# III Crystal symmetry

## 3-1 Symmetry elements

### (1) Rotation symmetry

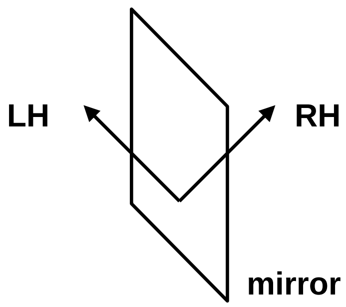
(a) two fold (diad ) 2

(b) three fold (triad ) 3

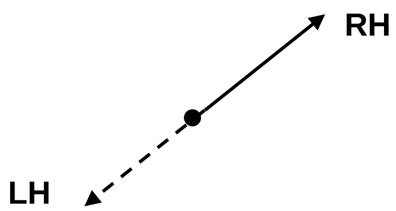
(c) four fold (tetrad ) 4

(d) six fold (hexad ) 6

### (2) Reflection (mirror) symmetry m



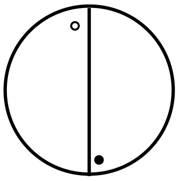

### (3) Inversion symmetry (center of symmetry) $\bar{1}$



## (4) Rotation-Inversion axis

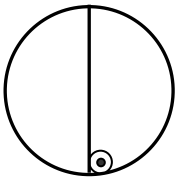
= Rotate by $\frac{360^o}{n}$ , then invert.

(a) one fold rotation inversion ($\bar{1}$)

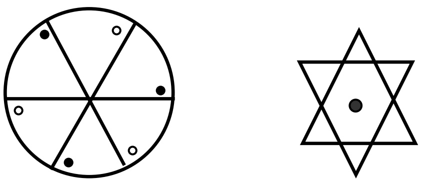


(b) two fold rotation inversion ($\bar{2}$)

= mirror symmetry = m

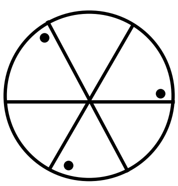


(c) inversion triad ($\bar{3}$)



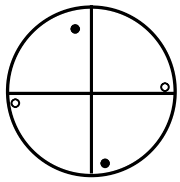
= Octahedral site in an octahedron

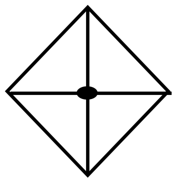
Note:



$3$

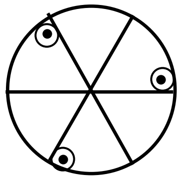
(d) inversion tetrad ($\bar{4}$)

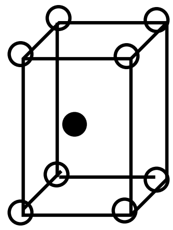




= tetrahedral site in a tetrahedron

(e) inversion hexad ($\bar{6}$)





Hexagonal close-packed (hcp) lattice

## 3-2 Fourteen Bravais lattice structures

Construct Bravais lattices from symmetrical point of view

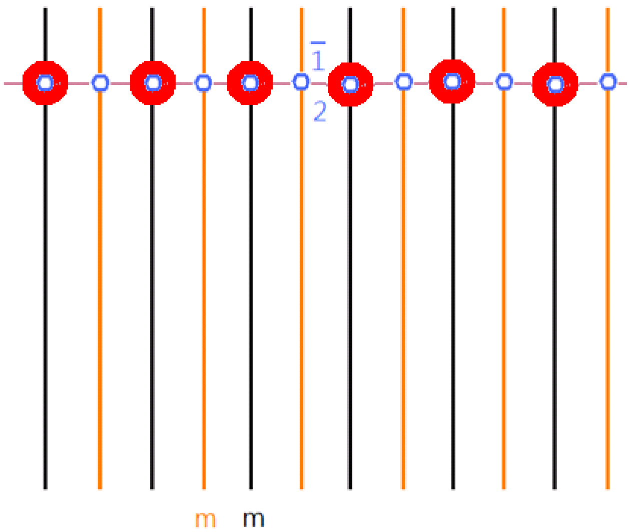
### 3-2-1 1-D lattice

3 types of symmetry can be arranged in a 1-D lattice

(1) mirror symmetry (m)

(2) 2-fold rotation (2)

(3) center of symmetry ($\bar{1}$)




### 3-2-2 2-D lattice

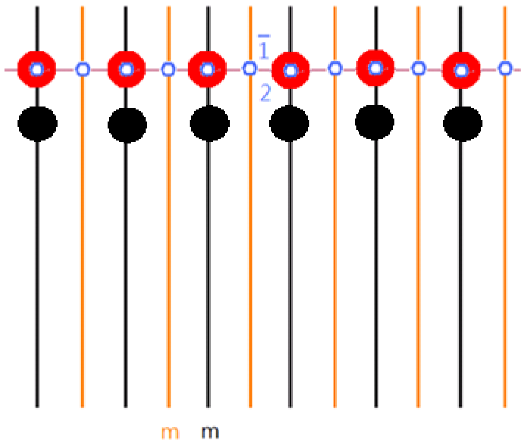
Two ways to repeat 1-D $\Rightarrow$ 2-D

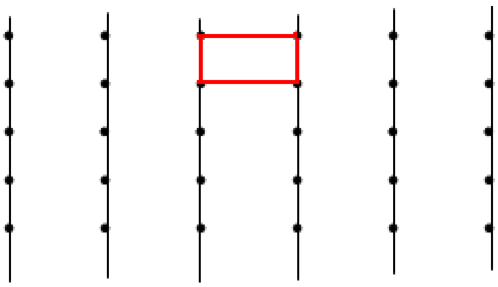
(1) maintain 1-D symmetry

(2) destroy 1-D symmetry

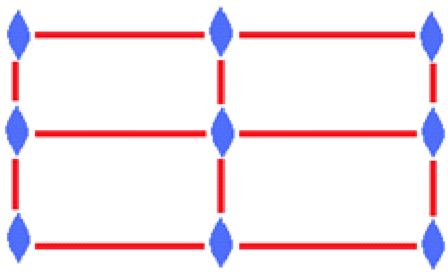
### (a) Rectangular lattice ($a \neq b$, $\gamma = 90^o$)

Maintain mirror symmetry m



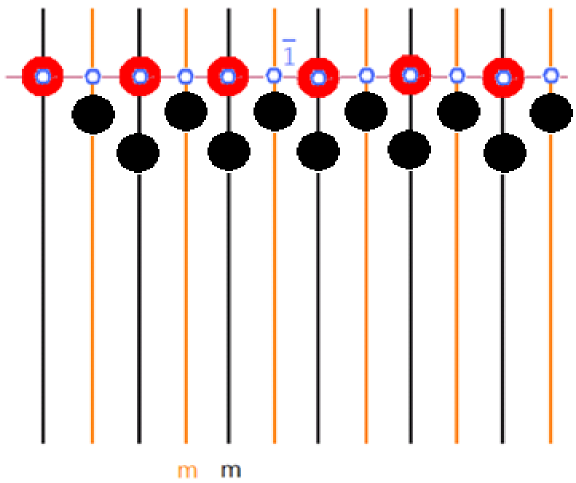
Symmetry elements in a rectangular lattice

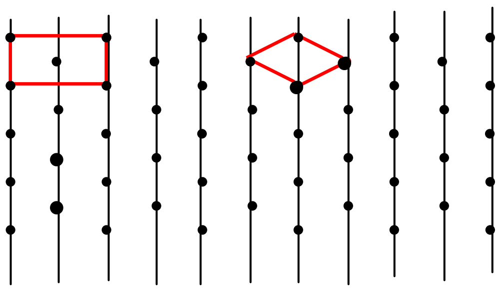


Unit cell $a \neq b$, $\gamma = 90^o$

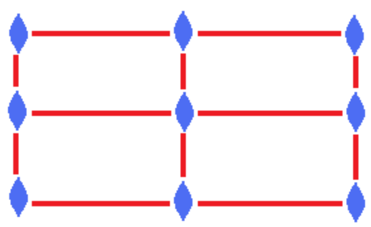
## (b) Center Rectangular lattice ( $a \neq b$ , $\gamma = 90^o$ )

Maintain mirror symmetry m

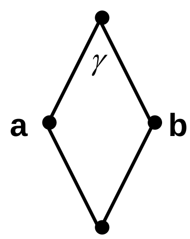


Symmetry elements in a center rectangular lattice



Unit cell

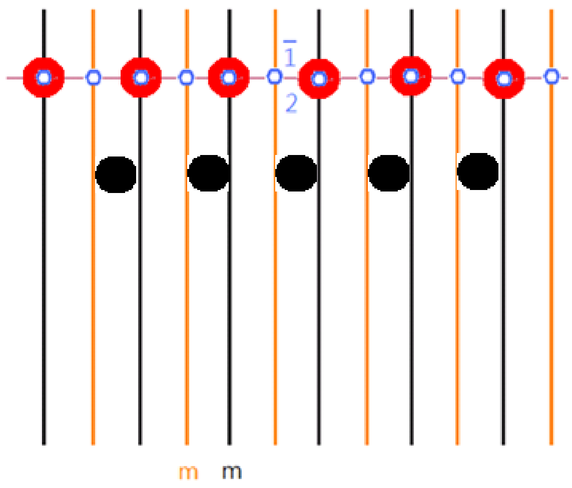


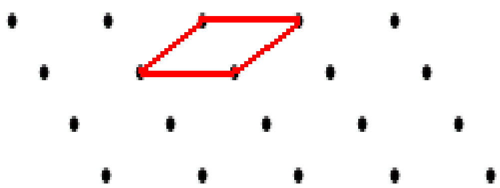
Rhombus cell (Primitive unit cell)

$$a = b \ , \ \gamma \neq 90^o$$

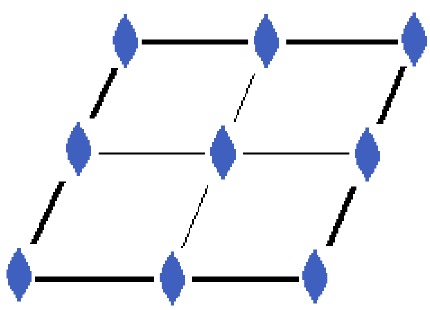
## (c) Parallelogram lattice ($a \neq b$ , $\gamma \neq 90^o$)

Destroy mirror symmetry



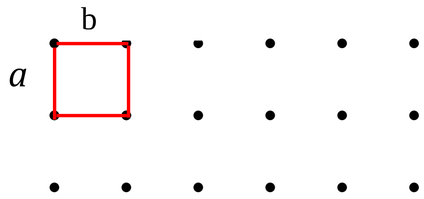



Symmetry elements in a parallelogram lattice

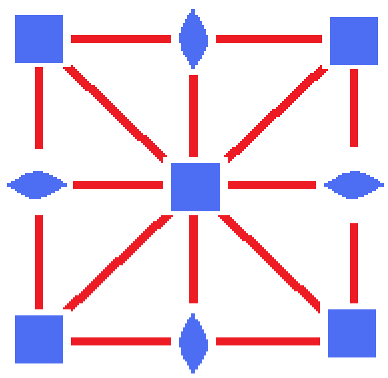


Unit cell

(d) square lattice ($a = b$ · $\gamma = 90^o$)

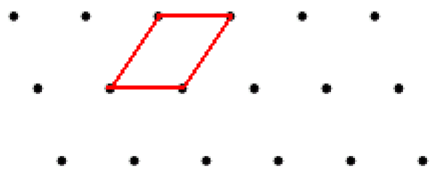



Symmetry elements in a square lattice

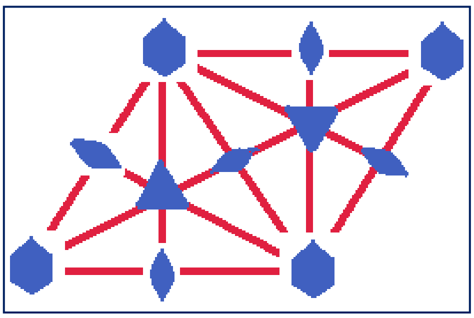


Unit cell

(e) hexagonal lattice ($a = b$, $\gamma = 120^o$)



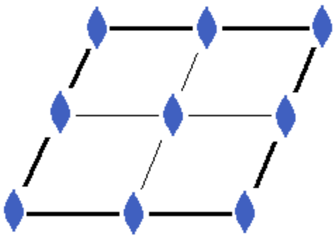
Symmetry elements in a hexagonal lattice



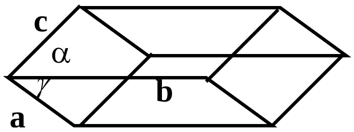
Unit cell

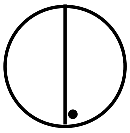
## 3-2-3 3-D lattice ： 7 systems，14 Bravais lattices

Starting from parallelogram lattice $a \neq b$，$\gamma \neq 90^o$



(1)Triclinic system 1-fold rotation (1)

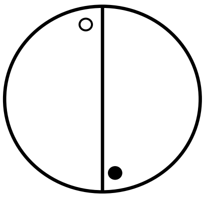


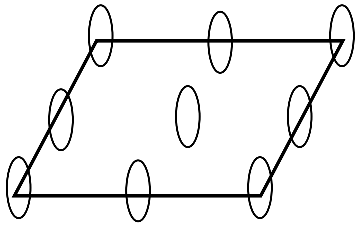
$$a \neq b \neq c \text{ , } \alpha \neq \beta \neq \gamma \neq 90^o$$

lattice center symmetry at lattice point as shown above which

the molecule is isotropic $(\bar{1})$



## (2) Monoclinic system



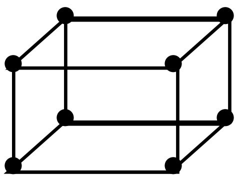
$a \neq b \neq c$ , $\alpha = \beta = 90^o \neq \gamma$

one diad axis

(only one axis perpendicular to the drawing plane ≡

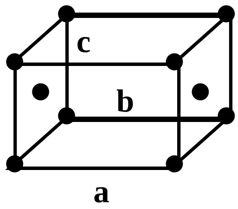
maintain 2-fold symmetry in a parallelogram lattice)

(1) Primitive monoclinic lattice (P cell)



Primitive monoclinic lattice (P cell)

(2) Base centered monoclinic lattice

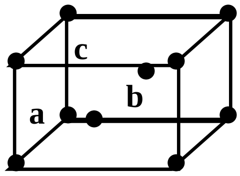



B-face centered monoclinic lattice

The second layer coincident to the middle of the

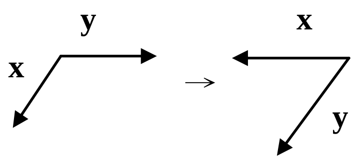
first layer，and maintain 2-fold symmetry

Note: other ways to maintain 2-fold symmetry




A-face centered monoclinic lattice

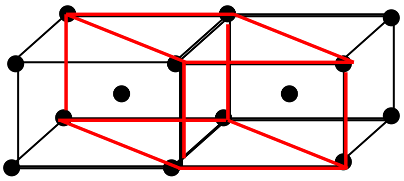
If relabeling lattice coordination




then A-face centered monoclinic lattice = B-face centered

monoclinic lattice

(3) Body centered monoclinic = Base centered monoclinic

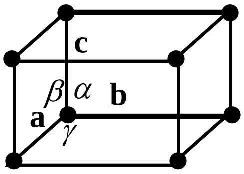


So monoclinic has two types

1. Primitive monoclinic

2. Base centered monoclinic

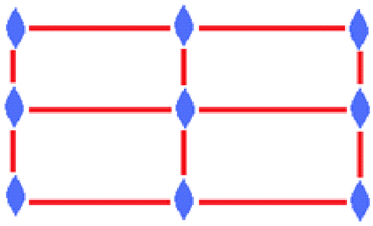
## (3) Orthorhombic system




$$a \neq b \neq c \text{，} \alpha = \beta = \gamma = 90^o$$

## 3 -diad axes

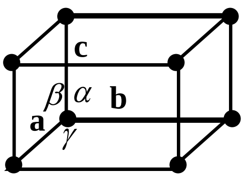
(1) Derived from rectangular lattice ($a \neq b$ ， $\gamma = 90^o$)

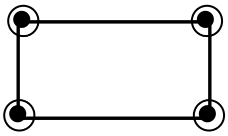


→ to maintain 2 fold symmetry

The second layer superposes directly on the first layer

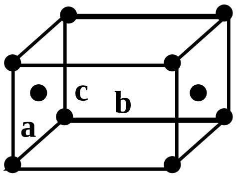
(a) Primitive orthorhombic lattice

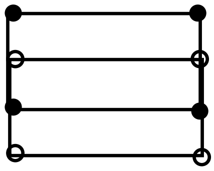


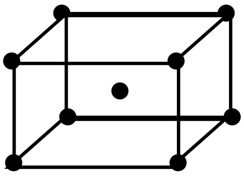
(b) B- face centered orthorhombic

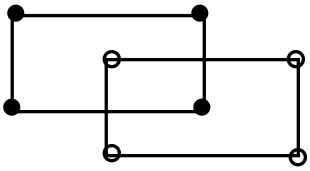
= A -face centered orthorhombic



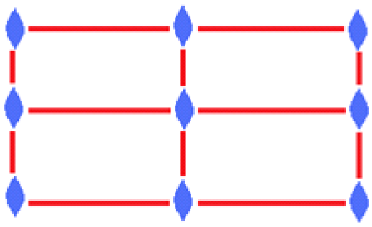



(c) Body-centered orthorhombic (I- cell)

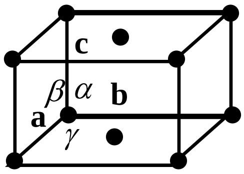


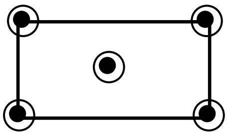


(2) Derived from centered rectangular lattice ( $a \neq b$ ， $\gamma = 90^o$ )



(a) C-face centered Orthorhombic

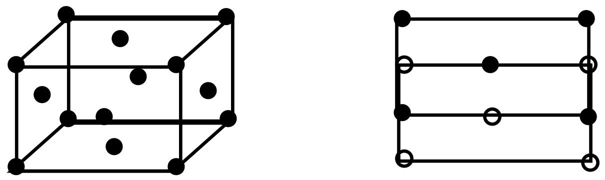


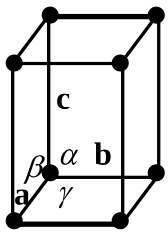
C- face centered orthorhombic

= B- face centered orthorhombic

(b) Face-centered Orthorhombic (F-cell)



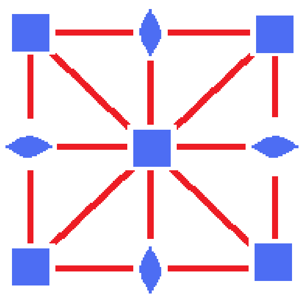
## (4) Tetragonal system




$$a = b \neq c \text{ ， } \alpha = \beta = \gamma = 90^o$$

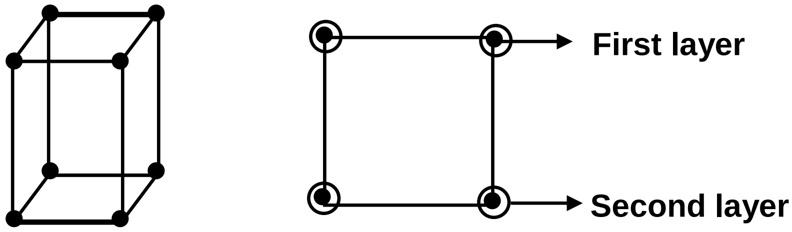
One tetrad axis

starting from square lattice ( $a = b$ ， $\gamma = 90^o$ )

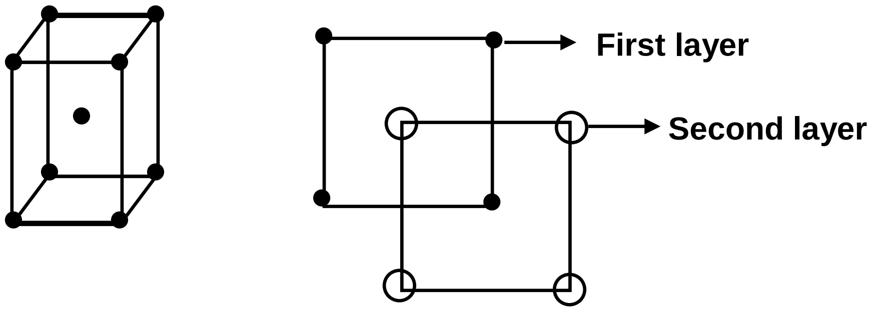


(1) maintain 4-fold symmetry

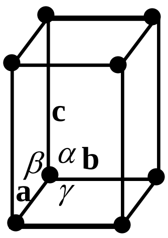
(a) Primitive tetragonal lattice




(b) Body-centered tetragonal lattice



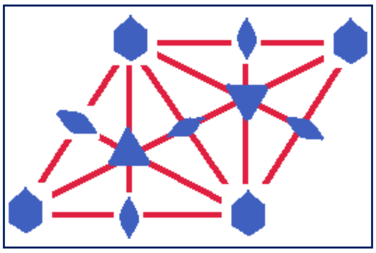

## (5) Hexagonal system




$$a = b \neq c \text{，} \alpha = \beta = 90^o \text{，} \gamma = 120^o$$

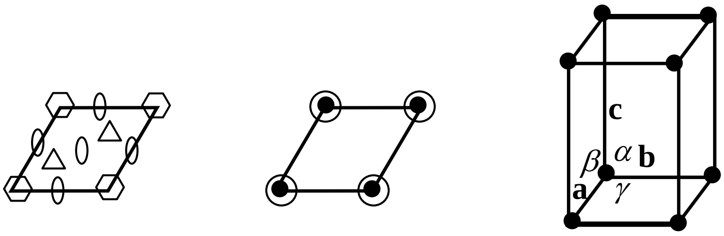
One hexad axis

starting from hexagonal lattice ($a = b$ ， $\gamma = 90^o$)

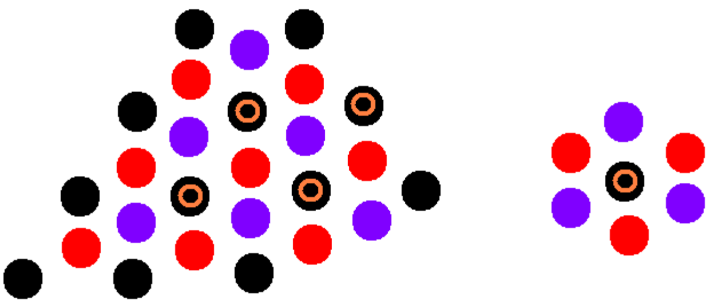


(1) maintain 6-fold symmetry

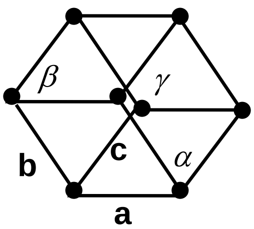
Primitive hexagonal lattice




(2) maintain 3-fold symmetry

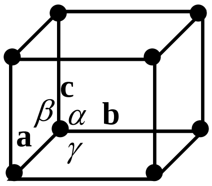


## Rhombohedral lattice




$$a = b = c \text{ ， } \alpha = \beta = \gamma \neq 90^o$$

## (6) Cubic system



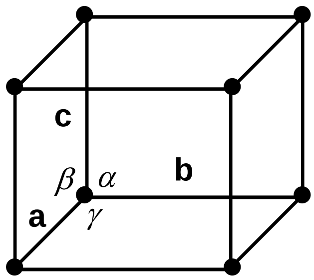

$a=b=c$ ， $\alpha=\beta=\gamma=90^{o}$

4 triad axes ( triad axis=cube diagonal )

## Cubic is a special form of Rhombohedral lattice

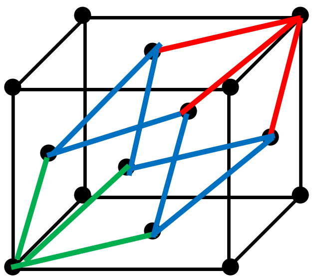
Cubic system has 4 triad axes mutually inclined along cube diagonal

(a) $\alpha=90^{o}$ Primitive cubic




$a=b=c$ ， $\alpha=\beta=\gamma=90^{o}$

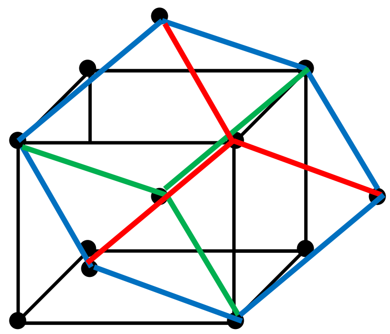
(b) $\alpha=60^{o}$ Face-centered cubic



$a=b=c$ ， $\alpha=\beta=\gamma=60^{o}$

≡ 2 regular tetrahedral

(c) $\alpha = 109^o$ Body-centered cubic



$a = b = c$ , $\alpha = \beta = \gamma = 109^o$