3.012 Fund of Mat Sci: Structure – Lecture 15

TILES, TILES, TILES, TILES, TILES, TILES

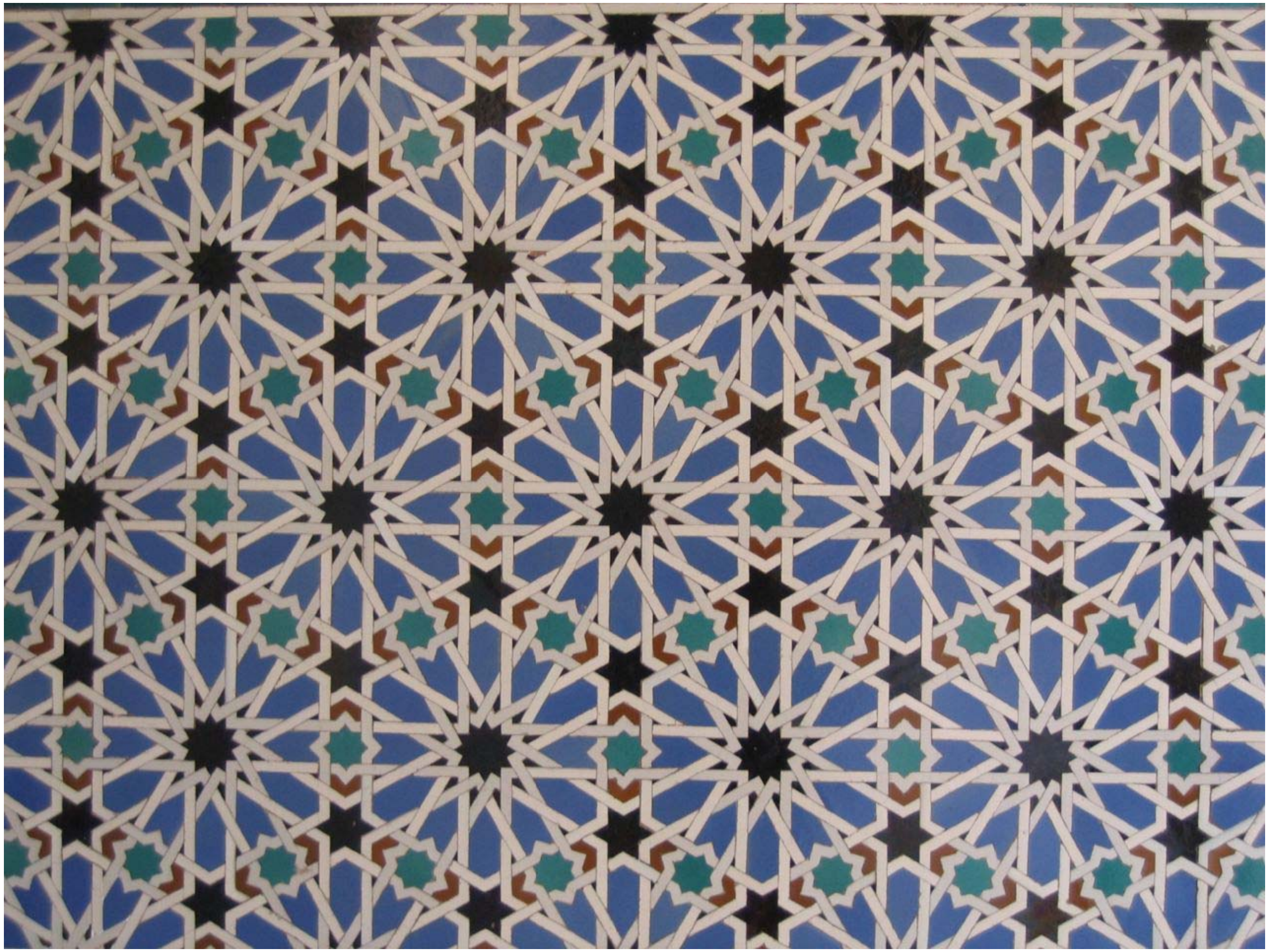


Photo courtesy of Chris Applegate.

Homework for Fri Nov 4

- Study: Allen and Thomas from 3.1.1 to 3.1.4 and 3.2.1, 3.2.4 (just read), and 3.2.5 (only crystal systems, Bravais lattices, unit cells)

Last time:

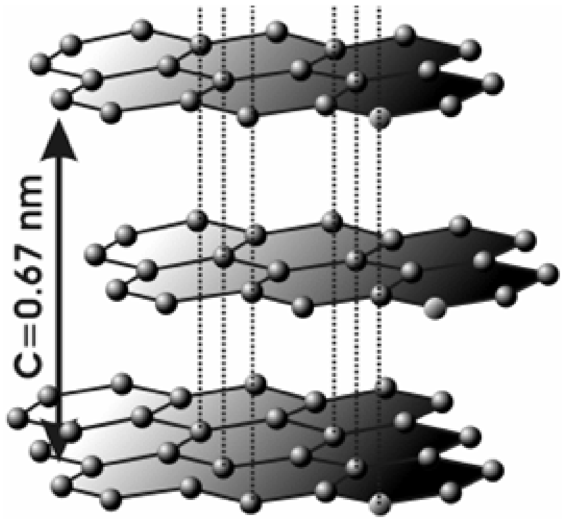
1. Symmetry operations forming a group, and symmetry operations as matrices
2. Molecular symmetries: rotation, inversion, rotoinversion
3. Examples of C_{2v}(water), D_{2h}(ethene)
4. Basic ideas about 3d, crystals, and lattices

Why do we do this ?

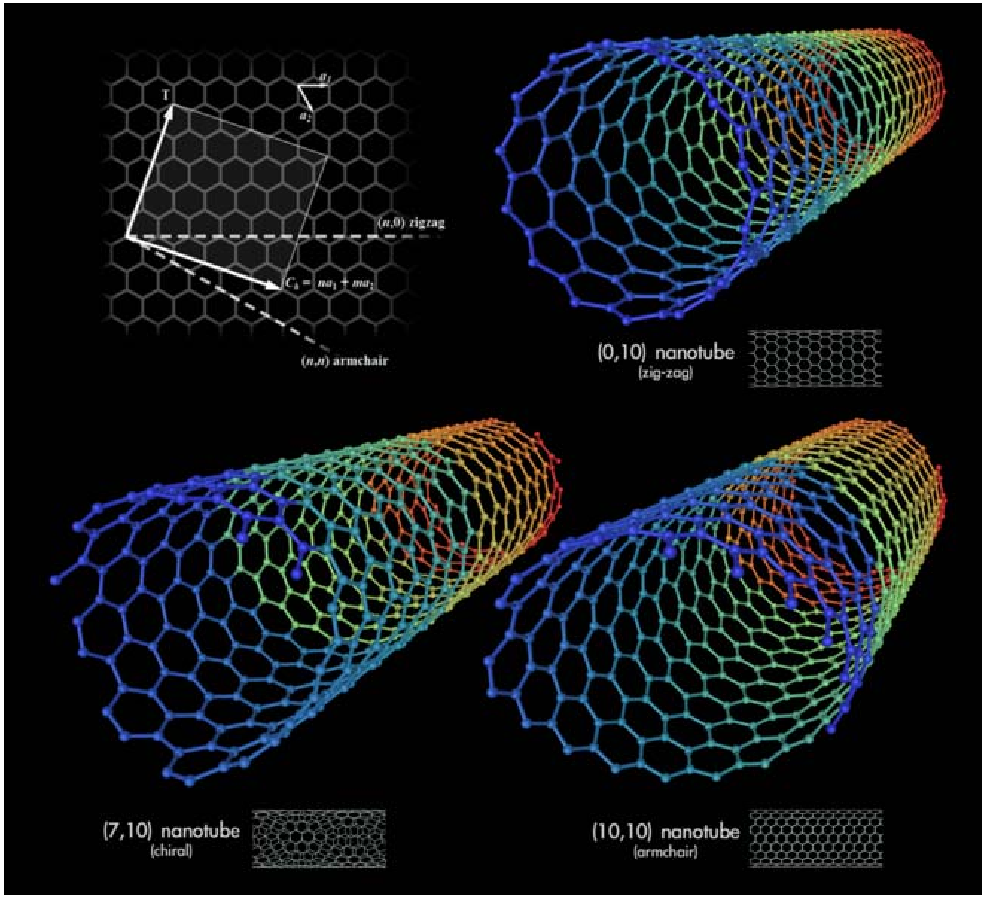
- Constraints on physical properties
- Crystal structures from spectroscopies
- Captures universal properties

From graphite to nanotubes

Photos of apples arranged to resemble atoms in graphite and carbon nanotubes removed for copyright reasons.



Source: Wikipedia



Point group symmetries in 3 dim:
1) Rotations (axis: diad, triad...)

Diagrams of various rotational symmetries removed for copyright reasons.
See pages 100-101, Figures 3.10 and 3.11, in Allen, S. M., and E. L. Thomas. *The Structure of Materials*. New York, NY: J. Wiley & Sons, 1999.

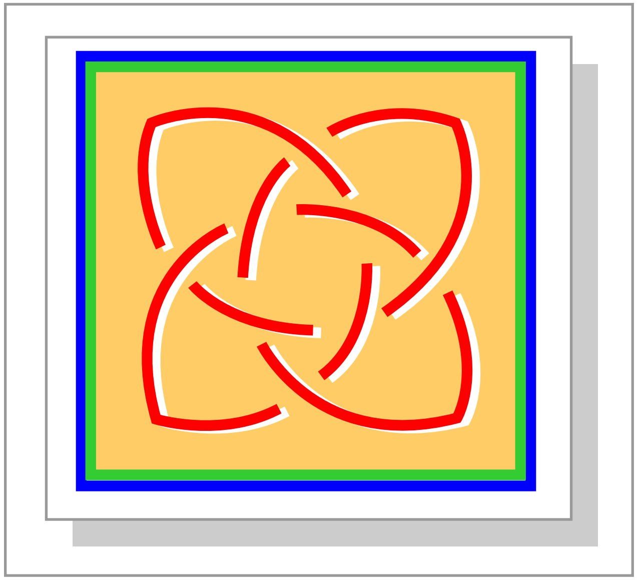


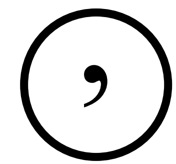
Figure by MIT OCW.

International notation:

1, 2, 3, 4, 6

Schoenflies: C_i

Point group symmetries in 3 dim:
2) Reflections (mirror)



Diagrams of reflectional symmetry removed for copyright reasons.
See p. 98, figure 3.7 in Allen, S. M., and E. L. Thomas.
The Structure of Materials. New York, NY: J. Wiley & Sons, 1999.

International: *m*

Point group symmetries in 3 dim:

3) Inversion, rotoinversion, rotoreflection

Diagrams of rotoinversion axes removed for copyright reasons. See p. 128, figures 3.34 and 3.35, in Allen, S. M., and E. L. Thomas. *The Structure of Materials*. New York, NY: J. Wiley & Sons, 1999.

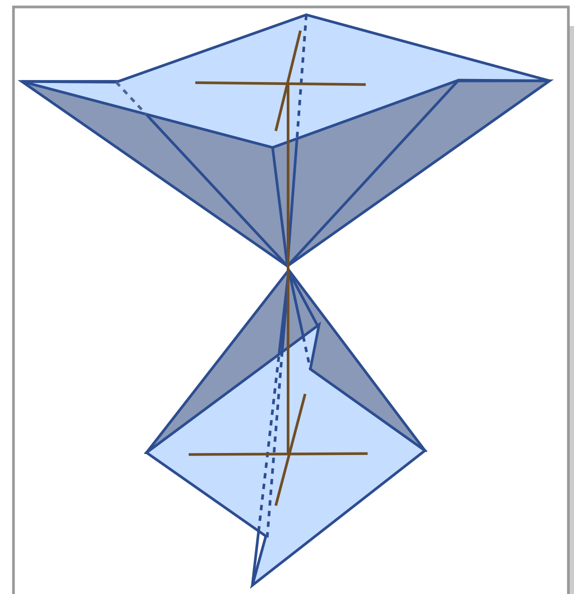


Figure by MIT OCW.

Rotoinversion: $\bar{1}, \bar{2}, \bar{3}\ldots$

Rotoreflection: $\tilde{1}, \tilde{2}, \tilde{3}\ldots$

(Inversion: $\bar{1}$)

Two mirror planes → rotation axis

Image of reflectional symmetry and rotation removed for copyright reasons.
See p. 104, figure 3.14 in Allen, S. M., and E. L. Thomas. *The Structure of Materials*. New York, NY: J. Wiley & Sons, 1999.

Translational Symmetry

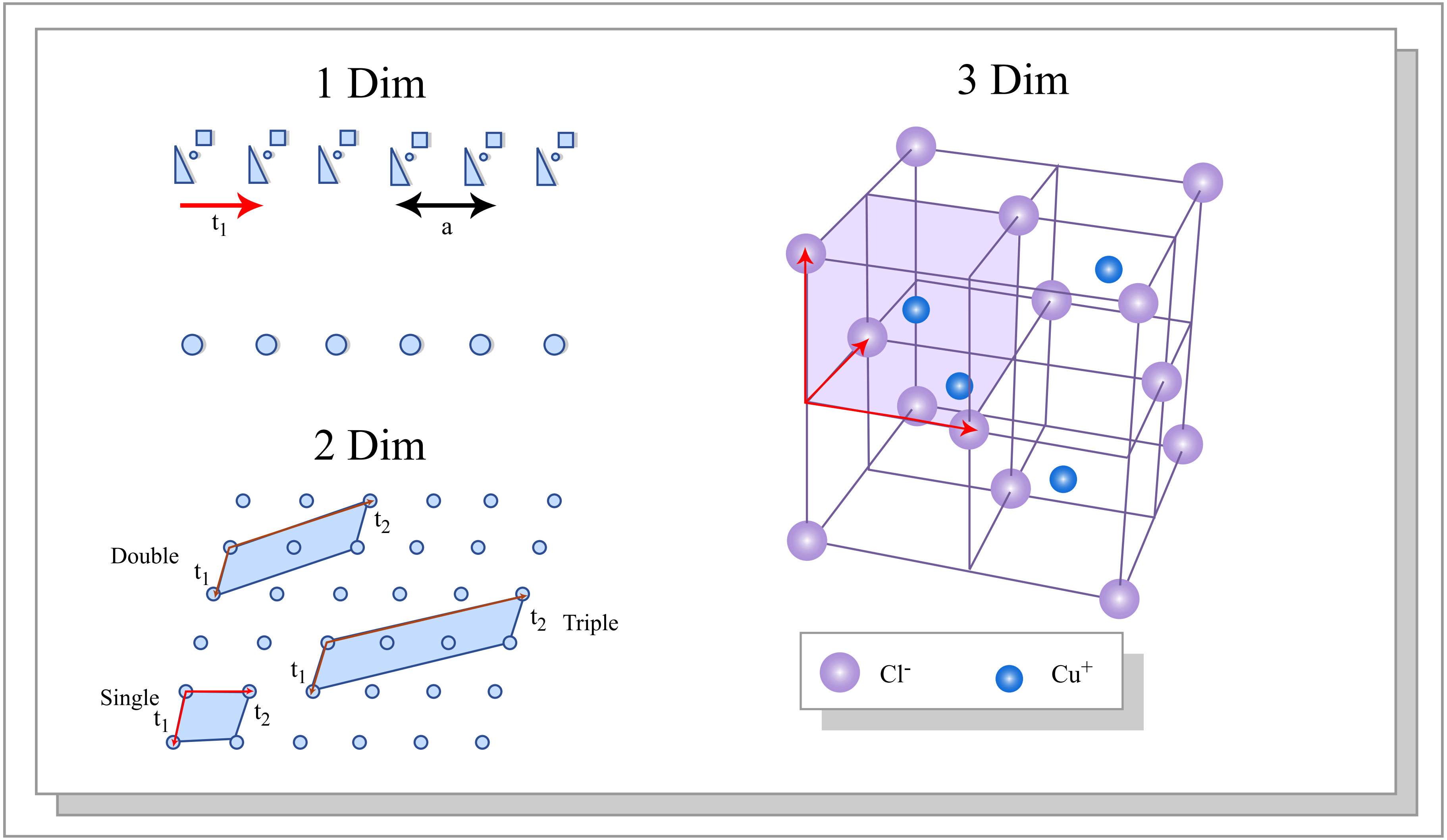


Figure by MIT OCW.

Rotations compatible with translations

Images removed for copyright reasons.
See p. 102, figures 3.12 and 3.13, in Allen, S. M., and E. L. Thomas. *The Structure of Materials*. New York, NY: J. Wiley & Sons, 1999.

$$mT = T - 2\left(T\cos\alpha\right)$$

Ten *crystallographic* point groups in 2d

Illustrations of the ten crystallographic point groups removed for copyright reasons.
See p. 106, figure 3.18, in Allen, S. M., and E. L. Thomas. *The Structure of Materials*. New York, NY: J. Wiley & Sons, 1999.

Bravais Lattices

- Infinite array of points with an arrangement and orientation that appears exactly the same regardless of the point from which the array is viewed.

$$\vec{R} = l\vec{a} + m\vec{b} + n\vec{c}$$ l,m and n integers

$\vec{a}, \vec{b}, \vec{c}$ primitive lattice vectors

- 14 Bravais lattices exist in 3 dimensions (1848)
- M. L. Frankenheimer in 1842 thought they were 15. So, so naïve…

Bravais Lattices

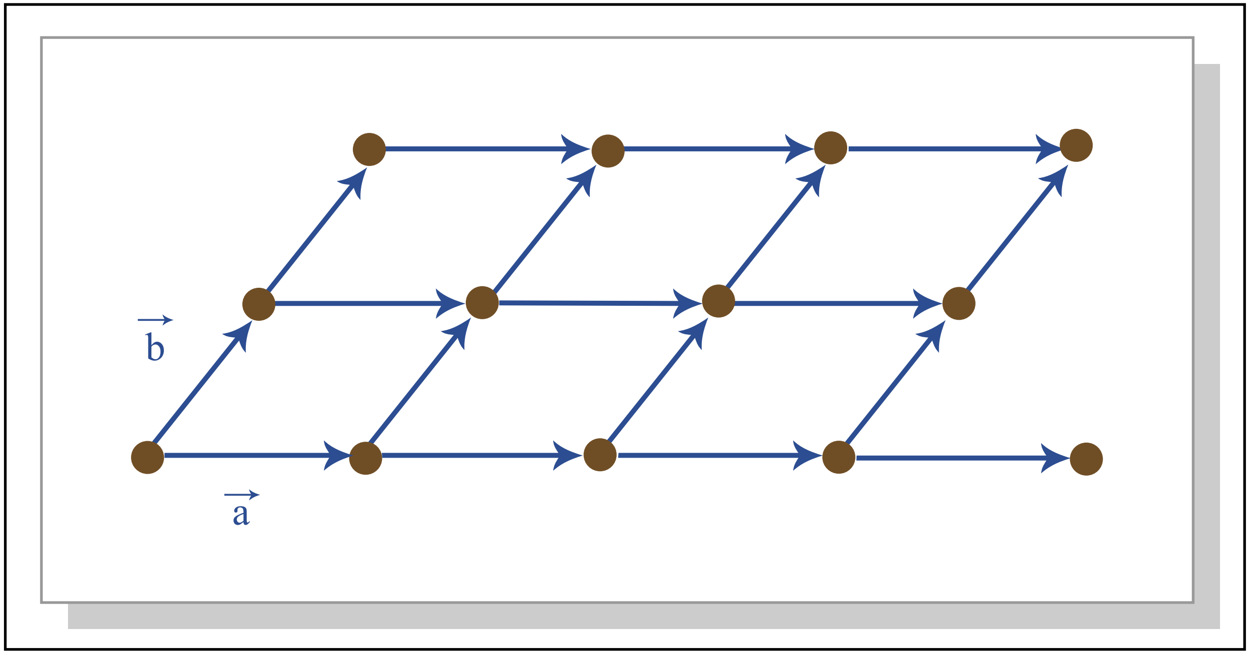


Figure by MIT OCW.

4 Lattice Types

7 Crystal Classes

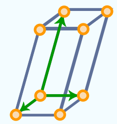
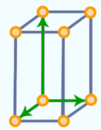
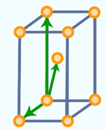
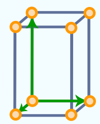
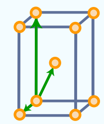
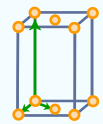
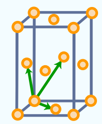
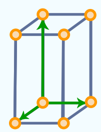
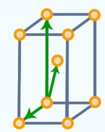
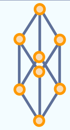
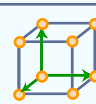
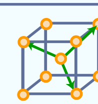
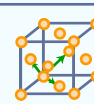
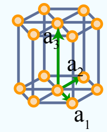
Bravais Lattice	Parameters	Simple (P)	Volume Centered (I)	Base Centered (C)	Face Centered (F)
Triclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} \neq \alpha_{23} \neq \alpha_{31}$				
Monoclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{23} = \alpha_{31} = 90^0$ $\alpha_{12} \neq 90^0$				
Orthorhombic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90^0$				
Tetragonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90^0$				
Trigonal	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} < 120^0$				
Cubic	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90^0$				
Hexagonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = 120^0$ $\alpha_{23} = \alpha_{31} = 90^0$				

Figure by MIT OCW.

32 *crystallographic* point groups in 3d

The Crystallographic Point Groups and the Lattice Types.

Crystal System	Schoenflies Symbol	Hermann-Mauguin Symbol	Order of the group	Laue Group
Triclinic	C_1	1	1	$\bar{1}$
	C_i	$\bar{1}$	2	
Monoclinic	C_2	2	2	2/*m*
	C_s	*m*	2	
	C_{2h}	2/*m*	4	
Orthorhombic	D_2	222	4	*mmm*
	C_{2v}	*mm*2	4	
	D_{2h}	*mmm*	8	
Tetragonal	C_4	4	4	4/*m*
	S_4	$\bar{4}$	4	
	C_{4h}	4/*m*	8	
	D_4	422	8	4/*m mm*
	C_{4v}	4*mm*	8	
	D_{2d}	$\bar{4}2m$	8	
	D_{4h}	4/*m mm*	16	
Trigonal	C_3	3	3	$\bar{3}$
	C_{3i}	$\bar{3}$	6	
	D_3	32	6	$\bar{3}m$
	C_{3v}	3*m*	6	
	D_{3d}	$\bar{3}m$	12	
Hexagonal	C_6	6	6	6/*m*
	C_{3h}	$\bar{6}$	6	
	C_{6h}	6/*m*	12	
	D_6	622	12	6/*m mm*
	C_{6v}	6*mm*	12	
	D_{3h}	$\bar{6}m2$	12	
	D_{6h}	6/*m mm*	24	
Cubic	T	23	12	$m\bar{3}$
	T_h	$m\bar{3}$	24	
	O	432	24	$m\bar{3}m$
	T_d	$\bar{4}3m$	24	
	O_h	$m\bar{3}m$	48	

Figure by MIT OCW.

Schoenflies notation

A_{nx} , where

- A:{C,D,T,O,S}
- n:{□,2,3,4,6} (□ means no symbol}
- x:{□,s,i,h,v,d}

Reading the International Tables

Figure removed for copyright reasons.
See p. 157, figure 3.59 in Allen, S. M., and E. L. Thomas. *The Structure of Materials*. New York, NY: J. Wiley & Sons, 1999.