Lattice and Crystal

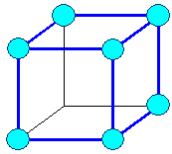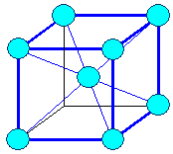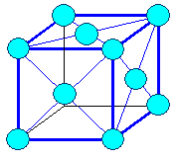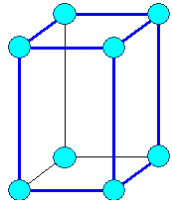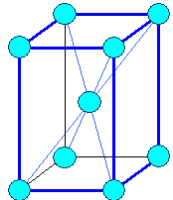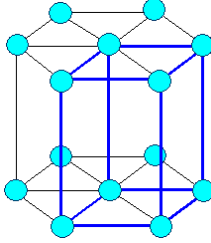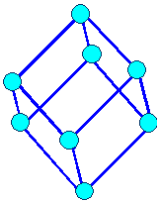An ideal crystal is a repetition of identical structural units in three dimensional space. The periodicity is described by a mathematical **lattice** (which are mathematical points at specific coordinates in space), the identical structural units (or **base** of the crystal) are the atoms in some specific arrangement which are unambiguously placed at every lattice point. Note that *a lattice is not a crystal*, even so the two words are often used synonymously in colloquial language, especially in the case of elemental crystals where the base consists of one atom only.
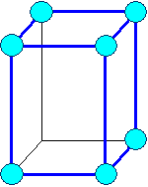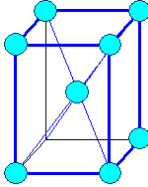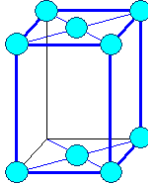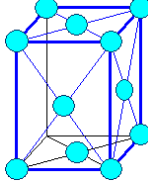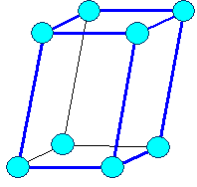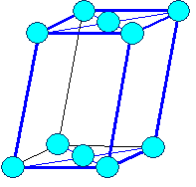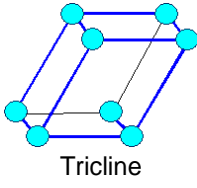
- All possible *lattices* can be described by a set of three linearly independent vectors $\underline{a}_1$, $\underline{a}_2$, and $\underline{a}_3$, the unit vectors of the lattice. Each lattice point than can be reached by a translation vector $\underline{T}$ of the lattice given by

$$\underline{T} = (u \cdot \underline{a}_1, v \cdot \underline{a}_1, w \cdot \underline{a}_3)$$
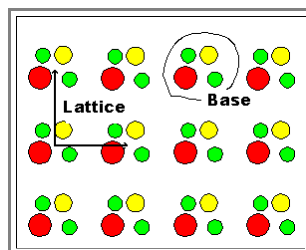
- With u, v, w = integers.

It is convenient, to classify lattices according to some basic symmetry groups. This yields the **14 Bravais lattices** , which are commonly used to describe lattice types. Their basic features are shown below (For sake of clarity, the lattice points are shown as little spheres and occasionally only "visible" lattice points are shown. These are *not* atoms, however!)

Name of crystal system Length of Base vectors	Angles between axes	Bravais Lattices		
Cubic $a_1 = a_2 = a_3$	$\alpha = \beta = \gamma = 90^0$	**cubic primitive**	**cubic body centered (*bcc*)**	**cubic face centered (*fcc*)**
Tetragonal $a_1 = a_2 \neq a_3$	$\alpha = \beta = \gamma = 90^0$	Tetragonal primitive	Tetragonal body centered	
Hexagonal $a_1 = a_2 \neq a_3$	$\alpha = \beta = 90^0$, $\gamma = 120^0$	Hexagonal (elementary cell continued to show hex. symmetry)		
Rhombohedral $a_1 = a_2 = a_3$	$\alpha = \beta = \gamma \neq 90^0$	Rhombohedral		
Orthorhombic $a_1 \neq a_2 \neq a_3$	$\alpha = \beta = \gamma \neq 90^0$			

Basics

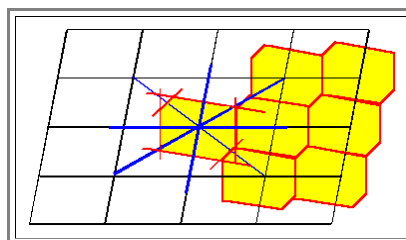| Orthorhombic $a_1 \neq a_2 \neq a_3$	$\alpha = \beta = \gamma \neq 90^0$	Orthorhombic primitive	Orthorhombic body centered	Orthorhombic base face centered / Orthorhombic face centered
Monoclinic $a_1 \neq a_2 \neq a_3$	$\alpha = \beta = 90^0, \gamma \neq 90^0$	Monocline primitive		Monocline base face centered
Tricline $a_1 \neq a_2 \neq a_3$	$\alpha \neq \beta \neq \gamma \neq 90^0$	Tricline		

A *crystal* now is obtained by taking a **Bravais lattice** *and* adding a **base**!

- The base can just be one atom (as in the case of many elemental crystals, most noteworthy the metals), two identical atoms (e.g. **Si**, **Ge**, **C**(diamond)), two different atoms (**NaCl**, **GaAs**, ...) three atoms, ... up to huge complex molecules as in the case of protein crystals.
- An arbitrary example is shown below

For certain applications, a Bravais lattice may not be the best choice. Whereas, for example, it shows best the cubic symmetry of the cubic lattices, its **elementary cell** is not a **primitive unit cell** of the lattice, i.e. there are unit cells with a smaller volume (but without the cubic symmetry). For other cases (especially if working in reciprocal lattices) the choice of a **Wigner**-**Seitz** cell may be appropriate, which is obtained by intersecting all lines from one lattice point to neighboring points at half the distance with planes at right angles to the lines

- This is shown schematically below: The blue lines connect lattice points, the red lines denote the intersection at right angles. The resulting Wigner-Seitz cell and its use in constructing the lattice are shown in yellow.

In practical work, one oftens refers to **crystal types** instead of lattices by using the name of prominent crystals, crystallographers or minerals etc.; e.g. "diamond type, Perovskites, "Zinkblende" structure and so on. A few examples are given in the link.