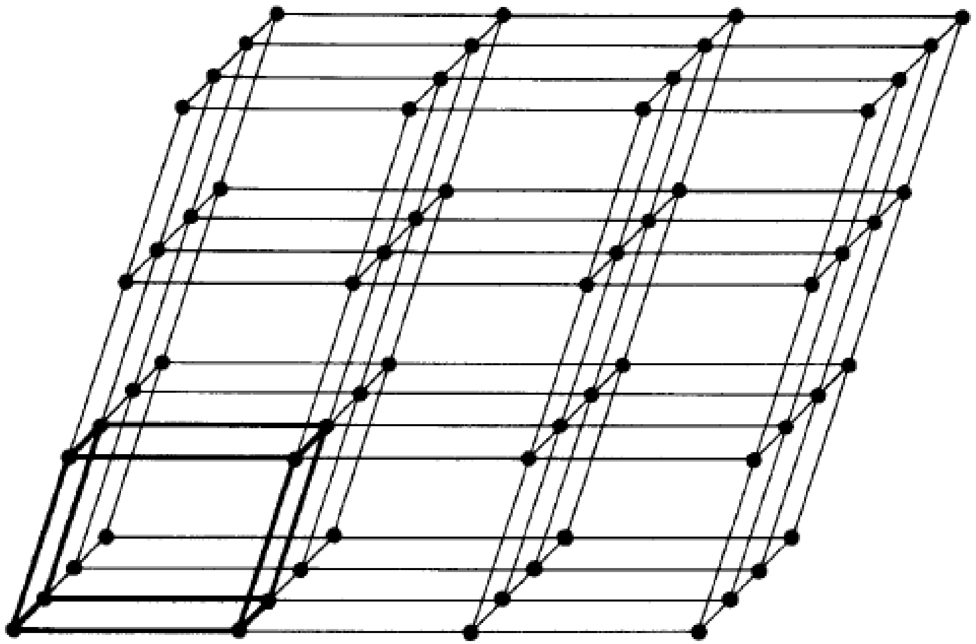
دانشگاه کاشان

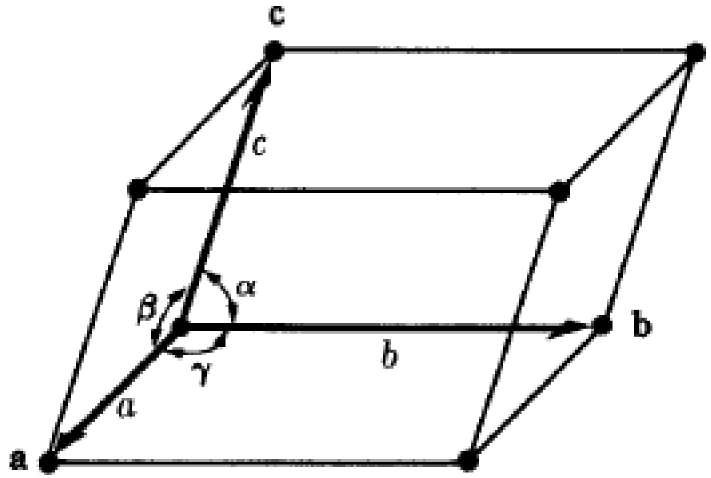
Crystallography

Mohammad Eghbali

شبکه و یکایاخته

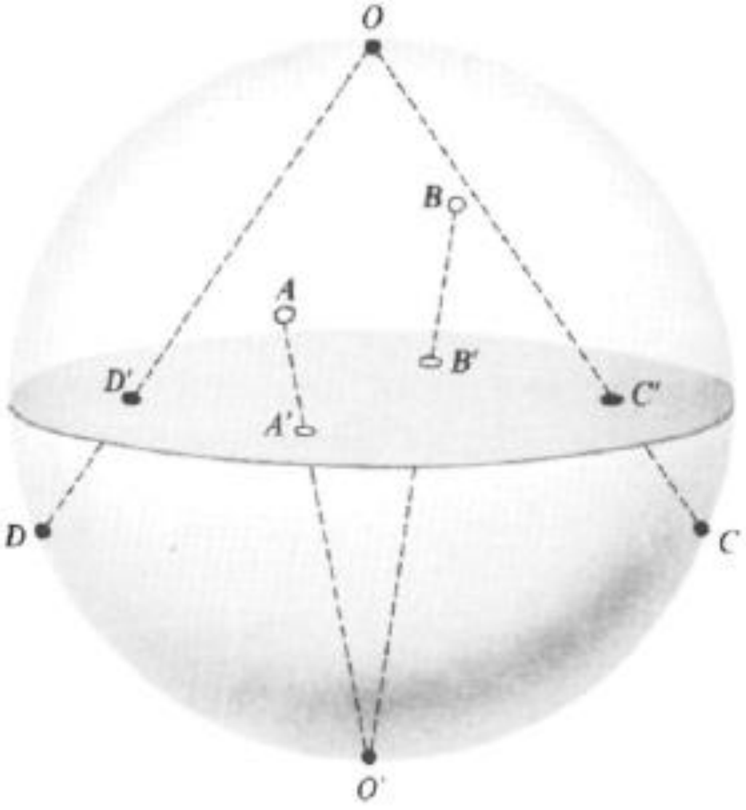


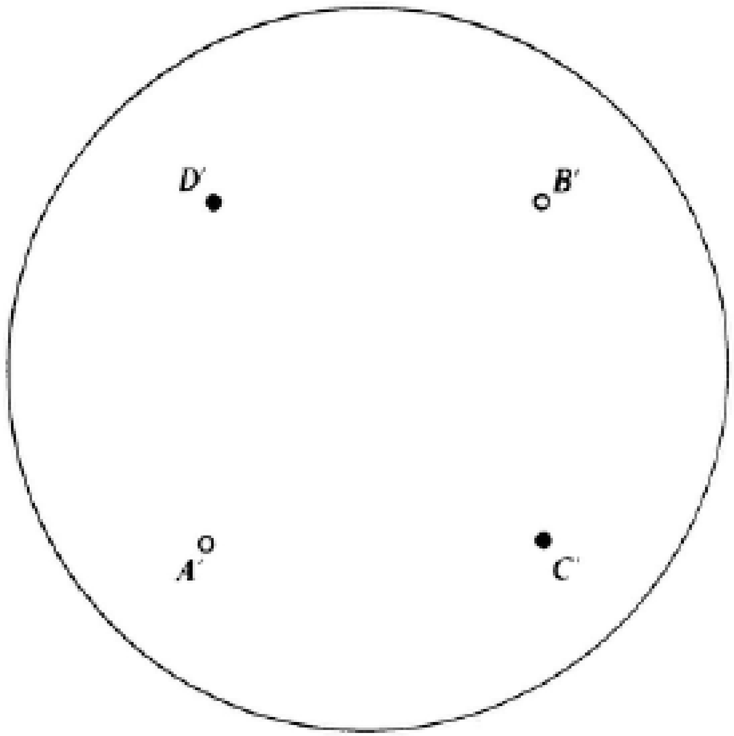
شبکه نقطه ای



یکا یاخته

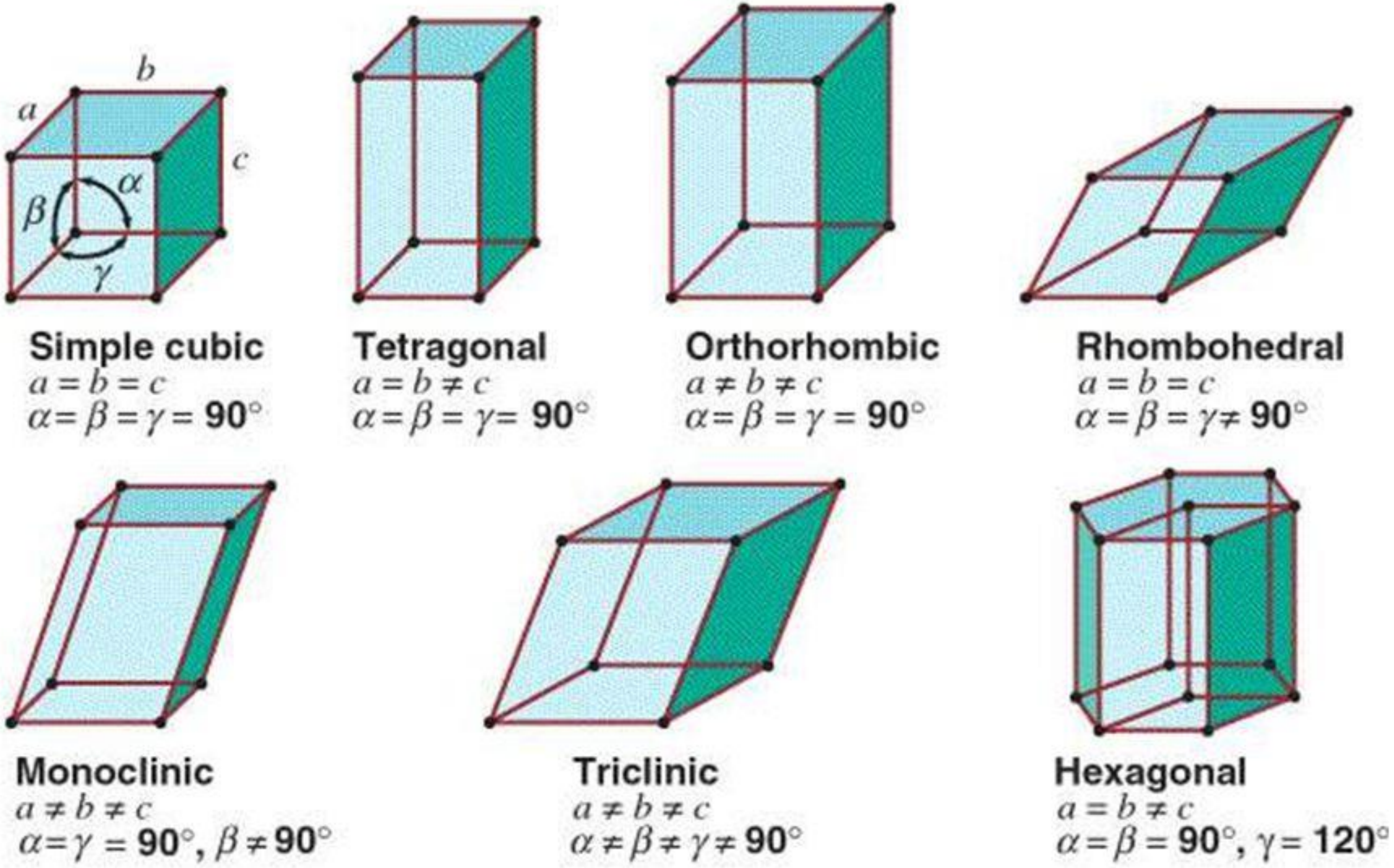
symmetry of crystals



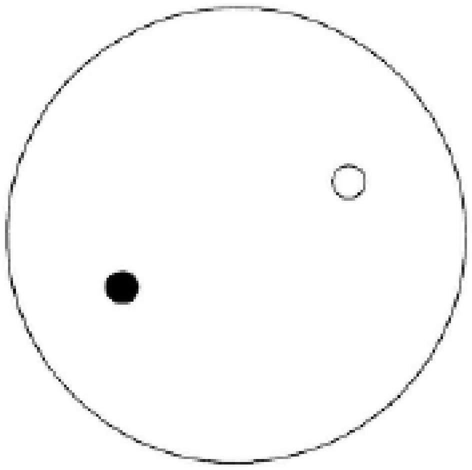


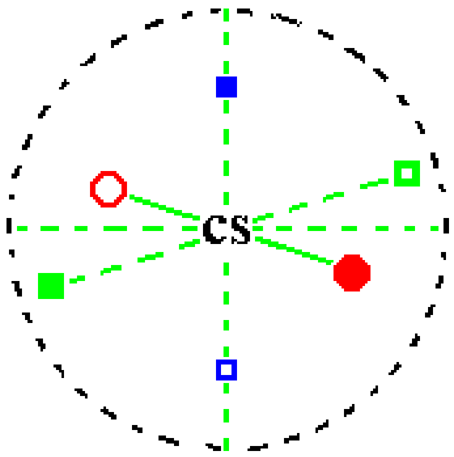
The stereographic projection

Seven Types of Unit Cells

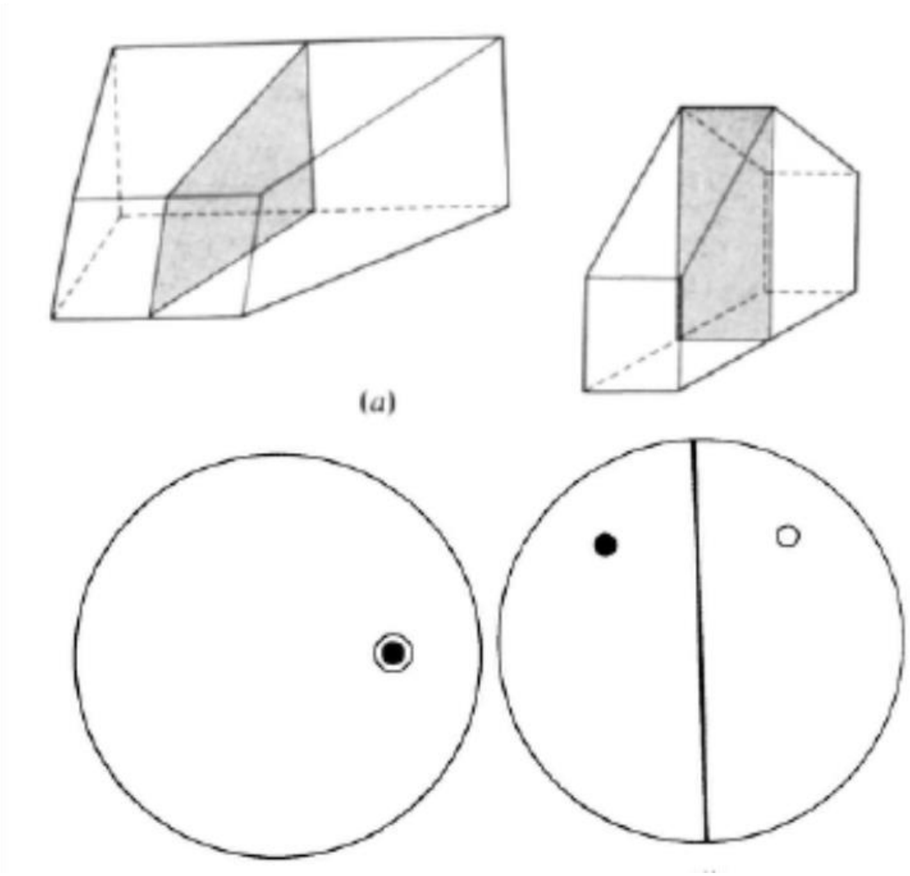


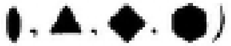
Centre of symmetry

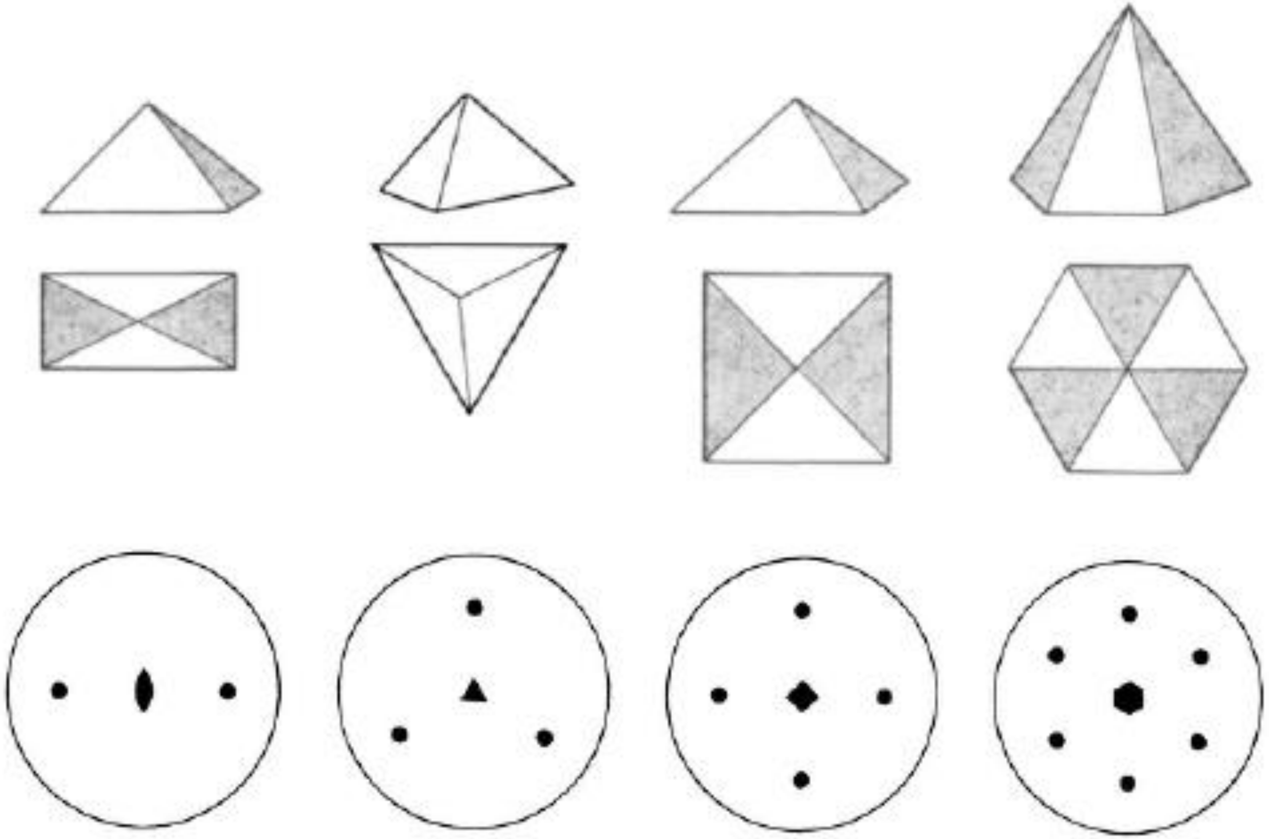




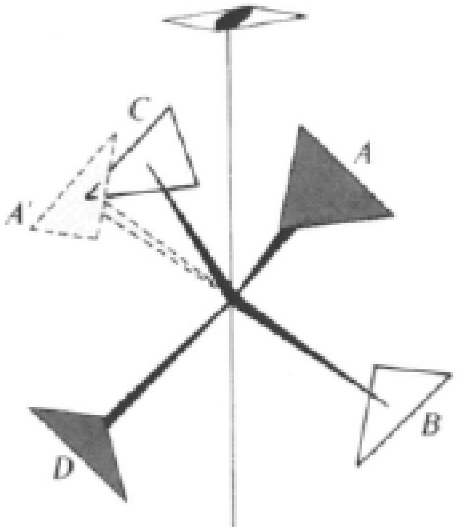
Mirror plane (written symbol m; graphical symbol —)

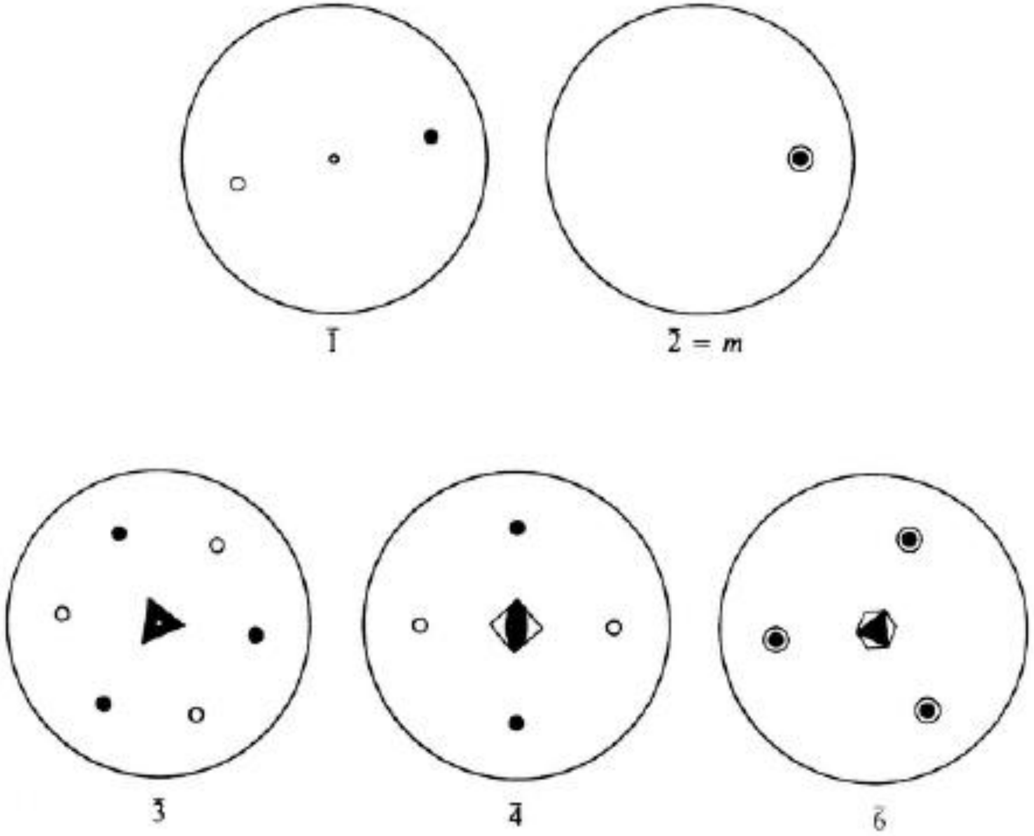


Rotation axes (written symbols 2, 3, 4, 6; graphical symbols )



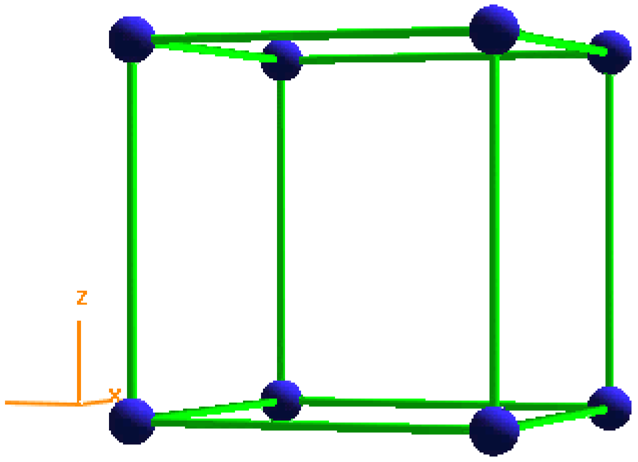
Inversion axes (written symbols 1, 2, 3, 4, 6; graphical symbols o, none,)

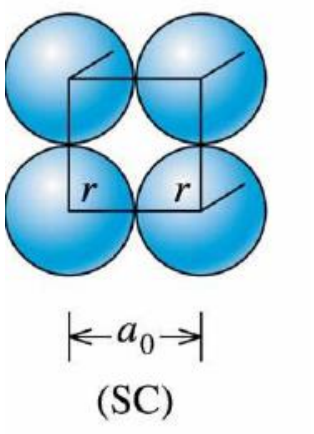




Bravais lattice

simple cubic (sc) *a=b=c* *α=β=γ =90*

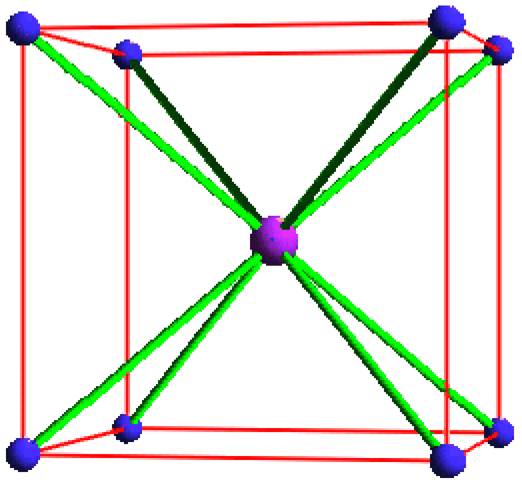


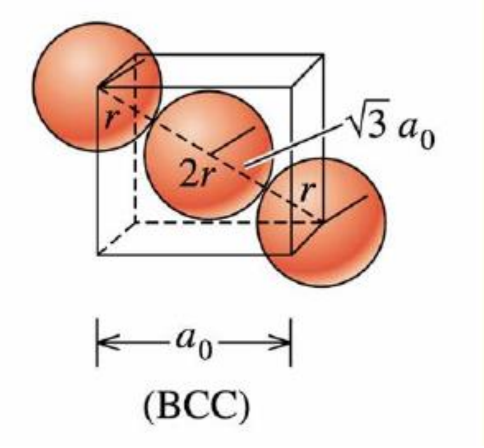


$$APF = \frac{\frac{4}{3}\pi\left(\frac{a}{2}\right)^3}{a^3} = \frac{\pi}{6}$$

Bravais lattice

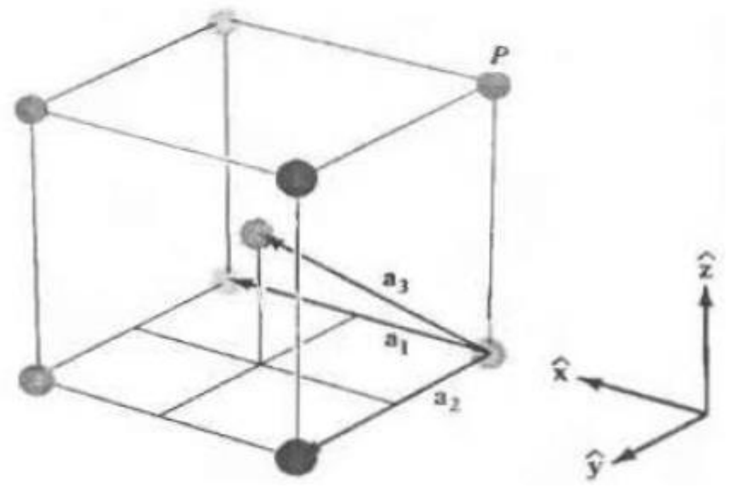
bace centered cubic (bcc) *a=b=c* *α=β=γ =90*



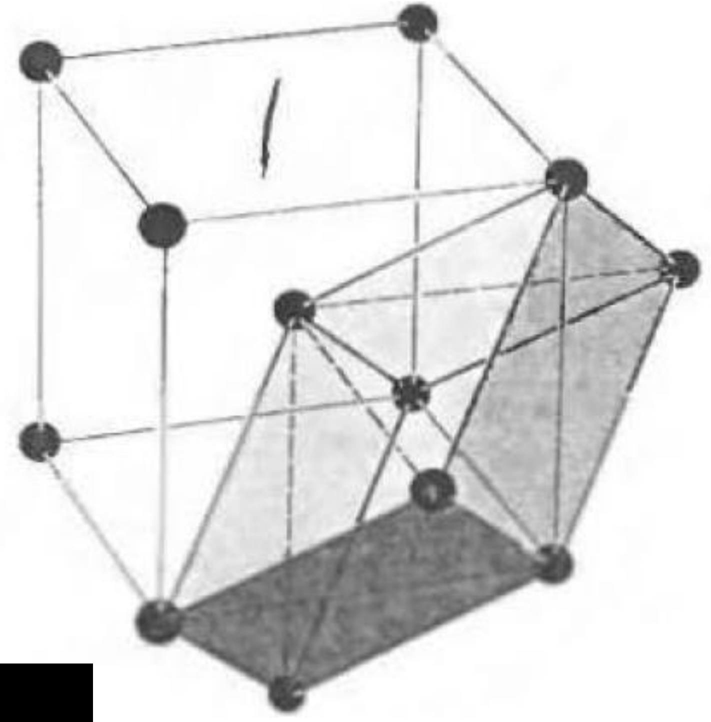


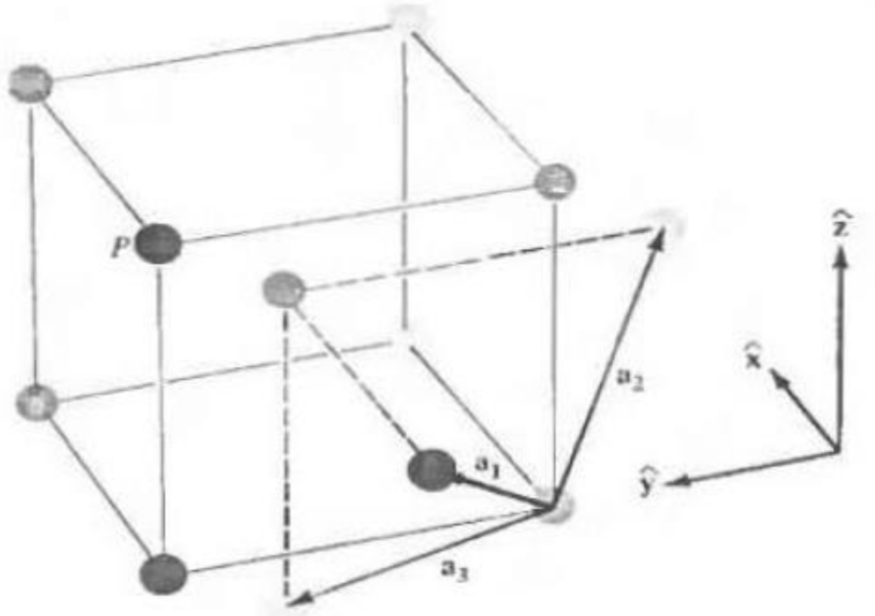
$$APF = \frac{2 \times \frac{4}{3}\pi\left(\frac{\sqrt{3}}{4}a\right)^3}{a^3} = \frac{\sqrt{3}}{8}\pi$$

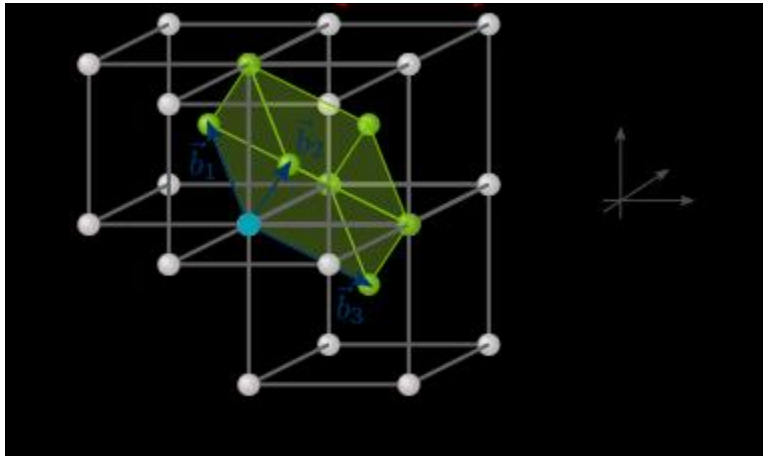
bcc



$$\mathbf{a}_1 = a\hat{\mathbf{x}}, \quad \mathbf{a}_2 = a\hat{\mathbf{y}}, \quad \mathbf{a}_3 = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}}).$$



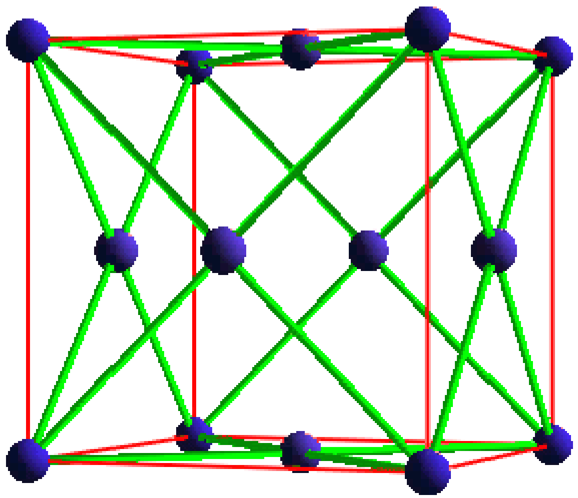


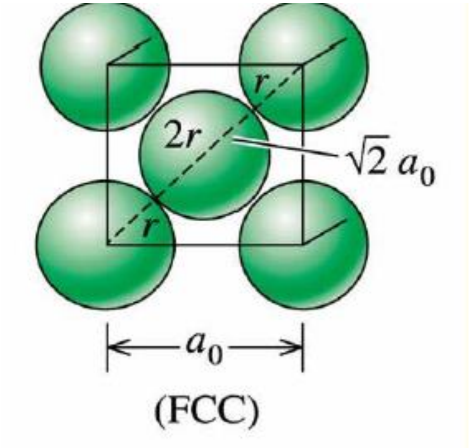


$$\mathbf{a}_1 = \frac{a}{2}(\hat{\mathbf{y}} + \hat{\mathbf{z}} - \hat{\mathbf{x}}), \quad \mathbf{a}_2 = \frac{a}{2}(\hat{\mathbf{z}} + \hat{\mathbf{x}} - \hat{\mathbf{y}}), \quad \mathbf{a}_3 = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}).$$

Bravais lattice

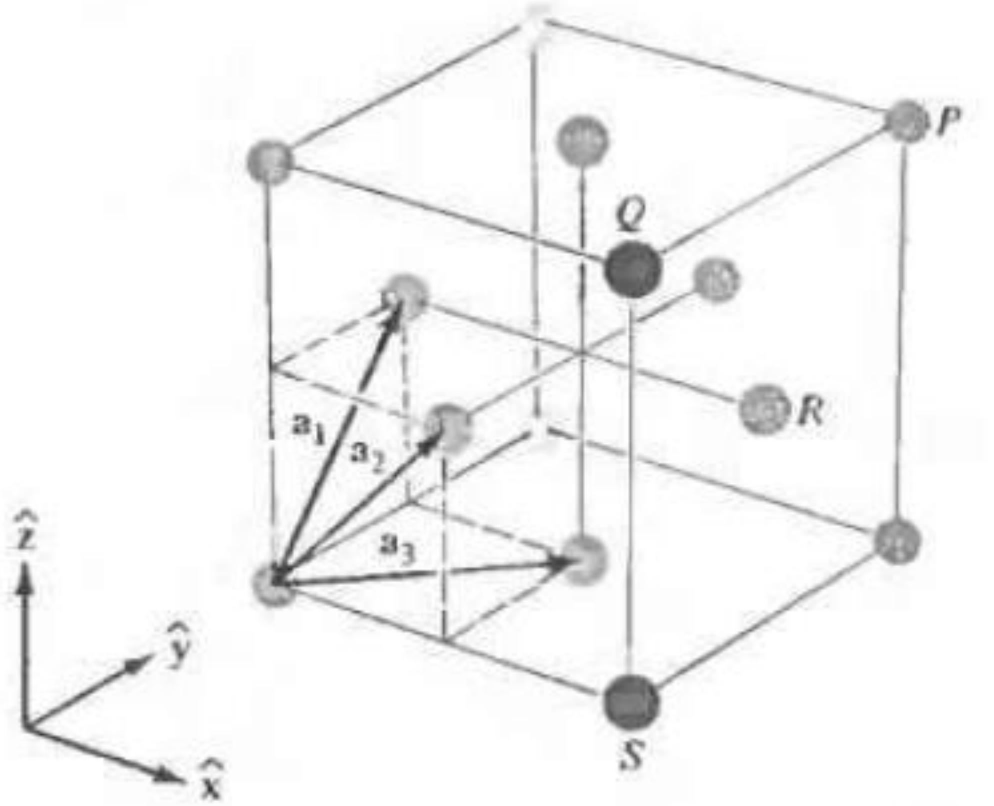
face centered cubic (fcc) $a=b=c$ $\alpha=\beta=\gamma=90$

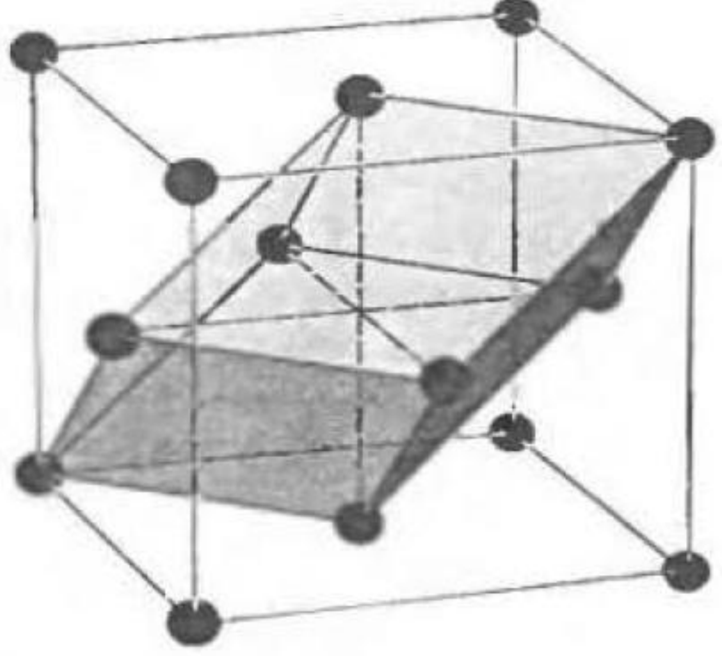


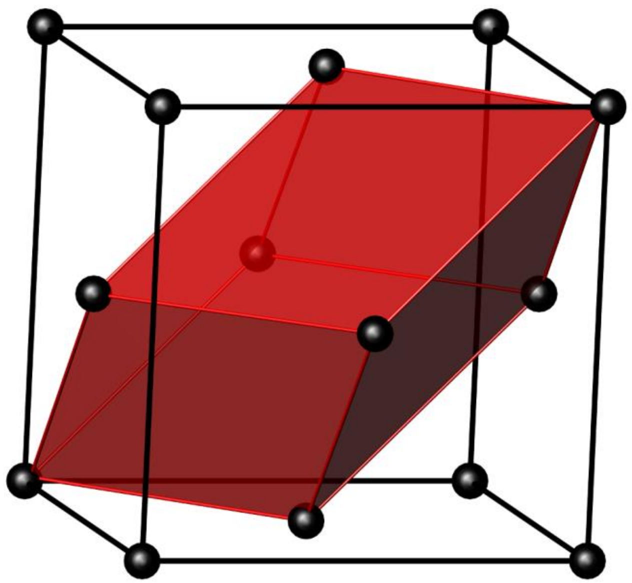


$$APF = \frac{4\times \frac{4}{3}\pi\left(\frac{\sqrt{2}}{4}a\right)^3}{a^3} = \frac{\sqrt{2}}{6}\pi$$

fcc



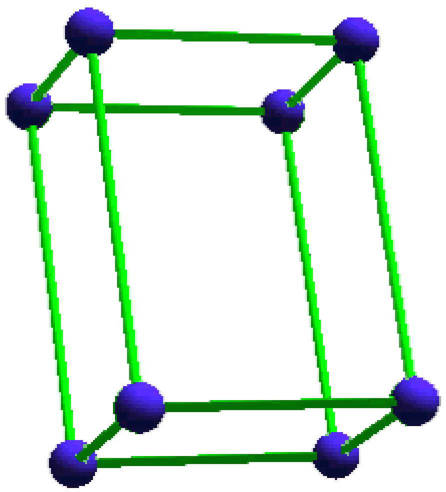




$$\mathbf{a}_1 = \frac{a}{2}(\hat{y} + \hat{z}), \quad \mathbf{a}_2 = \frac{a}{2}(\hat{z} + \hat{x}), \quad \mathbf{a}_3 = \frac{a}{2}(\hat{x} + \hat{y}).$$

Bravais lattice

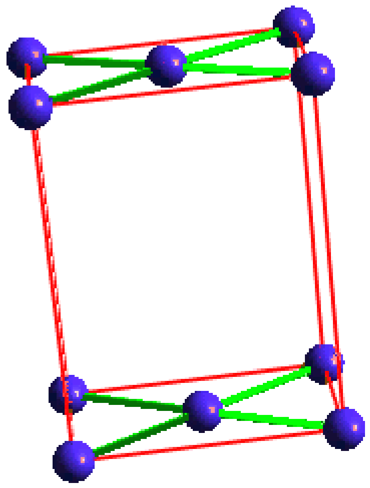
orthohombic (p) $a \neq b \neq c$ $\alpha = \beta = \gamma = 90$



$$APF = \frac{\frac{4}{3}\pi\left(\frac{a}{2}\right)^3}{abc}$$

Bravais lattice

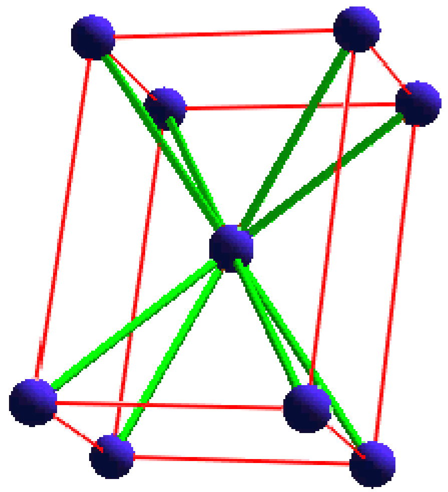
orthohombic (c) $a \neq b \neq c$ $\alpha=\beta=\gamma=90$



$$APF = \frac{2 \times \frac{4}{3} \pi \left(\frac{\sqrt{a^2 + b^2}}{4} \right)^3}{abc}$$

Bravais lattice

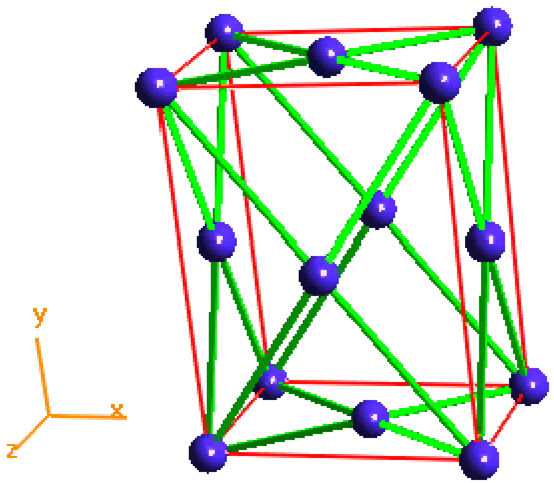
orthohombic (I) $a \neq b \neq c$ $\alpha=\beta=\gamma=90$



$$APF = \frac{2 \times \frac{4}{3}\pi\left(\frac{\sqrt{a^2+b^2+c^2}}{4}\right)^3}{abc}$$

Bravais lattice

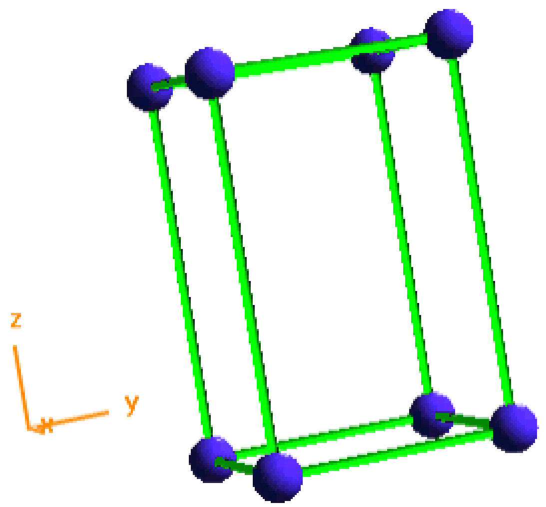
orthohombic (f) $a \neq b \neq c$ $\alpha=\beta=\gamma=90$



$$APF = \frac{4 \times \frac{4}{3}\pi \left(\frac{\sqrt{a^2 + b^2}}{4} \right)^3}{abc}$$

Bravais lattice

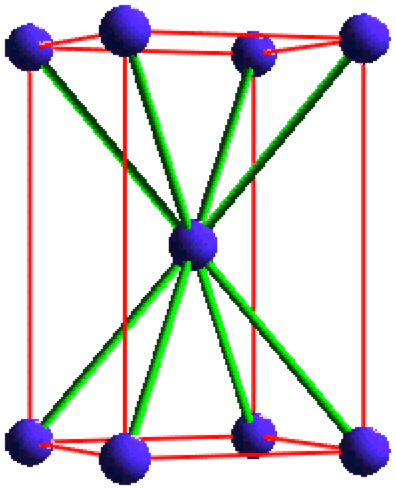
tetragonal (p) $a=b\neq c$ $\alpha=\beta=\gamma=90$



$$APF=\frac{\frac{4}{3}\pi\left(\frac{a}{2}\right)^{3}}{a^{2}c}=\frac{\pi}{6}\frac{a}{c}$$

Bravais lattice

tetragonal (I) $a=b\neq c$ $\alpha=\beta=\gamma=90$

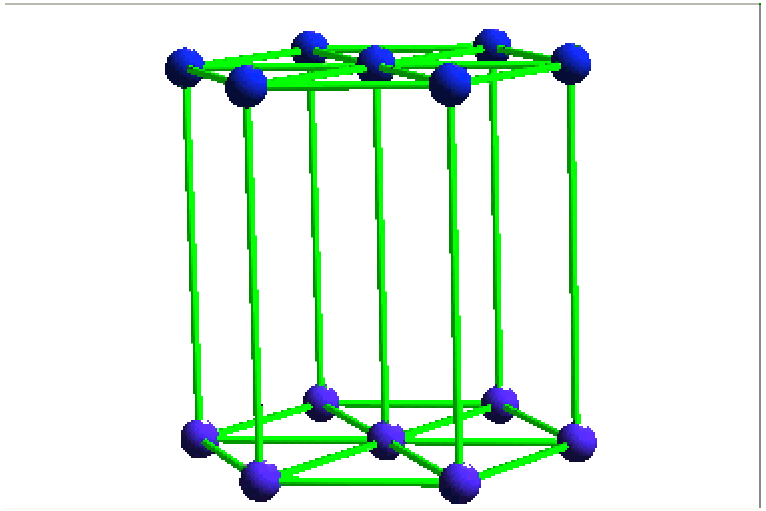


$$APF = \frac{2\times {}^{4}\!/_{3}\,\pi\left(\frac{a}{2}\right)^3}{a^2c}$$

$$APF = \frac{2\times {}^{4}\!/_{3}\,\pi\left(\frac{\sqrt{2a^2+c^2}}{4}\right)^3}{a^2c}$$

Bravais lattice

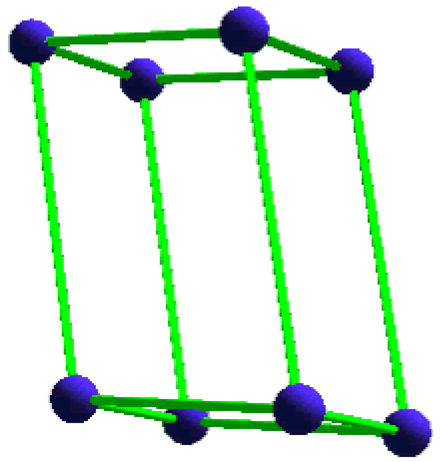
hexagonal $a=b\neq c$ $\alpha=\beta=90$, $\gamma=120$



$$APF = \frac{3\times \frac{4}{3}\pi\left(\frac{a}{2}\right)^3}{3\times\sqrt{3}/2a^2c}$$

Bravais lattice

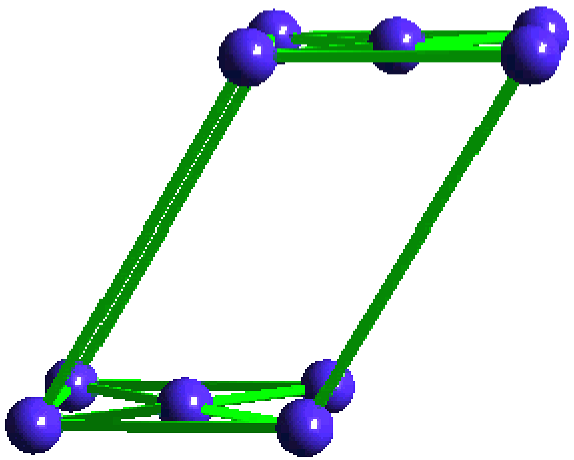
monoclinic *a≠b≠c* *α=γ=90* *,β=is not equal 90*



$$APF = \frac{\frac{4}{3}\pi\left(\frac{a}{2}\right)^3}{abc\sin\beta}$$

Bravais lattice

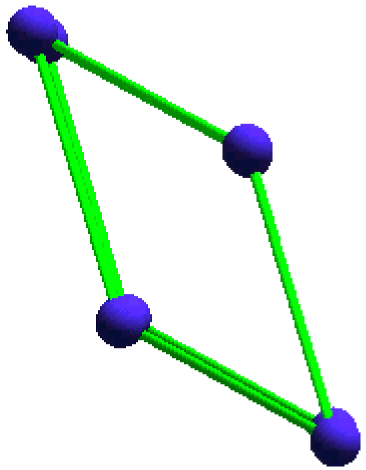
monoclinic $a \neq b \neq c$ $\alpha = \gamma = 90$,β=is not equal 90



$$APF = \frac{2 \times \frac{4}{3}\pi\left(\frac{a}{2}\right)^3}{abc\sin\beta}$$

Bravais lattice

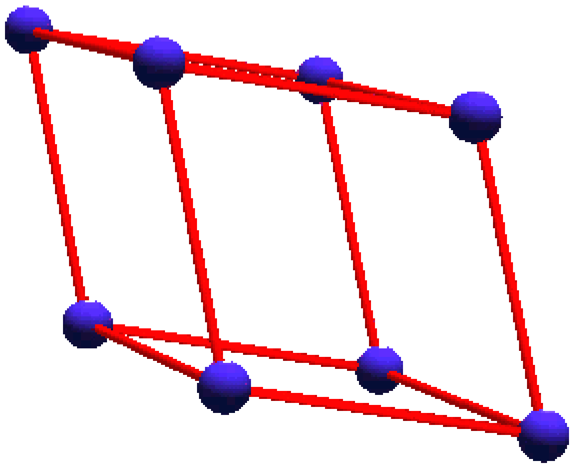
triclinic *a≠b≠c* *α≠β≠γ≠90*



$$AFP = \frac{\frac{4}{3}\pi\left(\frac{a}{2}\right)^3}{abc\sqrt{1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma}}$$

Bravais lattice

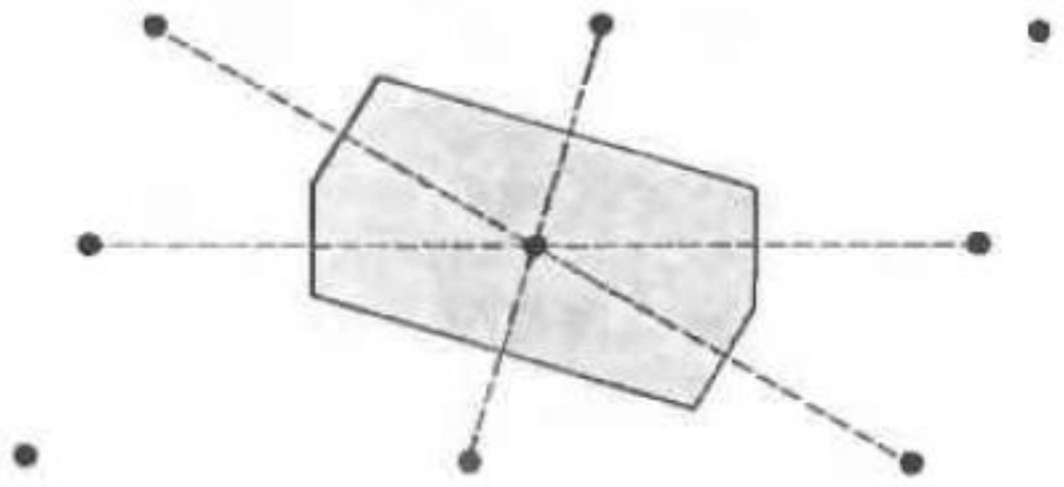
trigonal(rhombohedral) $a=b=c$ $\alpha=\beta=\gamma \neq 90$

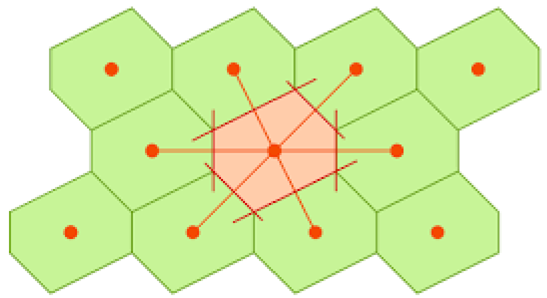


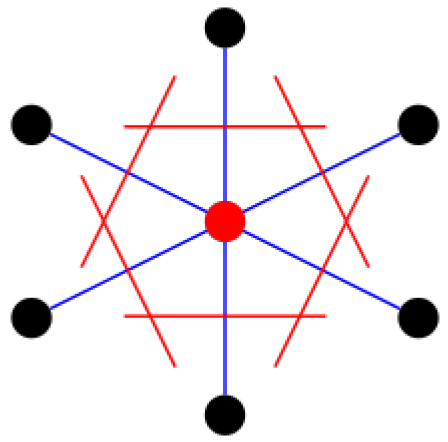
$$APF = \frac{\frac{4}{3}\pi\left(\frac{a}{2}\right)^3}{a^3\sqrt{1-3\cos^2\alpha+2\cos^3\alpha}}$$

	BRAVAIS LATTICE (BASIS OF SPHERICAL SYMMETRY)	CRYSTAL STRUCTURE (BASIS OF ARBITRARY SYMMETRY)
Number of point groups:	7 ("the 7 crystal systems")	32 ("the 32 crystallographic point groups")
Number of space groups:	14 ("the 14 Bravais lattices")	230 ("the 230 space groups")

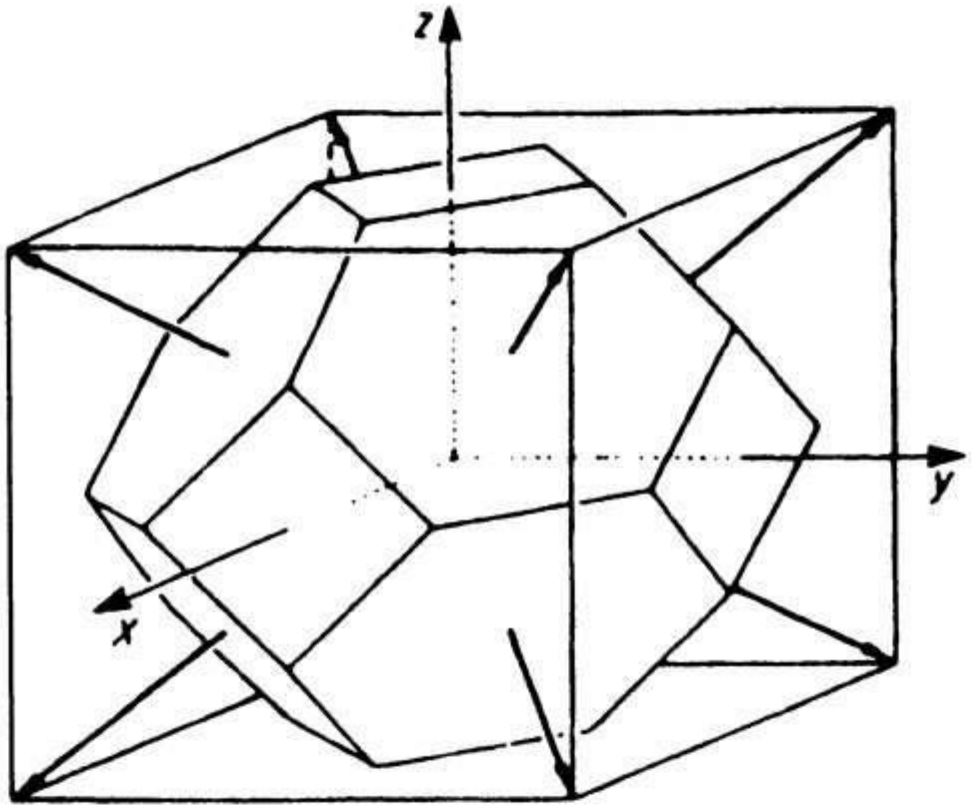
Wigner-Seitz cell

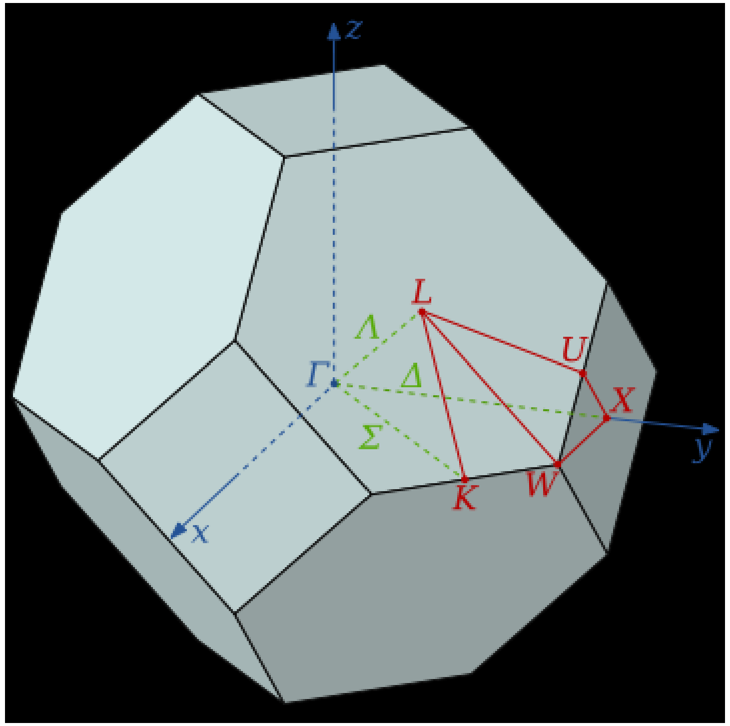




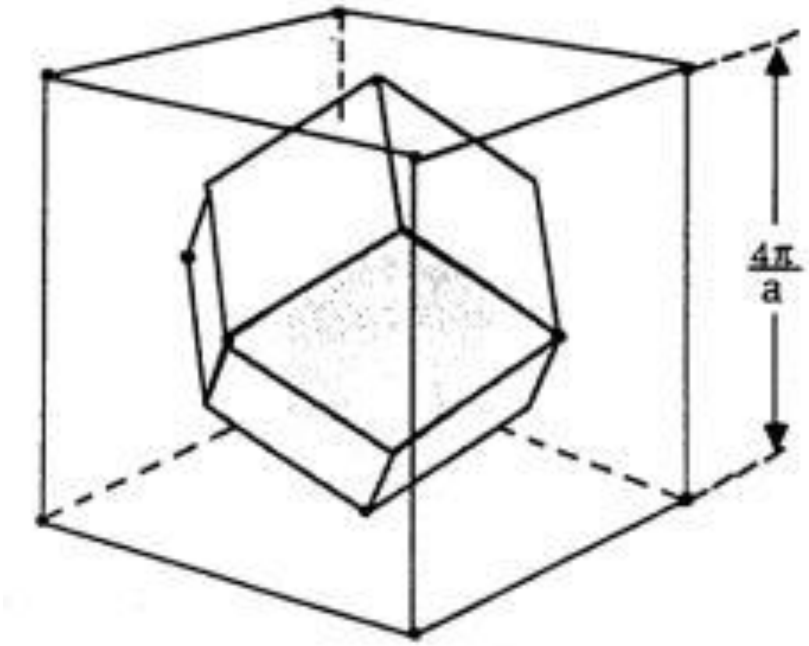


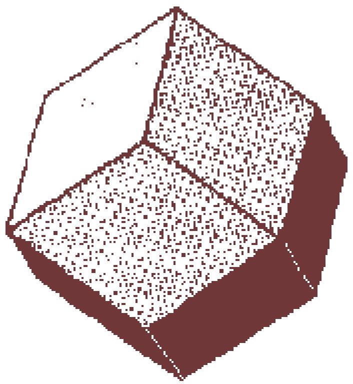
Wigner-Seitz cell of bcc



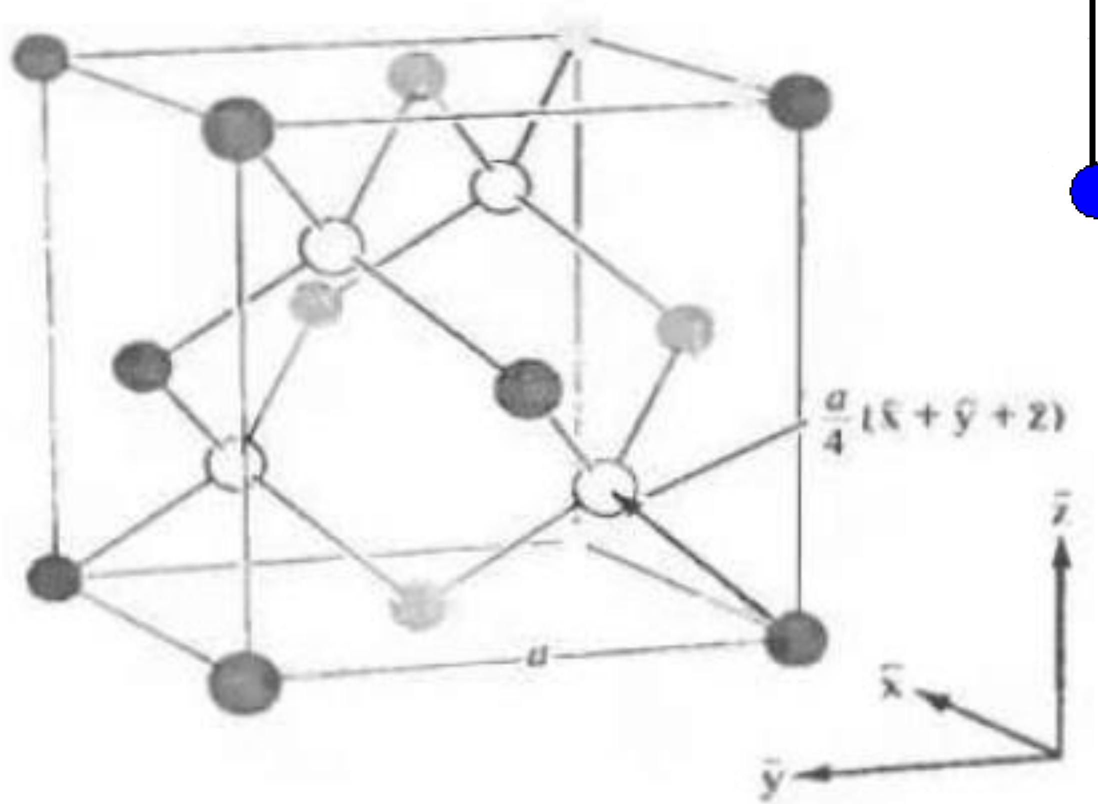


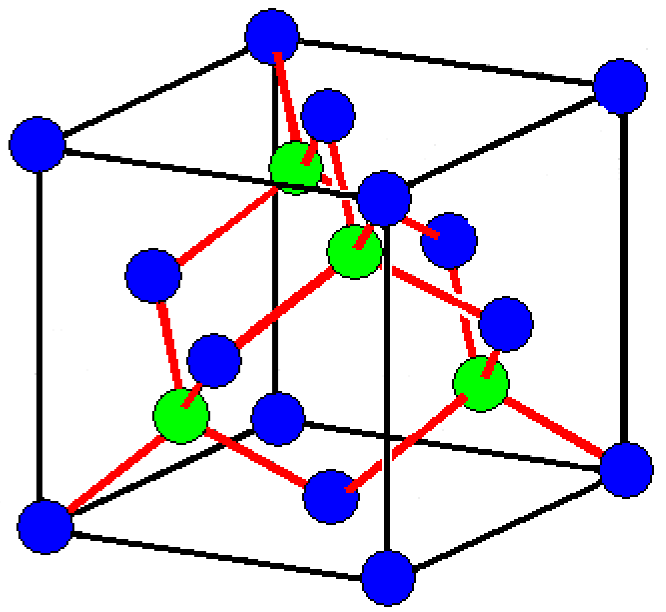
Wigner-Seitz cell of fcc





Diamond



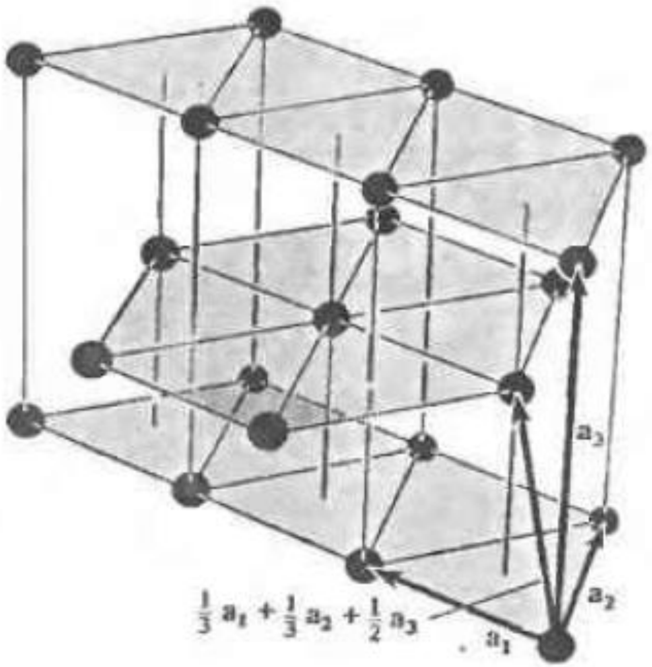


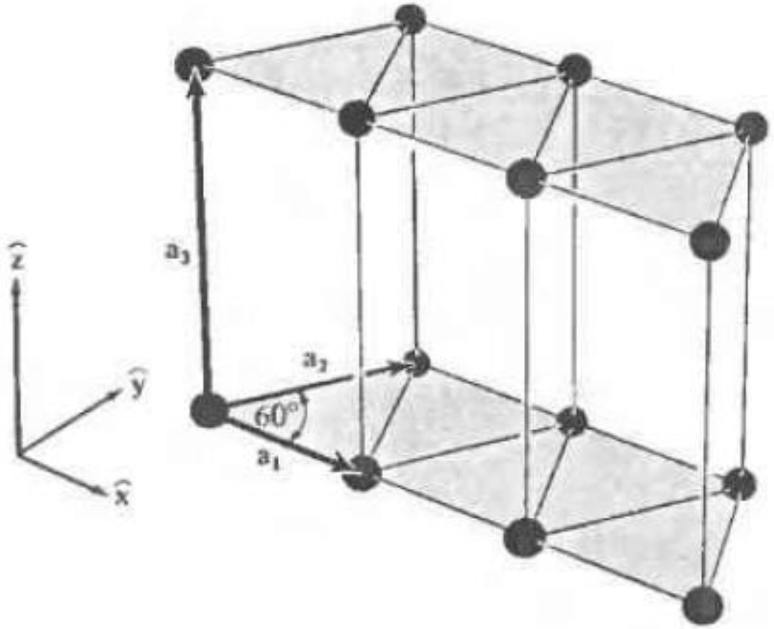
a face--centered cubic lattice with the two-point basis 0 and (a/ 4)(x + y + z).

Hexagonal Close-Packed Structure (hcp)

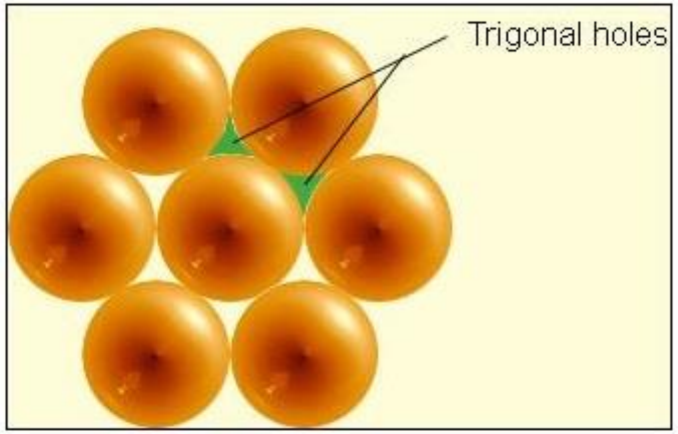
$$\mathbf{a}_1 = a\hat{\mathbf{x}}, \quad \mathbf{a}_2 = \frac{a}{2}\hat{\mathbf{x}} + \frac{\sqrt{3}a}{2}\hat{\mathbf{y}}, \quad \mathbf{a}_3 = c\hat{\mathbf{z}}.$$

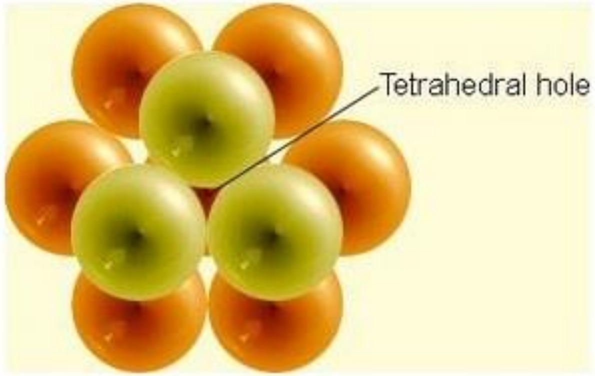
The hexagonal close-packed structure consists of two interpenetrating simple hexagonal Bravais lattices, displaced from one another by $\mathbf{a_1}/3 + \mathbf{a_2}/3 + \mathbf{a_3}/2$

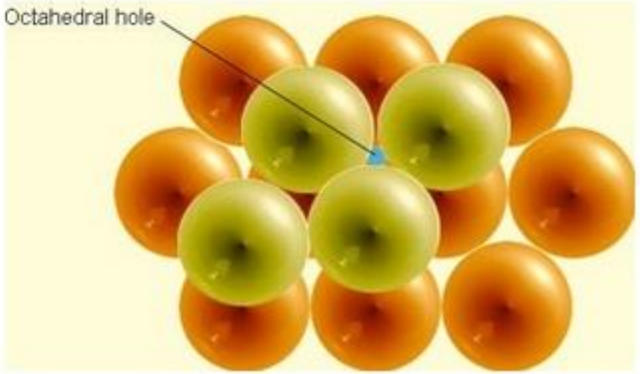


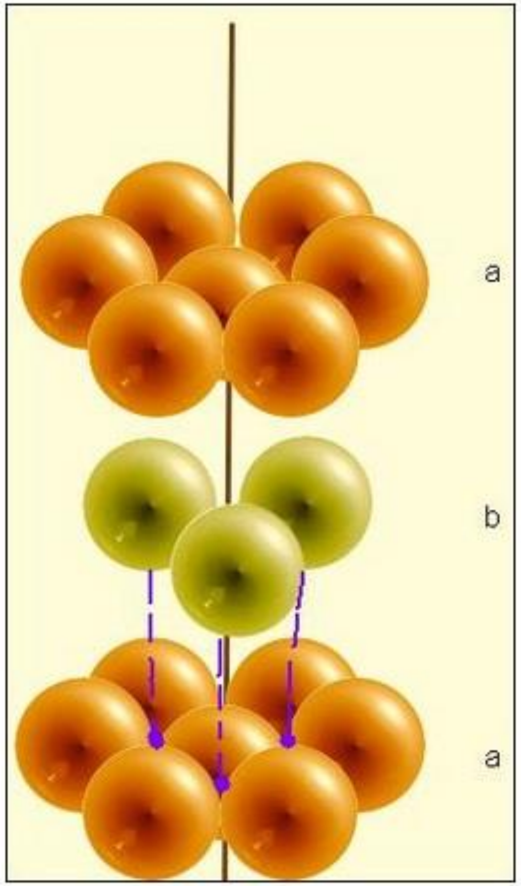


hcp









hcp