Crystal Systems

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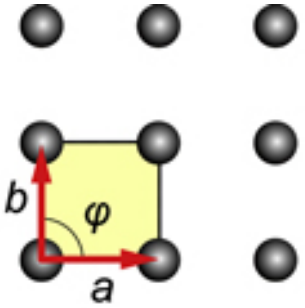
Two Dimensional Bravais Lattices

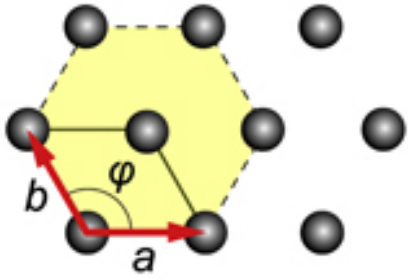
Lattice parameters are a,b and ϕ

5 distinct types of lattices.



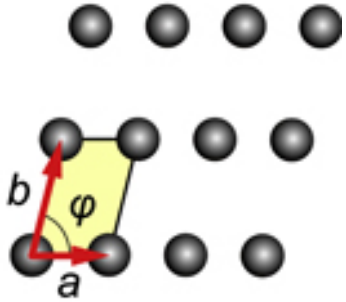
$|a| = |b|, \varphi = 90°$

Square



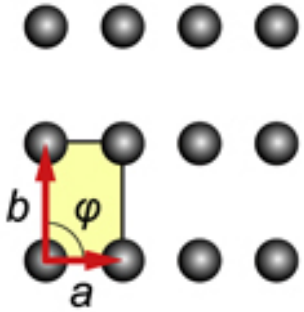
$|a| = |b|, \varphi = 120°$

Hexagonal



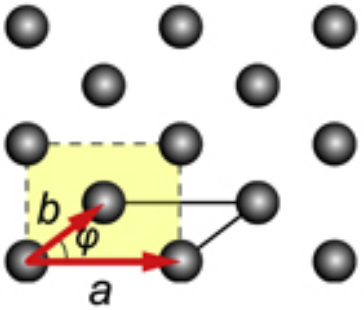
$|a| \neq |b|, \varphi \neq 90°$

Oblique



$|a| \neq |b|, \varphi = 90°$

Rectangular

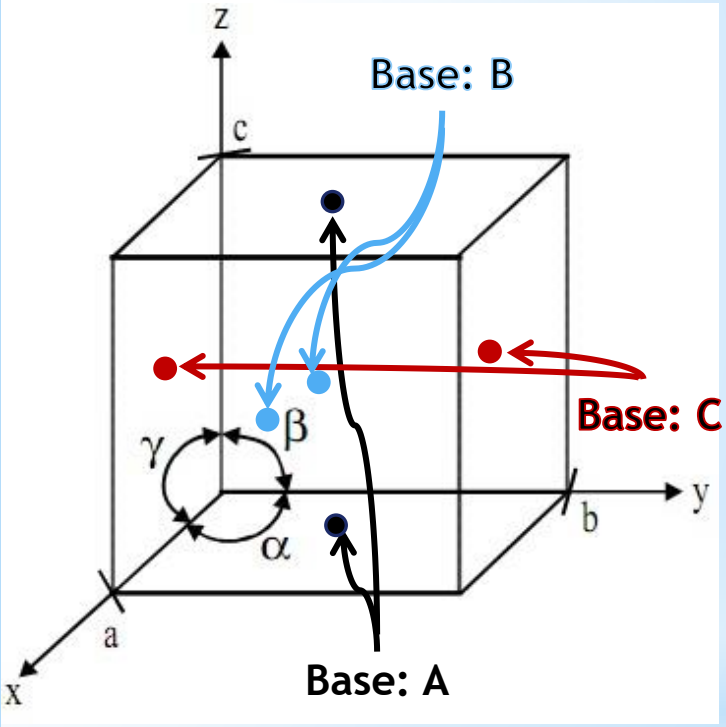


$|a| \neq |b|, \varphi \neq 90°$

Centerd Rectangular

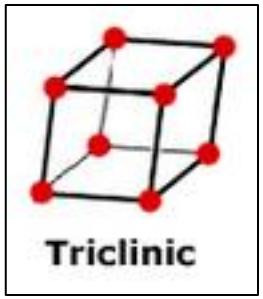
Symbols of Primitive and Non-primitive cell

- P → Primitive (it has atoms only at the corners of the parallelepiped)
- A, B, C → Base-centered (it has extra atom at the center of the base)
- I → Body centered (From German word Innenzentriete)
- F → Face-centered

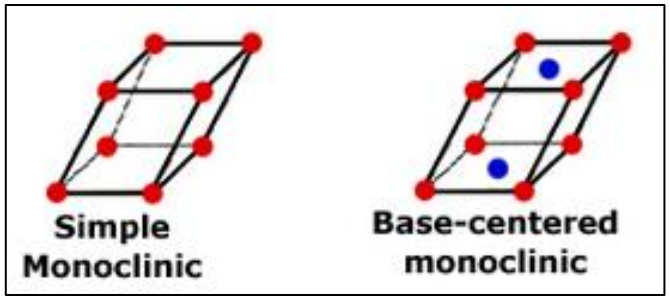


Three Dimensional Bravais Lattices

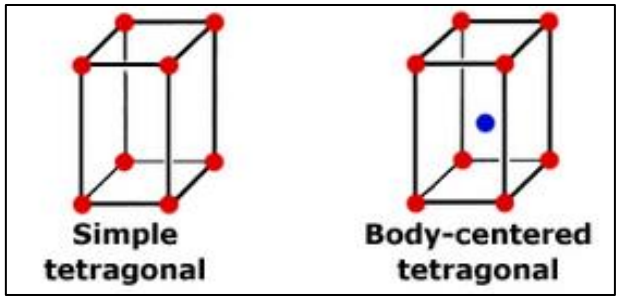
Lattice parameters are **a, b, c, α, β, and γ**, 14 distinct types of lattices.



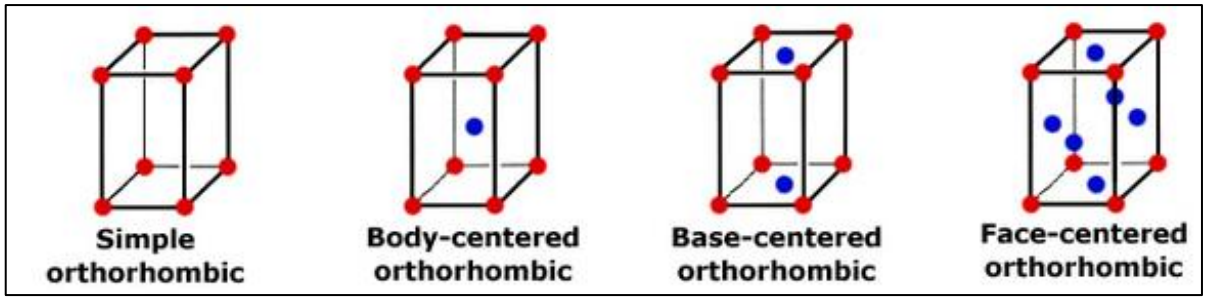
$a \neq b \neq c$, $\alpha \neq \beta \neq \gamma$, (P)



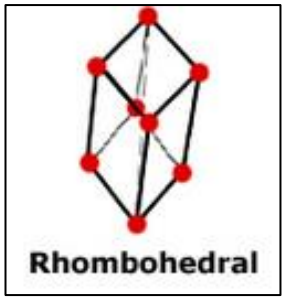
$a \neq b \neq c$, $\alpha = \gamma = 90^o \neq \beta$, (P, A)



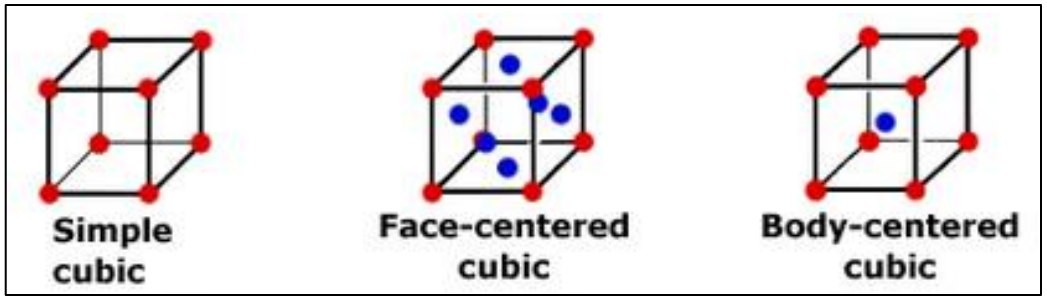
$a = b \neq c$, $\alpha = \beta = \gamma = 90^o$, (P, I)



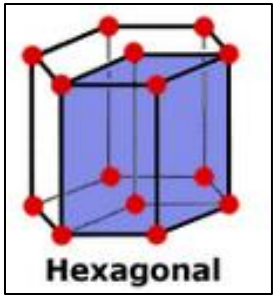
$a \neq b \neq c$, $\alpha = \beta = \gamma = 90^o$, (P, I, A, F)



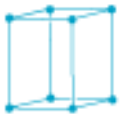
$a = b = c$, $\alpha = \beta = \gamma \neq 90^o$, (P)



$a = b = c$, $\alpha = \beta = \gamma = 90^o$, (P, F, I)



$a = b \neq c$, $\alpha = \beta = 90^o$, $\gamma = 120^o$, (Conventional)

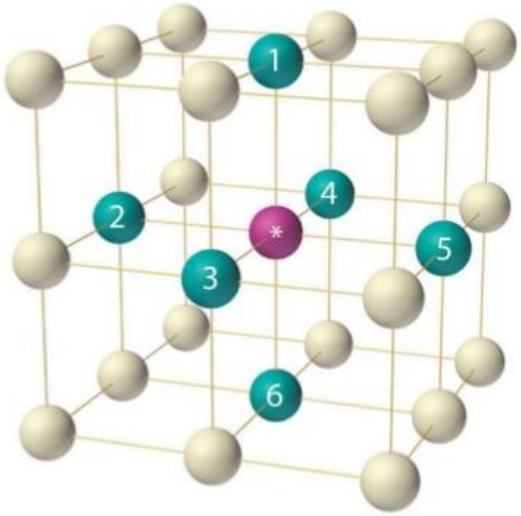
Bravais lattice cells	Axes and interaxial angles	Examples
 Cubic P Cubic I Cubic F	Three axes at right angles; all equal: $a = b = c$; $\alpha = \beta = \gamma = 90°$	Copper (Cu), silver (Ag), sodium chloride (NaCl)
 Tetragonal P Tetragonal I	Three axes at right angles; two equal: $a = b \neq c$; $\alpha = \beta = \gamma = 90°$	White tin (Sn), rutile (TiO_2), β-spodumene ($LiAlSi_2O_6$)
 P C I F Orthorhombic	Three axes at right angles; all unequal: $a \neq b \neq c$; $\alpha = \beta = \gamma = 90°$	Gallium (Ga), perovskite ($CaTiO_3$)
 Monoclinic P Monoclinic C	Three axes, one pair not at right angles, of any lengths: $a \neq b \neq c$; $\alpha = \gamma = 90° \neq \beta$	Gypsum ($CaSO_4 \cdot 2H_2O$)
 Triclinic P	Three axes not at right angles, of any lengths: $a \neq b \neq c$; $\alpha \neq \beta \neq \gamma \neq 90°$	Potassium chromate (K_2CrO_7)
 Trigonal R (rhombohedral)	Rhombohedral: three axes equally inclined, not at right angles; all equal: $a = b = c$; $\alpha = \beta = \gamma \neq 90°$	Calcite ($CaCO_3$), arsenic (As), bismuth (Bi)
 Trigonal and hexagonal C (or P)	Hexagonal: three equal axes coplanar at 120°, fourth axis at right angles to these: $a_1 = a_2 = a_3 \neq c$; $\alpha = \beta = 90°$, $\gamma = 120°$	Zinc (Zn), cadmium (Cd), quartz (SiO_2) [P]

Volume of a unit cell, $V = \vec{a}.(\vec{b} \times \vec{c})$

This relation is obtained by elementary vector analysis

Lattice system	Volume
Triclinic	$abc\sqrt{1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma}$
Monoclinic	$abc\sin\alpha$
Orthorhombic	abc
Tetragonal	a^2c
Rhombohedral	$a^3\sqrt{1-3\cos^2\alpha+2\cos^3\alpha}$
Hexagonal	$\frac{\sqrt{3}}{2}a^2c$
Cubic	a^3

SC-coordination number



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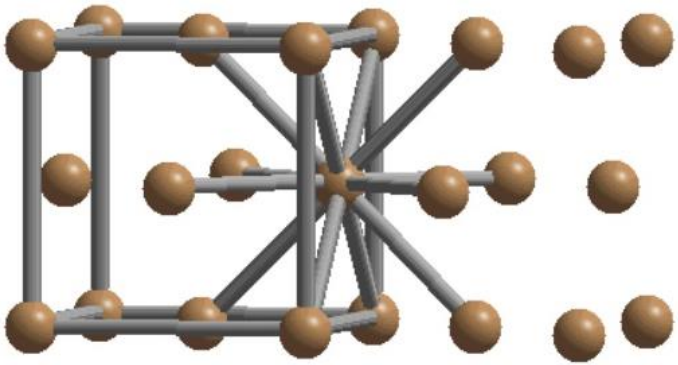
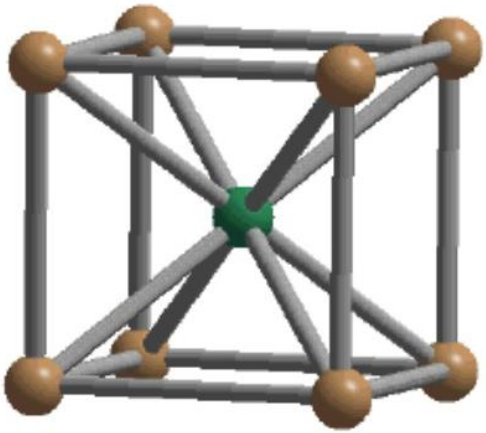
FCC-coordination number



4+4+4=12

BCC-coordination number



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Characteristics of Cubic Crystals

Type of lattice	Simple cubic (SC)	Body centered cubic (BCC)	Face centered cubic (FCC)
Volume	a^3		
Lattice points per unit cell	1	2	4
Volume of the primitive cell	a^3	$a^3/2$	$a^3/4$
Lattice points per unit volume	$1/a^3$	$2/a^3$	$4/a^3$
Coordination number	6	8	12
Nearest neighbor distance	a	$a\sqrt{3}/2$	$a/\sqrt{2}$
Number of 2nd nearest neighbors	12	6	6
2nd neighbor distance	$\sqrt{2}a$	a	a
Packing factor	$\pi/6=0.52$	$\sqrt{3}\pi/8=0.68$	$\sqrt{2}\pi/6=0.74$