$F\,d\,\bar{3}\,c$ No. 228 $F\,4_1/d\,\bar{3}\,2/c$ O_h^8

ORIGIN CHOICE 1, Origin at $2\,3$, at $-\frac{3}{8},-\frac{3}{8},-\frac{3}{8}$ from centre $(\bar{3})$

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); (25)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates

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

192   h 1

(1) x,y,z (2) $\bar{x},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (4) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$

(5) z,x,y (6) $z+\frac{1}{2},\bar{x},\bar{y}+\frac{1}{2}$ (7) $\bar{z},\bar{x}+\frac{1}{2},y+\frac{1}{2}$ (8) $\bar{z}+\frac{1}{2},x+\frac{1}{2},\bar{y}$

(9) y,z,x (10) $\bar{y}+\frac{1}{2},z+\frac{1}{2},\bar{x}$ (11) $y+\frac{1}{2},\bar{z},\bar{x}+\frac{1}{2}$ (12) $\bar{y},\bar{z}+\frac{1}{2},x+\frac{1}{2}$

(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{3}{4}$ (14) $\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4}$ (15) $y+\frac{1}{4},\bar{x}+\frac{3}{4},z+\frac{3}{4}$ (16) $\bar{y}+\frac{3}{4},x+\frac{3}{4},z+\frac{1}{4}$

(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}+\frac{3}{4}$ (18) $\bar{x}+\frac{3}{4},z+\frac{3}{4},y+\frac{1}{4}$ (19) $\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4},\bar{y}+\frac{1}{4}$ (20) $x+\frac{1}{4},\bar{z}+\frac{3}{4},y+\frac{3}{4}$

(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}+\frac{3}{4}$ (22) $z+\frac{1}{4},\bar{y}+\frac{3}{4},x+\frac{3}{4}$ (23) $\bar{z}+\frac{3}{4},y+\frac{3}{4},x+\frac{1}{4}$ (24) $\bar{z}+\frac{1}{4},\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4}$

(25) $\bar{x}+\frac{3}{4},\bar{y}+\frac{3}{4},\bar{z}+\frac{3}{4}$ (26) $x+\frac{3}{4},y+\frac{1}{4},\bar{z}+\frac{1}{4}$ (27) $x+\frac{1}{4},\bar{y}+\frac{1}{4},z+\frac{3}{4}$ (28) $\bar{x}+\frac{1}{4},y+\frac{3}{4},z+\frac{1}{4}$

(29) $\bar{z}+\frac{3}{4},\bar{x}+\frac{3}{4},\bar{y}+\frac{3}{4}$ (30) $\bar{z}+\frac{1}{4},x+\frac{3}{4},y+\frac{1}{4}$ (31) $z+\frac{3}{4},x+\frac{1}{4},\bar{y}+\frac{1}{4}$ (32) $z+\frac{1}{4},\bar{x}+\frac{1}{4},y+\frac{3}{4}$

(33) $\bar{y}+\frac{3}{4},\bar{z}+\frac{3}{4},\bar{x}+\frac{3}{4}$ (34) $y+\frac{1}{4},\bar{z}+\frac{1}{4},x+\frac{3}{4}$ (35) $\bar{y}+\frac{1}{4},z+\frac{3}{4},x+\frac{1}{4}$ (36) $y+\frac{3}{4},z+\frac{1}{4},\bar{x}+\frac{1}{4}$

(37) $\bar{y},\bar{x}+\frac{1}{2},z$ (38) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$ (39) $\bar{y}+\frac{1}{2},x,\bar{z}$ (40) $y,\bar{x},\bar{z}+\frac{1}{2}$

(41) $\bar{x},\bar{z}+\frac{1}{2},y$ (42) $x,\bar{z},\bar{y}+\frac{1}{2}$ (43) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$ (44) $\bar{x}+\frac{1}{2},z,\bar{y}$

(45) $\bar{z},\bar{y}+\frac{1}{2},x$ (46) $\bar{z}+\frac{1}{2},y,\bar{x}$ (47) $z,\bar{y},\bar{x}+\frac{1}{2}$ (48) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $F\bar{4}3c$ (219)   (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] $F4_132$ (210)   (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] $Fd\bar{3}1$ (203, $Fd\bar{3}$)   (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] $F4_1/d12/c$ (142, $I4_1/acd$)   (1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40)+ $1/2(\mathbf{a}-\mathbf{b}),1/2(\mathbf{a}+\mathbf{b}),\mathbf{c}$ $0,0,1/4$

[3] $F4_1/d12/c$ (142, $I4_1/acd$)   (1; 4; 2; 3; 18; 19; 17; 20; 25; 28; 26; 27; 42; 43; 41; 44)+ $1/2(\mathbf{b}-\mathbf{c}),1/2(\mathbf{b}+\mathbf{c}),\mathbf{a}$ $1/4,0,0$

[3] $F4_1/d12/c$ (142, $I4_1/acd$)   (1; 3; 4; 2; 22; 24; 23; 21; 25; 27; 28; 26; 46; 48; 47; 45)+ $1/2(-\mathbf{a}+\mathbf{c}),1/2(\mathbf{a}+\mathbf{c}),\mathbf{b}$ $0,1/4,0$

[4] $F1\bar{3}2/c$ (167, $R\bar{3}c$)   (1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48)+ $1/2(-\mathbf{a}+\mathbf{b}),1/2(-\mathbf{b}+\mathbf{c}),\mathbf{a}+\mathbf{b}+\mathbf{c}$ $3/8,3/8,3/8$

[4] $F1\bar{3}2/c$ (167, $R\bar{3}c$)   (1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48)+ $1/2(\mathbf{a}+\mathbf{b}),1/2(-\mathbf{b}-\mathbf{c}),-\mathbf{a}+\mathbf{b}-\mathbf{c}$ $1/8,3/8,1/8$

[4] $F1\bar{3}2/c$ (167, $R\bar{3}c$)   (1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46)+ $1/2(-\mathbf{a}-\mathbf{b}),1/2(\mathbf{b}-\mathbf{c}),\mathbf{a}-\mathbf{b}-\mathbf{c}$ $3/8,1/8,1/8$

[4] $F1\bar{3}2/c$ (167, $R\bar{3}c$)   (1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46)+ $1/2(\mathbf{a}-\mathbf{b}),1/2(\mathbf{b}+\mathbf{c}),-\mathbf{a}-\mathbf{b}+\mathbf{c}$ $1/8,1/8,3/8$

II Maximal *klassengleiche* subgroups

• **Loss of centring translations**   none

• **Enlarged unit cell**   none

• **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}' = p\mathbf{a}$, $\mathbf{b}' = p\mathbf{b}$, $\mathbf{c}' = p\mathbf{c}$

$F d\bar{3}c$ (228) $\quad \langle 2+(\frac{1}{2}+2u, \frac{p}{2}+2v, \frac{p}{2}-\frac{1}{2}); 3+(\frac{p}{2}+2u, \frac{p}{2}-\frac{1}{2}, \frac{1}{2}+2w);$ $\quad p\mathbf{a}, p\mathbf{b}, p\mathbf{c} \quad 1/4+u, 1/4+v, 1/4+w$
$\quad 5+(u-w, -u+v, -v+w);$
$\quad 13+(\frac{3p}{4}-\frac{3}{4}+u-v, \frac{p}{4}-\frac{1}{4}-u+v, \frac{3p}{4}-\frac{1}{4}+2w);$
$\quad 25+(\frac{3p}{4}-\frac{1}{4}+2u, \frac{3p}{4}-\frac{1}{4}+2v, \frac{3p}{4}-\frac{1}{4}+2w)\rangle$
$\quad p > 2;\ 0 \leq u < p;\ 0 \leq v < p;\ 0 \leq w < p$
$\quad p^3$ conjugate subgroups for prime $p \equiv 3 \pmod 4$

$F d\bar{3}c$ (228) $\quad \langle 2+(2u, \frac{p}{2}-\frac{1}{2}+2v, \frac{p}{2}-\frac{1}{2}); 3+(\frac{p}{2}-\frac{1}{2}+2u, \frac{p}{2}-\frac{1}{2}, 2w);$ $\quad p\mathbf{a}, p\mathbf{b}, p\mathbf{c} \quad u, v, w$
$\quad 5+(u-w, -u+v, -v+w);$
$\quad 13+(\frac{3p}{4}-\frac{3}{4}+u-v, \frac{p}{4}-\frac{1}{4}-u+v, \frac{3p}{4}-\frac{3}{4}+2w);$
$\quad 25+(\frac{3p}{4}-\frac{3}{4}+2u, \frac{3p}{4}-\frac{3}{4}+2v, \frac{3p}{4}-\frac{3}{4}+2w)\rangle$
$\quad p > 4;\ 0 \leq u < p;\ 0 \leq v < p;\ 0 \leq w < p$
$\quad p^3$ conjugate subgroups for prime $p \equiv 1 \pmod 4$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

• **Additional centring translations** none

• **Decreased unit cell**

$[2]$ $\mathbf{a}' = \frac{1}{2}\mathbf{a}$, $\mathbf{b}' = \frac{1}{2}\mathbf{b}$, $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $Pn\bar{3}m$ (224)

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• **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}' = p\mathbf{a}$, $\mathbf{b}' = p\mathbf{b}$, $\mathbf{c}' = p\mathbf{c}$

$F d\bar{3}c$ (228) $\quad \langle 2+(\frac{p}{4}-\frac{1}{4}+2u, \frac{3p}{4}-\frac{3}{4}+2v, \frac{p}{2}-\frac{1}{2});$ $\quad\quad\quad p\mathbf{a}, p\mathbf{b}, p\mathbf{c} \quad\quad u, v, w$
$\quad 3+(\frac{3p}{4}-\frac{3}{4}+2u, \frac{p}{2}-\frac{1}{2}, \frac{p}{4}-\frac{1}{4}+2w);$
$\quad 5+(u-w, -u+v, -v+w);$
$\quad 13+(\frac{3p}{4}-\frac{3}{4}+u-v, \frac{p}{4}-\frac{1}{4}-u+v, 2w); 25+(2u, 2v, 2w)\rangle$
$\quad p > 2;\ 0 \leq u < p;\ 0 \leq v < p;\ 0 \leq w < p$
$\quad p^3$ conjugate subgroups for the prime p

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

• **Additional centring translations** none

• **Decreased unit cell**

$[2]$ $\mathbf{a}' = \frac{1}{2}\mathbf{a}$, $\mathbf{b}' = \frac{1}{2}\mathbf{b}$, $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $Pn\bar{3}m$ (224)