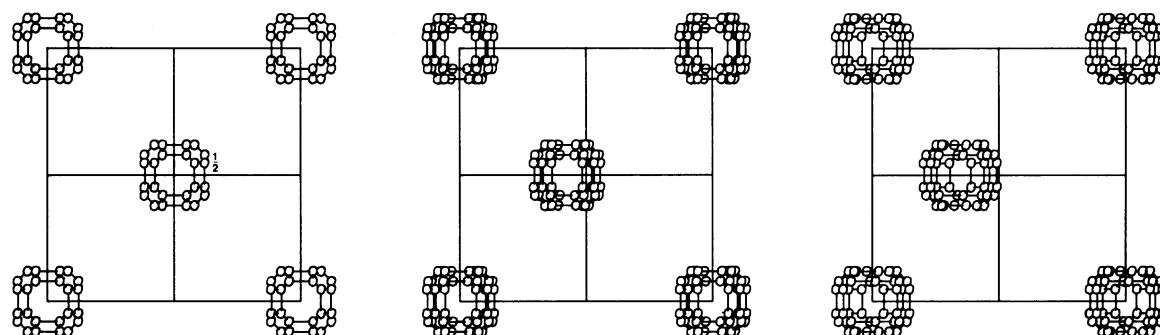
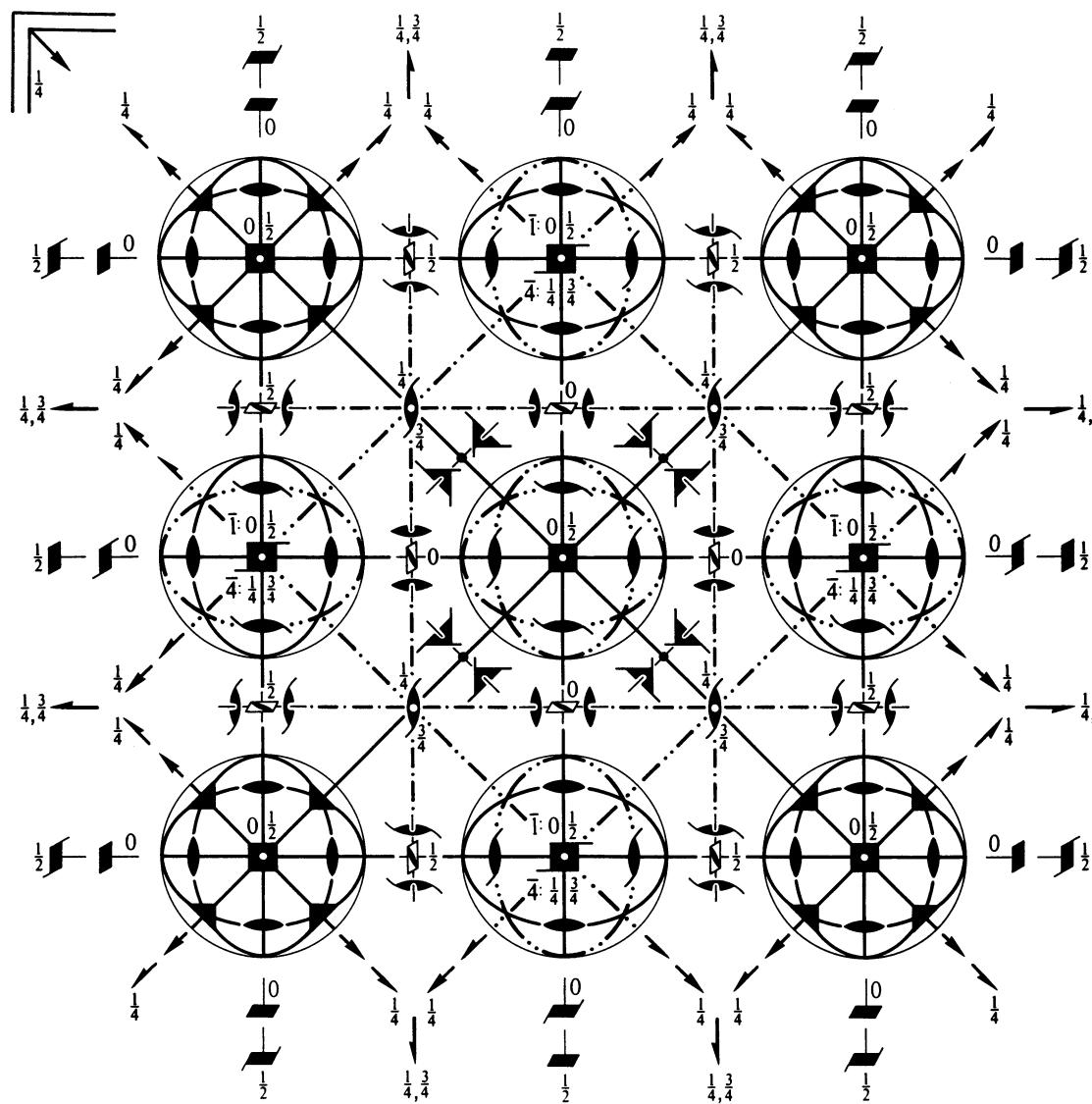


$I\bar{m}\bar{3}m$ O_h^9 $m\bar{3}m$

Cubic

No. 229

 $I\ 4/m\ \bar{3}\ 2/m$ Patterson symmetry $I\bar{m}\bar{3}m$ Origin at centre ($m\bar{3}m$)

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

Symmetry operations

(given on page 714)

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); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	(0,0,0)+	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			h,k,l permutable General:
96 <i>l</i> 1	(1) x,y,z (5) z,x,y (9) y,z,x (13) y,x,\bar{z} (17) x,z,\bar{y} (21) z,y,\bar{x} (25) \bar{x},\bar{y},\bar{z} (29) \bar{z},\bar{x},\bar{y} (33) \bar{y},\bar{z},\bar{x} (37) \bar{y},\bar{x},z (41) \bar{x},\bar{z},y (45) \bar{z},\bar{y},x	(2) \bar{x},\bar{y},z (6) z,\bar{x},\bar{y} (10) \bar{y},z,\bar{x} (14) \bar{y},\bar{x},\bar{z} (18) \bar{x},z,y (22) z,\bar{y},x (26) x,y,\bar{z} (30) \bar{z},x,y (34) y,\bar{z},x (38) y,x,z (42) x,\bar{z},\bar{y} (46) \bar{z},y,\bar{x}	(3) \bar{x},y,\bar{z} (7) \bar{z},\bar{x},y (11) y,\bar{z},\bar{x} (15) y,\bar{x},z (19) \bar{x},\bar{z},\bar{y} (23) \bar{z},y,x (27) x,\bar{y},z (31) z,x,\bar{y} (35) \bar{y},z,x (39) \bar{y},x,\bar{z} (43) x,z,y (47) z,\bar{y},\bar{x}	(4) x,\bar{y},\bar{z} (8) \bar{z},x,\bar{y} (12) \bar{y},\bar{z},x (16) \bar{y},x,z (20) x,\bar{z},y (24) \bar{z},\bar{y},\bar{x} (28) \bar{x},y,z (32) z,\bar{x},y (36) y,z,\bar{x} (40) y,\bar{x},\bar{z} (44) \bar{x},z,\bar{y} (48) z,y,x	$hkl : h+k+l=2n$ $0kl : k+l=2n$ $hh\bar{l} : l=2n$ $h00 : h=2n$
48 <i>k</i> . . <i>m</i>	x,x,z \bar{z},\bar{x},x x,x,\bar{z} \bar{x},\bar{z},\bar{x}	\bar{x},\bar{x},z \bar{z},x,\bar{x} \bar{x},\bar{x},\bar{z} x,\bar{z},x	\bar{x},x,\bar{z} x,z,\bar{x} x,\bar{x},z z,x,\bar{x}	x,\bar{x},\bar{z} \bar{x},z,\bar{x} \bar{x},x,z z,\bar{x},x	z,x,x \bar{x},\bar{z},\bar{x} \bar{x},z,x \bar{z},x,\bar{x}
48 <i>j</i> <i>m</i> . .	$0,y,z$ $\bar{z},0,y$ $y,0,\bar{z}$ $0,\bar{z},\bar{y}$	$0,\bar{y},z$ $\bar{z},0,\bar{y}$ $\bar{y},0,\bar{z}$ $0,\bar{z},y$	$0,y,\bar{z}$ $y,z,0$ $y,0,z$ $z,y,0$	$0,\bar{y},\bar{z}$ $\bar{y},z,0$ $\bar{y},0,z$ $z,\bar{y},0$	$z,0,y$ $\bar{y},\bar{z},0$ $0,z,\bar{y}$ $\bar{z},y,0$
48 <i>i</i> . . 2	$\frac{1}{4},y,\bar{y}+\frac{1}{2}$ $\bar{y}+\frac{1}{2},\frac{1}{4},y$ $y,\bar{y}+\frac{1}{2},\frac{1}{4}$ $\frac{3}{4},\bar{y},y+\frac{1}{2}$ $y+\frac{1}{2},\frac{3}{4},\bar{y}$ $\bar{y},y+\frac{1}{2},\frac{3}{4}$ $\bar{y},y+\frac{1}{2},\frac{3}{4}$	$\frac{3}{4},\bar{y},\bar{y}+\frac{1}{2}$ $\bar{y}+\frac{1}{2},\frac{3}{4},\bar{y}$ $y+\frac{1}{2},\frac{3}{4},y$ $\frac{1}{4},y,y+\frac{1}{2}$ $y+\frac{1}{2},\frac{3}{4},y$ $\bar{y},y+\frac{1}{2},\frac{3}{4}$ $y,y+\frac{1}{2},\frac{3}{4}$	$\frac{3}{4},y,y+\frac{1}{2}$ $y+\frac{1}{2},\frac{3}{4},y$ $y,y+\frac{1}{2},\frac{3}{4}$ $\frac{1}{4},\bar{y},\bar{y}+\frac{1}{2}$ $\bar{y}+\frac{1}{2},\frac{3}{4},\bar{y}$ $\bar{y},y+\frac{1}{2},\frac{3}{4}$ $\bar{y},\bar{y}+\frac{1}{2},\frac{3}{4}$	$\frac{1}{4},\bar{y},y+\frac{1}{2}$ $y+\frac{1}{2},\frac{1}{4},\bar{y}$ $\bar{y},y+\frac{1}{2},\frac{1}{4}$ $\frac{3}{4},y,\bar{y}+\frac{1}{2}$ $\bar{y}+\frac{1}{2},\frac{1}{4},y$ $\bar{y}+\frac{1}{2},\frac{1}{4},\bar{y}$ $y,\bar{y}+\frac{1}{2},\frac{1}{4}$	Special: as above, plus no extra conditions
24 <i>h</i> <i>m</i> . <i>m</i> 2	$0,y,y$ $\bar{y},0,y$	$0,\bar{y},y$ $\bar{y},0,\bar{y}$	$0,y,\bar{y}$ $y,y,0$	$0,\bar{y},\bar{y}$ $\bar{y},y,0$	$y,0,\bar{y}$ $\bar{y},\bar{y},0$
24 <i>g</i> <i>m m</i> 2..	$x,0,\frac{1}{2}$ $0,x,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$ $0,\bar{x},\frac{1}{2}$	$\frac{1}{2},x,0$ $x,\frac{1}{2},0$	$\frac{1}{2},\bar{x},0$ $\bar{x},\frac{1}{2},0$	$0,\frac{1}{2},x$ $\frac{1}{2},0,\bar{x}$
16 <i>f</i> . 3 <i>m</i>	x,x,x x,x,\bar{x}	\bar{x},\bar{x},x \bar{x},\bar{x},\bar{x}	\bar{x},x,\bar{x} x,\bar{x},x	x,\bar{x},\bar{x} \bar{x},x,x	no extra conditions
12 <i>e</i> 4 <i>m</i> . <i>m</i>	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$
12 <i>d</i> 4̄ <i>m</i> . 2	$\frac{1}{4},0,\frac{1}{2}$	$\frac{3}{4},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{4},0$	$\frac{1}{2},\frac{3}{4},0$	$0,\frac{1}{2},\frac{1}{4}$
8 <i>c</i> . 3̄ <i>m</i>	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$hkl : k,l=2n$
6 <i>b</i> 4/m <i>m</i> . <i>m</i>	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$		no extra conditions
2 <i>a</i> <i>m</i> 3̄ <i>m</i>	$0,0,0$				no extra conditions

Symmetry of special projections

$$\text{Along } [001] p4mm \\ \mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b}) \\ \text{Origin at } 0,0,z$$

$$\text{Along } [111] p6mm \\ \mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c}) \quad \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c}) \\ \text{Origin at } x,x,x$$

$$\text{Along } [110] p2mm \\ \mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b}) \quad \mathbf{b}' = \frac{1}{2}\mathbf{c} \\ \text{Origin at } x,x,0$$

Maximal non-isomorphic subgroups

I	[2] $I\bar{4}3m$ (217)	(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] $I432$ (211)	(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] $Im\bar{3}1$ ($Im\bar{3}$, 204)	(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] $I4/m12/m$ ($I4/mmm$, 139) }	(1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40) +
	{ [3] $I4/m12/m$ ($I4/mmm$, 139) }	(1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44) +
	{ [3] $I4/m12/m$ ($I4/mmm$, 139) }	(1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48) +
	{ [4] $I1\bar{3}2/m$ ($R\bar{3}m$, 166) }	(1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48) +
	{ [4] $I1\bar{3}2/m$ ($R\bar{3}m$, 166) }	(1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48) +
	{ [4] $I1\bar{3}2/m$ ($R\bar{3}m$, 166) }	(1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46) +
	{ [4] $I1\bar{3}2/m$ ($R\bar{3}m$, 166) }	(1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46) +
IIa	[2] $Pn\bar{3}m$ (224)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48; (13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $Pm\bar{3}n$ (223)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36; (13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $Pn\bar{3}n$ (222)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24; (25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[2] $Pm\bar{3}m$ (221)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48

IIb none**Maximal isomorphic subgroups of lowest index**

IIc	[27] $Im\bar{3}m$ ($a' = 3a, b' = 3b, c' = 3c$) (229)
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Minimal non-isomorphic supergroups**I** none**II** [4] $Pm\bar{3}m$ ($a' = \frac{1}{2}a, b' = \frac{1}{2}b, c' = \frac{1}{2}c$) (221)**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) 2 $x, x, 0$	(14) 2 $x, \bar{x}, 0$	(15) 4 ⁻ 0,0,z	(16) 4 ⁺ 0,0,z
(17) 4 ⁻ $x, 0, 0$	(18) 2 0,y,y	(19) 2 0,y, \bar{y}	(20) 4 ⁺ x,0,0
(21) 4 ⁺ 0,y,0	(22) 2 x,0,x	(23) 4 ⁻ 0,y,0	(24) 2 $\bar{x}, 0, x$
(25) $\bar{1}$ 0,0,0	(26) m x,y,0	(27) m x,0,z	(28) m 0,y,z
(29) $\bar{3}^+$ $x, x, x; 0, 0, 0$	(30) $\bar{3}^+$ $\bar{x}, x, \bar{x}; 0, 0, 0$	(31) $\bar{3}^+$ $x, \bar{x}, \bar{x}; 0, 0, 0$	(32) $\bar{3}^+$ $\bar{x}, \bar{x}, x; 0, 0, 0$
(33) $\bar{3}^-$ $x, x, x; 0, 0, 0$	(34) $\bar{3}^-$ $\bar{x}, x, \bar{x}; 0, 0, 0$	(35) $\bar{3}^-$ $\bar{x}, \bar{x}, x; 0, 0, 0$	(36) $\bar{3}^-$ $\bar{x}, x, \bar{x}; 0, 0, 0$
(37) m x, \bar{x}, z	(38) m x, x, z	(39) 4 ⁻ 0,0,z; 0,0,0	(40) 4 ⁺ 0,0,z; 0,0,0
(41) 4 ⁻ $x, 0, 0; 0, 0, 0$	(42) m x,y, \bar{y}	(43) m x,y,y	(44) 4 ⁺ x,0,0; 0,0,0
(45) 4 ⁺ 0,y,0; 0,0,0	(46) m \bar{x}, y, x	(47) 4 ⁻ 0,y,0; 0,0,0	(48) m x,y,x

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

(1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	(2) 2(0,0, $\frac{1}{2}$) $\frac{1}{4}, \frac{1}{4}, z$	(3) 2(0, $\frac{1}{2}, 0$) $\frac{1}{4}, y, \frac{1}{4}$	(4) 2($\frac{1}{2}, 0, 0$) $x, \frac{1}{4}, \frac{1}{4}$
(5) $3^+(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x, x, x	(6) $3^+(\frac{1}{6}, -\frac{1}{6}, \frac{1}{6})$ $\bar{x} + \frac{1}{3}, x + \frac{1}{3}, \bar{x} + \frac{1}{3}$	(7) $3^+(\frac{1}{6}, -\frac{1}{6}, \frac{1}{6})$ $x + \frac{2}{3}, \bar{x} - \frac{1}{3}, \bar{x}$	(8) $3^+(\frac{1}{6}, -\frac{1}{6}, -\frac{1}{6})$ $\bar{x} + \frac{1}{3}, \bar{x} + \frac{2}{3}, x$
(9) $3^-(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ x, x, x	(10) $3^-(\frac{1}{6}, \frac{1}{6}, \frac{1}{6})$ $x + \frac{1}{3}, \bar{x} + \frac{1}{3}, \bar{x} + \frac{1}{3}$	(11) $3^-(\frac{1}{6}, \frac{1}{6}, \frac{1}{6})$ $\bar{x} - \frac{1}{3}, \bar{x} + \frac{2}{3}, x + \frac{1}{3}$	(12) $3^-(\frac{1}{6}, \frac{1}{6}, \frac{1}{6})$ $\bar{x} - \frac{1}{3}, x + \frac{2}{3}, \bar{x}$
(13) 2($\frac{1}{2}, \frac{1}{2}, 0$) $x, x, \frac{1}{4}$	(14) 2 $x, \bar{x} + \frac{1}{2}, \frac{1}{4}$	(15) 4 ⁻ (0,0, $\frac{1}{2}$) $\frac{1}{2}, 0, z$	(16) 4 ⁺ (0,0, $\frac{1}{2}$) $0, \frac{1}{2}, z$
(17) 4 ⁻ ($\frac{1}{2}, 0, 0$) $x, \frac{1}{2}, 0$	(18) 2($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$) $\frac{1}{4}, y, y$	(19) 2 $\frac{1}{4}, y + \frac{1}{2}, \bar{y}$	(20) 4 ⁺ ($\frac{1}{2}, 0, 0$) $x, 0, \frac{1}{2}$
(21) 4 ⁺ (0, $\frac{1}{2}, 0$) $\frac{1}{2}, y, 0$	(22) 2($\frac{1}{2}, 0, \frac{1}{2}$) $x, \frac{1}{4}, x$	(23) 4 ⁻ (0, $\frac{1}{2}, 0$) $0, y, \frac{1}{2}$	(24) 2 $\bar{x} + \frac{1}{2}, \frac{1}{4}, x$
(25) $\bar{1}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	(26) n($\frac{1}{2}, \frac{1}{2}, 0$) $x, y, \frac{1}{4}$	(27) n($\frac{1}{2}, 0, \frac{1}{2}$) $x, \frac{1}{4}, z$	(28) n($0, \frac{1}{2}, \frac{1}{2}$) $\frac{1}{4}, y, z$
(29) $\bar{3}^+$ $x, x, x; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	(30) $\bar{3}^+$ $\bar{x} - 1, x + 1, \bar{x}; -\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	(31) $\bar{3}^+$ $x, \bar{x} + 1, \bar{x}; \frac{1}{4}, \frac{3}{4}, -\frac{1}{4}$	(32) $\bar{3}^+$ $\bar{x} + 1, \bar{x}, x; \frac{3}{4}, -\frac{1}{4}, \frac{1}{4}$
(33) $\bar{3}^-$ $x, x, x; \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	(34) $\bar{3}^-$ $\bar{x} + 1, \bar{x} - 1, \bar{x}; \frac{1}{4}, -\frac{1}{4}, \frac{3}{4}$	(35) $\bar{3}^-$ $\bar{x}, \bar{x} + 1, x; -\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	(36) $\bar{3}^-$ $\bar{x} + 1, x, \bar{x}; \frac{3}{4}, \frac{1}{4}, -\frac{1}{4}$
(37) c $x + \frac{1}{2}, \bar{x}, z$	(38) n($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$) x, x, z	(39) 4 ⁻ 0, $\frac{1}{2}, z$; 0, $\frac{1}{2}, \frac{1}{4}$	(40) 4 ⁺ $\frac{1}{2}, 0, z$; $\frac{1}{2}, 0, \frac{1}{2}$
(41) 4 ⁻ $x, 0, \frac{1}{2}$; $\frac{1}{4}, 0, \frac{1}{2}$	(42) a $x, y + \frac{1}{2}, \bar{y}$	(43) n($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$) x, y, y	(44) 4 ⁺ $x, \frac{1}{2}, 0$; $\frac{1}{2}, \frac{1}{2}, 0$
(45) 4 ⁺ 0, $y, \frac{1}{2}$; 0, $\frac{1}{4}, \frac{1}{2}$	(46) b $\bar{x} + \frac{1}{2}, y, x$	(47) 4 ⁻ $\frac{1}{2}, y, 0$; $\frac{1}{2}, \frac{1}{4}, 0$	(48) n($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$) x, y, x