

$Pn\bar{3}n$

$O_h^2$

$m\bar{3}m$

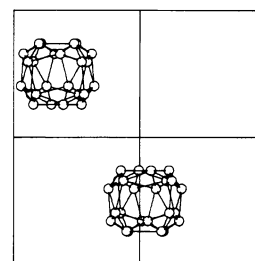
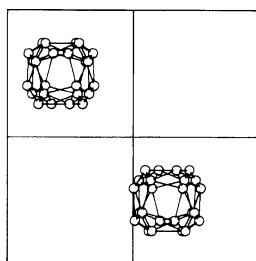
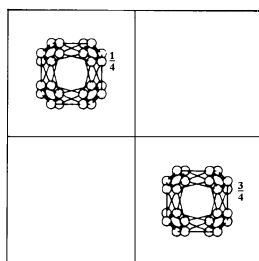
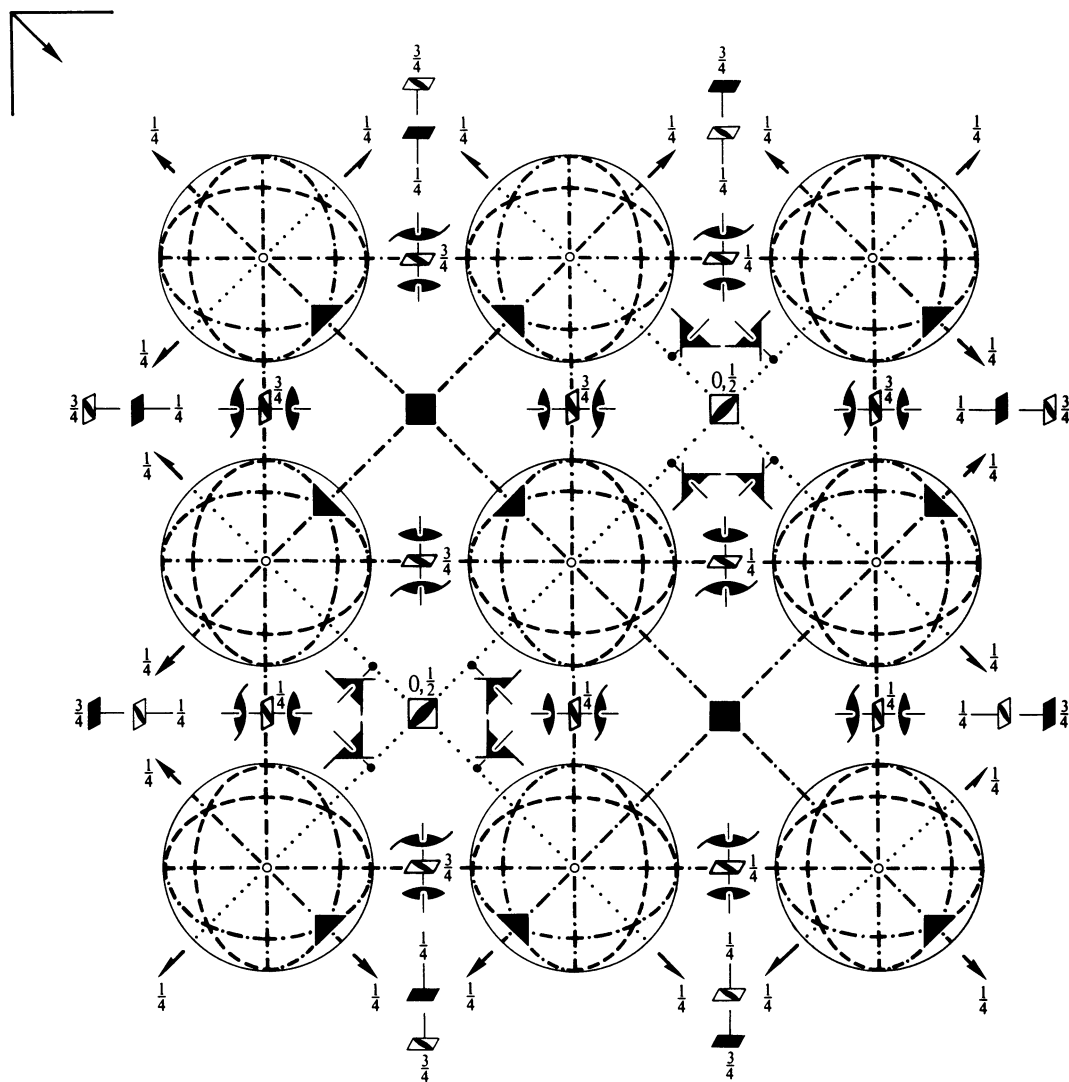
Cubic

No. 222

$P 4/n \bar{3} 2/n$

Patterson symmetry  $Pm\bar{3}m$

ORIGIN CHOICE 2



Origin at centre ( $\bar{3}$ ), at  $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$  from 432

Asymmetric unit  $\frac{1}{4} \leq x \leq \frac{3}{4}; \frac{1}{4} \leq y \leq \frac{3}{4}; \frac{1}{4} \leq z \leq \frac{3}{4}; y \leq x; z \leq y$

Vertices  $\frac{1}{4}, \frac{1}{4}, \frac{1}{4} \quad \frac{3}{4}, \frac{1}{4}, \frac{1}{4} \quad \frac{3}{4}, \frac{3}{4}, \frac{1}{4} \quad \frac{3}{4}, \frac{3}{4}, \frac{3}{4}$

## Symmetry operations

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

Generators selected (1);  $t(1, 0, 0)$ ;  $t(0, 1, 0)$ ;  $t(0, 0, 1)$ ; (2); (3); (5); (13); (25)

## Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions							
48 $i$ 1	(1) $x, y, z$ (2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ (3) $\bar{x} + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ (4) $x, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (5) $z, x, y$ (6) $z, \bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (7) $\bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}, y$ (8) $\bar{z} + \frac{1}{2}, x, \bar{y} + \frac{1}{2}$ (9) $y, z, x$ (10) $\bar{y} + \frac{1}{2}, z, \bar{x} + \frac{1}{2}$ (11) $y, \bar{z} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (12) $\bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}, x$ (13) $y, x, \bar{z} + \frac{1}{2}$ (14) $\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (15) $y, \bar{x} + \frac{1}{2}, z$ (16) $\bar{y} + \frac{1}{2}, x, z$ (17) $x, z, \bar{y} + \frac{1}{2}$ (18) $\bar{x} + \frac{1}{2}, z, y$ (19) $\bar{x} + \frac{1}{2}, \bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ (20) $x, \bar{z} + \frac{1}{2}, y$ (21) $z, y, \bar{x} + \frac{1}{2}$ (22) $z, \bar{y} + \frac{1}{2}, x$ (23) $\bar{z} + \frac{1}{2}, y, x$ (24) $\bar{z} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ (25) $\bar{x}, \bar{y}, \bar{z}$ (26) $x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ (27) $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ (28) $\bar{x}, y + \frac{1}{2}, z + \frac{1}{2}$ (29) $\bar{z}, \bar{x}, \bar{y}$ (30) $\bar{z}, x + \frac{1}{2}, y + \frac{1}{2}$ (31) $z + \frac{1}{2}, x + \frac{1}{2}, \bar{y}$ (32) $z + \frac{1}{2}, \bar{x}, y + \frac{1}{2}$ (33) $\bar{y}, \bar{z}, \bar{x}$ (34) $y + \frac{1}{2}, \bar{z}, x + \frac{1}{2}$ (35) $\bar{y}, z + \frac{1}{2}, x + \frac{1}{2}$ (36) $y + \frac{1}{2}, z + \frac{1}{2}, \bar{x}$ (37) $\bar{y}, \bar{x}, z + \frac{1}{2}$ (38) $y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (39) $\bar{y}, x + \frac{1}{2}, \bar{z}$ (40) $y + \frac{1}{2}, \bar{x}, \bar{z}$ (41) $\bar{x}, \bar{z}, y + \frac{1}{2}$ (42) $x + \frac{1}{2}, \bar{z}, \bar{y}$ (43) $x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}$ (44) $\bar{x}, z + \frac{1}{2}, \bar{y}$ (45) $\bar{z}, \bar{y}, x + \frac{1}{2}$ (46) $\bar{z}, y + \frac{1}{2}, \bar{x}$ (47) $z + \frac{1}{2}, \bar{y}, \bar{x}$ (48) $z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}$	$Ok_l : k + l = 2n$ $hhl : l = 2n$ $h00 : h = 2n$							
24 $h$ ..2	$\frac{1}{4}, y, y$ $y, \frac{1}{4}, y$ $y, y, \frac{1}{4}$ $\frac{3}{4}, \bar{y}, \bar{y}$ $\bar{y}, \frac{3}{4}, \bar{y}$ $\bar{y}, \bar{y}, \frac{3}{4}$	$\frac{1}{4}, \bar{y} + \frac{1}{2}, y$ $y, \frac{1}{4}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, y, \frac{1}{4}$ $\frac{3}{4}, y + \frac{1}{2}, \bar{y}$ $\bar{y}, \frac{3}{4}, y + \frac{1}{2}$ $y + \frac{1}{2}, \bar{y}, \frac{3}{4}$	$\frac{1}{4}, y, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{1}{4}, y$ $\bar{y} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \frac{1}{4}$ $\frac{3}{4}, \bar{y}, y + \frac{1}{2}$ $y + \frac{1}{2}, \frac{3}{4}, \bar{y}$ $\bar{y}, y + \frac{1}{2}, \frac{3}{4}$	$\frac{1}{4}, \bar{y} + \frac{1}{2}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \frac{1}{4}, \bar{y} + \frac{1}{2}$ $\bar{y} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \frac{1}{4}$ $\frac{3}{4}, y + \frac{1}{2}, y + \frac{1}{2}$ $y + \frac{1}{2}, \frac{3}{4}, y + \frac{1}{2}$ $y + \frac{1}{2}, y + \frac{1}{2}, \frac{3}{4}$	$hkl : h + k + l = 2n$				
24 $g$ 2..	$x, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, x, \frac{1}{4}$ $\bar{x}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, \bar{x}, \frac{3}{4}$	$\bar{x} + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $x + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}$ $\frac{1}{4}, x + \frac{1}{2}, \frac{3}{4}$	$\frac{1}{4}, x, \frac{3}{4}$ $x, \frac{1}{4}, \frac{3}{4}$ $\frac{3}{4}, \bar{x}, \frac{1}{4}$ $\bar{x}, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, \bar{x} + \frac{1}{2}, \frac{3}{4}$ $\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}$ $\frac{3}{4}, x + \frac{1}{2}, \frac{1}{4}$ $x + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{1}{4}, x$ $\frac{1}{4}, \frac{3}{4}, \bar{x} + \frac{1}{2}$ $\frac{1}{4}, \frac{3}{4}, \bar{x}$ $\frac{3}{4}, \frac{1}{4}, x + \frac{1}{2}$	$hkl : h + k + l = 2n$			
16 $f$ .3.	$x, x, x$ $x, x, \bar{x} + \frac{1}{2}$ $\bar{x}, \bar{x}, \bar{x}$ $\bar{x}, \bar{x}, x + \frac{1}{2}$	$\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, x$ $\bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $x + \frac{1}{2}, x + \frac{1}{2}, \bar{x}$ $x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}$	$\bar{x} + \frac{1}{2}, x, \bar{x} + \frac{1}{2}$ $x, \bar{x} + \frac{1}{2}, x$ $x + \frac{1}{2}, \bar{x}, x + \frac{1}{2}$ $\bar{x}, x + \frac{1}{2}, \bar{x}$	$x, \bar{x} + \frac{1}{2}, \bar{x} + \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x, x$ $\bar{x}, x + \frac{1}{2}, x + \frac{1}{2}$ $x + \frac{1}{2}, \bar{x}, \bar{x}$	$hkl : h + k + l = 2n$				
12 $e$ 4..	$x, \frac{1}{4}, \frac{1}{4}$ $\bar{x}, \frac{3}{4}, \frac{3}{4}$	$\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}$ $x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}$	$\frac{1}{4}, x, \frac{1}{4}$ $\frac{3}{4}, \bar{x}, \frac{3}{4}$	$\frac{1}{4}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ $\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}$	$\frac{1}{4}, \frac{1}{4}, x$ $\frac{3}{4}, \frac{3}{4}, \bar{x}$ $\frac{1}{4}, \frac{1}{4}, \bar{x} + \frac{1}{2}$ $\frac{3}{4}, \frac{3}{4}, x + \frac{1}{2}$	$hkl : h + k + l = 2n$			
12 $d$ $\bar{4}$ ..	$0, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, 0, \frac{1}{4}$	$\frac{1}{2}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \frac{1}{2}, \frac{1}{4}$	$\frac{1}{4}, 0, \frac{3}{4}$ $0, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{1}{2}, \frac{3}{4}$ $\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$	$\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$ $\frac{1}{4}, \frac{3}{4}, 0$	$hkl : h + k + l = 2n$			
8 $c$ . $\bar{3}$ .	0,0,0	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	0, $\frac{1}{2}, \frac{1}{2}$	0, $\frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	0, $\frac{1}{2}, 0$	$\frac{1}{2}, 0, 0$	$hkl : h, k, l = 2n$
6 $b$ 42.2	$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$	$hkl : h + k + l = 2n$		
2 $a$ 432	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$				$hkl : h + k + l = 2n$			

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