Course BT 631

Protein Structure, Function and Crystallography

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Why do we need a crystal?

- The diffraction from a single molecule would be too weak to measure. So, an ordered three-dimensional array of molecules is required, in other words a crystal, to magnify the signal. Even a small protein crystal might contain a billion molecules.

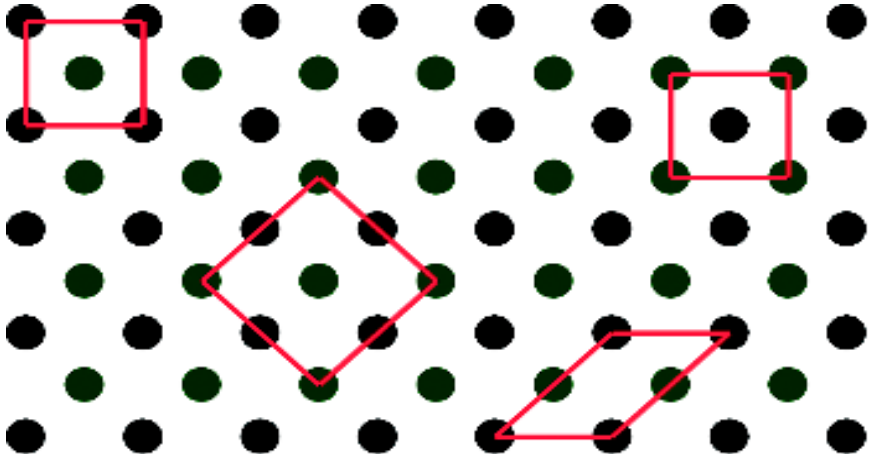
- If the internal order of the crystal is poor, then the X-rays will not be diffracted to high angles or high resolution and the data will not yield a detailed structure.

- If the crystal is well ordered, then diffraction will be measurable at high angles or high resolution and a detailed structure should result.

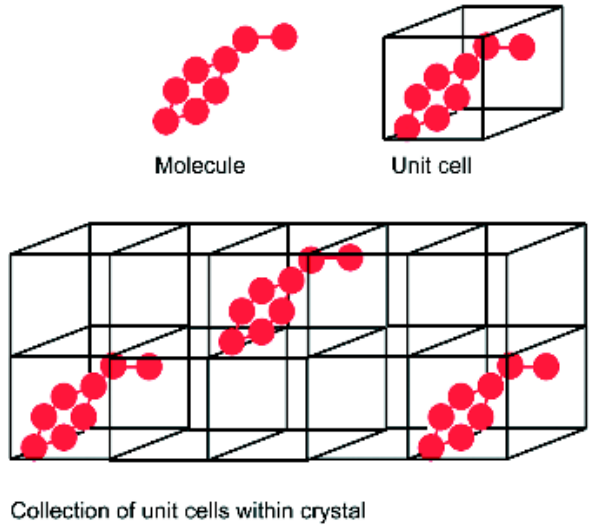
What is Unit cell in a crystal?

- With in any crystal the basic repeating pattern is the *unit cell* (Fig.) and in some crystals more than one unit cell is recognised. The simplest unit is chosen by a series of selection rules.

- The unit cell can be translated (moved side ways but not rotated) in any direction with in the crystal to yield an identical arrangement (Fig.).



Possible unit cells in a two-dimensional lattice

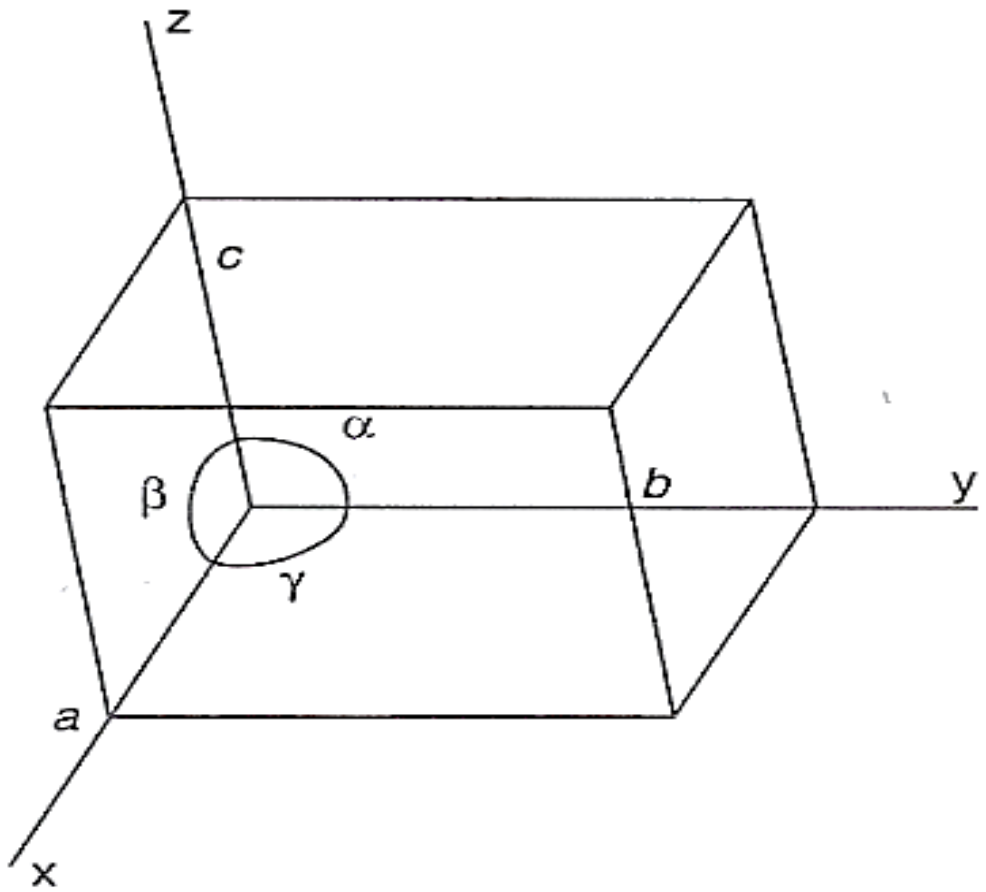


A unit cell for a simple molecule

What is Unit cell in a crystal?

- **The unit cell, the basic building block of a crystal is repeated infinitely in three dimensions but is characterized by three vectors *a, b, c.***

- **The unit cell is also defined by three angles between these three vectors:**
  α, the angel between b and c;
  β, angle between a and c;
  γ, the angle between a and b).

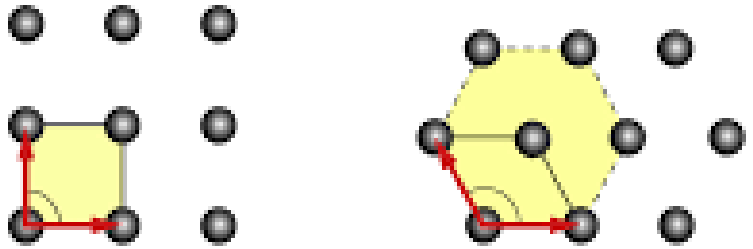


The angles and vectors defining any unit cell

2D-Bravais Lattices

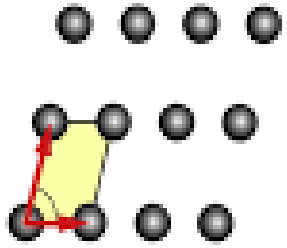
The recognition of different arrangements within a unit cell was recognized by Auguste Bravais.

In 2-Dimensions there are 5 distinct Bravais lattices

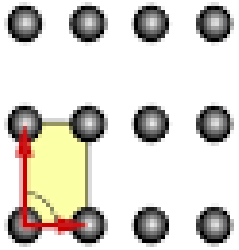


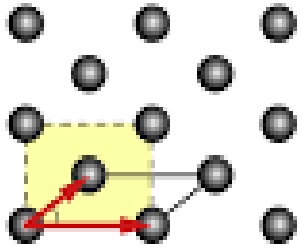
(a) square

(b) hexagonal



c) oblique





(d) Reactangular (e) Centered Rectangular

(2-Dimensional 5-Bravais Lattices)

Auguste Bravais
1811-1863 France

3D-Bravais Lattices

In 3-Dimensions there are 7 crystal systems

i) Triclinic,
ii) Monoclinic,
iii) Ortho-rhombic,
iv) Tetragonal,
v) Rhombohedral,
vi) Hexagonal and
vii) Cubic

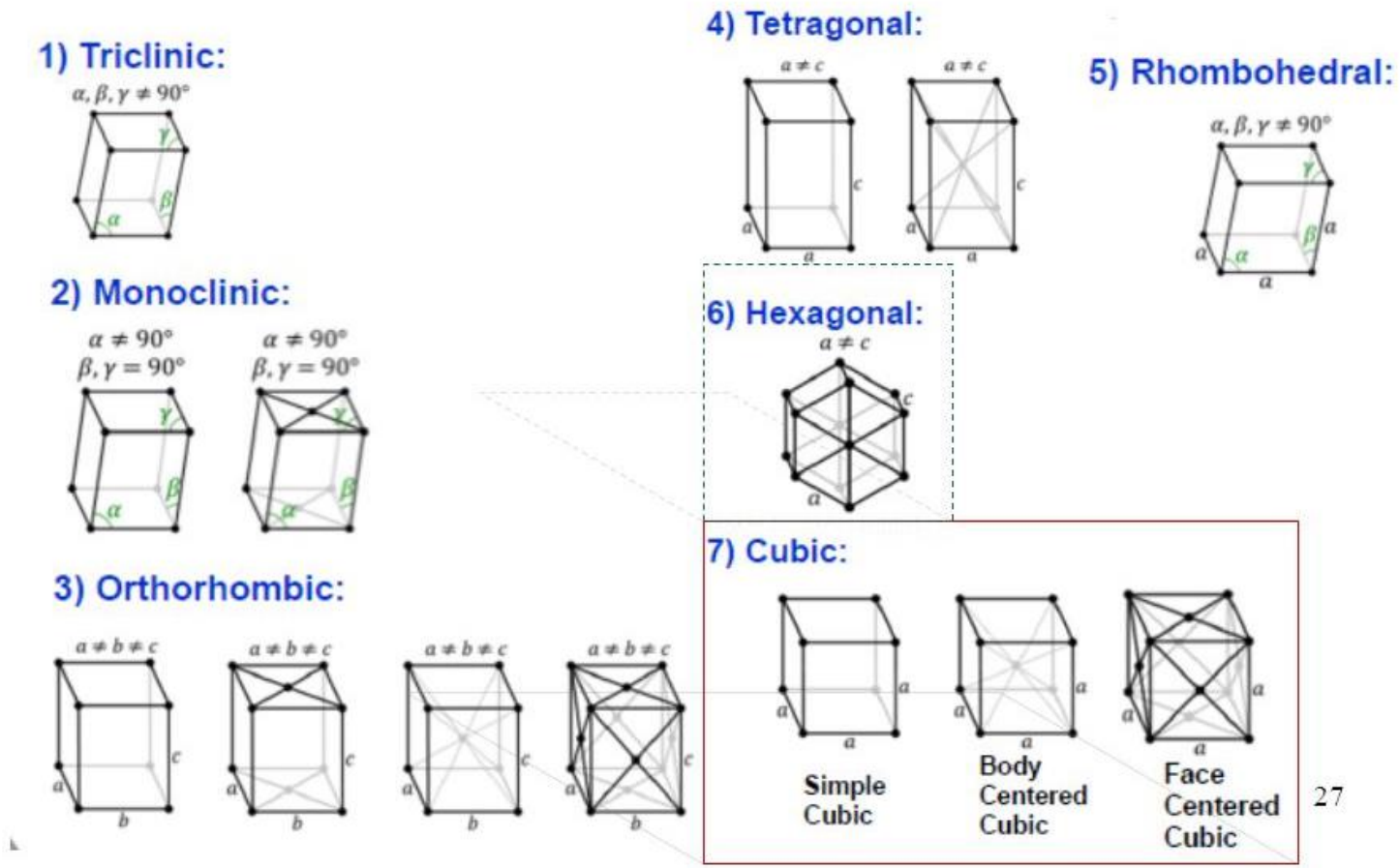
And total number extends to 14, usually classified into crystal types.

Any crystal will belong to one of the seven possible designs and the symmetry of these systems introduces constraints on the possible values of the unit cell parameters.

3D-Bravais Lattices

Bravais Lattices in 3D

There are 14 different Bravais lattices in 3D that are classified into 7 different crystal systems (only the unit cells are shown below)



The parameters (*a*, *b*, *c* and α, β, γ) govern different crystal lattices together with their simpler arrangement.

Introduction to X-ray Crystallography ?