

2. BASIC CRYSTALLOGRAPHY

Table 2.1.3.4. *The seven crystal systems*

Crystal system	Conditions imposed on cell geometry	Minimum point-group symmetry
Triclinic	None	1
Monoclinic	Unique axis $b: \alpha = \gamma = 90^\circ$	2
Orthorhombic	$\alpha = \beta = \gamma = 90^\circ$	222
Tetragonal	$a = b; \alpha = \beta = \gamma = 90^\circ$	4
Trigonal	Hexagonal axes: $a = b; \alpha = \beta = 90^\circ; \gamma = 120^\circ$ Rhombohedral axes: $a = b = c; \alpha = \beta = \gamma^*$	3
Hexagonal	$a = b; \alpha = \beta = 90^\circ; \gamma = 120^\circ$	6
Cubic	$a = b = c; \alpha = \beta = \gamma = 90^\circ$	23

* A rhombohedral unit cell can be regarded as a cube extended or compressed along the body diagonal (the threefold axis) (see Fig. 2.1.3.2).

occur either as primitive unit cells or as centred unit cells (Section 2.1.1). A total of 14 different types of unit cell exist, depicted in Fig. 2.1.3.3. Their corresponding crystal lattices are commonly called Bravais lattices.

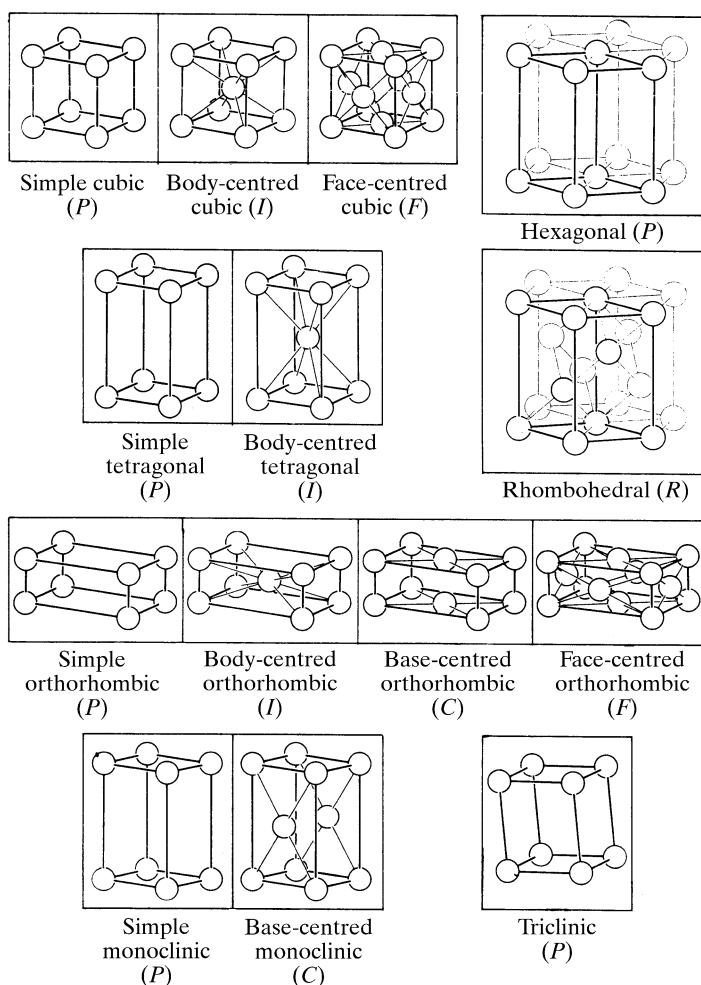


Fig. 2.1.3.3. The 14 Bravais lattices. Reproduced with permission from Burzlaff & Zimmermann (1995). Copyright (1995) International Union of Crystallography.

2.1.4. Basic diffraction physics

2.1.4.1. Diffraction by one electron

The scattering of an X-ray beam by a crystal results from interaction between the electric component of the beam and the electrons in the crystal. The magnetic component has hardly any effect and can be disregarded.

If a monochromatic polarized beam hits an electron, the electron starts to oscillate in the direction of the electric vector of the incident beam (Fig. 2.1.4.1). This oscillating electron acts as the aerial of a transmitter and radiates X-rays with the same or lower frequency as the incident beam. The frequency change is due to the Compton effect: the photons of the incident beam collide with the electron and lose part of their energy. This is inelastic scattering, and the scattered radiation is incoherent with the incident beam. Compton scattering contributes to the background in a diffraction experiment. In elastic scattering, the scattered radiation has the same wavelength as the incident radiation, and this is the radiation responsible for the interference effects in diffraction. It was shown by Thomson that if the electron is completely free the following hold:

(1) The phase difference between the incident and the scattered beam is π , because the scattered radiation is proportional to the displacement of the electron, which differs by π in phase with its acceleration imposed by the electric vector.

(2) The amplitude of the electric component of the scattered wave at a distance r which is large in comparison with the wavelength of the radiation is

$$E_{\text{el}} = E_o \frac{1}{r} \frac{e^2}{mc^2} \sin \varphi,$$

where E_o is the amplitude of the electric vector of the incident beam, e is the electron charge, m is its mass, c is the speed of light and φ is the angle between the oscillation direction of the electron and the scattering direction (Fig. 2.1.4.1). Note that $E_o \sin \varphi$ is the component of E_o perpendicular to the scattering direction.

In terms of energy,

$$I_{\text{el}} = I_o \frac{1}{r^2} \left(\frac{e^2}{mc^2} \right)^2 \sin^2 \varphi. \quad (2.1.4.1a)$$

The scattered energy per unit solid angle is