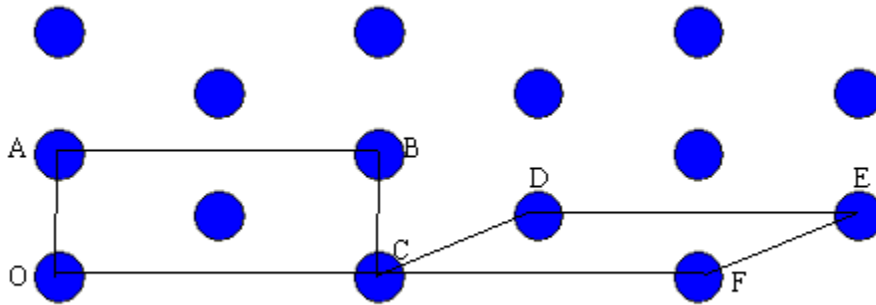


Lecture 7: Conventional Unit Cell, Bravais Lattice Classification, and Symmetry Groups

1. Conventional Unit Cell

As mentioned previously, the smallest repeating cell in a lattice is called the primitive cell. However, it is important to emphasize that the primitive cell does not necessarily exhibit the full symmetry of the crystal.



In the figure, the cell CDEF is a primitive cell, but it does not display the complete symmetry of the crystal. If instead we choose the cell OABC, we observe that this cell possesses the full symmetry of the crystal. **Nevertheless, this cell is not a primitive cell.**

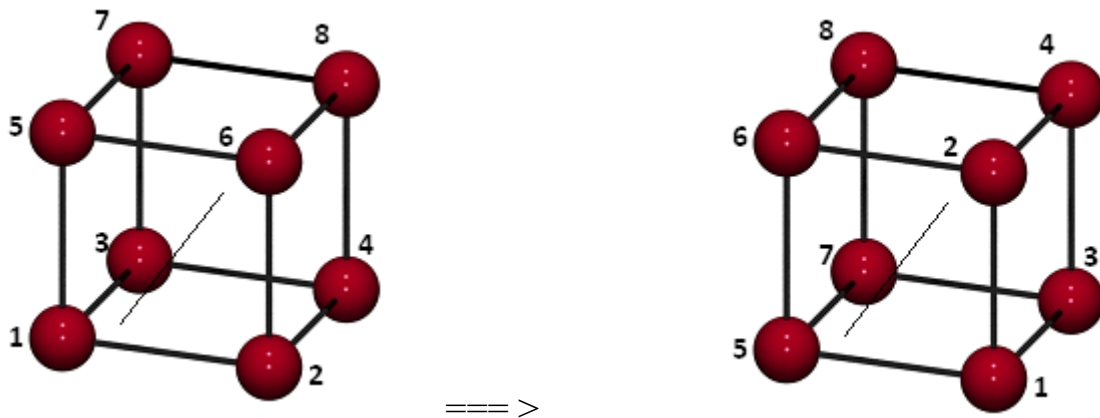
A unit cell that exhibits the full symmetry of the crystal, but is not necessarily the smallest possible cell, is called the *conventional unit cell*.

The main advantage of using the conventional unit cell is that it allows us **to clearly visualize the crystal's full symmetry.**

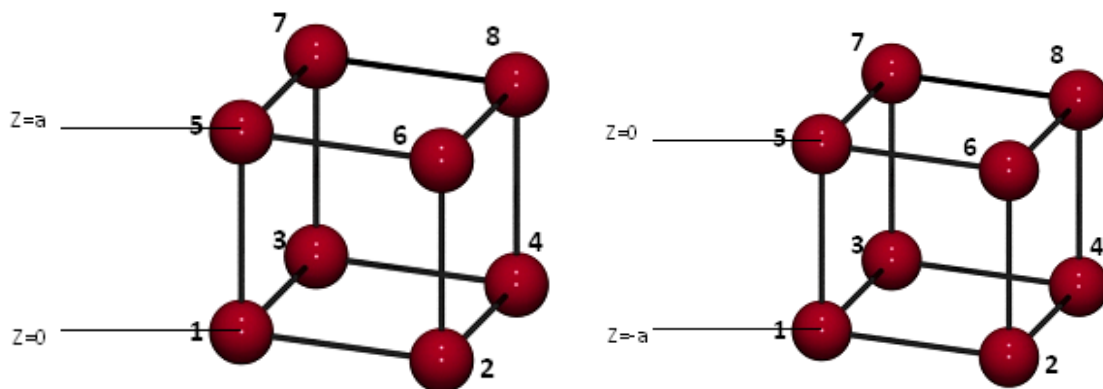
2. Bravais Lattice Classification

In this section, we explain how Bravais lattices can be classified from the viewpoint of symmetry (rather than from the structure point of view). A Bravais lattice can be classified according to the limited set of symmetry operations that leave the lattice invariant.

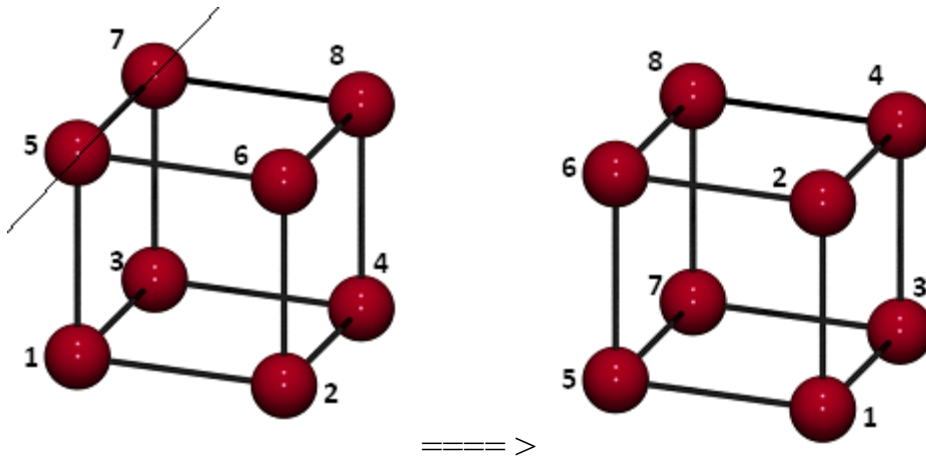
- ✓ For example, a cube may be rotated by a certain angle ($\pi/2$) about an axis passing through its center and still coincide with itself.



- ✓ In another example, the cube may be translated by a Bravais lattice vector ($\vec{R} = -a\hat{z}$) and remain unchanged.



- ✓ Similarly, rotating the cube by $\pi/2$ about an axis passing through atoms labeled 5 and 7 leaves these atoms unchanged, indicating a valid symmetry operation.



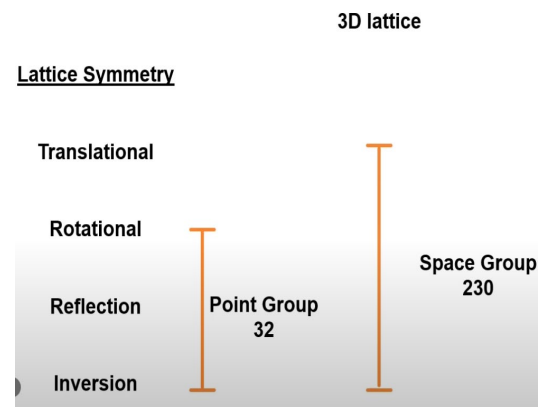
Therefore, any symmetry operation of a Bravais lattice can be classified as one of the following:

- **Rotation about an axis.**
- **Translation by a Bravais lattice vector.**
- **A rigid operation that leaves at least one part of the lattice unchanged.**

3. Point Groups and Space Groups

- Symmetry operations that leave at least one point in the lattice unchanged are called **point-group** symmetry operations. These usually include **rotation, reflection, and inversion**.
- It has been shown that there are exactly 32 possible crystallographic point groups.
- When **translational symmetry** is included along with point-group symmetry operations, the resulting set of symmetries is called a **space group**.

➤ There are 230 distinct space groups in three-dimensional crystals.



Remember

- **7 crystal systems:** point symmetry of external lattice
- **14 Bravais lattices:** translational symmetry of lattice points
- **32 point groups:** point symmetry of external crystal
- **230 space groups:** translational symmetry inside crystal molecules

Optional:

4. Crystallographic Symmetry Notation:

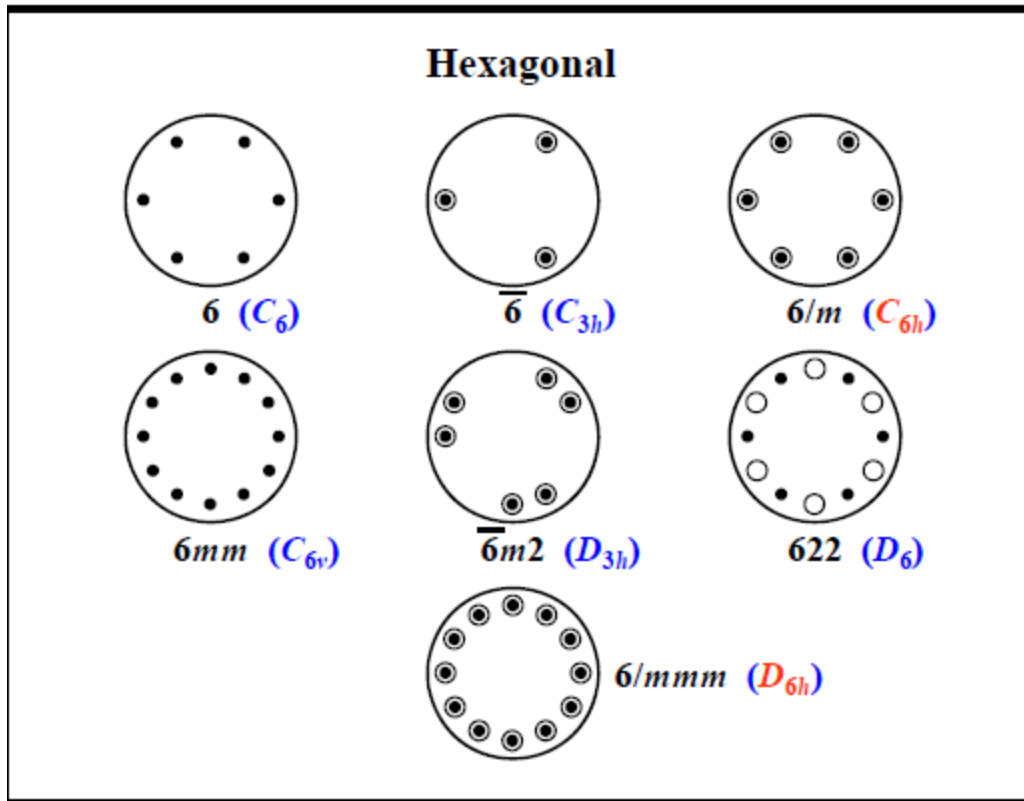
Hermann–Mauguin (H–M) notation, or international notation, describes the symmetry elements of a crystal and their orientations with respect to crystallographic directions and planes. It uses symbols such as 1,2,3,4,6 for rotation axes, $\bar{n}$ for roto-inversion axes, and m for mirror planes.

Schoenflies notation classifies crystal point groups according to their principal symmetry axis and associated symmetry operations. It uses symbols such as C_n , C_{nv} , C_{nh} , D_n , and D_{nh} .

Both notations describe the same point-group symmetry, but they emphasize different aspects of that symmetry.

Example:

- **Hermann–Mauguin (H–M) notation:** the black notation, e.g. $6mm$, 622 , $6/mmm$.
- **Schoenflies notation:** the blue notation in parentheses, e.g. C_{6v} , D_6 , D_{6h} .



Hermann–Mauguin	Schoenflies	Main symmetry elements
6	C_6	One 6-fold rotation axis
$\bar{6}$	C_{3h}	6-fold roto-inversion axis
6/m	C_{6h}	6-fold axis + horizontal mirror plane
6mm	C_{6v}	6-fold axis + vertical mirror planes
$\bar{6}m2$	D_{3h}	$\bar{6}$ axis + mirror planes + perpendicular 2-fold axes
622	D_6	6-fold axis + perpendicular 2-fold axes
6/mmm	D_{6h}	6-fold axis + horizontal/vertical mirrors + perpendicular 2-fold axes + inversion