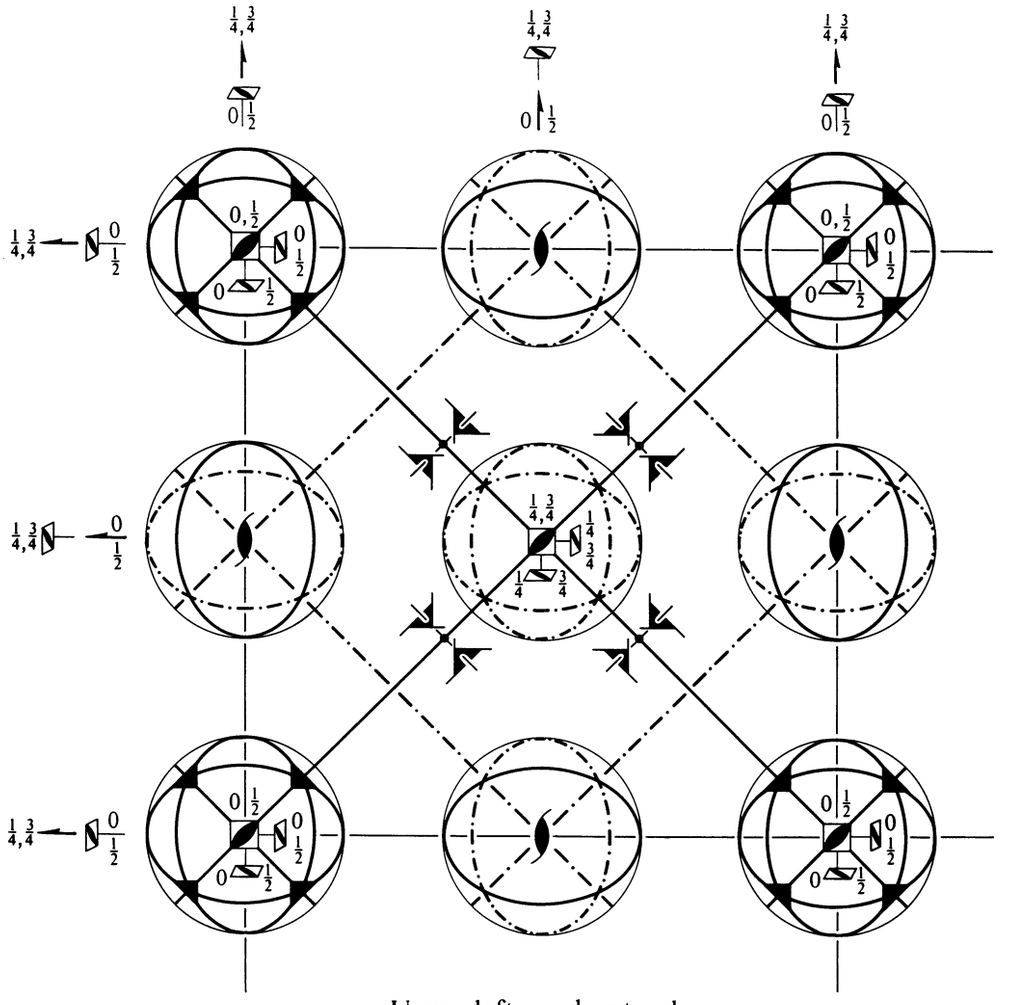
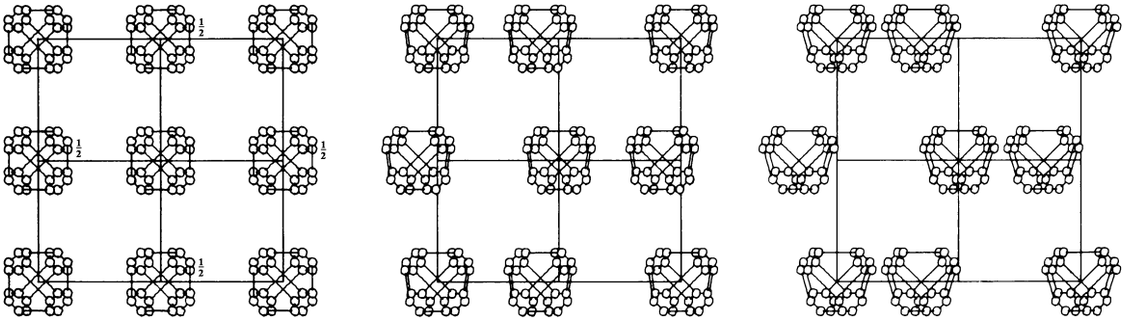
# $F\bar{4}3m$ $T_d^2$ $\bar{4}3m$ Cubic

No. 216 $F\bar{4}3m$ Patterson symmetry $Fm\bar{3}m$



Upper left quadrant only



**Origin** at $\bar{4}3m$

**Asymmetric unit** $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{4}$; $-\frac{1}{4} \le z \le \frac{1}{4}$; $y \le \min(x, \frac{1}{2} - x)$; $-y \le z \le y$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{1}{4},\frac{1}{4},-\frac{1}{4}$

**Symmetry operations**

For (0,0,0)+ set

| | | | |
|---|---|---|---|
| (1) 1 | (2) 2 0,0,$z$ | (3) 2 0,$y$,0 | (4) 2 $x$,0,0 |
| (5) $3^+$ $x,x,x$ | (6) $3^+$ $\bar{x},x,\bar{x}$ | (7) $3^+$ $x,\bar{x},\bar{x}$ | (8) $3^+$ $\bar{x},\bar{x},x$ |
| (9) $3^-$ $x,x,x$ | (10) $3^-$ $x,\bar{x},\bar{x}$ | (11) $3^-$ $\bar{x},\bar{x},x$ | (12) $3^-$ $\bar{x},x,\bar{x}$ |
| (13) $m$ $x,x,z$ | (14) $m$ $x,\bar{x},z$ | (15) $\bar{4}^+$ 0,0,$z$; 0,0,0 | (16) $\bar{4}^-$ 0,0,$z$; 0,0,0 |
| (17) $m$ $x,y,y$ | (18) $\bar{4}^+$ $x$,0,0; 0,0,0 | (19) $\bar{4}^-$ $x$,0,0; 0,0,0 | (20) $m$ $x,y,\bar{y}$ |
| (21) $m$ $x,y,x$ | (22) $\bar{4}^-$ 0,$y$,0; 0,0,0 | (23) $m$ $\bar{x},y,x$ | (24) $\bar{4}^+$ 0,$y$,0; 0,0,0 |

For $(0,\frac{1}{2},\frac{1}{2})+$ set

| | | | |
|---|---|---|---|
| (1) $t(0,\frac{1}{2},\frac{1}{2})$ | (2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$ | (3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$ | (4) 2 $x,\frac{1}{4},\frac{1}{4}$ |
| (5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{3},x-\frac{1}{6},x$ | (6) $3^+$ $\bar{x},x+\frac{1}{2},\bar{x}$ | (7) $3^+(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$ | (8) $3^+$ $\bar{x},\bar{x}+\frac{1}{2},x$ |
| (9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x+\frac{1}{6},x$ | (10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ | (11) $3^-$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$ | (12) $3^-$ $\bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$ |
| (13) $g(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x-\frac{1}{4},x,z$ | (14) $g(-\frac{1}{4},\frac{1}{4},\frac{1}{2})$ $x+\frac{1}{4},\bar{x},z$ | (15) $\bar{4}^+$ $\frac{1}{4},\frac{1}{4},z$; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ | (16) $\bar{4}^-$ $-\frac{1}{4},\frac{1}{4},z$; $-\frac{1}{4},\frac{1}{4},\frac{1}{4}$ |
| (17) $g(0,\frac{1}{2},\frac{1}{2})$ $x,y,y$ | (18) $\bar{4}^+$ $x,\frac{1}{2},0$; $0,\frac{1}{2},0$ | (19) $\bar{4}^-$ $x,0,\frac{1}{2}$; $0,0,\frac{1}{2}$ | (20) $m$ $x,y+\frac{1}{2},\bar{y}$ |
| (21) $g(\frac{1}{4},\frac{1}{2},\frac{1}{4})$ $x-\frac{1}{4},y,x$ | (22) $\bar{4}^-$ $\frac{1}{4},y,\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ | (23) $g(-\frac{1}{4},\frac{1}{2},\frac{1}{4})$ $\bar{x}+\frac{1}{4},y,x$ | (24) $\bar{4}^+$ $-\frac{1}{4},y,\frac{1}{4}$; $-\frac{1}{4},\frac{1}{4},\frac{1}{4}$ |

For $(\frac{1}{2},0,\frac{1}{2})+$ set

| | | | |
|---|---|---|---|
| (1) $t(\frac{1}{2},0,\frac{1}{2})$ | (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$ | (3) 2 $\frac{1}{4},y,\frac{1}{4}$ | (4) $2(\frac{1}{2},0,0)$ $x,0,\frac{1}{4}$ |
| (5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x-\frac{1}{6},x$ | (6) $3^+(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$ | (7) $3^+$ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$ | (8) $3^+$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$ |
| (9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x-\frac{1}{3},x$ | (10) $3^-$ $x+\frac{1}{2},\bar{x},\bar{x}$ | (11) $3^-$ $\bar{x}+\frac{1}{2},\bar{x},x$ | (12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$ |
| (13) $g(\frac{1}{4},\frac{1}{4},\frac{1}{2})$ $x+\frac{1}{4},x,z$ | (14) $g(\frac{1}{4},-\frac{1}{4},\frac{1}{2})$ $x+\frac{1}{4},\bar{x},z$ | (15) $\bar{4}^+$ $\frac{1}{4},-\frac{1}{4},z$; $\frac{1}{4},-\frac{1}{4},\frac{1}{4}$ | (16) $\bar{4}^-$ $\frac{1}{4},\frac{1}{4},z$; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ |
| (17) $g(\frac{1}{2},\frac{1}{4},\frac{1}{4})$ $x,y-\frac{1}{4},y$ | (18) $\bar{4}^+$ $x,\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ | (19) $\bar{4}^-$ $x,-\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},-\frac{1}{4},\frac{1}{4}$ | (20) $g(\frac{1}{2},-\frac{1}{4},\frac{1}{4})$ $x,y+\frac{1}{4},\bar{y}$ |
| (21) $g(\frac{1}{2},0,\frac{1}{2})$ $x,y,x$ | (22) $\bar{4}^-$ $\frac{1}{2},y,0$; $\frac{1}{2},0,0$ | (23) $m$ $\bar{x}+\frac{1}{2},y,x$ | (24) $\bar{4}^+$ 0,$y$,$\frac{1}{2}$; 0,0,$\frac{1}{2}$ |

For $(\frac{1}{2},\frac{1}{2},0)+$ set

| | | | |
|---|---|---|---|
| (1) $t(\frac{1}{2},\frac{1}{2},0)$ | (2) 2 $\frac{1}{4},\frac{1}{4},z$ | (3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$ | (4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$ |
| (5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x+\frac{1}{3},x$ | (6) $3^+$ $\bar{x}+\frac{1}{2},x,\bar{x}$ | (7) $3^+$ $x+\frac{1}{2},\bar{x},\bar{x}$ | (8) $3^+(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$ |
| (9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},x+\frac{1}{6},x$ | (10) $3^-$ $x,\bar{x}+\frac{1}{2},\bar{x}$ | (11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$ | (12) $3^-$ $\bar{x},x+\frac{1}{2},\bar{x}$ |
| (13) $g(\frac{1}{2},\frac{1}{2},0)$ $x,x,z$ | (14) $m$ $x+\frac{1}{2},\bar{x},z$ | (15) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,0$ | (16) $\bar{4}^-$ 0,$\frac{1}{2}$,$z$; 0,$\frac{1}{2}$,0 |
| (17) $g(\frac{1}{2},\frac{1}{4},\frac{1}{4})$ $x,y+\frac{1}{4},y$ | (18) $\bar{4}^+$ $x,\frac{1}{4},-\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},-\frac{1}{4}$ | (19) $\bar{4}^-$ $x,\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ | (20) $g(\frac{1}{2},\frac{1}{4},-\frac{1}{4})$ $x,y+\frac{1}{4},\bar{y}$ |
| (21) $g(\frac{1}{4},\frac{1}{2},\frac{1}{4})$ $x+\frac{1}{4},y,x$ | (22) $\bar{4}^-$ $\frac{1}{4},y,-\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},-\frac{1}{4}$ | (23) $g(\frac{1}{4},\frac{1}{2},-\frac{1}{4})$ $\bar{x}+\frac{1}{4},y,x$ | (24) $\bar{4}^+$ $\frac{1}{4},y,\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ |

**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); (5); (13)

**Positions**

| Multiplicity, Wyckoff letter, Site symmetry | | | Coordinates (0,0,0)+ | (0,$\frac{1}{2}$,$\frac{1}{2}$)+ | ($\frac{1}{2}$,0,$\frac{1}{2}$)+ | ($\frac{1}{2}$,$\frac{1}{2}$,0)+ | Reflection conditions |
|---|---|---|---|---|---|---|---|
| | | | | | | | $h,k,l$ permutable |
| | | | | | | | General: |
| 96 | $i$ | 1 | (1) $x,y,z$ | (2) $\bar{x},\bar{y},z$ | (3) $\bar{x},y,\bar{z}$ | (4) $x,\bar{y},\bar{z}$ | $hkl$ : $h+k,h+l,k+l=2n$ |
| | | | (5) $z,x,y$ | (6) $z,\bar{x},\bar{y}$ | (7) $\bar{z},\bar{x},y$ | (8) $\bar{z},x,\bar{y}$ | $0kl$ : $k,l=2n$ |
| | | | (9) $y,z,x$ | (10) $\bar{y},z,\bar{x}$ | (11) $y,\bar{z},\bar{x}$ | (12) $\bar{y},\bar{z},x$ | $hhl$ : $h+l=2n$ |
| | | | (13) $y,x,z$ | (14) $\bar{y},\bar{x},z$ | (15) $y,\bar{x},\bar{z}$ | (16) $\bar{y},x,\bar{z}$ | $h00$ : $h=2n$ |
| | | | (17) $x,z,y$ | (18) $\bar{x},z,\bar{y}$ | (19) $\bar{x},\bar{z},y$ | (20) $x,\bar{z},\bar{y}$ | |
| | | | (21) $z,y,x$ | (22) $z,\bar{y},\bar{x}$ | (23) $\bar{z},y,\bar{x}$ | (24) $\bar{z},\bar{y},x$ | |
| | | | | | | | Special: no extra conditions |
| 48 | $h$ | . . $m$ | $x,x,z$ | $\bar{x},\bar{x},z$ | $\bar{x},x,\bar{z}$ | $x,\bar{x},\bar{z}$ | $z,x,x$ $z,\bar{x},\bar{x}$ |
| | | | $\bar{z},\bar{x},x$ | $\bar{z},x,\bar{x}$ | $x,z,x$ | $\bar{x},z,\bar{x}$ | $x,\bar{z},\bar{x}$ $\bar{x},\bar{z},x$ |
| 24 | $g$ | 2 . $mm$ | $x,\frac{1}{4},\frac{1}{4}$ | $\bar{x},\frac{3}{4},\frac{1}{4}$ | $\frac{1}{4},x,\frac{1}{4}$ | $\frac{1}{4},\bar{x},\frac{3}{4}$ | $\frac{1}{4},\frac{1}{4},x$ $\frac{3}{4},\frac{1}{4},\bar{x}$ |
| 24 | $f$ | 2 . $mm$ | $x,0,0$ | $\bar{x},0,0$ | $0,x,0$ | $0,\bar{x},0$ | $0,0,x$ $0,0,\bar{x}$ |
| 16 | $e$ | . 3 $m$ | $x,x,x$ | $\bar{x},\bar{x},x$ | $\bar{x},x,\bar{x}$ | $x,\bar{x},\bar{x}$ | |
| 4 | $d$ | $\bar{4}$ 3 $m$ | $\frac{3}{4},\frac{3}{4},\frac{3}{4}$ | | | | |
| 4 | $c$ | $\bar{4}$ 3 $m$ | $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ | | | | |
| 4 | $b$ | $\bar{4}$ 3 $m$ | $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ | | | | |
| 4 | $a$ | $\bar{4}$ 3 $m$ | $0,0,0$ | | | | |

### Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [111] $p31m$
$\mathbf{a}' = \frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at $x,x,x$

Along [110] $c1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

### Maximal non-isomorphic subgroups

**I**
[2] $F231$ ($F23$, 196) (1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+
[3] $F\bar{4}1m$ ($I\bar{4}m2$, 119) (1; 2; 3; 4; 13; 14; 15; 16)+
[3] $F\bar{4}1m$ ($I\bar{4}m2$, 119) (1; 2; 3; 4; 17; 18; 19; 20)+
[3] $F\bar{4}1m$ ($I\bar{4}m2$, 119) (1; 2; 3; 4; 21; 22; 23; 24)+
[4] $F13m$ ($R3m$, 160) (1; 5; 9; 13; 17; 21)+
[4] $F13m$ ($R3m$, 160) (1; 6; 12; 14; 20; 21)+
[4] $F13m$ ($R3m$, 160) (1; 7; 10; 14; 17; 23)+
[4] $F13m$ ($R3m$, 160) (1; 8; 11; 13; 20; 23)+

**IIa**
[4] $P\bar{4}3m$ (215) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24
[4] $P\bar{4}3m$ (215) 1; 2; 3; 4; 13; 14; 15; 16; (9; 10; 11; 12; 17; 18; 19; 20) + $(0,\frac{1}{2},\frac{1}{2})$; (5; 6; 7; 8; 21; 22; 23; 24) + $(\frac{1}{2},0,\frac{1}{2})$
[4] $P\bar{4}3m$ (215) 1; 2; 3; 4; 17; 18; 19; 20; (9; 10; 11; 12; 21; 22; 23; 24) + $(\frac{1}{2},0,\frac{1}{2})$; (5; 6; 7; 8; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},0)$
[4] $P\bar{4}3m$ (215) 1; 2; 3; 4; 21; 22; 23; 24; (5; 6; 7; 8; 17; 18; 19; 20) + $(0,\frac{1}{2},\frac{1}{2})$; (9; 10; 11; 12; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},0)$
[4] $P\bar{4}3m$ (215) 1; 5; 9; 13; 17; 21; (4; 6; 11; 15; 20; 22) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 8; 10; 16; 18; 23) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 7; 12; 14; 19; 24) + $(\frac{1}{2},\frac{1}{2},0)$
[4] $P\bar{4}3m$ (215) 1; 6; 12; 14; 20; 21; (4; 5; 10; 16; 17; 22) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 7; 11; 15; 19; 23) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 8; 9; 13; 18; 24) + $(\frac{1}{2},\frac{1}{2},0)$
[4] $P\bar{4}3m$ (215) 1; 7; 10; 14; 17; 23; (4; 8; 12; 16; 20; 24) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 6; 9; 15; 18; 21) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 5; 11; 13; 19; 22) + $(\frac{1}{2},\frac{1}{2},0)$
[4] $P\bar{4}3m$ (215) 1; 8; 11; 13; 20; 23; (4; 7; 9; 15; 17; 24) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 5; 12; 16; 19; 21) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 6; 10; 14; 18; 22) + $(\frac{1}{2},\frac{1}{2},0)$

**IIb** none

### Maximal isomorphic subgroups of lowest index

**IIc** [27] $F\bar{4}3m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (216)

### Minimal non-isomorphic supergroups

**I** [2] $Fm\bar{3}m$ (225); [2] $Fd\bar{3}m$ (227)

**II** [2] $P\bar{4}3m$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (215)