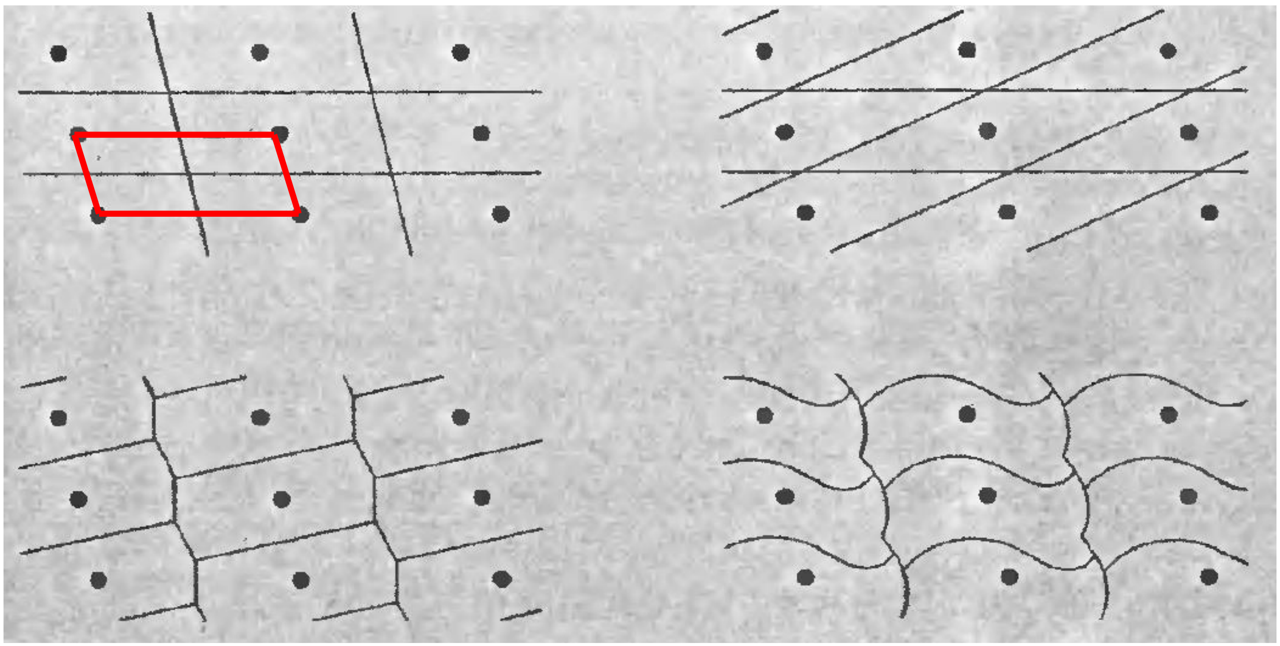
Primitive Unit-cell

A volume of space which when translated through all the vectors in a Bravais lattice just fills all of space without either overlapping itself or leaving voids is called a primitive cell or primitive unit-cell of the lattice.

Choice again is not unique



Several choices of primitive cell for a single 2D Bravais lattice

Primitive cell must precisely contain one lattice point. Thus if "n" is no. density of lattice points and "v" is volume of primitive cell, then nv =1

Volume of primitive cell is fixed between various choices

Primitive Unit-cell

The obvious primitive cell to be associated with a particular choice of primitive vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ is the set of all points $\boldsymbol{r}$ of the form –

$$\boldsymbol{r} = x_1\, \mathbf{a}_1 + x_2\, \mathbf{a}_2 + x_3\, \mathbf{a}_3$$

(x_i ranging continuously between 0 and 1)

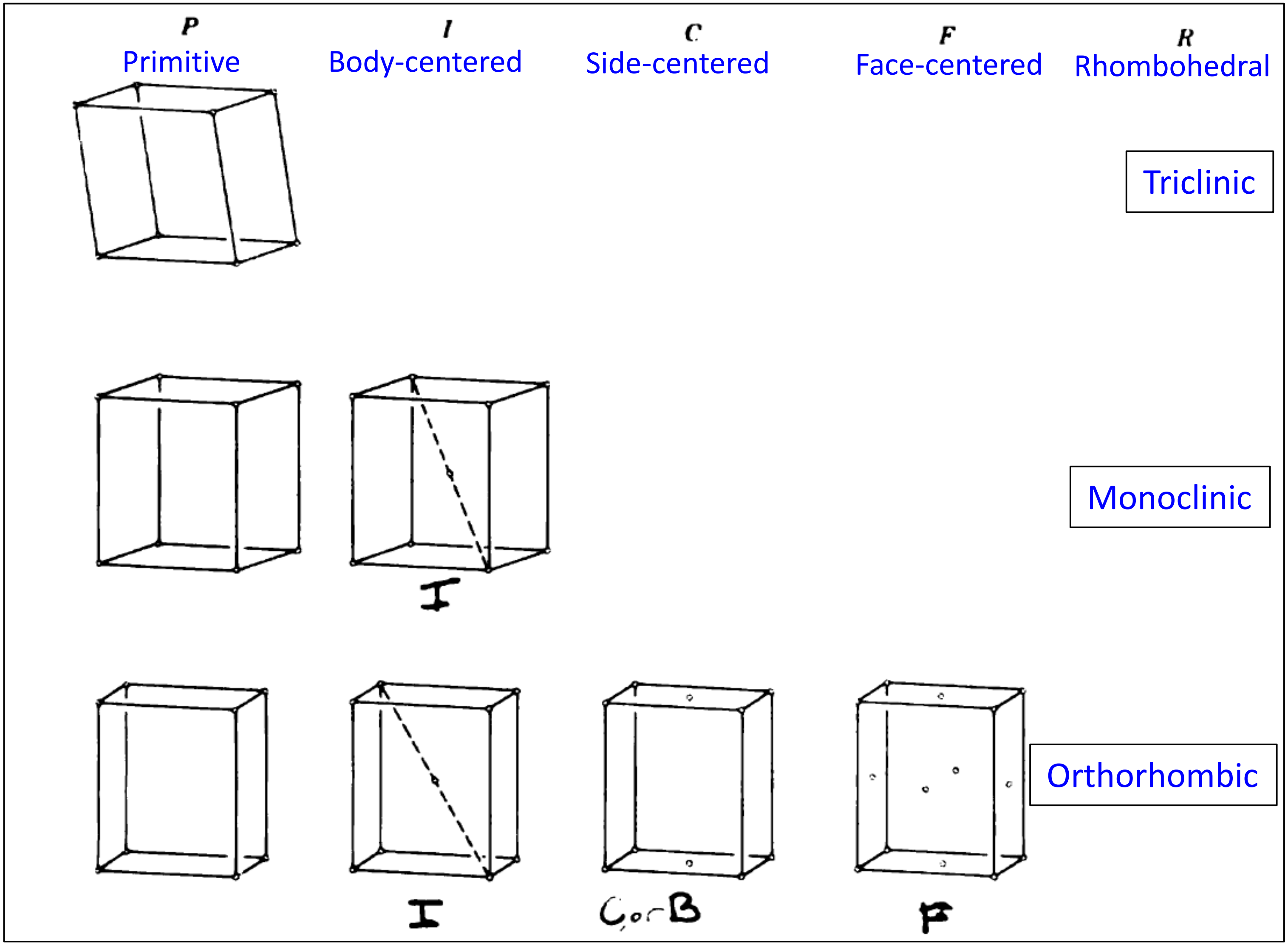
Primitive cells often do not represent the full symmetry of the Bravais lattice

Conventional Unit-cell

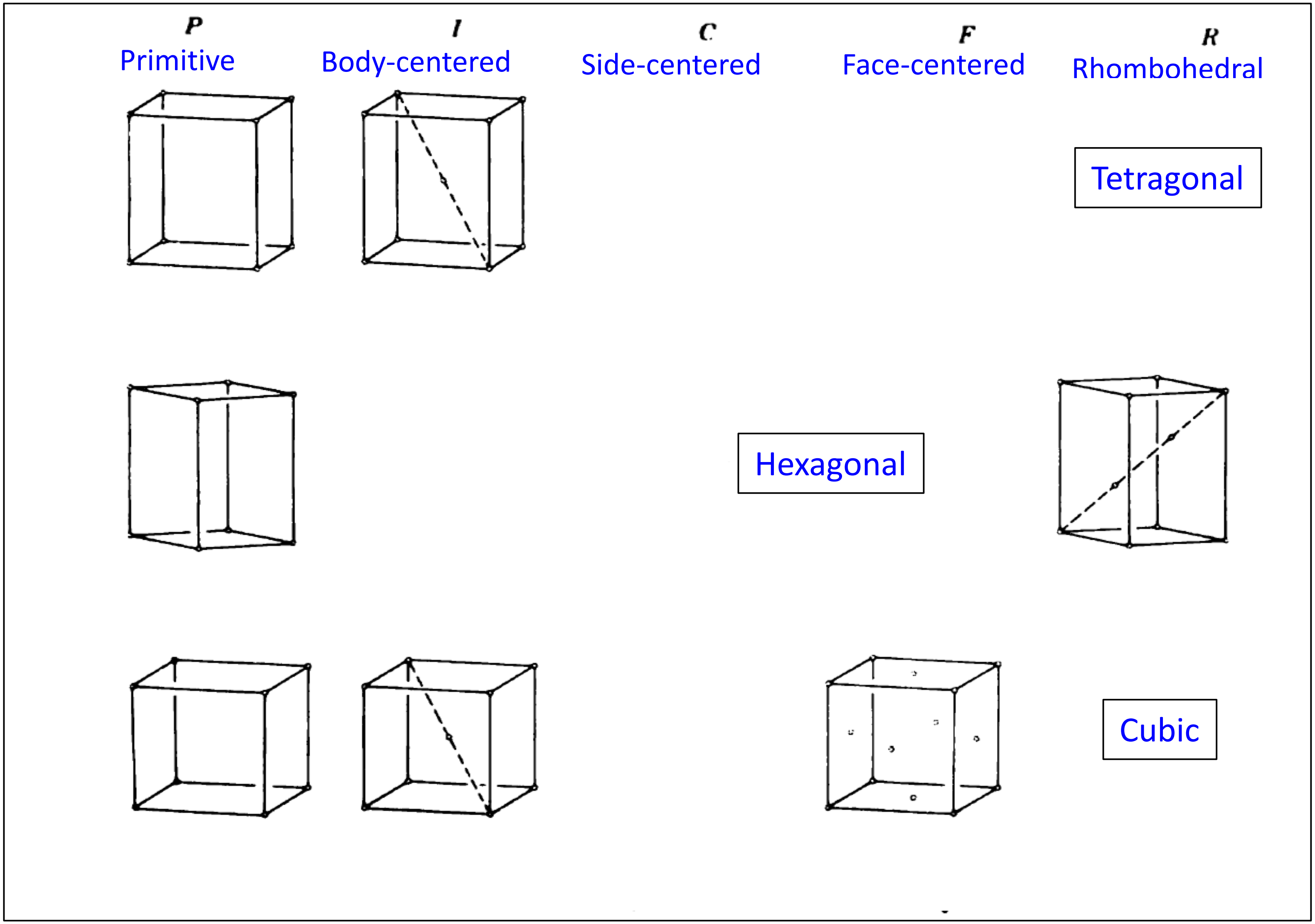
Space can also be filled up with non-primitive unit cells (also known as unit cells)

A conventional unit cell is usually chosen bigger than the primitive cell to have the symmetry of the Bravais lattice

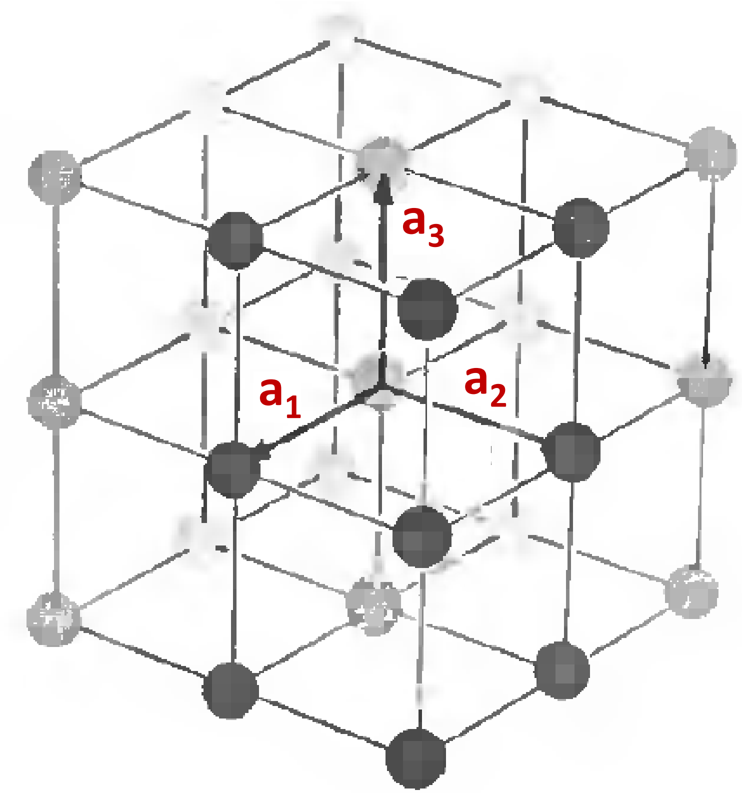
Six Crystal systems and Fourteen Bravais Lattices



Six crystal systems and Fourteen Bravais Lattices



Simple cubic Bravais Lattice



A simple cubic 3D Bravais lattice (Note point no. 1 in definition)
One choice – Take mutually perpendicular primitive vectors of equal length

Body-centered Bravais Lattice

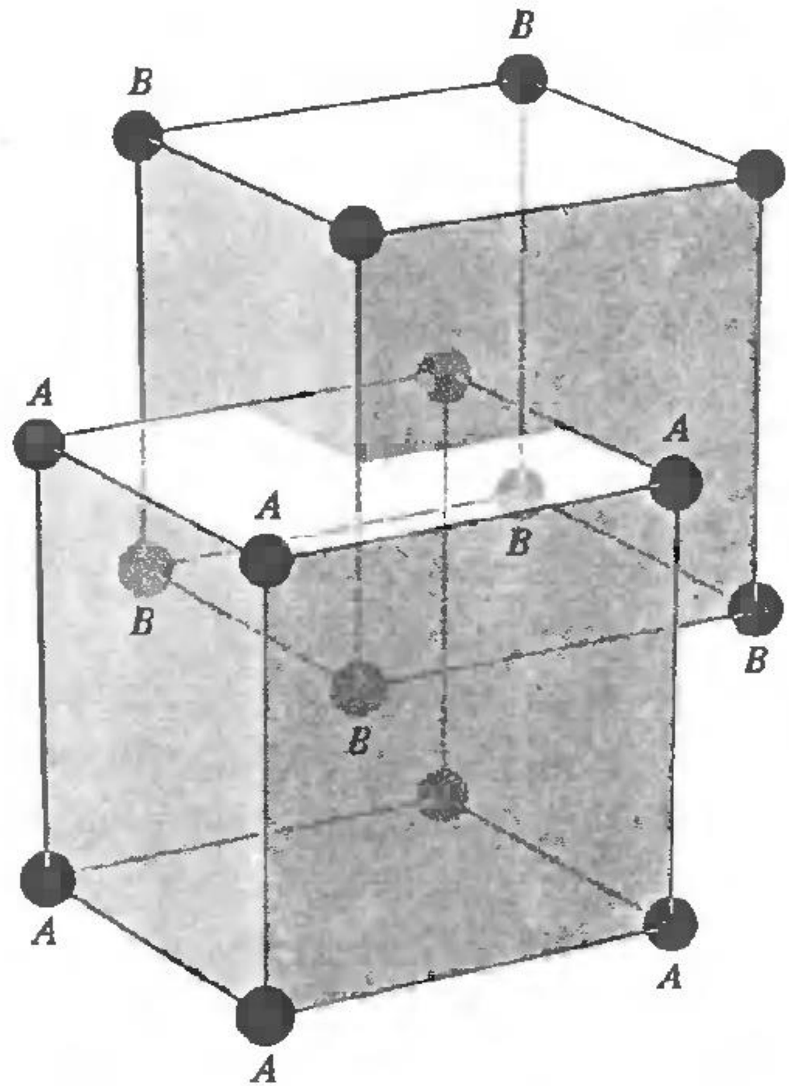
<u>Two ways to visualize</u>

Simple cubic lattice of A with points B at the body-center

OR

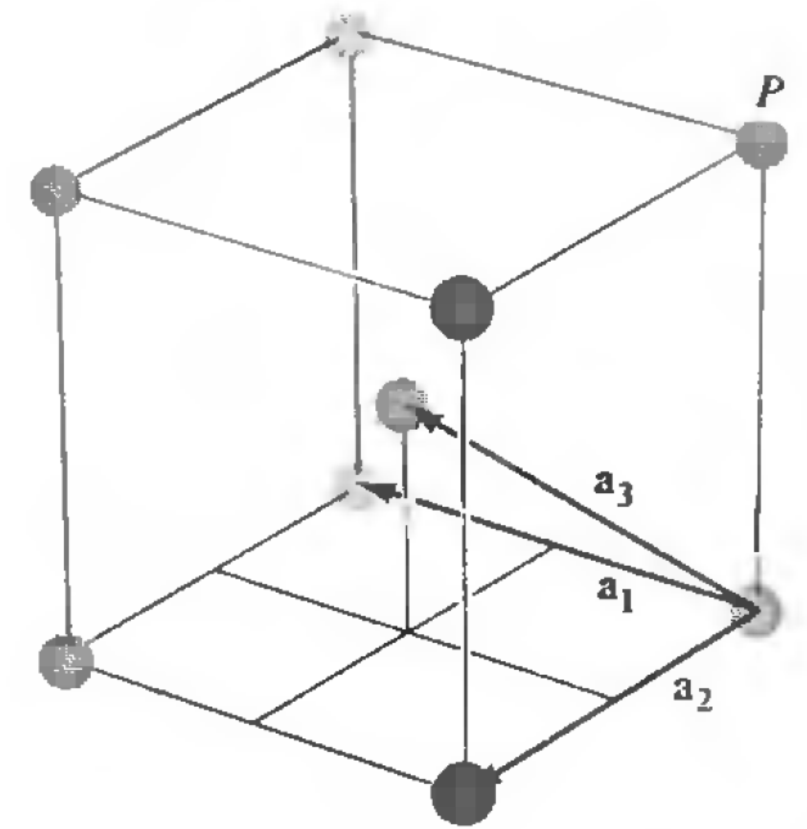
Simple cubic lattice of B with points A at the body-center.

(Definition 1 is satisfied)



Body-centered Bravais Lattice

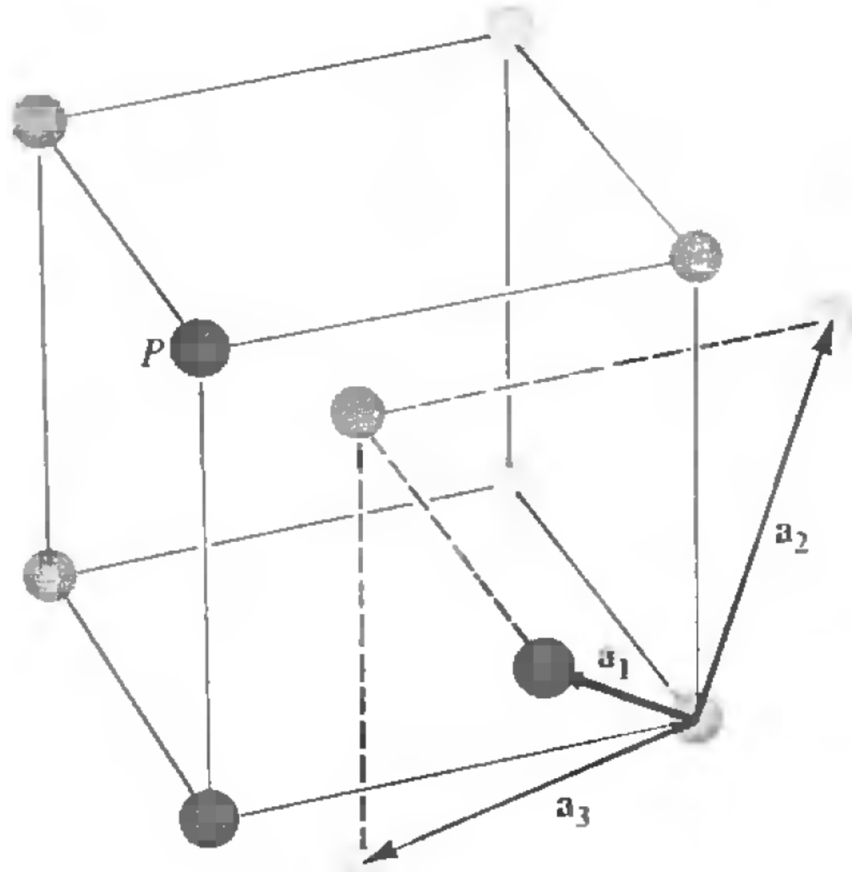
Possible primitive vectors



$\mathbf{a_1} = a \underset{x}{\rightarrow}$, $\mathbf{a_2} = a \underset{y}{\rightarrow}$, $\mathbf{a_3} = a/2 \left(\underset{x}{\rightarrow} + \underset{y}{\rightarrow} + \underset{z}{\rightarrow} \right)$

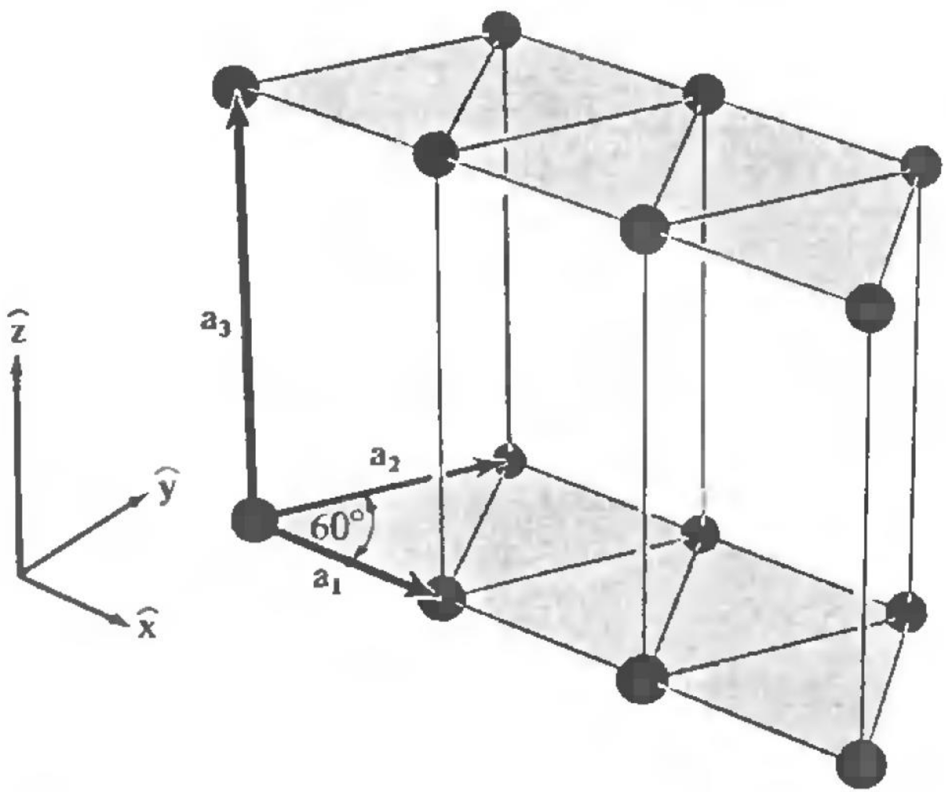
Body-centered Bravais Lattice

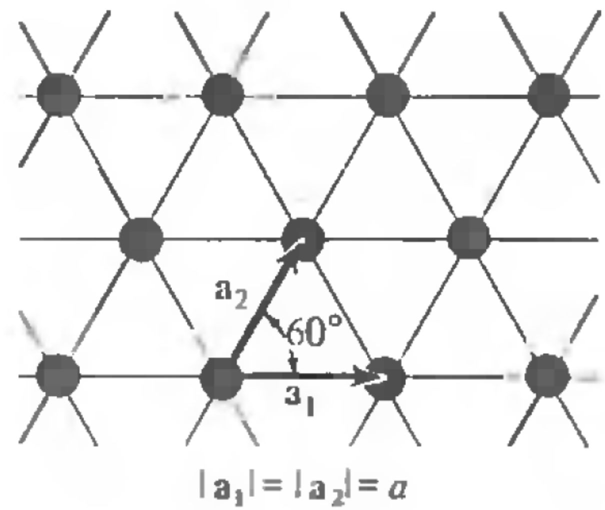
More symmetric set of primitive vectors



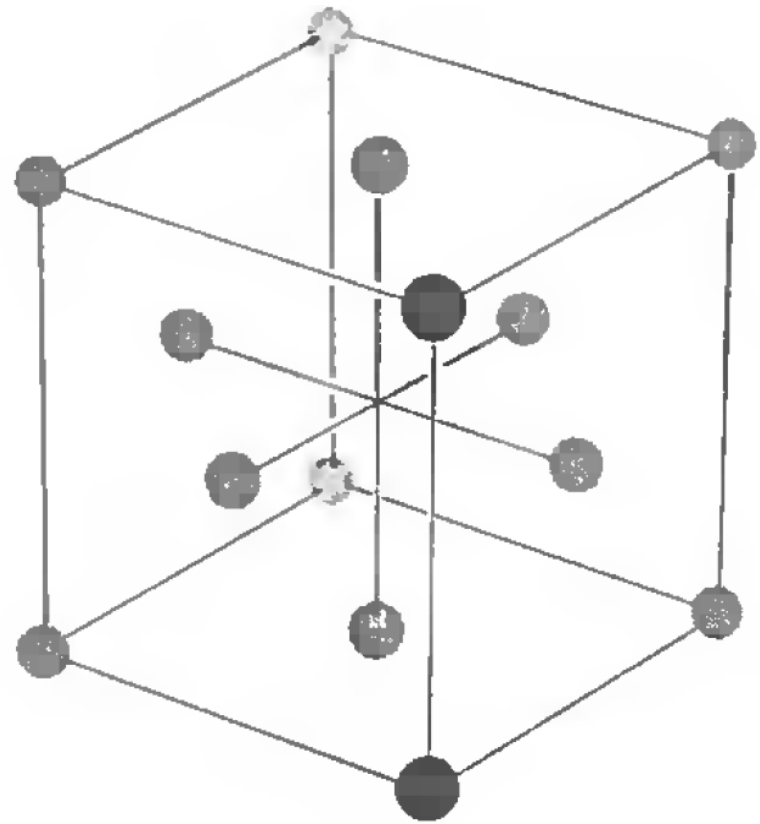
$$\mathbf{a_1} = a/2\,(\vec{y} + \vec{z} - \vec{x})\,,\ \mathbf{a_2} = a/2\,(\vec{z} + \vec{x} - \vec{y})\,,\ \mathbf{a_3} = a/2\,(\vec{x} + \vec{y} - \vec{z})$$

Hexagonal Bravais lattice



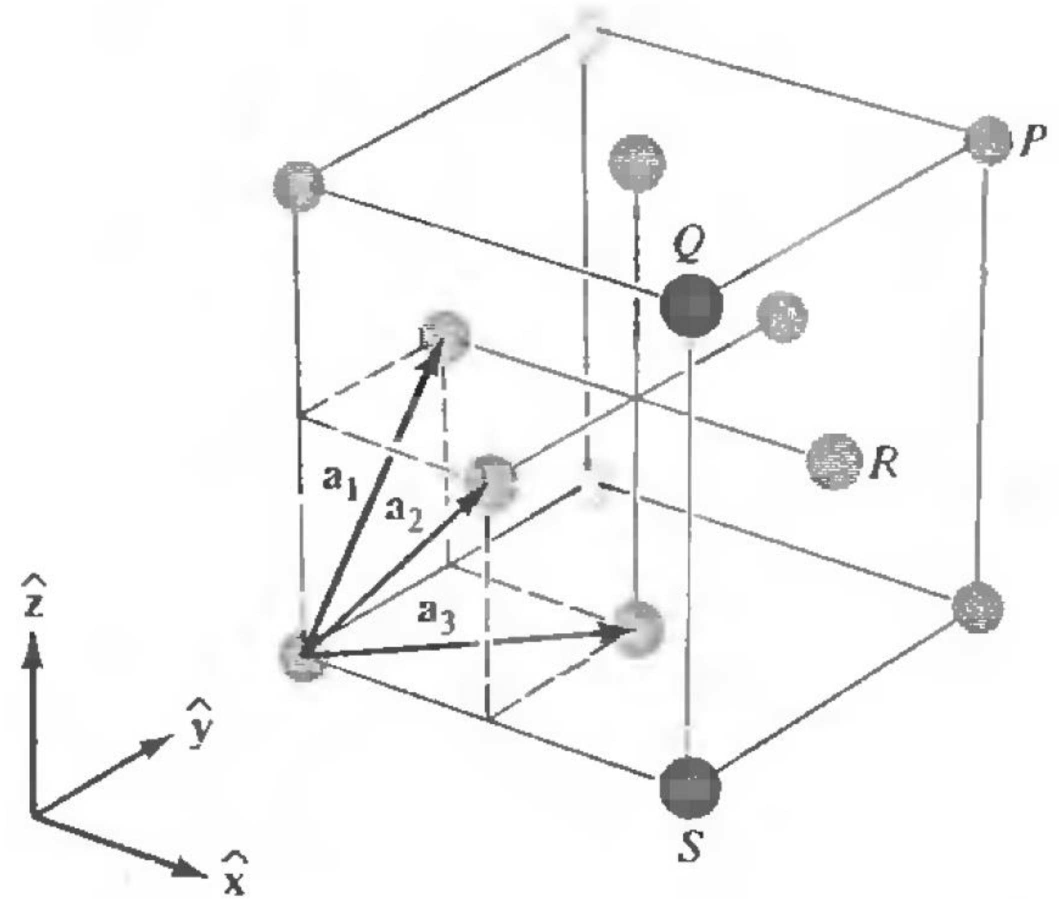


Face-centered Bravais Lattice



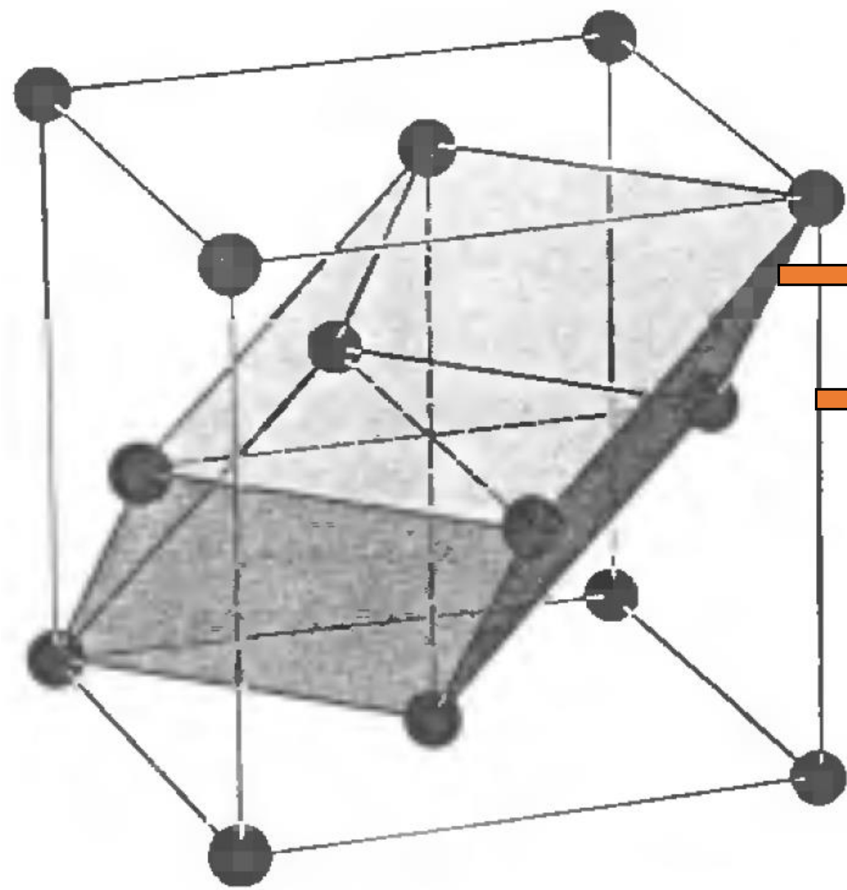
Face-centered Bravais Lattice

Possible primitive vectors



$\mathbf{a_1} = a/2\,(\vec{y} + \vec{z})$, $\mathbf{a_2} = a/2\,(\vec{z} + \vec{x})$, $\mathbf{a_3} = a/2\,(\vec{x} + \vec{y})$

Different Unit-cells for FCC Bravais lattice

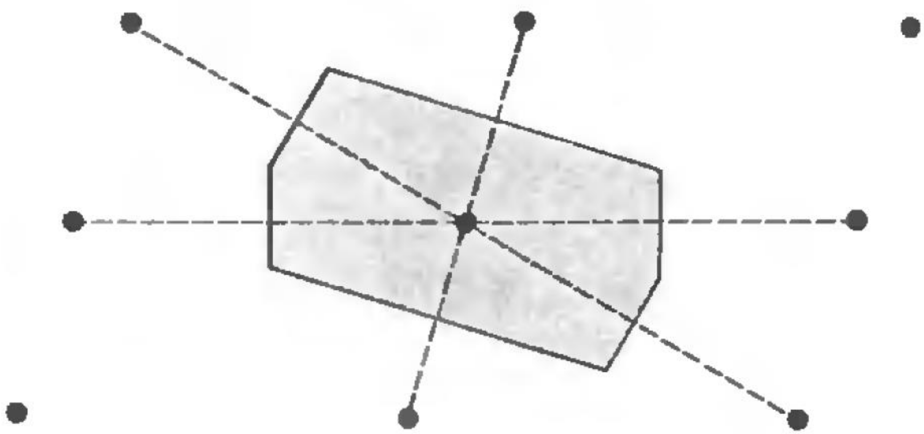


Primitive unit-cell

Conventional unit-cell

Is it possible to construct a primitive cell with Bravais lattice symmetry ?

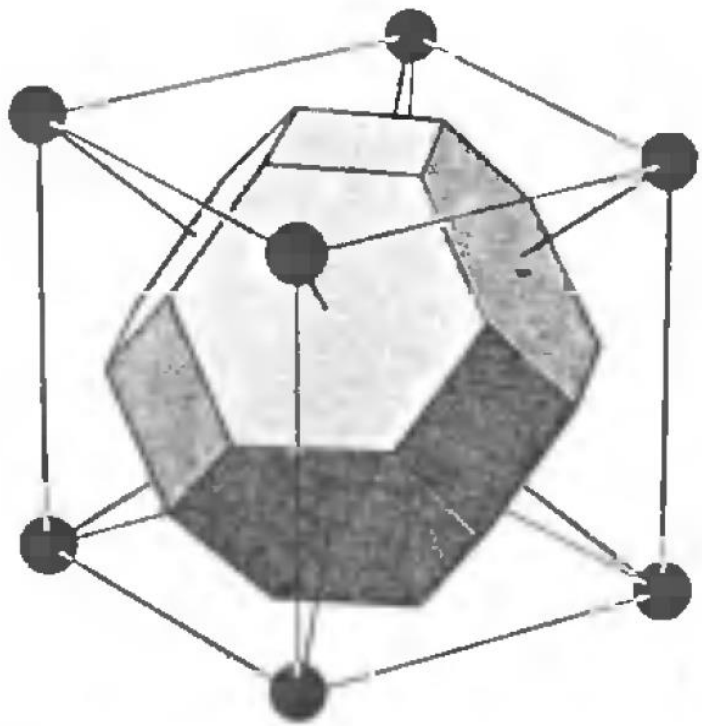
Yes ! A Wigner-Seitz primitive cell.



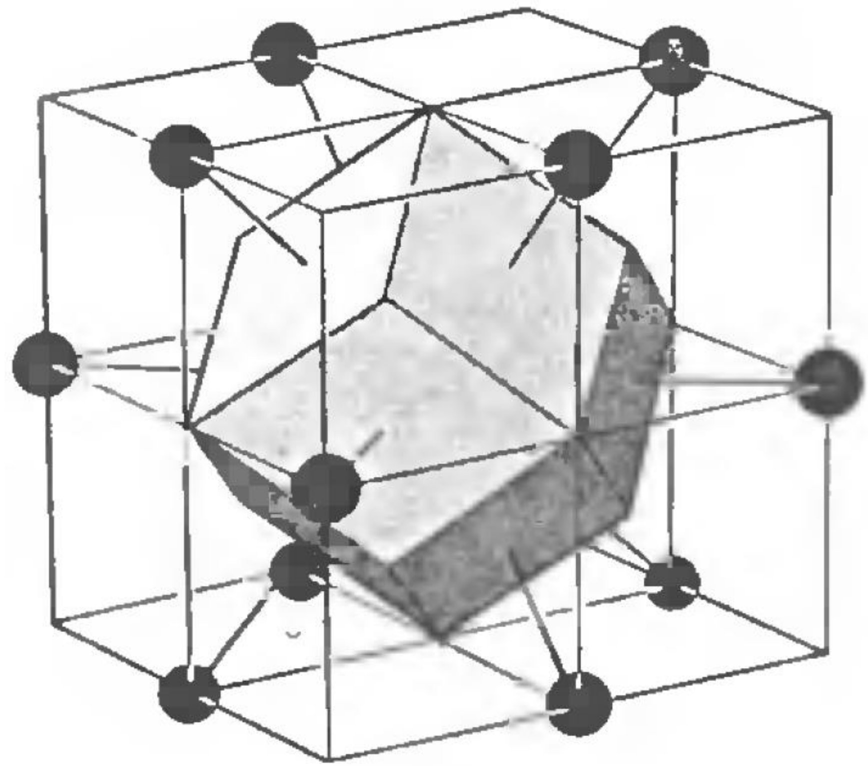
A Wigner-Seitz cell about a point is a region of space that is closer to that point than to any other lattice point

Wigner-Seitz cells

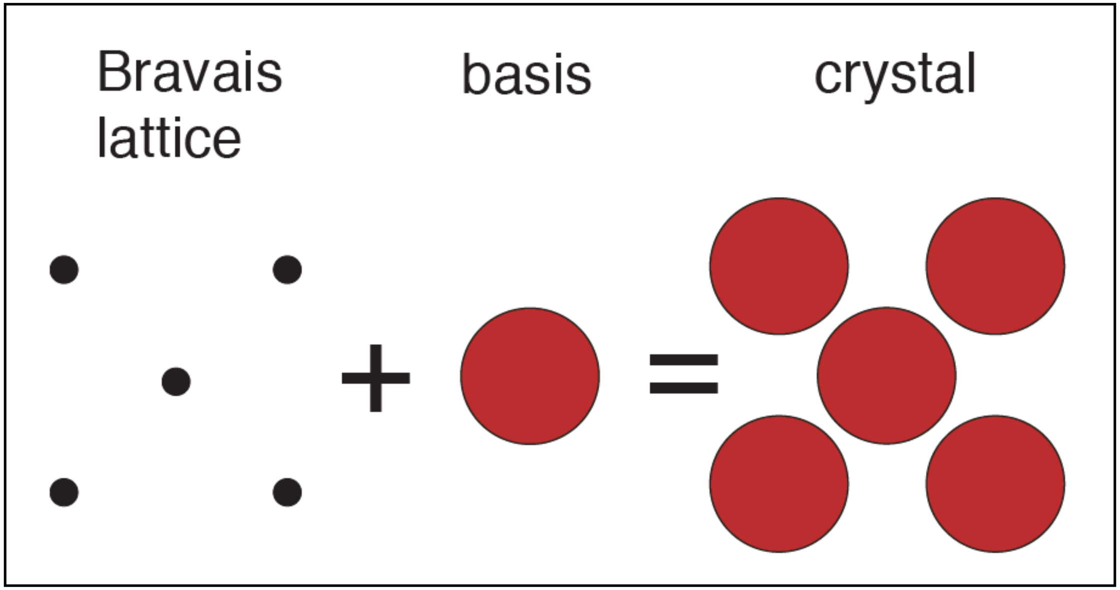
BCC Bravais Lattice



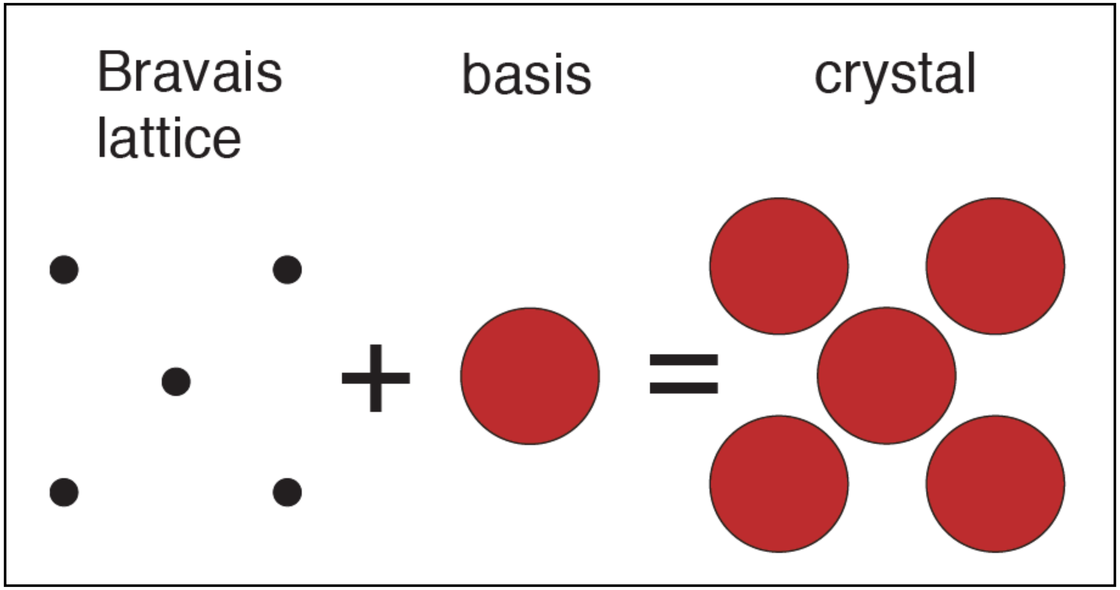
FCC Bravais Lattice

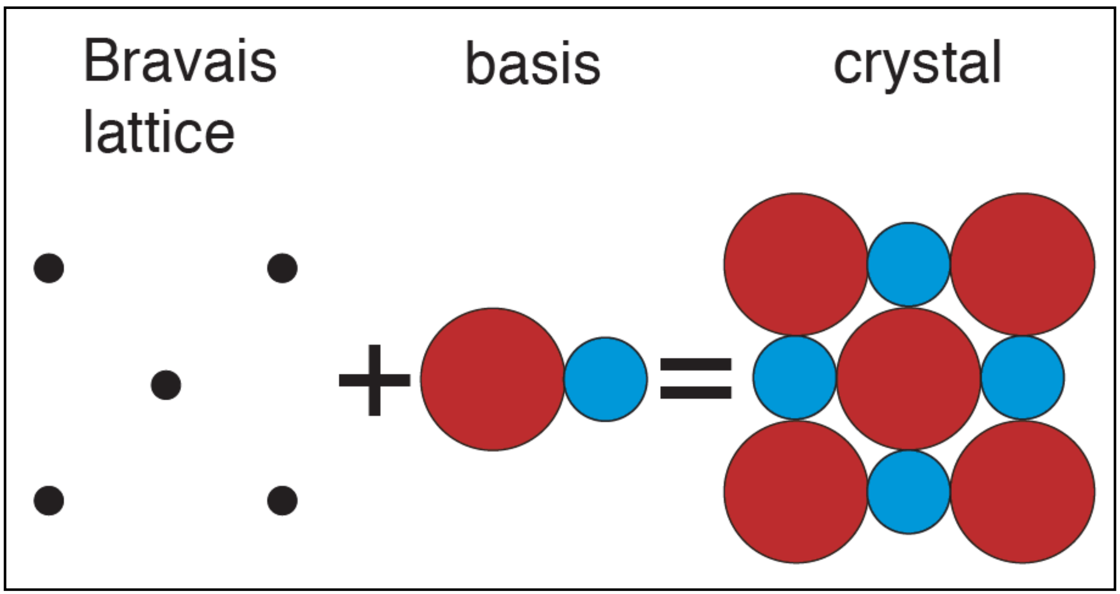


Crystal Lattice



Crystal Lattice





Lattice with a basis

Cuprate high-temperature superconductor