

$Pn\bar{3}m$

No. 224

 $P4_2/n\bar{3}2/m$ O_h^4 ORIGIN CHOICE 1, Origin at $\bar{4}\bar{3}m$, at $-\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4}$ from centre ($\bar{3}m$)**Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)**General position**

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

48	l	1	(1) x, y, z	(2) \bar{x}, \bar{y}, z	(3) \bar{x}, y, \bar{z}	(4) x, \bar{y}, \bar{z}
			(5) z, x, y	(6) z, \bar{x}, \bar{y}	(7) \bar{z}, \bar{x}, y	(8) \bar{z}, x, \bar{y}
			(9) y, z, x	(10) \bar{y}, z, \bar{x}	(11) y, \bar{z}, \bar{x}	(12) \bar{y}, \bar{z}, x
			(13) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(14) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(15) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$	(16) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$
			(17) $x + \frac{1}{2}, z + \frac{1}{2}, \bar{y} + \frac{1}{2}$	(18) $\bar{x} + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}$	(19) $\bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}$	(20) $x + \frac{1}{2}, \bar{z} + \frac{1}{2}, y + \frac{1}{2}$
			(21) $z + \frac{1}{2}, y + \frac{1}{2}, \bar{x} + \frac{1}{2}$	(22) $z + \frac{1}{2}, \bar{y} + \frac{1}{2}, x + \frac{1}{2}$	(23) $\bar{z} + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}$	(24) $\bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}$
			(25) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(26) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$	(27) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	(28) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$
			(29) $\bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}$	(30) $\bar{z} + \frac{1}{2}, x + \frac{1}{2}, y + \frac{1}{2}$	(31) $z + \frac{1}{2}, x + \frac{1}{2}, \bar{y} + \frac{1}{2}$	(32) $z + \frac{1}{2}, \bar{x} + \frac{1}{2}, y + \frac{1}{2}$
			(33) $\bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}$	(34) $y + \frac{1}{2}, \bar{z} + \frac{1}{2}, x + \frac{1}{2}$	(35) $\bar{y} + \frac{1}{2}, z + \frac{1}{2}, x + \frac{1}{2}$	(36) $y + \frac{1}{2}, z + \frac{1}{2}, \bar{x} + \frac{1}{2}$
			(37) \bar{y}, \bar{x}, z	(38) y, x, z	(39) \bar{y}, x, \bar{z}	(40) y, \bar{x}, \bar{z}
			(41) \bar{x}, \bar{z}, y	(42) x, \bar{z}, \bar{y}	(43) x, z, y	(44) \bar{x}, z, \bar{y}
			(45) \bar{z}, \bar{y}, x	(46) \bar{z}, y, \bar{x}	(47) z, y, \bar{x}	(48) z, y, x

I Maximal translationengleiche subgroups

[2] $P\bar{4}3m$ (215)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48
[2] $P4_232$ (208)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
[2] $Pn\bar{3}1$ (201, $Pn\bar{3}$)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36
{ [3] $P4_2/n12/m$ (134, $P4_2/nnm$)	1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40
{ [3] $P4_2/n12/m$ (134, $P4_2/nnm$)	1; 4; 2; 3; 18; 19; 17; 20; 25; 28; 26; 27; 42; 43; 41; 44
{ [3] $P4_2/n12/m$ (134, $P4_2/nnm$)	1; 3; 4; 2; 22; 24; 23; 21; 25; 27; 28; 26; 46; 48; 47; 45
{ [4] $P1\bar{3}2/m$ (166, $R\bar{3}m$)	1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48
{ [4] $P1\bar{3}2/m$ (166, $R\bar{3}m$)	1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48
{ [4] $P1\bar{3}2/m$ (166, $R\bar{3}m$)	1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46
{ [4] $P1\bar{3}2/m$ (166, $R\bar{3}m$)	1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46

II Maximal klassengleiche subgroups**• Enlarged unit cell**

[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$	
$Fd\bar{3}c$ (228)	$\langle 2; 3; 5; 25; 13 + (1, 1, 1) \rangle$
$Fd\bar{3}c$ (228)	$\langle 2; 3; 5; 13; 25 + (1, 1, 1) \rangle$
$Fd\bar{3}m$ (227)	$\langle 2; 3; 5; 13; 25 \rangle$
$Fd\bar{3}m$ (227)	$\langle 2; 3; 5; (13; 25) + (0, 0, 1) \rangle$

• Series of maximal isomorphic subgroups

[p^3] $\mathbf{a}' = p\mathbf{a}$, $\mathbf{b}' = p\mathbf{b}$, $\mathbf{c}' = p\mathbf{c}$	
$Pn\bar{3}m$ (224)	$\langle 2 + (2u, 2v, 0); 3 + (2u, 0, 2w);$ $5 + (u - w, -u + v, -v + w);$ $13 + (\frac{p}{2} - \frac{1}{2} + u - v, \frac{p}{2} - \frac{1}{2} - u + v, \frac{p}{2} - \frac{1}{2} + 2w);$ $25 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2v, \frac{p}{2} - \frac{1}{2} + 2w) \rangle$ $p > 2; 0 \leq u < p; 0 \leq v < p; 0 \leq w < p$ p^3 conjugate subgroups for the prime p
	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$
	u, v, w

CONTINUED

No. 224

ORIGIN CHOICE 1 $Pn\bar{3}m$

I Minimal *translationengleiche* supergroups

none

II Minimal non-isomorphic *klassengleiche* supergroups

- Additional centring translations

[2] $Im\bar{3}m$ (229); [4] $Fm\bar{3}m$ (225)

- Decreased unit cell

none

(Continued from the following page)

No. 224

ORIGIN CHOICE 2 $Pn\bar{3}m$

I Minimal *translationengleiche* supergroups

none

II Minimal non-isomorphic *klassengleiche* supergroups

- Additional centring translations

[2] $Im\bar{3}m$ (229); [4] $Fm\bar{3}m$ (225)

- Decreased unit cell

none

ORIGIN CHOICE 2, Origin at centre ($\bar{3}m$), at $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ from $\bar{4}3m$ **Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25)**General position**Multiplicity,
Wyckoff letter,
Site symmetry**Coordinates**

48	<i>l</i>	1	(1) x, y, z	(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	(3) $\bar{x} + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$	(4) $x, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$
			(5) z, x, y	(6) $z, \bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}$	(7) $\bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}, y$	(8) $\bar{z} + \frac{1}{2}, x, \bar{y} + \frac{1}{2}$
			(9) y, z, x	(10) $\bar{y} + \frac{1}{2}, z, \bar{x} + \frac{1}{2}$	(11) $y, \bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}$	(12) $\bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}, x$
			(13) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$	(14) $\bar{y}, \bar{x}, \bar{z}$	(15) $y + \frac{1}{2}, \bar{x}, z + \frac{1}{2}$	(16) $\bar{y}, x + \frac{1}{2}, z + \frac{1}{2}$
			(17) $x + \frac{1}{2}, z + \frac{1}{2}, \bar{y}$	(18) $\bar{x}, z + \frac{1}{2}, y + \frac{1}{2}$	(19) $\bar{x}, \bar{z}, \bar{y}$	(20) $x + \frac{1}{2}, \bar{z}, y + \frac{1}{2}$
			(21) $z + \frac{1}{2}, y + \frac{1}{2}, \bar{x}$	(22) $z + \frac{1}{2}, \bar{y}, x + \frac{1}{2}$	(23) $\bar{z}, y + \frac{1}{2}, x + \frac{1}{2}$	(24) $\bar{z}, \bar{y}, \bar{x}$
			(25) $\bar{x}, \bar{y}, \bar{z}$	(26) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$	(27) $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$	(28) $\bar{x}, y + \frac{1}{2}, z + \frac{1}{2}$
			(29) $\bar{z}, \bar{x}, \bar{y}$	(30) $\bar{z}, x + \frac{1}{2}, y + \frac{1}{2}$	(31) $z + \frac{1}{2}, x + \frac{1}{2}, \bar{y}$	(32) $z + \frac{1}{2}, \bar{x}, y + \frac{1}{2}$
			(33) $\bar{y}, \bar{z}, \bar{x}$	(34) $y + \frac{1}{2}, \bar{z}, x + \frac{1}{2}$	(35) $\bar{y}, z + \frac{1}{2}, x + \frac{1}{2}$	(36) $y + \frac{1}{2}, z + \frac{1}{2}, \bar{x}$
			(37) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, z$	(38) y, x, z	(39) $\bar{y} + \frac{1}{2}, x, \bar{z} + \frac{1}{2}$	(40) $y, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$
			(41) $\bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}, y$	(42) $x, \bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}$	(43) x, z, y	(44) $\bar{x} + \frac{1}{2}, z, \bar{y} + \frac{1}{2}$
			(45) $\bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}, x$	(46) $\bar{z} + \frac{1}{2}, y, \bar{x} + \frac{1}{2}$	(47) $z, \bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}$	(48) z, y, x

I Maximal translationengleiche subgroups

[2] P $\bar{4}3m$ (215)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39;	1/4, 1/4, 1/4
[2] P4 ₂ 32 (208)	40; 41; 42; 43; 44; 45; 46; 47; 48	
[2] Pn $\bar{3}$ 1 (201, Pn $\bar{3}$)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36	1/4, 1/4, 1/4
{ [3] P4 ₂ /n12/m (134, P4 ₂ /nnm)	1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40	0, 1/2, 0
{ [3] P4 ₂ /n12/m (134, P4 ₂ /nnm)	1; 4; 2; 3; 18; 19; 17; 20; 25; 28; 26; 27; 42; 43; 41; 44	0, 0, 1/2
{ [3] P4 ₂ /n12/m (134, P4 ₂ /nnm)	1; 3; 4; 2; 22; 24; 23; 21; 25; 27; 28; 26; 46; 48; 47; 45	1/2, 0, 0
{ [4] P1 $\bar{3}$ 2/m (166, R $\bar{3}$ m)	1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48	$\mathbf{a} - \mathbf{b}, \mathbf{b} - \mathbf{c}, \mathbf{a} + \mathbf{b} + \mathbf{c}$
{ [4] P1 $\bar{3}$ 2/m (166, R $\bar{3}$ m)	1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48	$-\mathbf{a} - \mathbf{b}, \mathbf{b} + \mathbf{c}, -\mathbf{a} + \mathbf{b} - \mathbf{c}$
{ [4] P1 $\bar{3}$ 2/m (166, R $\bar{3}$ m)	1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46	1/2, 0, 1/2
{ [4] P1 $\bar{3}$ 2/m (166, R $\bar{3}$ m)	1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46	$\mathbf{a} + \mathbf{b}, -\mathbf{b} + \mathbf{c}, \mathbf{a} - \mathbf{b} - \mathbf{c}$
		0, 1/2, 1/2
		$-\mathbf{a} + \mathbf{b}, -\mathbf{b} - \mathbf{c}, -\mathbf{a} - \mathbf{b} + \mathbf{c}$
		1/2, 1/2, 0

II Maximal klassengleiche subgroups**• Enlarged unit cell**

[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$		
Fd $\bar{3}c$ (228)	$\langle 2; 3; 5; 25; 13 + (1, 1, 1) \rangle$	2 \mathbf{a} , 2 \mathbf{b} , 2 \mathbf{c}
Fd $\bar{3}c$ (228)	$\langle 2; 3; 5; 13; 25 + (1, 1, 1) \rangle$	2 \mathbf{a} , 2 \mathbf{b} , 2 \mathbf{c}
Fd $\bar{3}m$ (227)	$\langle 2; 3; 5; 13; 25 \rangle$	2 \mathbf{a} , 2 \mathbf{b} , 2 \mathbf{c}
Fd $\bar{3}m$ (227)	$\langle 2; 3; 5; (13; 25) + (0, 0, 1) \rangle$	2 \mathbf{a} , 2 \mathbf{b} , 2 \mathbf{c}
		1/2, 1/2, 1/2

• Series of maximal isomorphic subgroups

[p ³] $\mathbf{a}' = p\mathbf{a}$, $\mathbf{b}' = p\mathbf{b}$, $\mathbf{c}' = p\mathbf{c}$		
Pn $\bar{3}m$ (224)	$\langle 2 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2v, 0);$ $3 + (\frac{p}{2} - \frac{1}{2} + 2u, 0, \frac{p}{2} - \frac{1}{2} + 2w);$ $5 + (u - w, -u + v, -v + w);$ $13 + (\frac{p}{2} - \frac{1}{2} + u - v, \frac{p}{2} - \frac{1}{2} - u + v, 2w);$ $25 + (2u, 2v, 2w) \rangle$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$
	$p > 2; 0 \leq u < p; 0 \leq v < p; 0 \leq w < p$	u, v, w
	p^3 conjugate subgroups for the prime p	

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No. 224

ORIGIN CHOICE 1 $Pn\bar{3}m$

I Minimal *translationengleiche* supergroups

none

II Minimal non-isomorphic *klassengleiche* supergroups

- Additional centring translations

[2] $Im\bar{3}m$ (229); [4] $Fm\bar{3}m$ (225)

- Decreased unit cell

none

(Continued from the following page)

No. 224

ORIGIN CHOICE 2 $Pn\bar{3}m$

I Minimal *translationengleiche* supergroups

none

II Minimal non-isomorphic *klassengleiche* supergroups

- Additional centring translations

[2] $Im\bar{3}m$ (229); [4] $Fm\bar{3}m$ (225)

- Decreased unit cell

none