International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 125, pp. 252–253.

$P4/nbm$ No. 125 $P4/n2/b2/m$ D_{4h}^3

ORIGIN CHOICE 1, Origin at 422 at $4/n22/g$, at $-\frac{1}{4},-\frac{1}{4},0$ from centre $(2/m)$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
16 n 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) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	(12) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}$
	(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(16) $y+\frac{1}{2},x+\frac{1}{2},z$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}b2$ (117)	1; 2; 7; 8; 11; 12; 13; 14		$0,1/2,0$
[2] $P\bar{4}2m$ (111)	1; 2; 5; 6; 11; 12; 15; 16		$0,1/2,0$
[2] $P4bm$ (100)	1; 2; 3; 4; 13; 14; 15; 16		
[2] $P422$ (89)	1; 2; 3; 4; 5; 6; 7; 8		
[2] $P4/n11$ (85, $P4/n$)	1; 2; 3; 4; 9; 10; 11; 12		$0,1/2,0$
[2] $P2/n12/m$ (67, $Cmme$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/4,3/4,0$
[2] $P2/n2/b1$ (50, $Pban$)	1; 2; 5; 6; 9; 10; 13; 14		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P4_2/nnm$ (134)	$\langle 2;\ 9;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,1/2,1/2$
$P4_2/nnm$ (134)	$\langle 2;\ 5;\ (3;\ 9)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,1/2,0$
$P4_2/nbc$ (133)	$\langle 2;\ 5;\ 9;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,1/2,1/2$
$P4_2/nbc$ (133)	$\langle 2;\ (3;\ 5;\ 9)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,1/2,0$
$P4/nnc$ (126)	$\langle 2;\ 3;\ 9;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P4/nnc$ (126)	$\langle 2;\ 3;\ 5;\ 9+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4/nbm$ (125)	$\langle 2;\ 3;\ 5;\ 9\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4/nbm$ (125)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P4/nbm$ (125)	$\langle 2;\ 3;\ 5;\ 9\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4/nbm$ (125)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P4/nbm$ (125)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P4/nbm$ (125)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P4/nbm$ (125)	$\langle 2+(2u,2v,0);\ 3+(u+v,-u+v,0);\ 5+(2u,0,0);$ $9+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4/mmm$ (123, $P4/mmm$); [2] $I4/mcm$ (140)

- **Decreased unit cell** none

ORIGIN CHOICE 2, Origin at centre $(2/m)$ at $n(b,a)(2_1/g,2/m)$, at $\frac{1}{4},\frac{1}{4},0$ from 422

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
16 n 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{y}+\frac{1}{2},x,z$	(4) $y,\bar{x}+\frac{1}{2},z$
	(5) $\bar{x}+\frac{1}{2},y,\bar{z}$	(6) $x,\bar{y}+\frac{1}{2},\bar{z}$	(7) $y,x,\bar{z}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$
	(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x},\bar{z}$	(12) $\bar{y},x+\frac{1}{2},\bar{z}$
	(13) $x+\frac{1}{2},\bar{y},z$	(14) $\bar{x},y+\frac{1}{2},z$	(15) $\bar{y},\bar{x},z$	(16) $y+\frac{1}{2},x+\frac{1}{2},z$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}b2$ (117)	1; 2; 7; 8; 11; 12; 13; 14		$1/4,3/4,0$
[2] $P\bar{4}2m$ (111)	1; 2; 5; 6; 11; 12; 15; 16		$1/4,3/4,0$
[2] $P4bm$ (100)	1; 2; 3; 4; 13; 14; 15; 16		$1/4,1/4,0$
[2] $P422$ (89)	1; 2; 3; 4; 5; 6; 7; 8		$1/4,1/4,0$
[2] $P4/n11$ (85, $P4/n$)	1; 2; 3; 4; 9; 10; 11; 12		
[2] $P2/n12/m$ (67, $Cmme$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,0$
[2] $P2/n2/b1$ (50, $Pban$)	1; 2; 5; 6; 9; 10; 13; 14		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P4_2/nnm$ (134)	$\langle 2;\ 9;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4_2/nnm$ (134)	$\langle 2;\ 5;\ (3;\ 9)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P4_2/nbc$ (133)	$\langle 2;\ 5;\ 9;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4_2/nbc$ (133)	$\langle 2;\ (3;\ 5;\ 9)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P4/nnc$ (126)	$\langle 2;\ 3;\ 9;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4/nnc$ (126)	$\langle 2;\ 3;\ 5;\ 9+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P4/nbm$ (125)	$\langle 2;\ 3;\ 5;\ 9\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4/nbm$ (125)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P4/nbm$ (125)	$\langle 2;\ 3;\ 5;\ 9\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4/nbm$ (125)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P4/nbm$ (125)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P4/nbm$ (125)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P4/nbm$ (125)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0);$ $3+(\frac{p}{2}-\frac{1}{2}+u+v,-u+v,0);\ 5+(\frac{p}{2}-\frac{1}{2}+2u,0,0);$ $9+(2u,2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4/mmm$ (123, $P4/mmm$); [2] $I4/mcm$ (140)

- **Decreased unit cell** none