$I4_1/amd$ No. 141 $I4_1/a2/m2/d$ D_{4h}^{19}

ORIGIN CHOICE 1, Origin at $\bar{4}m2$, at $0,\frac{1}{4},-\frac{1}{8}$ from centre $(2/m)$

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); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry		Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			
32	i 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$
		(5) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{3}{4}$	(6) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}$
		(9) $\bar{x},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$	(10) $x+\frac{1}{2},y,\bar{z}+\frac{3}{4}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$
		(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{x},y,z$	(15) $\bar{y}+\frac{1}{2},\bar{x},z+\frac{3}{4}$	(16) $y,x+\frac{1}{2},z+\frac{1}{4}$

I Maximal *translationengleiche* subgroups

[2] $I\bar{4}2d$ (122)	(1; 2; 5; 6; 11; 12; 15; 16)+		
[2] $I\bar{4}m2$ (119)	(1; 2; 7; 8; 11; 12; 13; 14)+		
[2] $I4_1md$ (109)	(1; 2; 3; 4; 13; 14; 15; 16)+		
[2] $I4_122$ (98)	(1; 2; 3; 4; 5; 6; 7; 8)+		
[2] $I4_1/a11$ (88, $I4_1/a$)	(1; 2; 3; 4; 9; 10; 11; 12)+		
[2] $I2/a2/m1$ (74, $Imma$)	(1; 2; 5; 6; 9; 10; 13; 14)+		$0,1/4,1/8$
[2] $I2/a12/d$ (70, $Fddd$)	(1; 2; 7; 8; 9; 10; 15; 16)+	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,1/4$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** none

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$I4_1/amd$ (141)	$\langle(2;\ 9)+(1,0,1);\ 3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2});\ 5+(1,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/2,0,1/4$
$I4_1/amd$ (141)	$\langle 2+(1,0,1);\ 3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2});\ 5+(1,0,4);\ 9+(1,0,3)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/2,0,5/4$
$I4_1/amd$ (141)	$\langle 2+(1,0,1);\ 3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2});\ 5+(1,0,6);\ 9+(1,0,5)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/2,0,9/4$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$I4_1/amd$ (141)	$\langle 2+(1,0,\frac{p}{2}-\frac{1}{2});\ 3+(\frac{1}{2},-\frac{1}{2},\frac{p}{4}-\frac{1}{4});\ 5+(1,0,\frac{3p}{4}-\frac{1}{4}+2u);$ $9+(1,0,\frac{p}{4}+\frac{1}{4}+2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 3\ (\mathrm{mod}\ 4)$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$1/2,0,1/4+u$
$I4_1/amd$ (141)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{4}-\frac{1}{4});\ 5+(0,0,\frac{3p}{4}-\frac{3}{4}+2u);$ $9+(0,0,\frac{p}{4}-\frac{1}{4}+2u)\rangle$ $p>4;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1\ (\mathrm{mod}\ 4)$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$I4_1/amd$ (141)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0);\ 3+(u+v,\frac{p}{2}-\frac{1}{2}-u+v,0);$ $5+(\frac{p}{2}-\frac{1}{2}+2u,0,0);\ 9+(2u,\frac{p}{2}-\frac{1}{2}+2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[3] $Fd\bar{3}m$ (227)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $C4_2/emd$ (134, $P4_2/nnm$)

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ORIGIN CHOICE 2, Origin at centre $(2/m)$ at $b\,(2/m, 2_1/n)\,d$, at $0, -\frac{1}{4}, \frac{1}{8}$ from $\bar{4}m2$

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); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry		Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			
32	i 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{y}+\frac{1}{4},x+\frac{3}{4},z+\frac{1}{4}$	(4) $y+\frac{1}{4},\bar{x}+\frac{1}{4},z+\frac{3}{4}$
		(5) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(6) $x,\bar{y},\bar{z}$	(7) $y+\frac{1}{4},x+\frac{3}{4},\bar{z}+\frac{1}{4}$	(8) $\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4}$
		(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(11) $y+\frac{3}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4}$	(12) $\bar{y}+\frac{3}{4},x+\frac{3}{4},\bar{z}+\frac{1}{4}$
		(13) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(14) $\bar{x},y,z$	(15) $\bar{y}+\frac{3}{4},\bar{x}+\frac{1}{4},z+\frac{3}{4}$	(16) $y+\frac{3}{4},x+\frac{3}{4},z+\frac{1}{4}$

I Maximal *translationengleiche* subgroups

[2] $I\bar{4}2d$ (122)	(1; 2; 5; 6; 11; 12; 15; 16)+		$0,1/4,3/8$
[2] $I\bar{4}m2$ (119)	(1; 2; 7; 8; 11; 12; 13; 14)+		$0,1/4,3/8$
[2] $I4_1md$ (109)	(1; 2; 3; 4; 13; 14; 15; 16)+		$0,1/4,0$
[2] $I4_122$ (98)	(1; 2; 3; 4; 5; 6; 7; 8)+		$0,1/4,3/8$
[2] $I4_1/a11$ (88, $I4_1/a$)	(1; 2; 3; 4; 9; 10; 11; 12)+		$0,1/2,0$
[2] $I2/a2/m1$ (74, $Imma$)	(1; 2; 5; 6; 9; 10; 13; 14)+		
[2] $I2/a12/d$ (70, $Fddd$)	(1; 2; 7; 8; 9; 10; 15; 16)+	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/4,3/4,1/4$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** none

- **Enlarged unit cell**

[3] $\mathbf{c}' = 3\mathbf{c}$

$I4_1/amd$ (141)	$\langle(2;\,5)+(1,0,1);\,3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2});\,9+(1,0,0)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/2,0,0$
$I4_1/amd$ (141)	$\langle 2+(1,0,1);\,3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2});\,5+(1,0,3);\,9+(1,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/2,0,1$
$I4_1/amd$ (141)	$\langle 2+(1,0,1);\,3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2});\,5+(1,0,5);\,9+(1,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/2,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}' = p\mathbf{c}$

$I4_1/amd$ (141)	$\langle 2+(1,0,\frac{p}{2}-\frac{1}{2});\,3+(\frac{1}{2},-\frac{1}{2},\frac{p}{4}-\frac{1}{4});\,5+(1,0,\frac{p}{2}-\frac{1}{2}+2u);$ $9+(1,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 3\pmod 4$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$1/2,0,u$
$I4_1/amd$ (141)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\,3+(0,0,\frac{p}{4}-\frac{1}{4});\,5+(0,0,\frac{p}{2}-\frac{1}{2}+2u);$ $9+(0,0,2u)\rangle$ $p>4;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1\pmod 4$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}' = p\mathbf{a},\ \mathbf{b}' = p\mathbf{b}$

$I4_1/amd$ (141)	$\langle 2+(\frac{p}{2}+\frac{1}{2}+2u,2v,0);\,3+(\frac{p}{4}+\frac{1}{4}+u+v,\frac{3p}{4}-\frac{5}{4}-u+v,0);$ $5+(\frac{p}{2}+\frac{1}{2}+2u,0,0);\,9+(1+2u,2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 3\pmod 4$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$1/2+u,v,0$
$I4_1/amd$ (141)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,2v,0);\,3+(\frac{p}{4}-\frac{1}{4}+u+v,\frac{3p}{4}-\frac{3}{4}-u+v,0);$ $5+(\frac{p}{2}-\frac{1}{2}+2u,0,0);\,9+(2u,2v,0)\rangle$ $p>4;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 1\pmod 4$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[3] $Fd\bar{3}m$ (227)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $C4_2/emd$ (134, $P4_2/nnm$)