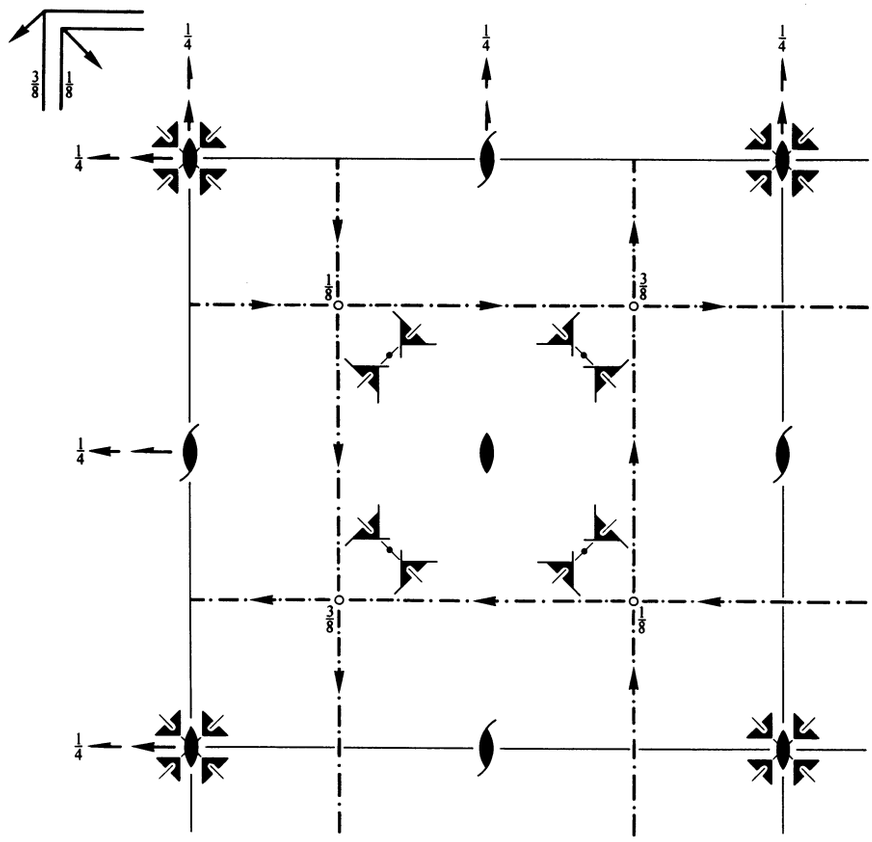
International Tables for Crystallography (2006). Vol. A, Space group 203, pp. 623–625.

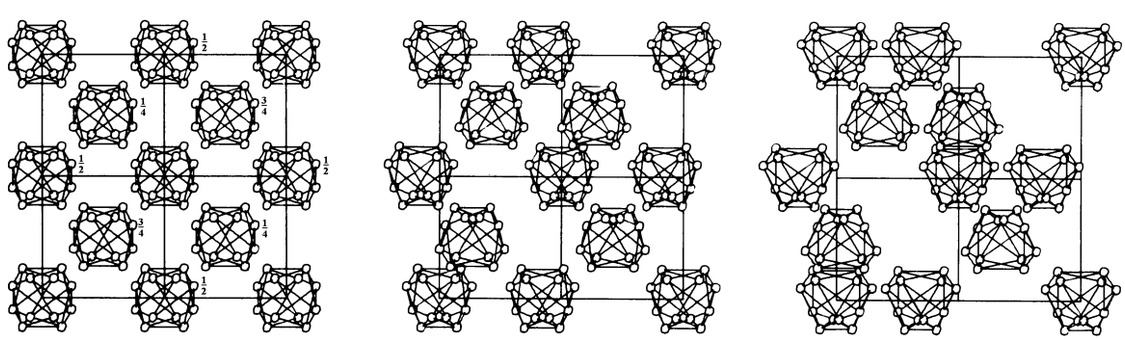
$F\,d\,\bar{3}$ $\quad T_h^4$ $\quad m\bar{3}$ $\quad$ Cubic

No. 203 $\quad F\,2/d\,\bar{3}$ $\quad$ Patterson symmetry $F\,m\,\bar{3}$

ORIGIN CHOICE 1



Upper left quadrant only



Origin at 23, at $-\frac{1}{8}, -\frac{1}{8}, -\frac{1}{8}$ from centre $(\bar{3})$

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

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

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Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2\quad 0,0,z$	(3) $2\quad 0,y,0$	(4) $2\quad x,0,0$
(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) $\bar{1}\quad \frac{1}{8},\frac{1}{8},\frac{1}{8}$	(14) $d(\frac{1}{4},\frac{1}{4},0)\quad x,y,\frac{1}{8}$	(15) $d(\frac{1}{4},0,\frac{1}{4})\quad x,\frac{1}{8},z$	(16) $d(0,\frac{1}{4},\frac{1}{4})\quad \frac{1}{8},y,z$
(17) $\bar{3}^{+}\ x,x,x;\ \frac{1}{8},\frac{1}{8},\frac{1}{8}$	(18) $\bar{3}^{+}\ \bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x};\ -\frac{1}{8},\frac{1}{8},\frac{3}{8}$	(19) $\bar{3}^{+}\ x,\bar{x}+\frac{1}{2},\bar{x};\ \frac{1}{8},\frac{3}{8},-\frac{1}{8}$	(20) $\bar{3}^{+}\ \bar{x}+\frac{1}{2},\bar{x},x;\ \frac{3}{8},-\frac{1}{8},\frac{1}{8}$
(21) $\bar{3}^{-}\ x,x,x;\ \frac{1}{8},\frac{1}{8},\frac{1}{8}$	(22) $\bar{3}^{-}\ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x};\ \frac{1}{8},-\frac{1}{8},\frac{3}{8}$	(23) $\bar{3}^{-}\ \bar{x},\bar{x}+\frac{1}{2},x;\ -\frac{1}{8},\frac{3}{8},\frac{1}{8}$	(24) $\bar{3}^{-}\ \bar{x}+\frac{1}{2},x,\bar{x};\ \frac{3}{8},\frac{1}{8},-\frac{1}{8}$

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

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

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

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

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

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

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 cyclically permutable
							General:
96	g	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	hkl : $h+k=2n$ and $h+l,k+l=2n$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$	$0kl$: $k+l=4n$ and $k,l=2n$
			(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) $\bar{x}+\frac{1}{4},\bar{y}+\frac{1}{4},\bar{z}+\frac{1}{4}$	(14) $x+\frac{1}{4},y+\frac{1}{4},\bar{z}+\frac{1}{4}$	(15) $x+\frac{1}{4},\bar{y}+\frac{1}{4},z+\frac{1}{4}$	(16) $\bar{x}+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	$h00$: $h=4n$
			(17) $\bar{z}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{y}+\frac{1}{4}$	(18) $\bar{z}+\frac{1}{4},x+\frac{1}{4},y+\frac{1}{4}$	(19) $z+\frac{1}{4},x+\frac{1}{4},\bar{y}+\frac{1}{4}$	(20) $z+\frac{1}{4},\bar{x}+\frac{1}{4},y+\frac{1}{4}$	
			(21) $\bar{y}+\frac{1}{4},\bar{z}+\frac{1}{4},\bar{x}+\frac{1}{4}$	(22) $y+\frac{1}{4},\bar{z}+\frac{1}{4},x+\frac{1}{4}$	(23) $\bar{y}+\frac{1}{4},z+\frac{1}{4},x+\frac{1}{4}$	(24) $y+\frac{1}{4},z+\frac{1}{4},\bar{x}+\frac{1}{4}$	
							Special: as above, plus
48	f	2 . .	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	hkl : $h=2n+1$
			$\bar{x}+\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$x+\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\bar{x}+\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},x+\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\bar{x}+\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},x+\frac{1}{4}$	or $h+k+l=4n$
32	e	. 3 .	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$	no extra conditions
			$\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4}$	$x+\frac{1}{4},x+\frac{1}{4},\bar{x}+\frac{1}{4}$	$x+\frac{1}{4},\bar{x}+\frac{1}{4},x+\frac{1}{4}$	$\bar{x}+\frac{1}{4},x+\frac{1}{4},x+\frac{1}{4}$	
16	d	. $\bar{3}$.	$\frac{5}{8},\frac{5}{8},\frac{5}{8}$	$\frac{3}{8},\frac{3}{8},\frac{5}{8}$	$\frac{3}{8},\frac{5}{8},\frac{3}{8}$	$\frac{5}{8},\frac{3}{8},\frac{3}{8}$	hkl : $h=2n+1$
16	c	. $\bar{3}$.	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	$\frac{7}{8},\frac{7}{8},\frac{1}{8}$	$\frac{7}{8},\frac{1}{8},\frac{7}{8}$	$\frac{1}{8},\frac{7}{8},\frac{7}{8}$	or $h,k,l=4n+2$ or $h,k,l=4n$
8	b	2 3 .	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	hkl : $h=2n+1$ or $h+k+l=4n$
8	a	2 3 .	$0,0,0$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	

(*Continued on page 623*)

ORIGIN CHOICE 1

Symmetry of special projections

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

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

Along [110] $c\,2\,m\,m$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, x, \frac{1}{8}$

ORIGIN CHOICE 2

Symmetry of special projections

Along [001] $c\,2\,m\,m$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $\frac{1}{8}, \frac{1}{8}, z$

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

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

ORIGIN CHOICES 1 AND 2

Maximal non-isomorphic subgroups

I [2] $F\,2\,3$ (196) (1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+
[3] $F\,d\,1$ ($F\,d\,d\,d$, 70) (1; 2; 3; 4; 13; 14; 15; 16)+
{ [4] $F\,1\,\bar{3}$ ($R\bar{3}$, 148) (1; 5; 9; 13; 17; 21)+
{ [4] $F\,1\,\bar{3}$ ($R\bar{3}$, 148) (1; 6; 12; 13; 18; 24)+
{ [4] $F\,1\,\bar{3}$ ($R\bar{3}$, 148) (1; 7; 10; 13; 19; 22)+
{ [4] $F\,1\,\bar{3}$ ($R\bar{3}$, 148) (1; 8; 11; 13; 20; 23)+

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [27] $F\,d\,\bar{3}$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (203)

Minimal non-isomorphic supergroups

I [2] $F\,d\,\bar{3}\,m$ (227); [2] $F\,d\,\bar{3}\,c$ (228)

II [2] $P\,n\,\bar{3}$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (201)