

No. 225 $Fm\bar{3}m$ CONTINUED

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

Site symmetry			$(0, 0, 0) +$	$(0, \frac{1}{2}, \frac{1}{2}) +$	$(\frac{1}{2}, 0, \frac{1}{2}) +$	$(\frac{1}{2}, \frac{1}{2}, 0) +$	h, k, l permutable		
General:									
192	l	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	$hkl : h + k, h + l, k + l = 2$ $Ok l : k, l = 2n$ $hhl : h + l = 2n$ $h00 : h = 2n$		
Special: as above, plus									
96	k	$.m$	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, 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 $x, \bar{z}, \bar{x}$ $x, z, \bar{x}$ $\bar{z}, x, x$	$z, \bar{x}, \bar{x}$ $\bar{x}, \bar{z}, x$ $\bar{x}, z, x$ $\bar{z}, \bar{x}, \bar{x}$	no extra conditions
96	j	$m..$	$0, y, z$ $\bar{z}, 0, y$ $y, 0, \bar{z}$ $0, \bar{z}, \bar{y}$	$0, \bar{y}, z$ $\bar{z}, 0, \bar{y}$ $\bar{y}, 0, \bar{z}$ $0, \bar{z}, y$	$0, y, \bar{z}$ $y, z, 0$ $y, 0, z$ $z, y, 0$	$0, \bar{y}, \bar{z}$ $\bar{y}, z, 0$ $\bar{y}, 0, z$ $z, \bar{y}, 0$	$z, 0, y$ $y, \bar{z}, 0$ $0, z, \bar{y}$ $\bar{z}, y, 0$	$z, 0, \bar{y}$ $\bar{y}, \bar{z}, 0$ $0, z, y$ $\bar{z}, \bar{y}, 0$	no extra conditions
48	i	$m.m2$	$\frac{1}{2}, y, y$ $\bar{y}, \frac{1}{2}, y$	$\frac{1}{2}, \bar{y}, y$ $\bar{y}, \frac{1}{2}, \bar{y}$	$\frac{1}{2}, y, \bar{y}$ $y, y, \frac{1}{2}$	$\frac{1}{2}, \bar{y}, \bar{y}$ $\bar{y}, y, \frac{1}{2}$	$y, \frac{1}{2}, y$ $y, \bar{y}, \frac{1}{2}$	$y, \frac{1}{2}, \bar{y}$ $\bar{y}, \bar{y}, \frac{1}{2}$	no extra conditions
48	h	$m.m2$	$0, y, y$ $\bar{y}, 0, y$	$0, \bar{y}, y$ $\bar{y}, 0, \bar{y}$	$0, y, \bar{y}$ $y, y, 0$	$0, \bar{y}, \bar{y}$ $\bar{y}, y, 0$	$y, 0, y$ $y, \bar{y}, 0$	$y, 0, \bar{y}$ $\bar{y}, \bar{y}, 0$	no extra conditions
48	g	$2.m m$	$x, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, x, \frac{3}{4}$	$\bar{x}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \bar{x}, \frac{3}{4}$	$\frac{1}{4}, x, \frac{1}{4}$ $x, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \bar{x}, \frac{3}{4}$ $\bar{x}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{1}{4}, x$ $\frac{1}{4}, \frac{1}{4}, \bar{x}$	$\frac{3}{4}, \frac{1}{4}, \bar{x}$ $\frac{1}{4}, \frac{3}{4}, x$	$hkl : h = 2n$
32	f	$.3m$	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
24	e	$4m.m$	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	$0, 0, x$	$0, 0, \bar{x}$	no extra conditions
24	d	$m.m m$	$0, \frac{1}{4}, \frac{1}{4}$	$0, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, 0, \frac{1}{4}$	$\frac{1}{4}, 0, \frac{3}{4}$	$\frac{1}{4}, \frac{1}{4}, 0$	$\frac{3}{4}, \frac{1}{4}, 0$	$hkl : h = 2n$
8	c	$\bar{4}3m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$					$hkl : h = 2n$
4	b	$m\bar{3}m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$						no extra conditions
4	a	$m\bar{3}m$	$0, 0, 0$						no extra conditions

No. 123 $P 4/m m m$ CONTINUED

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
16	u	1	(1) x, y, z (5) $\bar{x}, y, \bar{z}$ (9) $\bar{x}, \bar{y}, \bar{z}$ (13) $x, \bar{y}, z$	(2) $\bar{x}, \bar{y}, z$ (6) $x, \bar{y}, \bar{z}$ (10) $x, y, \bar{z}$ (14) $\bar{x}, y, z$	(3) $\bar{y}, x, z$ (7) $y, x, \bar{z}$ (11) $y, \bar{x}, \bar{z}$ (15) $\bar{y}, \bar{x}, z$	(4) $y, \bar{x}, z$ (8) $\bar{y}, \bar{x}, \bar{z}$ (12) $\bar{y}, x, \bar{z}$ (16) y, x, z	General: no conditions
8	t	$.m.$	$x, \frac{1}{2}, z$ $\bar{x}, \frac{1}{2}, \bar{z}$	$\bar{x}, \frac{1}{2}, z$ $x, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, x, z$ $\frac{1}{2}, x, \bar{z}$	$\frac{1}{2}, \bar{x}, z$ $\frac{1}{2}, \bar{x}, \bar{z}$	Special: no extra conditions
8	s	$.m.$	$x, 0, z$ $\bar{x}, 0, \bar{z}$	$\bar{x}, 0, z$ $x, 0, \bar{z}$	$0, x, z$ $0, x, \bar{z}$	$0, \bar{x}, z$ $0, \bar{x}, \bar{z}$	no extra conditions
8	r	$.m$	x, x, z $\bar{x}, x, \bar{z}$	$\bar{x}, \bar{x}, z$ $x, \bar{x}, \bar{z}$	$\bar{x}, x, z$ $x, x, \bar{z}$	$x, \bar{x}, z$ $\bar{x}, \bar{x}, \bar{z}$	no extra conditions
8	q	$m..$	$x, y, \frac{1}{2}$ $\bar{x}, y, \frac{1}{2}$	$\bar{x}, \bar{y}, \frac{1}{2}$ $x, \bar{y}, \frac{1}{2}$	$\bar{y}, x, \frac{1}{2}$ $y, x, \frac{1}{2}$	$y, \bar{x}, \frac{1}{2}$ $\bar{y}, \bar{x}, \frac{1}{2}$	no extra conditions
8	p	$m..$	$x, y, 0$ $\bar{x}, y, 0$	$\bar{x}, \bar{y}, 0$ $x, \bar{y}, 0$	$\bar{y}, x, 0$ $y, x, 0$	$y, \bar{x}, 0$ $\bar{y}, \bar{x}, 0$	no extra conditions
4	o	$m 2m.$	$x, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, x, \frac{1}{2}$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$	no extra conditions
4	n	$m 2m.$	$x, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, 0$	$\frac{1}{2}, x, 0$	$\frac{1}{2}, \bar{x}, 0$	no extra conditions
4	m	$m 2m.$	$x, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$	$0, x, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$	no extra conditions
4	l	$m 2m.$	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	no extra conditions
4	k	$m. 2m$	$x, x, \frac{1}{2}$	$\bar{x}, \bar{x}, \frac{1}{2}$	$\bar{x}, x, \frac{1}{2}$	$x, \bar{x}, \frac{1}{2}$	no extra conditions
4	j	$m. 2m$	$x, x, 0$	$\bar{x}, \bar{x}, 0$	$\bar{x}, x, 0$	$x, \bar{x}, 0$	no extra conditions
4	i	$2m m.$	$0, \frac{1}{2}, z$	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, \bar{z}$	$\frac{1}{2}, 0, \bar{z}$	$hkl: h + k = 2n$
2	h	$4m m$	$\frac{1}{2}, \frac{1}{2}, z$	$\frac{1}{2}, \frac{1}{2}, \bar{z}$			no extra conditions
2	g	$4m m$	$0, 0, z$	$0, 0, \bar{z}$			no extra conditions
2	f	$m m m.$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$			$hkl: h + k = 2n$
2	e	$m m m.$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$			$hkl: h + k = 2n$
1	d	$4/m m m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$				no extra conditions
1	c	$4/m m m$	$\frac{1}{2}, \frac{1}{2}, 0$				no extra conditions
1	b	$4/m m m$	$0, 0, \frac{1}{2}$				no extra conditions
1	a	$4/m m m$	$0, 0, 0$				no extra conditions