3.012 Fund of Mat Sci: Structure – Lecture 14

POINT GROUPS AND BRAVAIS LATTICES

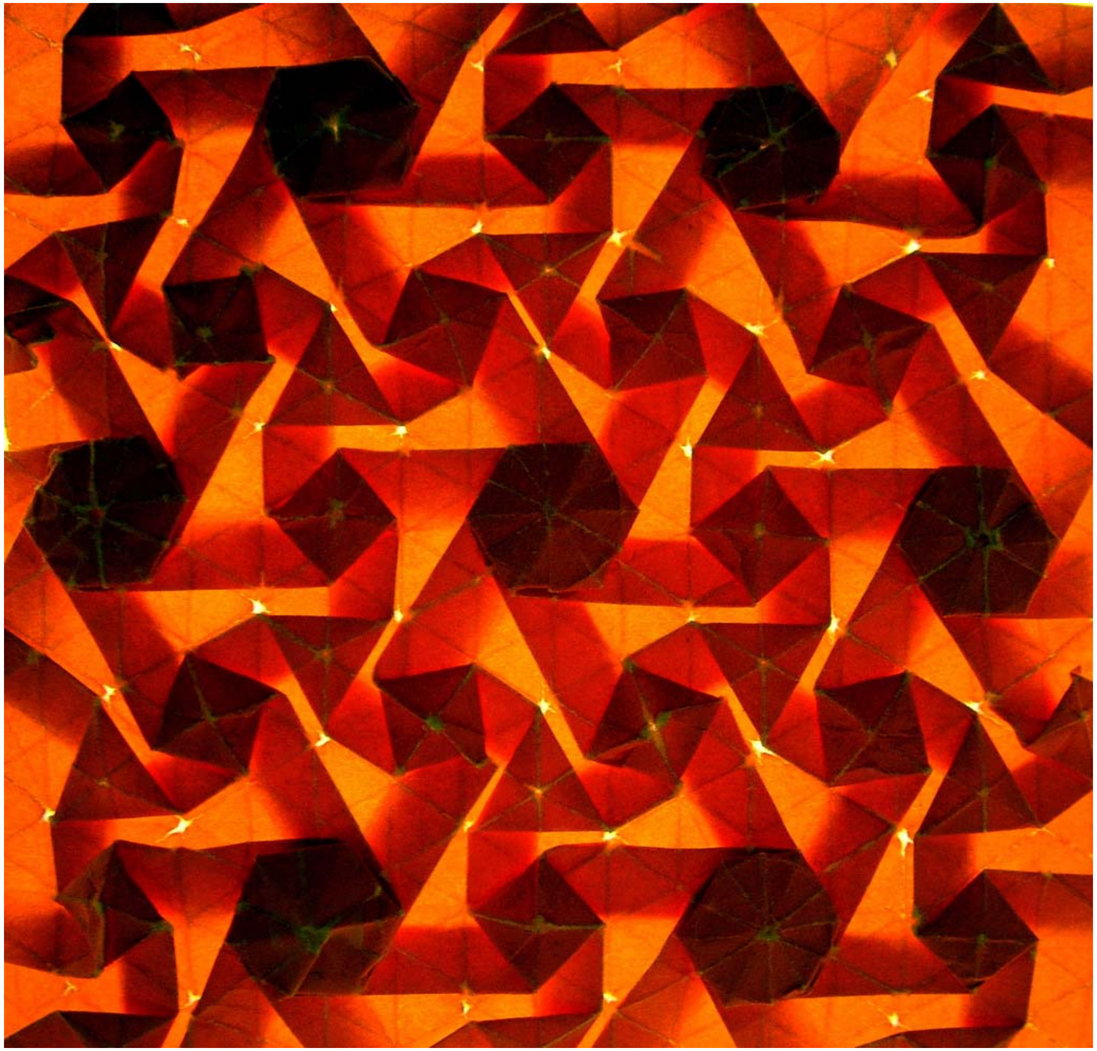


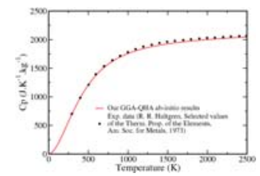
Photo courtesy of Eric Gjerde

Homework for Wed Nov 2

- Study: Allen and Thomas from 3.1.1 to 3.1.4 and 3.2.1, 3.2.4, and 3.2.5

Last time:

1. The quantization of vibrations: $E = \hbar\omega\left(n + \frac{1}{2}\right)$
2. Specific heat and excitations of a Bose-Einstein ensemble



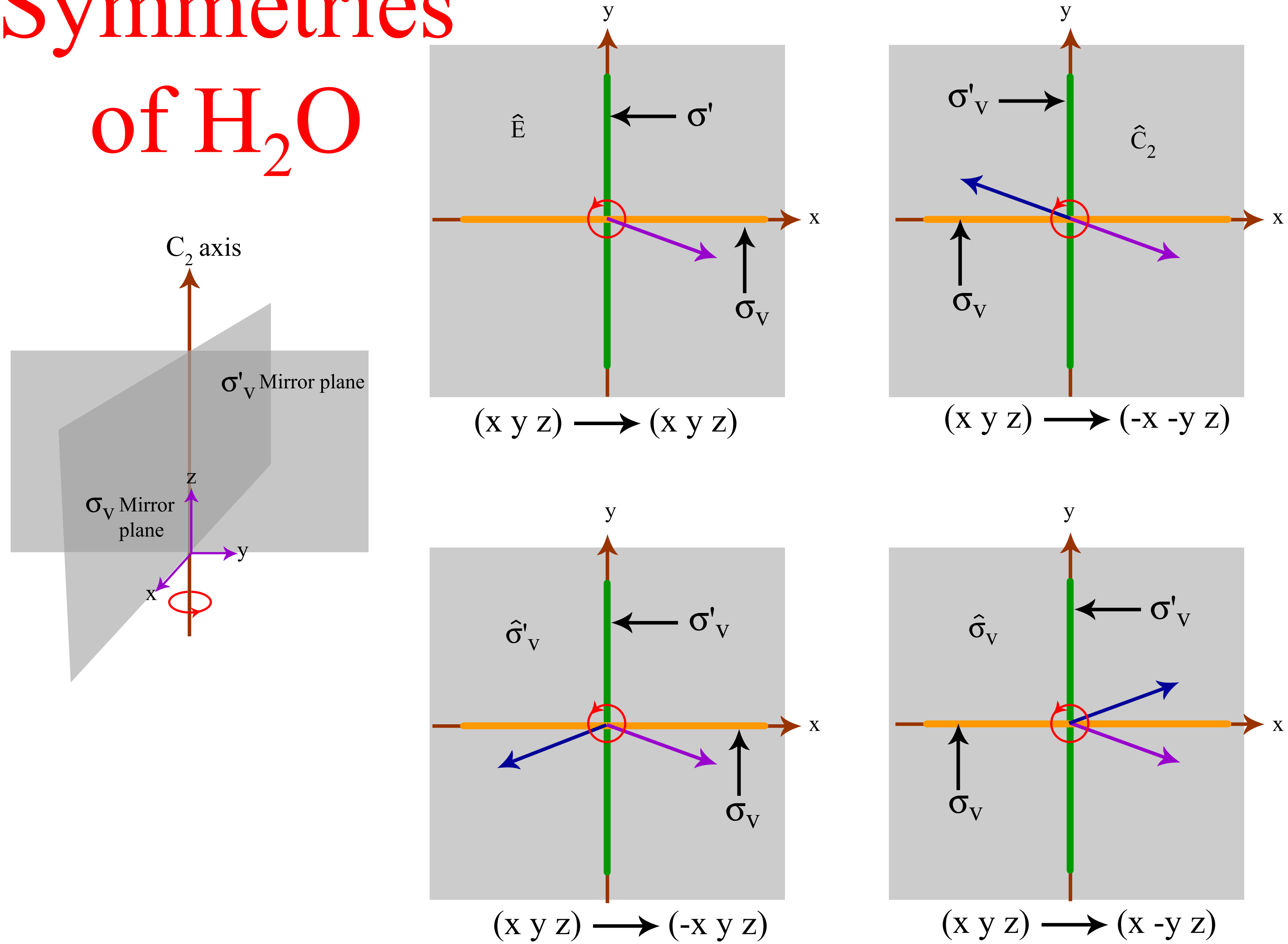
3. Symmetry operations (inversion, rotation, mirror…) and elements (points, axes, planes…)
4. Group theory

Possible symmetries in a molecule

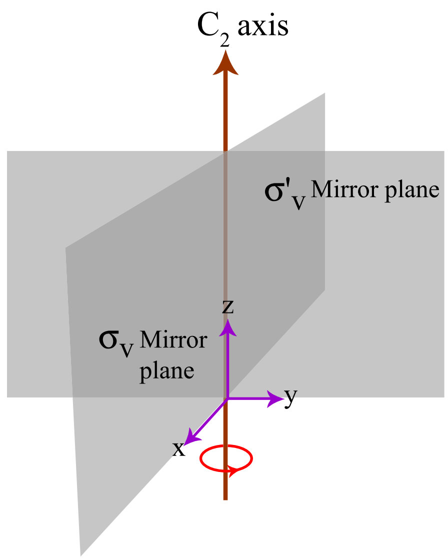
Table of symmetry elements and their corresponding operations removed for copyright reasons.

See Engel, T., and P. Reid. *Physical Chemistry*. Single volume ed. San Francisco, CA: Benjamin Cummings, 2005, p. 658, table 28.1.

Symmetries of H_2O



Symmetries of H_2O



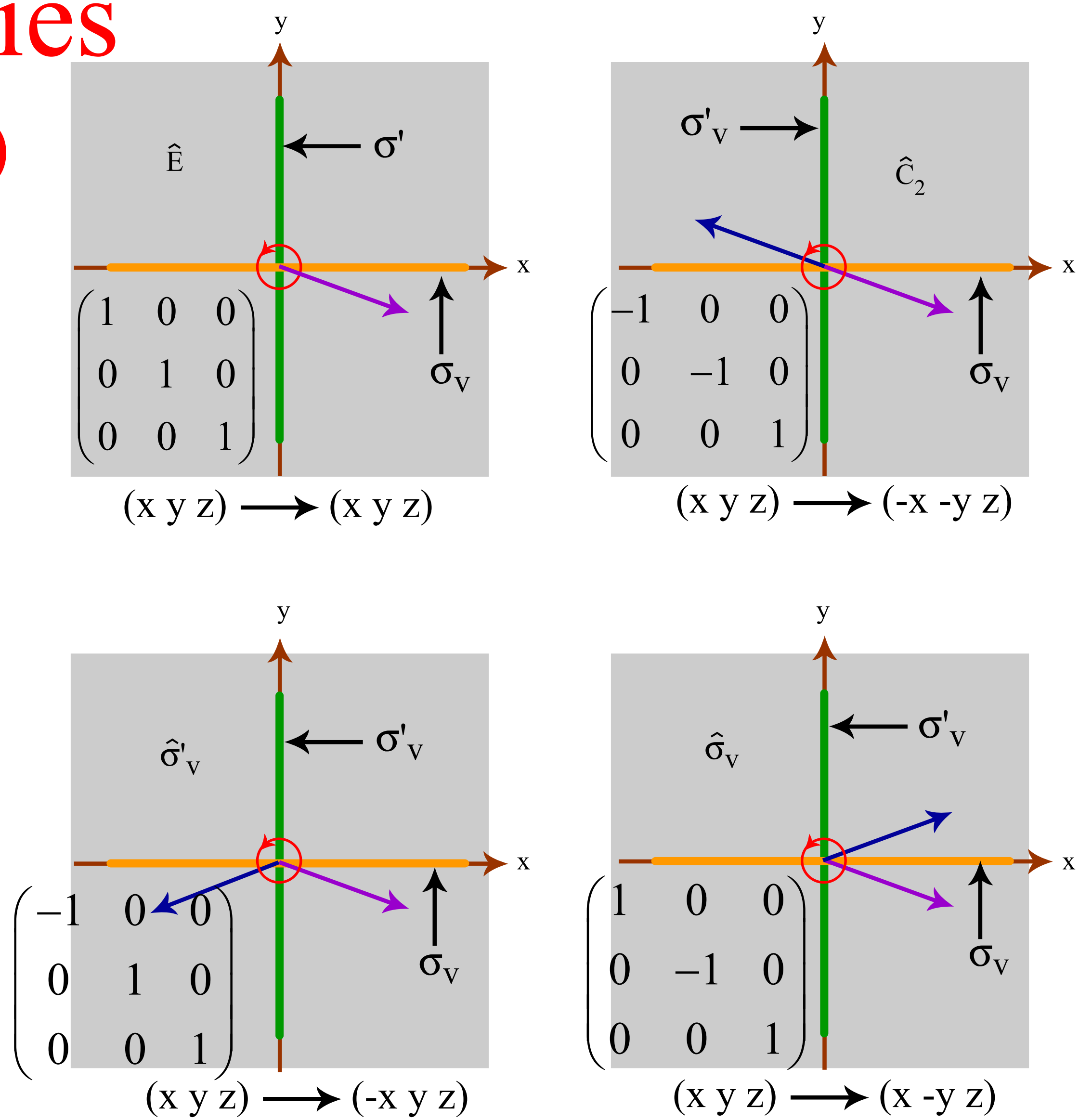


Figure by MIT OCW.

The 4 symmetry operations of H_2O form a group (called C_{2v})

1. Closure: A☼B is also in G.
2. Associativity: (A☼B) ☼C=A☼ (B☼C)
3. Identity: I☼A=A☼I
4. Inverse: A☼inv(A)=inv(A) ☼A=I

Multiplication Table for Operators of the C_{2V} Group removed for copyright reasons.

See Engel, T., and P. Reid. *Physical Chemistry*. Single volume ed. San Francisco, CA: Benjamin Cummings, 2005, p. 666, table 28.3.

D_{2h}

Image of the Symmetry elements of the D_{2h} group in ethene removed for copyright reasons.

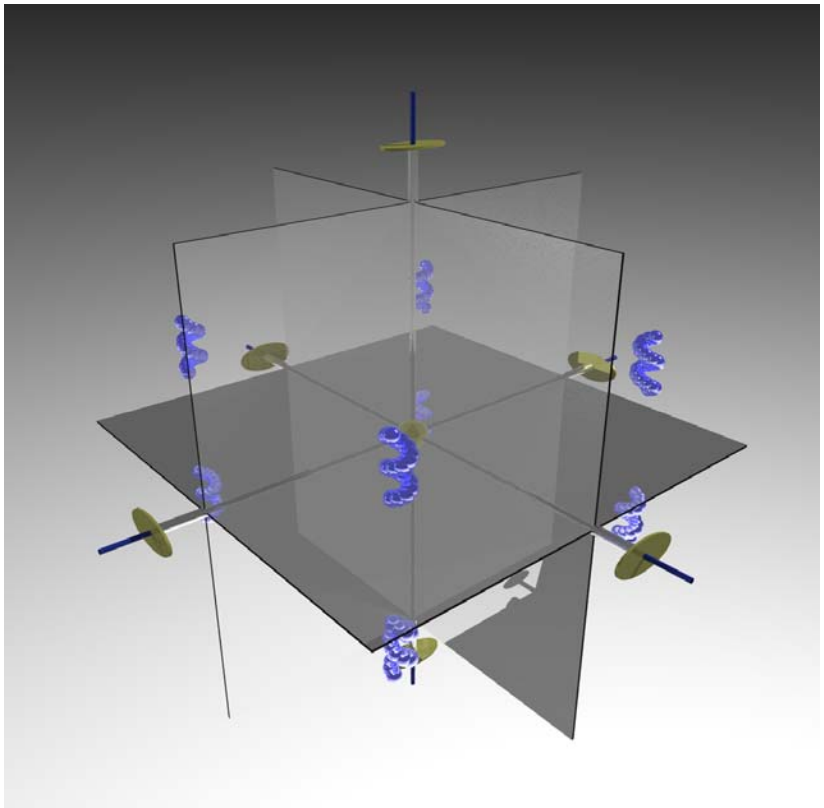
See Engel, T., and P. Reid. *Physical Chemistry*. Single volume ed. San Francisco, CA: Benjamin Cummings, 2005, p. 682, figure 28.10.

Representation of a proper rotation

Diagrams of various rotational axes removed for copyright reasons.

See Allen, S. M., and E. L. Thomas. *The Structure of Materials*. New York, NY: J. Wiley & Sons, 1999, pp. 100-101, figures 3.10 and 3.11.

Representation of D_{2h}



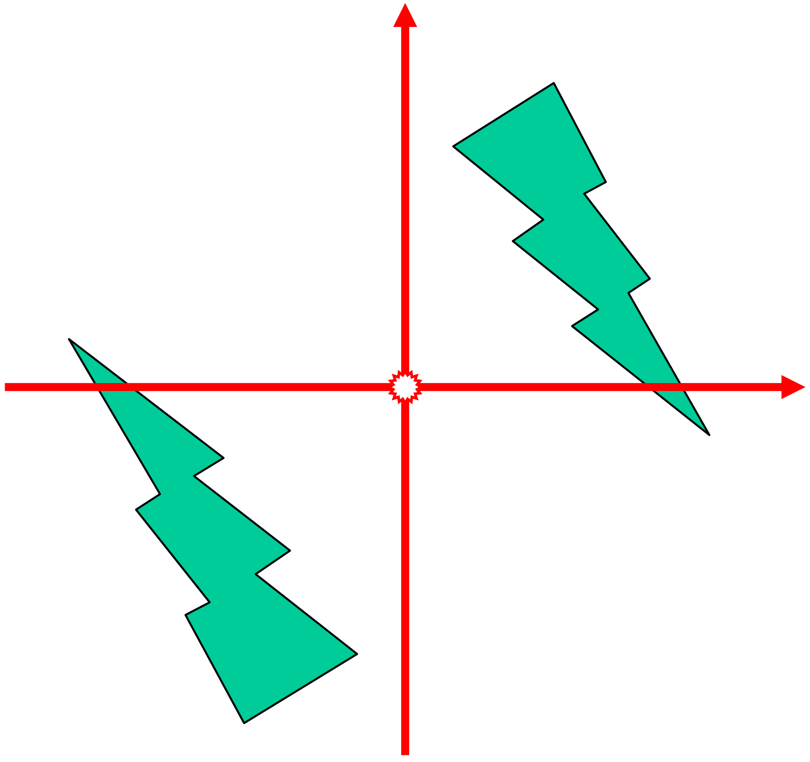
Courtesy of Marc De Graef. Used with permission.

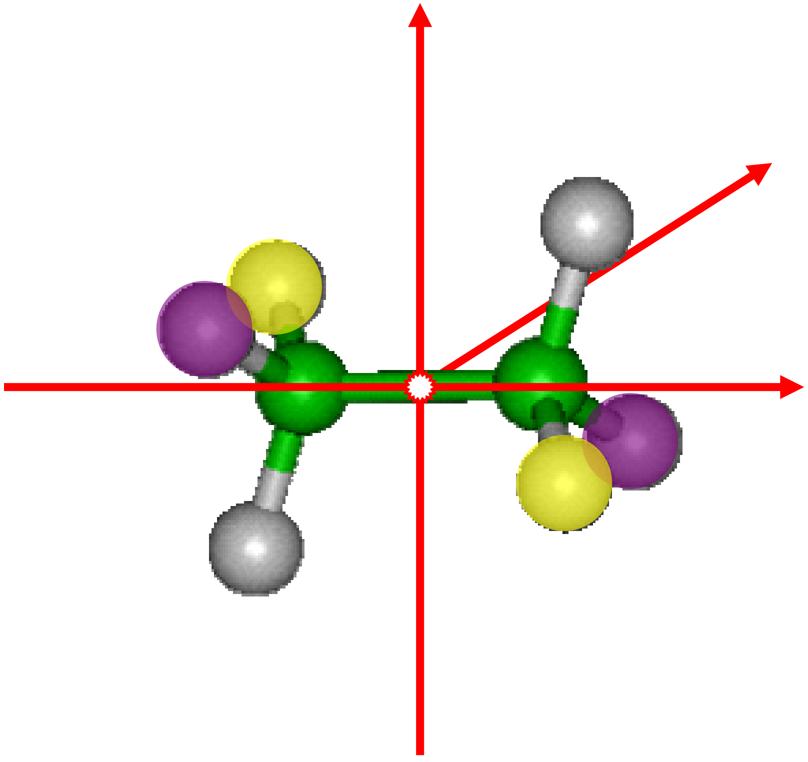
Image of the Symmetry elements of the D_{2h} group in ethene removed for copyright reasons.

See Engel, T., and P. Reid. *Physical Chemistry*. Single volume ed. San Francisco, CA: Benjamin Cummings, 2005, p. 682, figure 28.10.

Symmetry in three dimensions

- Inversion is only meaningful in 3-dim





Symmetry in three dimensions

- Roto-inversion (improper rotation)

Diagrams of rotoinversion axes removed for copyright reasons.

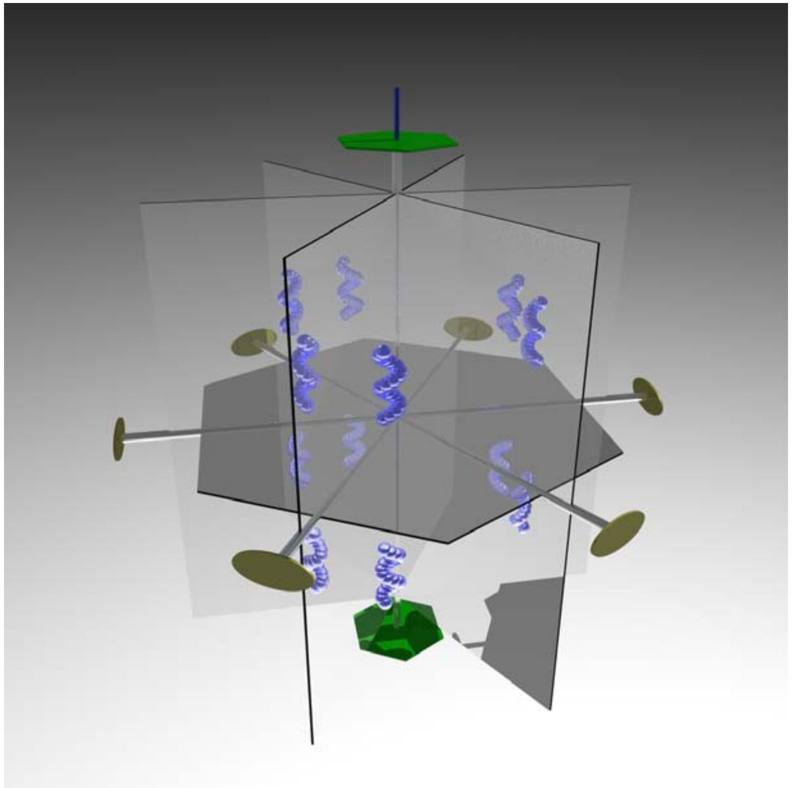
See Allen, S. M., and E. L. Thomas. *The Structure of Materials*. New York, NY: J. Wiley & Sons, 1999, p. 128, figures 3.34 and 3.35.

Symmetry in three dimensions

- Roto-reflection (improper rotation)

Diagrams of the operation of a threefold rotoreflection axis removed for copyright reasons.
See Allen, S. M., and E. L. Thomas. *The Structure of Materials*. New York, NY: J. Wiley & Sons, 1999, p. 129, figure 3.36.

Representation of D_{3h}



Courtesy of Marc De Graef. Used with permission.

Image of the symmetry elements of a PCL5 molecule removed for copyright reasons.
See Engel, T., and P. Reid. *Physical Chemistry*. Single volume ed. San Francisco, CA: Benjamin Cummings, 2005, page 658, figure 28.1(b).

Translational Symmetry

Diagrams of one-dimensional periodicity removed for copyright reasons.
See Allen, S. M., and E. L. Thomas. *The Structure of Materials*. New York, NY: J. Wiley & Sons, 1999, p. 92, figure 3.1.

Primitive, multiple, and unit cells

Diagrams of primitive and nonprimitive cells removed for copyright reasons.
See Allen, S. M., and E. L. Thomas. *The Structure of Materials*. New York, NY: J. Wiley & Sons, 1999, p. 94, figures 3.4 and 3.5.

4 Lattice Types

7 Crystal Classes

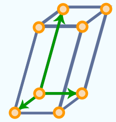
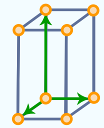
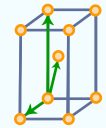
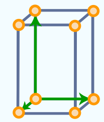
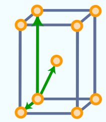
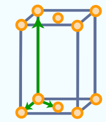
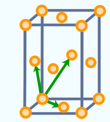
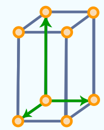
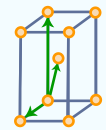
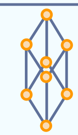
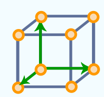
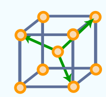
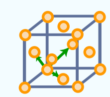
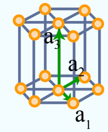
Bravais Lattice	Parameters	Simple (P)	Volume Centered (I)	Base Centered (C)	Face Centered (F)
Triclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} \neq \alpha_{23} \neq \alpha_{31}$				
Monoclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{23} = \alpha_{31} = 90^0$ $\alpha_{12} \neq 90^0$				
Orthorhombic	$a_1 \neq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

Mirror and glide planes

Figures of reflectional symmetry and symmetrical pattern generation removed for copyright reasons.
See Allen, S. M., and E. L. Thomas. *The Structure of Materials*. New York, NY: J. Wiley & Sons, 1999, pp. 98-99, figures 3.7 and 3.8.

Screw axes

Diagram of rotation axis and parallel translation removed for copyright reasons.
See page 130, Figure 3.38 in Allen, S. M., and E. L. Thomas. *The Structure of Materials*.
New York, NY: J. Wiley & Sons, 1999.

$$n\vec{\tau} = m\vec{\mathrm{T}}$$

Diagram of object repetitions by operation of 4_1, 4_2, and 4_3 screw axes. Removed for copyright reasons.
See page 133, Figure 3.39 in Allen, S. M., and E. L. Thomas. *The Structure of Materials.*
New York, NY: J. Wiley & Sons, 1999.

Combining rotations and translations

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

32 Crystallographic Point Groups

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}	$mm2$	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}	$4mm$	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}	$3m$	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}	$6mm$	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.