, \mathbf{b}, 3\mathbf{c}$ | |
| $Pcca$ (54) | $\langle 2; 3 + (0, 0, 3); 5 + (0, 0, 2) \rangle$ | $\mathbf{a}, \mathbf{b}, 3\mathbf{c}$ | 0, 0, 1 |
| $Pcca$ (54) | $\langle 2; 3 + (0, 0, 5); 5 + (0, 0, 4) \rangle$ | $\mathbf{a}, \mathbf{b}, 3\mathbf{c}$ | 0, 0, 2 |

• Series of maximal isomorphic subgroups

| | | | |
|-------------------------------------|---|---------------------------------------|-----------|
| [p] $\mathbf{a}' = p\mathbf{a}$ | | | |
| $Pcca$ (54) | $\langle 2 + (\frac{p}{2} - \frac{1}{2} + 2u, 0, 0); (3; 5) + (2u, 0, 0) \rangle$ | $p\mathbf{a}, \mathbf{b}, \mathbf{c}$ | $u, 0, 0$ |
| | prime $p > 2$; $0 \leq u < p$ | | |
| | p conjugate subgroups | | |
| [p] $\mathbf{b}' = p\mathbf{b}$ | | | |
| $Pcca$ (54) | $\langle 3; (2; 5) + (0, 2u, 0) \rangle$ | $\mathbf{a}, p\mathbf{b}, \mathbf{c}$ | $0, u, 0$ |
| | prime $p > 2$; $0 \leq u < p$ | | |
| | p conjugate subgroups | | |
| [p] $\mathbf{c}' = p\mathbf{c}$ | | | |
| $Pcca$ (54) | $\langle 2; 3 + (0, 0, \frac{p}{2} - \frac{1}{2} + 2u); 5 + (0, 0, 2u) \rangle$ | $\mathbf{a}, \mathbf{b}, p\mathbf{c}$ | $0, 0, u$ |
| | prime $p > 2$; $0 \leq u < p$ | | |
| | p conjugate subgroups | | |

I Minimal translationengleiche supergroups

none

II Minimal non-isomorphic klassengleiche supergroups

• Additional centring translations

[2] $Aema$ (64, $Cmce$); [2] $Bmem$ (67, $Cmme$); [2] $Ccce$ (68); [2] $Ibca$ (73)

• Decreased unit cell

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $Pccm$ (49); [2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $Pmma$ (51)