PHYSICS OF CRYSTALS

THE CRYSTAL LATTICE

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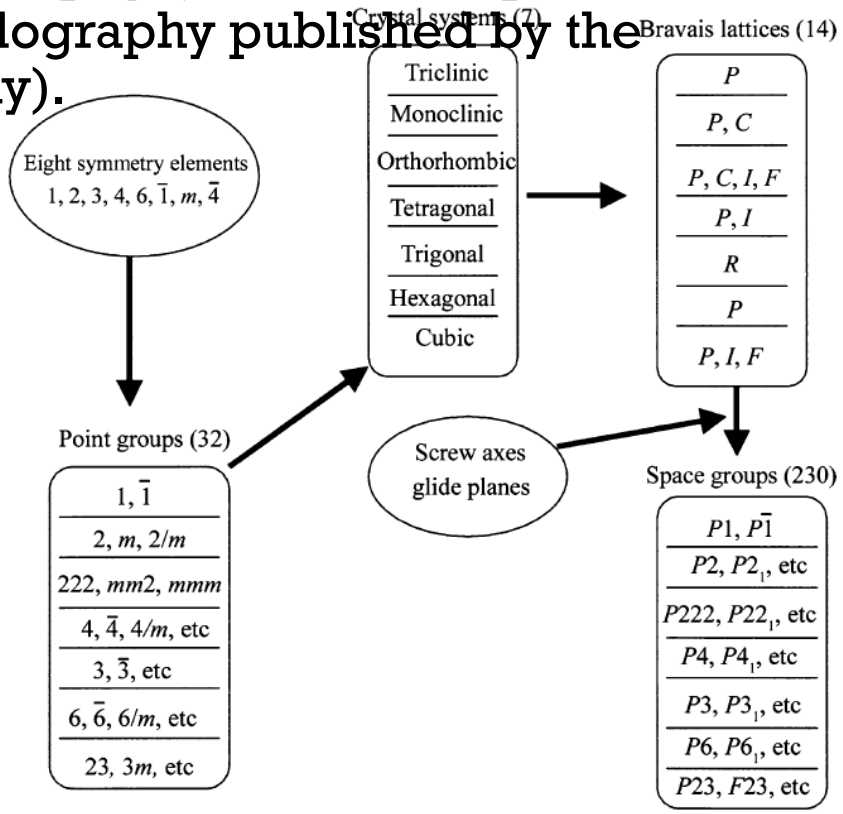
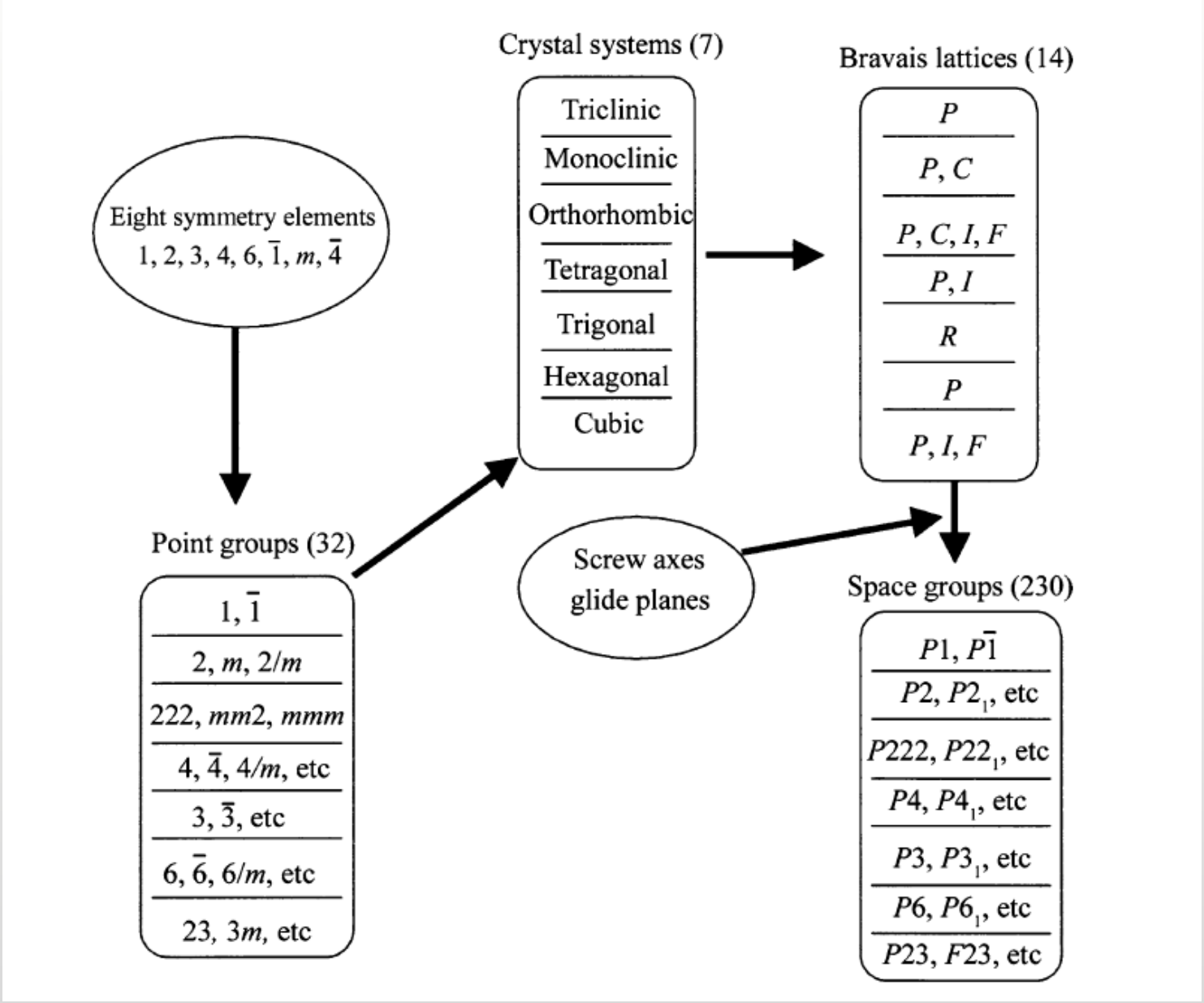
- The origin of crystallography can be traced to the study for the external appearance of natural minerals, such as quartz, fluorite, pyrite, and corundum, which are regular in shape and clearly exhibit a good deal of symmetry. A large amount of data for such minerals have been systematized by applying geometry and group theory.

- "Crystallography" involves the general consideration of how crystals can be built from small units. This corresponds to the infinite repetition of identical structural units (frequently referred to as a unit cell) in space. In other words, the structure of all crystals can be described by a lattice, with a group of atoms allocated to every lattice point.

CRYSTAL SYSTEMS

- Crystals can be classified into 32 point groups on the basis of eight kinds of symmetry elements. There are seven crystal systems for classification, which consist of 14 kinds of Bravais lattices. For convenience, these relations are illustrated in Fig. Furthermore, if it is extended to include space groups, by adding point groups, Bravais lattices, screw axis, and glide reflection axis, there will be 230 classifications in total. In other words, all crystals "belong to one of 230 space groups," the details available in other books on crystallography (see for example International Tables for X-ray Crystallography published by the International Union of Crystallography).




Crystal systems (7)
Bravais lattices (14)
Eight symmetry elements
1, 2, 3, 4, 6, $\bar{1}$, m, $\bar{4}$
Triclinic
Monoclinic
Orthorhombic
Tetragonal
Trigonal
Hexagonal
Cubic
P
P, C
P, C, I, F
P, I
R
P
P, I, F
Point groups (32)
Screw axes
glide planes
Space groups (230)
1, $\bar{1}$
2, m, 2/m
222, $mm2$, mmm
4, $\bar{4}$, 4/m, etc
3, $\bar{3}$, etc
6, $\bar{6}$, 6/m, etc
23, 3m, etc
$P1$, $P\bar{1}$
$P2$, $P2_1$, etc
$P222$, $P22_1$, etc
$P4$, $P4_1$, etc
$P3$, $P3_1$, etc
$P6$, $P6_1$, etc
$P23$, $F23$, etc

Lattice points: The highly repetitive order within the crystal lattice makes it is possible to identify positions within the lattice that are identical. These positions can then be marked with an imaginary point, referred to as a lattice point.

The key to selecting a lattice point is that the environment surrounding each point has to be the same. That is, the view from each lattice point is the same as that from every other point. In two dimensions, for example in Fig.(a), lattice points are selected at the tips of the dark petals and the surrounding environment of each lattice point consists primarily of the dark petals and the space between the 'flowers'.
In Fig. 1.9(b) however, the lattice points are defined in the middle of the space between the 'flowers' and the immediate surrounding environment of each lattice point is mainly the white space and the blue petals.

Figure 1.9 From Principles of Xray Crystallography, Oxford Press, L. Ooi

Lattice planes:In two dimensions, we can then join four adjoining or adjacent lattice points to form a latlice plane.

In Fig.a for example, it is possible to place a lattice point at the tip of the dark petals of each 'flower' and subsequently join the four lattice points to form a lattice plane that consists of two adjacent halves of the 'flower: In Fig.(b), however, the lattice points are connected to form a lattice plane that contains a whole «f1ower»

Figure 1.9 From Principles of Xray Crystallography, Oxford Press, L. Ooi

Figure 1.10 From Principles of Xray Crystallography, Oxford Uni. Press, L. Ooi

When considering objects in three dimensions, the adjoining lattice points that are
selected can be connected to form a 'box' or a container as illustrated in Fig.
The box
is known asa unit cell.

DEFINITION OF UNIT CELL

- A unit cell forms the basic building block of a crystal lattice. Each 'box' or container that defines the unit cell is related to the next unit cell by translation and the contents within each unit cell are exactly the same.

Figure 1.11 From Principles of Xray Crystallography, Oxford Uni Press, L. Ooi

Figure 1.13 From Principles of Xray Crystallography, Oxford Uni. Press, L. Ooi

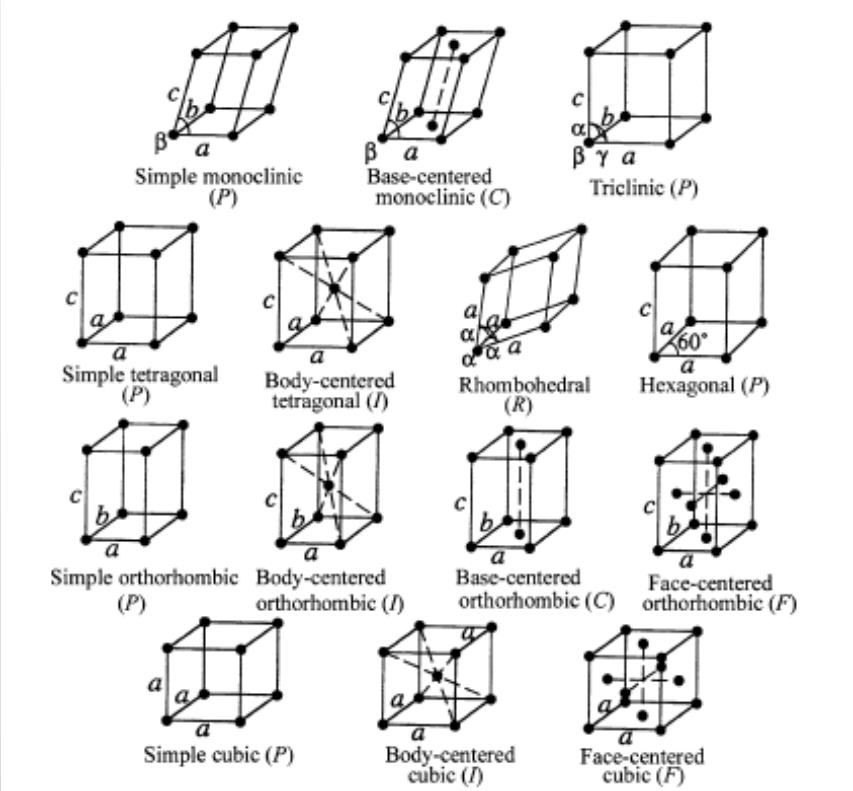
- there are again several possible ways to select a 'unit cell'; two examples are shown.
- If we are to compare the two, both are derived from adjacent lattice points.
- On closer examination, we will notice that the square has a higher internal symmetry than the diamond shape. We are able to divide the square into a greater number of smalle equivalent sections than the diamond. Hence, the square is a better 'unit cell'.

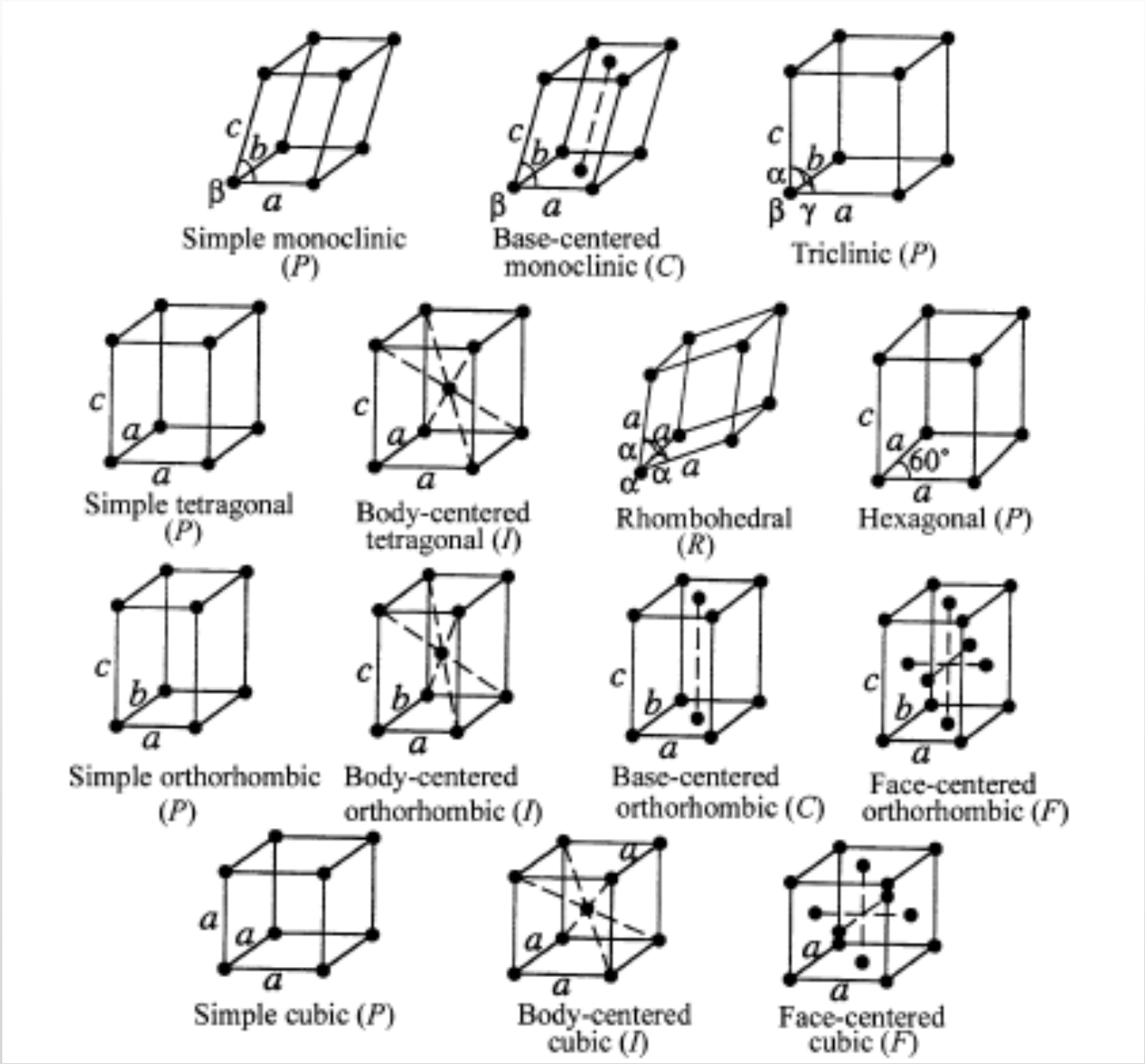
UNIT CELL NOMENCLATURE AND PARAMETERS

Figure 1.15 From Principles of Xray Crystallography, Oxford Uni. Press, L. Ooi

LATTICE TYPES

- Although it may seem that there is an infinite array of possibilities in selecting a unit cell. in reality there are only seven possible 'box' shapes that can be stacked together within a crystal lattice. These are known as the crystal systems. These seven crystal systems are cubic. tetragonal. orthorhombic, hexagonal, trigonal, monoclinic, and triclinic.




Simple monoclinic (P)
Base-centered monoclinic (C)
Triclinic (P)
Simple tetragonal (P)
Body-centered tetragonal (I)
Rhombohedral (R)
Hexagonal (P)
Simple orthorhombic (P)
Body-centered orthorhombic (I)
Base-centered orthorhombic (C)
Face-centered orthorhombic (F)
Simple cubic (P)
Body-centered cubic (I)
Face-centered cubic (F)

In some crystal lattices, it is also possible to identify lattice points other than those defining the unit cell.

- The primitive (P) lattice is a lattice type in which the lattice points lie only althe corners of the unit cell. found in all the crystal systems.
- The body-centered (I) lattice is a lattice type in which the lattice points lie at the corners of the unit cell and one lattice point lies in the middle of the unit cell. Found in the cubic, tetragonal, orthorhombic and monoclinic crystal systems.
- The face-centred (F) lattice is a lattice type in which the lattice pOints lie at the corners of the unit cell and one lattice pOint lies in the middle of every face of the unit cell. found in the cubic and orthorhombic crystal systems.
- The other single-face-centred (base-centred) lattice types are those in which the lattice points lie at the corners of the unit cell and a lattice point lies at each of the two relevant faces.

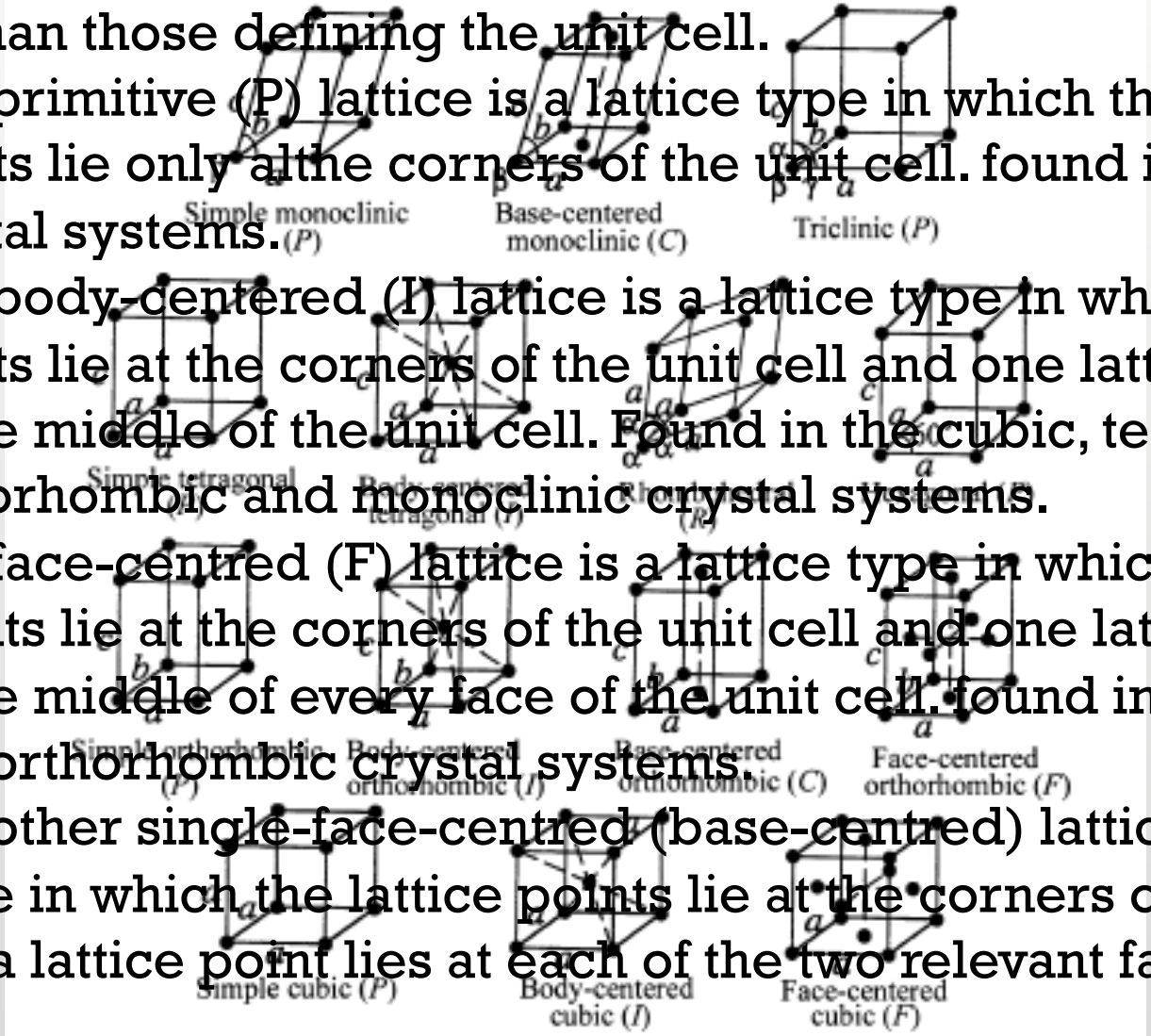


Table 1.1 From Principles of Xray Crystallography, Oxford Uni. Press, L. Ooi

LATTICE REDUCTION

Figure 1.17 From Principles of Xray Crystallography, Oxford Uni. Press, L. Ooi

- the C-type Bravais lattice does not occur for the cubic unit cell, as shown
- in Fig.
- In Figure the unit cells drawn in black denote a C-centred cubic lattice. However, this unit cell can be reduced further to a smaller unit cell with higher symmetry and this is shown with the lines in blue.
- The lines in blue are drawn to join the face-centred lattice points to the corners of the lattices. In doing so, a new lattice type can be found; the primitive-type (P) tetragonal lattice is obtained. This satisfies the rules for selecting the 'best' unit cell.