



# Analytical Methods for Materials

## Lesson 14

### Crystallography and Crystal Structures – continued

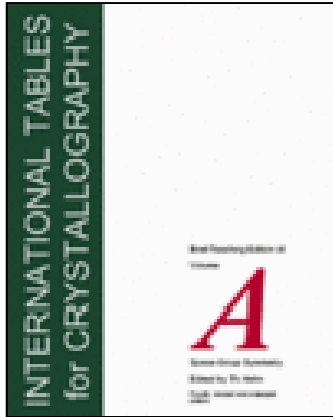
#### Suggested Reading

- Ch. 6 in Waseda
- Ch. 1 – C. Kittel, Introduction to Solid State Physics, 3<sup>rd</sup> Edition, Wiley (1956).
- Excerpt from ASM Metals Handbook.
- Chs. 1 and 3 – M. DeGraef and M.E. McHenry, Structure of Materials, Cambridge (2007).
- Chs. 1 and 3 – S.M. Allen and E.L. Thomas, The Structure of Materials, Wiley (1999).
- Chs. 3 and 4 – R. Tilley, Crystals and Crystal Structures, Wiley (2006).

# Graphical representation of space groups

- International Tables for Crystallography

- Expensive eight volume book series published by Springer. Volume A contains Space-group symmetry. You can access some of this information on line through the University of Alabama Libraries web site.
- An inexpensive Brief Teaching Edition of Volume A (ISBN 978-0-7923-6591-4) is available from the International Union of Crystallography (<http://www.iucr.org>).



- Information In Tables

- Diagrams of symmetry elements
  - One shows effect of operation of symmetry elements
  - One shows location of various symmetry elements
- Origin
- Asymmetric unit
- Symmetry operations
- Generators selected
- Positions, multiplicities, site symmetries, coordinates, reflection conditions
- Symmetry of special projections
- Maximal non-isomorphic subgroups
- Maximal isomorphic subgroups of lowest index
- Minimal non-isomorphic supergroups

Full H-M notation  $\rightarrow F m \bar{3} m$

SG number  $\rightarrow$  No. 225

$O_h^5$

$F 4/m \bar{3} 2/m$

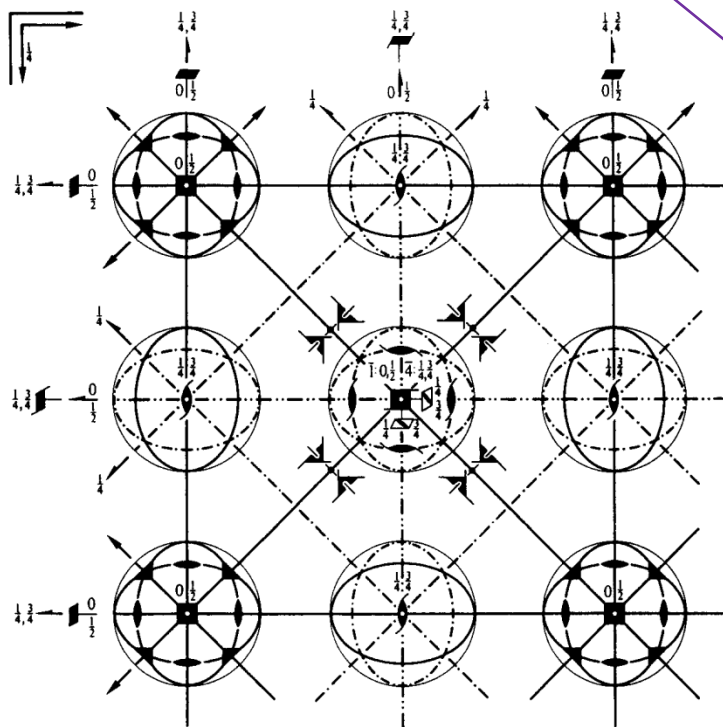
$m \bar{3} m$

Cubic  $\leftarrow$  **Lattice type**

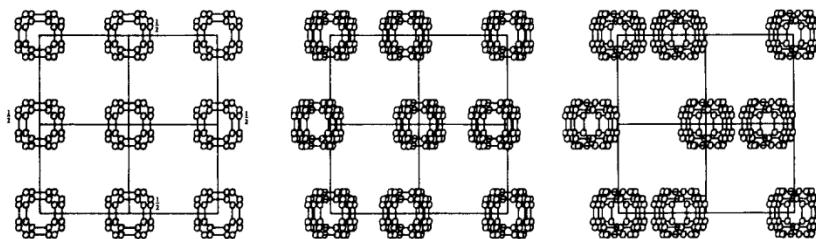
Patterson symmetry  $F m \bar{3} m$

**Short H-M notation**

**SG diagrams**



Upper left quadrant only



**Site symmetry of origin**

**Asymmetric unit**

**Location of motif**

Origin at centre ( $m \bar{3} m$ )

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

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

**Symmetry operations**

(given on page 153)

**Symmetry operations**



**Generators**

Determine sequence of coordinate triplets and reflection conditions

**Generators selected** (1);  $r(1,0,0)$ ;  $r(0,1,0)$ ;  $r(0,0,1)$ ;  $r(0, \frac{1}{2}, \frac{1}{2})$ ;  $r(\frac{1}{2}, 0, \frac{1}{2})$ ; (2); (3); (5); (13); (25)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry

Coordinates

Reflection conditions

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

$h, k, l$  permutable

General:

$hkl : h+k, h+l, k+l = 2n$

$OkI : k, l = 2n$

$hhl : h+l = 2n$

$h00 : h = 2n$

Special: as above, plus

no extra conditions

no extra conditions

no extra conditions

no extra conditions

$hkl : h = 2n$

no extra conditions

no extra conditions

$hkl : h = 2n$

$hkl : h = 2n$

no extra conditions

no extra conditions

192	<i>l</i>	1	(1) $x, y, z$	(2) $\bar{x}, \bar{y}, \bar{z}$	(3) $\bar{x}, y, \bar{z}$	(4) $x, \bar{y}, \bar{z}$
			(5) $z, \bar{x}, y$	(6) $z, \bar{x}, \bar{y}$	(7) $\bar{z}, \bar{x}, y$	(8) $\bar{z}, \bar{x}, \bar{y}$
			(9) $y, z, x$	(10) $\bar{y}, z, \bar{x}$	(11) $y, \bar{z}, \bar{x}$	(12) $\bar{y}, \bar{z}, x$
			(13) $y, x, \bar{z}$	(14) $\bar{y}, \bar{x}, \bar{z}$	(15) $y, \bar{x}, z$	(16) $\bar{y}, x, z$
			(17) $x, z, \bar{y}$	(18) $\bar{x}, z, y$	(19) $\bar{x}, \bar{z}, \bar{y}$	(20) $x, \bar{z}, y$
			(21) $z, y, \bar{x}$	(22) $z, \bar{y}, x$	(23) $\bar{z}, y, x$	(24) $\bar{z}, \bar{y}, \bar{x}$
			(25) $\bar{x}, \bar{y}, \bar{z}$	(26) $x, y, \bar{z}$	(27) $x, \bar{y}, z$	(28) $\bar{x}, y, z$
			(29) $\bar{z}, \bar{x}, \bar{y}$	(30) $\bar{z}, x, y$	(31) $z, x, \bar{y}$	(32) $z, \bar{x}, y$
			(33) $\bar{y}, \bar{z}, \bar{x}$	(34) $y, \bar{z}, x$	(35) $\bar{y}, z, x$	(36) $y, z, \bar{x}$
			(37) $\bar{y}, \bar{x}, z$	(38) $y, x, z$	(39) $\bar{y}, x, \bar{z}$	(40) $y, \bar{x}, \bar{z}$
			(41) $\bar{x}, \bar{z}, y$	(42) $x, \bar{z}, \bar{y}$	(43) $x, z, y$	(44) $\bar{x}, z, \bar{y}$
			(45) $\bar{z}, \bar{y}, x$	(46) $\bar{z}, y, \bar{x}$	(47) $z, \bar{y}, \bar{x}$	(48) $z, y, x$

96	<i>k</i>	$\dots m$	$x, x, z$ $\bar{x}, \bar{x}, x$ $x, x, \bar{z}$ $\bar{x}, \bar{z}, \bar{x}$	$\bar{x}, \bar{x}, z$ $\bar{z}, x, \bar{x}$ $\bar{x}, \bar{x}, \bar{z}$ $x, \bar{z}, x$	$\bar{x}, x, \bar{z}$ $x, z, x$ $x, \bar{x}, z$ $z, x, \bar{x}$	$x, \bar{x}, \bar{z}$ $\bar{x}, z, \bar{x}$ $\bar{x}, x, z$ $z, \bar{x}, x$	$z, x, x$ $x, \bar{z}, \bar{x}$ $x, z, \bar{x}$ $\bar{z}, x, x$	$z, \bar{x}, \bar{x}$ $\bar{x}, \bar{z}, x$ $\bar{x}, z, x$ $\bar{z}, \bar{x}, \bar{x}$	no extra conditions
96	<i>j</i>	$m \dots$	$0, y, z$ $\bar{z}, 0, y$ $y, 0, \bar{z}$ $0, \bar{z}, y$	$0, \bar{y}, z$ $\bar{z}, 0, \bar{y}$ $\bar{y}, 0, z$ $0, \bar{z}, y$	$0, y, \bar{z}$ $y, z, 0$ $y, 0, z$ $z, y, 0$	$0, \bar{y}, \bar{z}$ $\bar{y}, z, 0$ $\bar{y}, 0, z$ $z, \bar{y}, 0$	$z, 0, y$ $y, \bar{z}, 0$ $0, z, \bar{y}$ $\bar{z}, y, 0$	$z, 0, \bar{y}$ $\bar{y}, \bar{z}, 0$ $0, z, y$ $\bar{z}, \bar{y}, 0$	no extra conditions
48	<i>i</i>	$m \cdot m2$	$\frac{1}{2}, y, y$ $\bar{y}, \frac{1}{2}, y$	$\frac{1}{2}, \bar{y}, y$ $\bar{y}, \frac{1}{2}, \bar{y}$	$\frac{1}{2}, y, \bar{y}$ $y, y, \frac{1}{2}$	$\frac{1}{2}, \bar{y}, \bar{y}$ $\bar{y}, y, \frac{1}{2}$	$y, \frac{1}{2}, y$ $y, \bar{y}, \frac{1}{2}$	$y, \frac{1}{2}, \bar{y}$ $\bar{y}, \bar{y}, \frac{1}{2}$	no extra conditions
48	<i>h</i>	$m \cdot m2$	$0, y, y$ $\bar{y}, 0, y$	$0, \bar{y}, y$ $\bar{y}, 0, \bar{y}$	$0, y, \bar{y}$ $y, y, 0$	$0, \bar{y}, \bar{y}$ $\bar{y}, y, 0$	$y, 0, y$ $y, \bar{y}, 0$	$y, 0, \bar{y}$ $\bar{y}, \bar{y}, 0$	no extra conditions
48	<i>g</i>	$2 \cdot mm$	$x, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, x, \frac{1}{2}$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \bar{x}, \frac{1}{2}$	$\frac{1}{2}, x, \frac{1}{2}$ $x, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$ $\bar{x}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, x$ $\frac{1}{2}, \frac{1}{2}, \bar{x}$	$\frac{1}{2}, \frac{1}{2}, \bar{x}$ $\frac{1}{2}, \frac{1}{2}, x$	$hkl : h = 2n$
32	<i>f</i>	$\cdot 3m$	$x, x, x$ $x, x, \bar{x}$	$\bar{x}, \bar{x}, x$ $\bar{x}, \bar{x}, \bar{x}$	$\bar{x}, x, \bar{x}$ $x, \bar{x}, x$	$x, \bar{x}, \bar{x}$ $\bar{x}, x, x$			no extra conditions
24	<i>e</i>	$4m \cdot m$	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	$0, 0, x$	$0, 0, \bar{x}$	no extra conditions
24	<i>d</i>	$m \cdot mm$	$0, \frac{1}{2}, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, 0$	$hkl : h = 2n$
8	<i>c</i>	$\bar{4}3m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$					$hkl : h = 2n$
4	<i>b</i>	$m\bar{3}m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$						no extra conditions
4	<i>a</i>	$m\bar{3}m$	$0, 0, 0$						no extra conditions

**Symmetry of special projections**

Along [001]  $p4mm$   
 $a' = \frac{1}{2}a$   $b' = \frac{1}{2}b$   
Origin at  $0, 0, z$

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

Along [110]  $c2mm$   
 $a' = \frac{1}{2}(-a + b)$   $b' = c$   
Origin at  $x, x, 0$

**Wyckoff positions**  
with multiplicity, Wyckoff letter and site symmetry

If atoms are occupying position  $8c$ , there are two equivalent atoms at  $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$  and  $\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$

**Orthographic projections**  
along symmetry directions

**Wyckoff positions for Cu**



**Maximal non-isomorphic subgroups**

<b>I</b>	[2] $F\bar{4}3m$ (216)	(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] $F432$ (209)	(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] $Fm\bar{3}1$ ( $Fm\bar{3}$ , 202)	(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] $F4/m12/m(I4/mmm, 139)$	(1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40)+
		[3] $F4/m12/m(I4/mmm, 139)$	(1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44)+
	}	[3] $F4/m12/m(I4/mmm, 139)$	(1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48)+
		[4] $F1\bar{3}2/m(R\bar{3}m, 166)$	(1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48)+
	}	[4] $F1\bar{3}2/m(R\bar{3}m, 166)$	(1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48)+
		[4] $F1\bar{3}2/m(R\bar{3}m, 166)$	(1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46)+
	}	[4] $F1\bar{3}2/m(R\bar{3}m, 166)$	(1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46)+
<b>IIa</b>			
<b>IIa</b>	[4] $Pn\bar{3}m$ (224)	1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48; (4; 6; 11; 16; 18; 23; 28; 30; 35; 40; 42; 47) + $(0, \frac{1}{2}, \frac{1}{2})$ ; (3; 8; 10; 15; 20; 22; 27; 32; 34; 39; 44; 46) + $(\frac{1}{2}, 0, \frac{1}{2})$ ; (2; 7; 12; 13; 17; 21; 26; 31; 36; 37; 41; 45) + $(\frac{1}{2}, \frac{1}{2}, 0)$	
	[4] $Pn\bar{3}m$ (224)	1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48; (4; 5; 10; 15; 19; 23; 28; 29; 34; 39; 43; 47) + $(0, \frac{1}{2}, \frac{1}{2})$ ; (3; 7; 11; 16; 17; 22; 27; 31; 35; 40; 41; 46) + $(\frac{1}{2}, 0, \frac{1}{2})$ ; (2; 8; 9; 14; 20; 21; 26; 32; 33; 38; 44; 45) + $(\frac{1}{2}, \frac{1}{2}, 0)$	
	[4] $Pn\bar{3}m$ (224)	1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46; (4; 8; 12; 15; 18; 21; 28; 32; 36; 39; 42; 45) + $(0, \frac{1}{2}, \frac{1}{2})$ ; (3; 6; 9; 16; 20; 24; 27; 30; 33; 40; 44; 48) + $(\frac{1}{2}, 0, \frac{1}{2})$ ; (2; 5; 11; 14; 17; 23; 26; 29; 35; 38; 41; 47) + $(\frac{1}{2}, \frac{1}{2}, 0)$	
	[4] $Pn\bar{3}m$ (224)	1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46; (4; 7; 9; 16; 19; 21; 28; 31; 33; 40; 43; 45) + $(0, \frac{1}{2}, \frac{1}{2})$ ; (3; 5; 12; 15; 17; 24; 27; 29; 36; 39; 41; 48) + $(\frac{1}{2}, 0, \frac{1}{2})$ ; (2; 6; 10; 13; 20; 23; 26; 30; 34; 37; 44; 47) + $(\frac{1}{2}, \frac{1}{2}, 0)$	
	[4] $Pm\bar{3}m$ (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	
	[4] $Pm\bar{3}m$ (221)	1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40; (9; 10; 11; 12; 17; 18; 19; 20; 33; 34; 35; 36; 41; 42; 43; 44) + $(0, \frac{1}{2}, \frac{1}{2})$ ; (5; 6; 7; 8; 21; 22; 23; 24; 29; 30; 31; 32; 45; 46; 47; 48) + $(\frac{1}{2}, 0, \frac{1}{2})$	
	[4] $Pm\bar{3}m$ (221)	1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44; (9; 10; 11; 12; 21; 22; 23; 24; 33; 34; 35; 36; 45; 46; 47; 48) + $(\frac{1}{2}, 0, \frac{1}{2})$ ; (5; 6; 7; 8; 13; 14; 15; 16; 29; 30; 31; 32; 37; 38; 39; 40) + $(\frac{1}{2}, \frac{1}{2}, 0)$	
	[4] $Pm\bar{3}m$ (221)	1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48; (5; 6; 7; 8; 17; 18; 19; 20; 29; 30; 31; 32; 41; 42; 43; 44) + $(0, \frac{1}{2}, \frac{1}{2})$ ; (9; 10; 11; 12; 13; 14; 15; 16; 33; 34; 35; 36; 37; 38; 39; 40) + $(\frac{1}{2}, \frac{1}{2}, 0)$	
	<b>IIb</b>	none	

**Refer to relations between space groups**



**Maximal isomorphic subgroups of lowest index**

**IIc** [27]  $Fm\bar{3}m$  ( $a' = 3a, b' = 3b, c' = 3c$ ) (225)

**Minimal non-isomorphic supergroups**

**I** none  
**II** [2]  $Pm\bar{3}m$  ( $a' = \frac{1}{3}a, b' = \frac{1}{3}b, c' = \frac{1}{3}c$ ) (221)

**More information can be found in the international Tables!**

**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 <sup>+</sup> x,x,x         | (6) 3 <sup>+</sup> $\bar{x},x,\bar{x}$          | (7) 3 <sup>+</sup> x, $\bar{x},\bar{x}$         | (8) 3 <sup>+</sup> $\bar{x},\bar{x},x$         |
| (9) 3 <sup>-</sup> x,x,x         | (10) 3 <sup>-</sup> x, $\bar{x},\bar{x}$        | (11) 3 <sup>-</sup> $\bar{x},\bar{x},x$         | (12) 3 <sup>-</sup> $\bar{x},x,\bar{x}$        |
| (13) 2 x,x,0                     | (14) 2 x, $\bar{x},0$                           | (15) 4 <sup>-</sup> 0,0,z                       | (16) 4 <sup>-</sup> 0,0,z                      |
| (17) 4 <sup>-</sup> x,0,0        | (18) 2 0,y,y                                    | (19) 2 0,y, $\bar{y}$                           | (20) 4 <sup>+</sup> x,0,0                      |
| (21) 4 <sup>+</sup> 0,y,0        | (22) 2 x,0,x                                    | (23) 4 <sup>-</sup> 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) 3 <sup>+</sup> x,x,x; 0,0,0 | (30) 3 <sup>+</sup> $\bar{x},x,\bar{x}; 0,0,0$  | (31) 3 <sup>+</sup> x, $\bar{x},\bar{x}; 0,0,0$ | (32) 3 <sup>+</sup> $\bar{x},\bar{x},x; 0,0,0$ |
| (33) 3 <sup>-</sup> x,x,x; 0,0,0 | (34) 3 <sup>-</sup> x, $\bar{x},\bar{x}; 0,0,0$ | (35) 3 <sup>-</sup> $\bar{x},\bar{x},x; 0,0,0$  | (36) 3 <sup>-</sup> $\bar{x},x,\bar{x}; 0,0,0$ |
| (37) m x, $\bar{x},z$            | (38) m x,x,z                                    | (39) 4 <sup>-</sup> 0,0,z; 0,0,0                | (40) 4 <sup>-</sup> 0,0,z; 0,0,0               |
| (41) 4 <sup>-</sup> x,0,0; 0,0,0 | (42) m x,y, $\bar{y}$                           | (43) m x,y,y                                    | (44) 4 <sup>+</sup> x,0,0; 0,0,0               |
| (45) 4 <sup>+</sup> 0,y,0; 0,0,0 | (46) m $\bar{x},y,x$                            | (47) 4 <sup>-</sup> 0,y,0; 0,0,0                | (48) m x,y,x                                   |

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

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

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

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

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

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

← **Symmetry operations**  
Continued from first page

Transform the initial point x, y, z into point under consideration

# Other sources for information

- Pearson's Handbook of Crystallographic Data for Intermetallic Phases
  - Very inclusive
- Smithells Metals Reference Book
  - Information for many crystal structures
- Various other handbooks
- The information provided will allow you to build up crystal structures.



# Excerpt from Pearson's Handbook

---

Phase	Structure Type	Pearson Symbol and Space Group	$a, b, c$ (nm)	$\alpha, \beta, \gamma$ ( $^\circ$ )	Atoms	Point Set	$x$	$y$	$z$	$Occ$
<b>Cu</b>	Cu	$cF4 Fm\bar{3}m$ ( $Fm3m$ )	0.36148		$Cu$	$4a$	000	000	000	100

---

- A prototype (i.e., structure type) is provided for each phase.
- Pearson symbol and space group tell us Bravais lattice, basis, and symmetry.
- **Atoms**, **Point Set**,  $(x,y,z)$  and **Occ** are the **Wykoff generating sites**.

These are sites of specific atoms in the crystal structure that the space group symmetry operators act on.

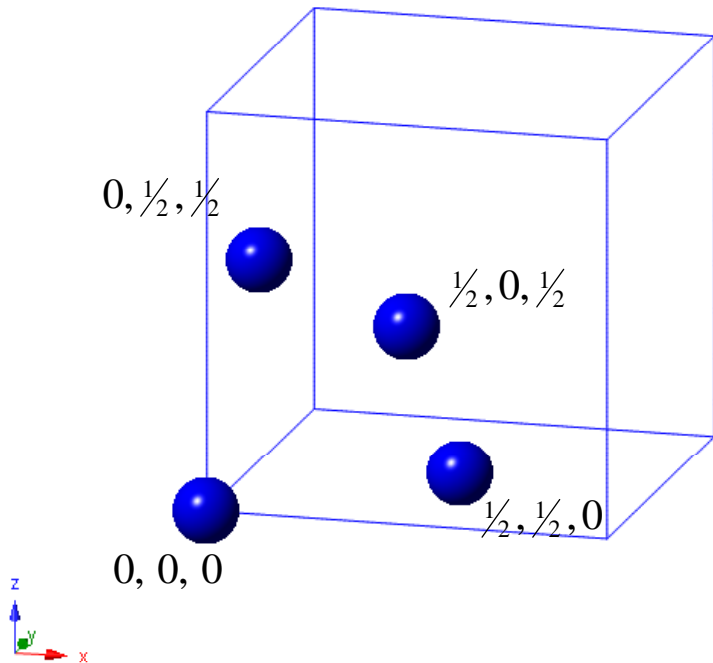
We find these sites in the *International Tables for Crystallography, Volume A, Space Group Symmetry*.

*Wyckoff sites and Point Sets  
are used to determine site  
occupancy.*

See this site for high resolution diagrams and tables  
<http://img.chem.ucl.ac.uk/sgp/mainmenu.htm>



# Example for Copper



FCC basis

Cu

$$(x, y, z) = (0, 0, 0)$$

+

$$(0, 0, 0)$$

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

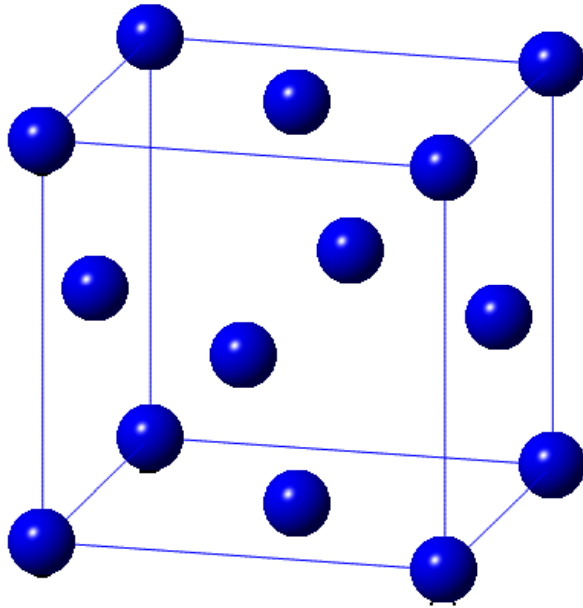
$$(\frac{1}{2}, 0, \frac{1}{2})$$

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

} Wyckoff  
Coords.

Stack on every corner

# Example for Copper - continued



Cu

$$(x, y, z) = (0, 0, 0)$$

+

$$(0, 0, 0)$$

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

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

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

} Wyckoff  
Coords.

Normal FCC unit cell

# What about Tungsten (W, atomic number = 74)

---

Phase	Structure Type	Pearson Symbol and Space Group	$a, b, c$ (nm)	$\alpha, \beta, \gamma$ ( $^\circ$ )	Atoms	Point Set	$x$	$y$	$z$	$Occ$
<b>W</b>	W	$cI2 Im\bar{3}m$ ( $Im3m$ )	0.3165		W	$2a$	000	000	000	100

---

- It is part of space group #229. I've presented relevant information on next 2 pages. You can also find this information online at:

<http://img.chem.ucl.ac.uk/sgp/mainmenu.htm>

$Im\bar{3}m$

$O_h^9$

$m\bar{3}m$

Cubic

CONTINUED

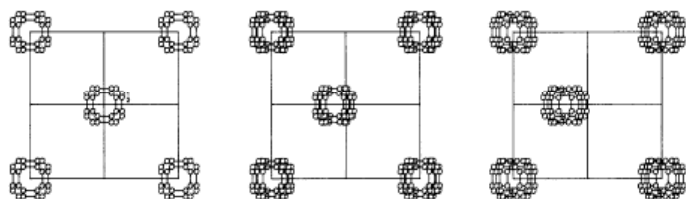
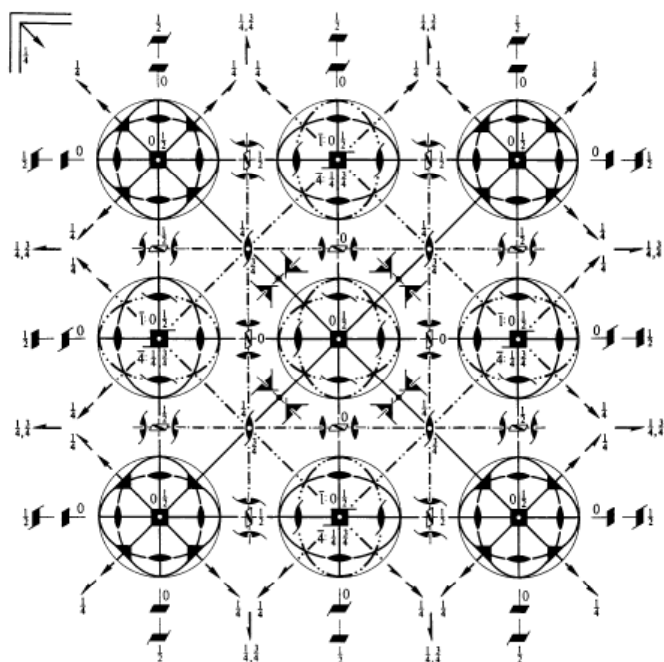
No. 229

$Im\bar{3}m$

No. 229

$I 4/m\bar{3}2/m$

Patterson symmetry  $Im\bar{3}m$



Origin at centre ( $m\bar{3}m$ )

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

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

Symmetry of special projections

Along  $[001]$   $p4mm$   $a' = \frac{1}{2}(a-b)$   $b' = \frac{1}{2}(a+b)$       Along  $[111]$   $p6mm$   $a' = \frac{1}{3}(2a-b-c)$   $b' = \frac{1}{3}(-a+2b-c)$       Along  $[110]$   $p2mm$   $a' = \frac{1}{2}(-a+b)$   $b' = \frac{1}{2}c$

**Maximal non-isomorphic subgroups**

<b>I</b>	[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] $I132/m(R\bar{3}m, 166)$	(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] $I132/m(R\bar{3}m, 166)$	(1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46)+
	[4] $I132/m(R\bar{3}m, 166)$	(1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46)+
<b>IIa</b>	[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; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48) + $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
	[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)

**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 <sup>+</sup> x,x,x	(6) 3 <sup>+</sup> x,x,x	(7) 3 <sup>+</sup> x,x,x	(8) 3 <sup>+</sup> x,x,x
(9) 3 <sup>-</sup> x,x,x	(10) 3 <sup>-</sup> x,x,x	(11) 3 <sup>-</sup> x,x,x	(12) 3 <sup>-</sup> x,x,x
(13) 2 x,x,0	(14) 2 x,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,y	(20) 4 <sup>+</sup> x,0,0
(21) 4 <sup>-</sup> 0,y,0	(22) 2 x,0,x	(23) 4 <sup>-</sup> 0,y,0	(24) 2 x,0,x
(25) I 0,0,0	(26) m x,y,0	(27) m x,0,z	(28) m 0,y,z
(29) 3 <sup>+</sup> x,x,x; 0,0,0	(30) 3 <sup>+</sup> x,x,x; 0,0,0	(31) 3 <sup>+</sup> x,x,x; 0,0,0	(32) 3 <sup>+</sup> x,x,x; 0,0,0
(33) 3 <sup>-</sup> x,x,x; 0,0,0	(34) 3 <sup>-</sup> x,x,x; 0,0,0	(35) 3 <sup>-</sup> x,x,x; 0,0,0	(36) 3 <sup>-</sup> x,x,x; 0,0,0
(37) m x,x,z	(38) m x,x,z	(39) 4 <sup>-</sup> 0,0,z; 0,0,0	(40) 4 <sup>-</sup> 0,0,z; 0,0,0
(41) 4 <sup>-</sup> x,0,0; 0,0,0	(42) m x,y,y	(43) m x,y,y	(44) 4 <sup>+</sup> x,0,0; 0,0,0
(45) 4 <sup>+</sup> 0,y,0; 0,0,0	(46) m x,y,x	(47) 4 <sup>-</sup> 0,y,0; 0,0,0	(48) m x,y,x

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

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