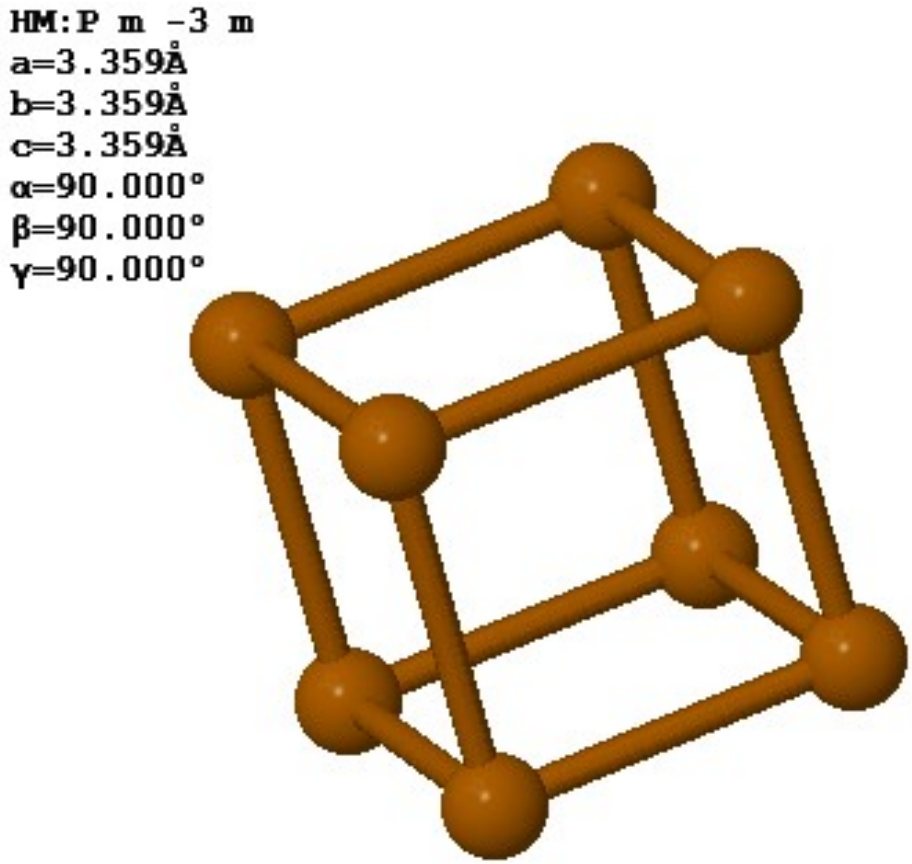
Crystal structure

simple cubic

Po



Number: 221

Primitive Vectors:

$$\vec{a}_1 = a\hat{x}$$

$$\vec{a}_2 = a\hat{y}$$

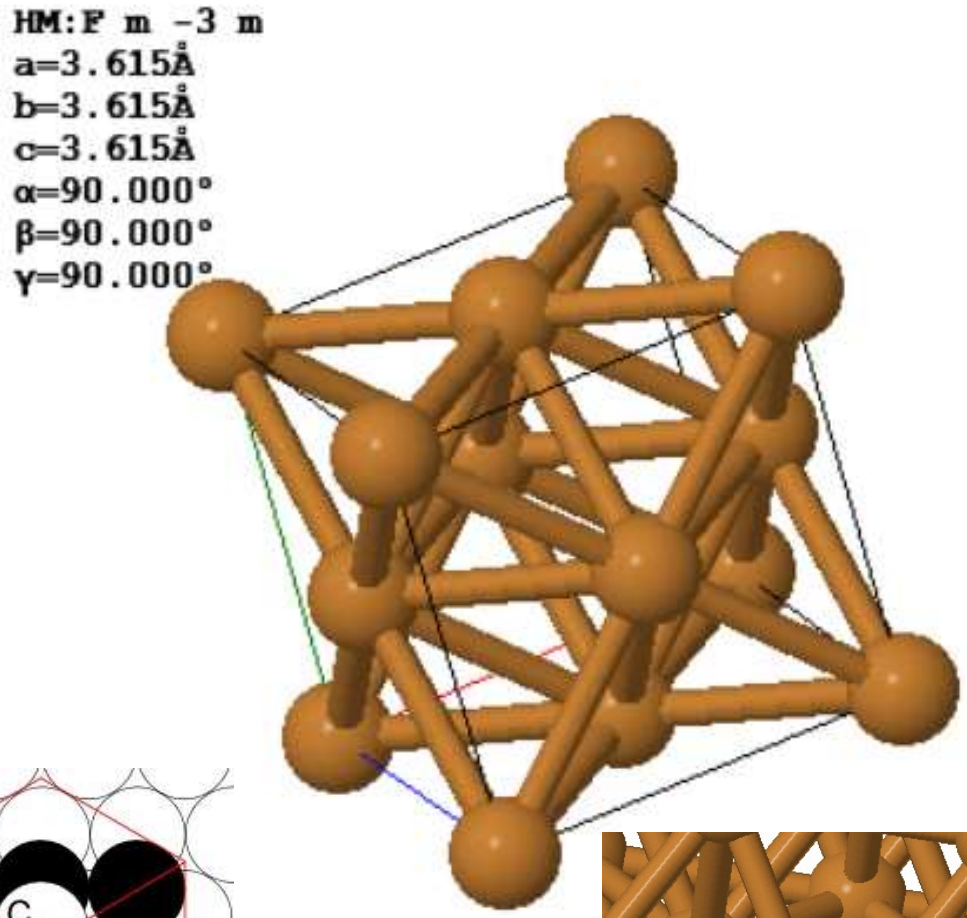
$$\vec{a}_3 = a\hat{z}$$

Basis Vector: $\vec{B}_1 = (0,0,0)$

fcc

Number 225

Al, Cu,
Ni, Sr,
Rh, Pd,
Ag, Ce,
Tb, Ir,
Pt, Au,
Pb, Th



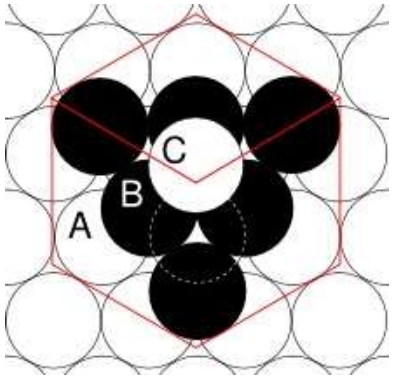
[111]

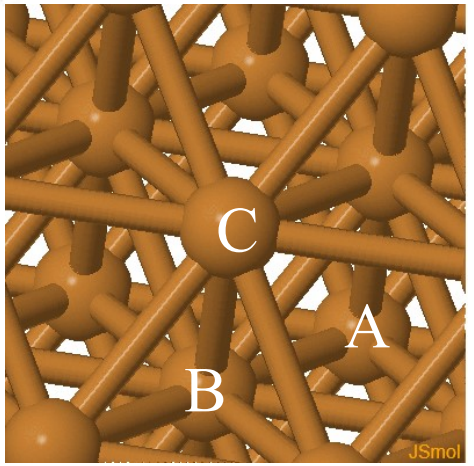
Primitive Vectors:

$$\vec{a}_1 = \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z}$$

$$\vec{a}_2 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{z}$$

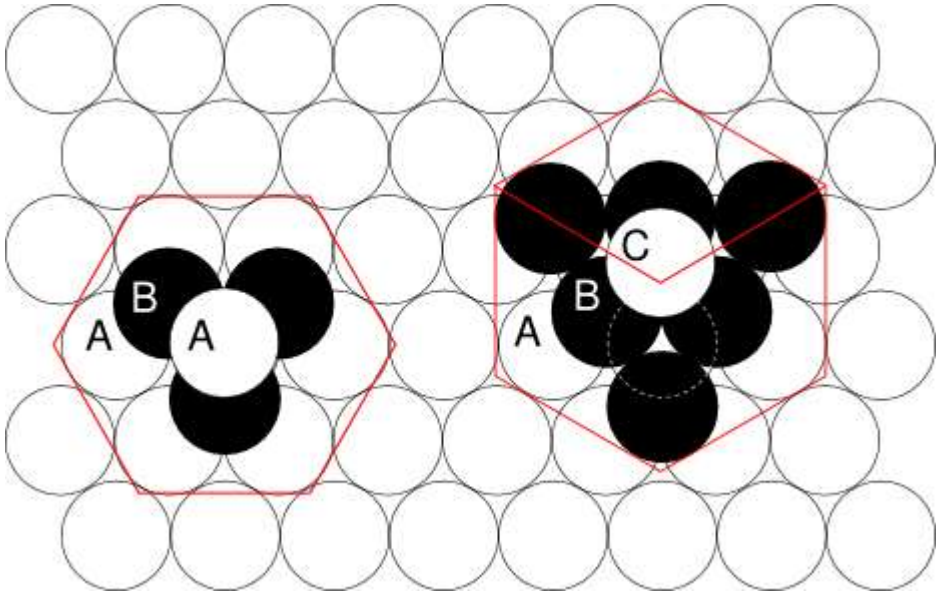
$$\vec{a}_3 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{y}$$



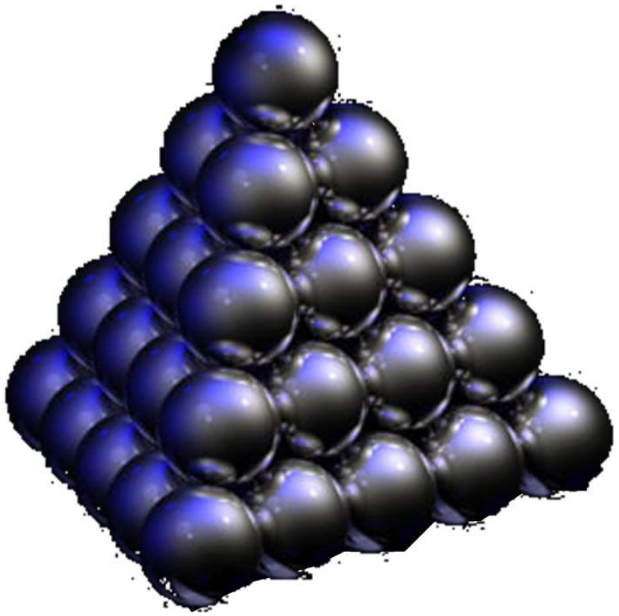


Basis Vector: $\vec{B}_1 = (0,0,0)$

Close packing



HCP FCC



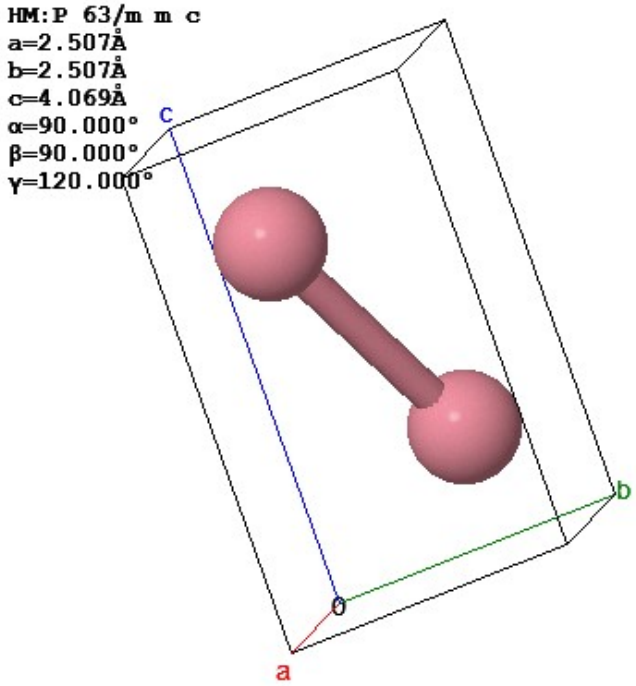
HCP = Hexagonal close pack
Hexagonal Bravais lattice with two atoms in the basis.

hcp

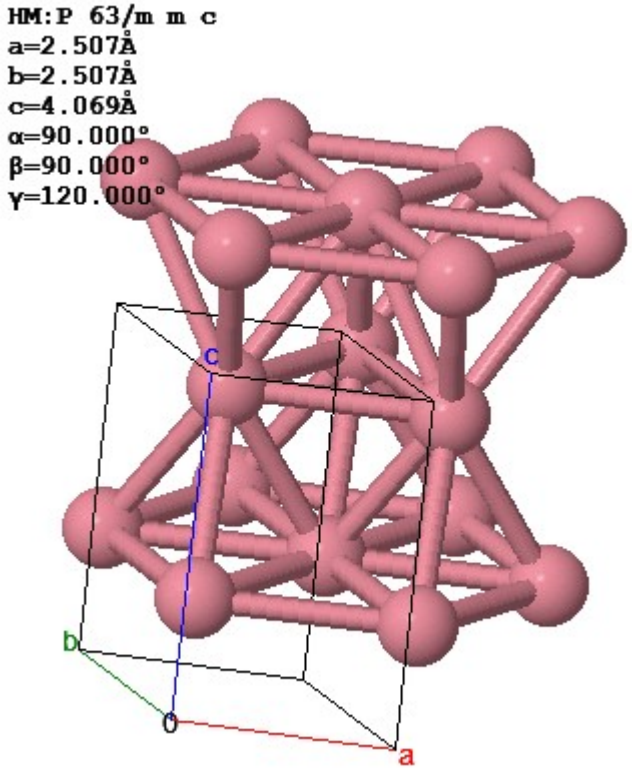
Space group 194

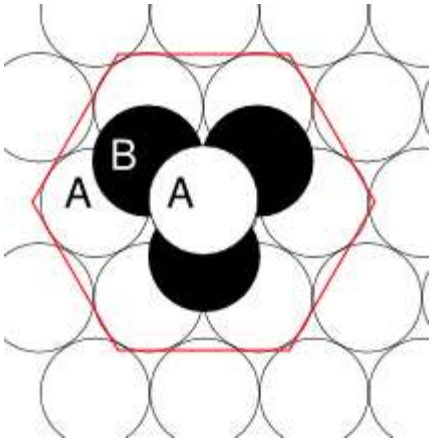
Mg, Be,
Sc, Ti,
Co, Zn,
Y, Zr, Tc,
Ru, Cd,
Gd, Tb,
Dy, Ho,
Er, Tm,
Lu, Hf,
Re, Os,
Tl

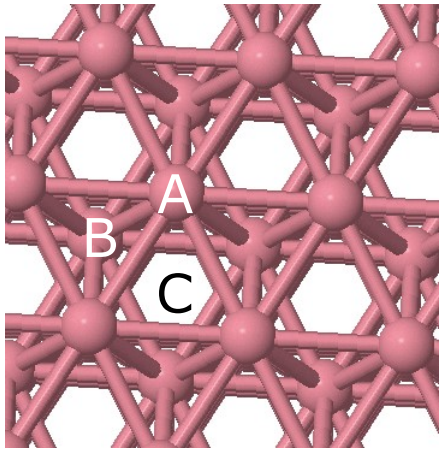
Crystallographic unit cell



Hexagonal unit cell







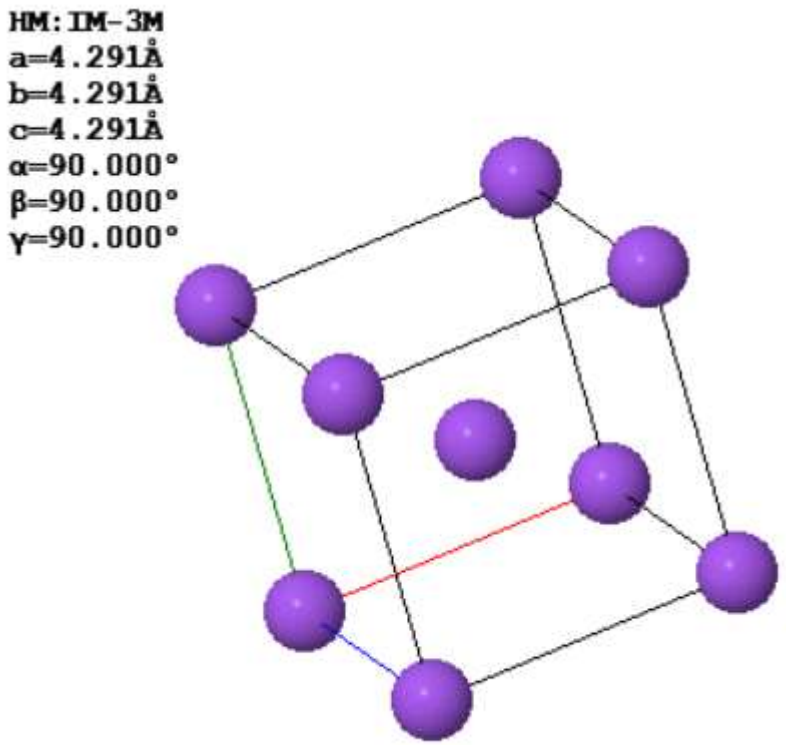
Hexagonal Bravais lattice
Basis vectors:

$$\vec{B}_1 = (0,0,0) \quad \vec{B}_2 = (\tfrac{2}{3},\tfrac{1}{3},\tfrac{1}{2})$$

bcc

W
Na
K
V
Cr
Fe
Rb
Nb
Mo
Cs
Ba
Eu
Ta

Number 229



Primitive Vectors:

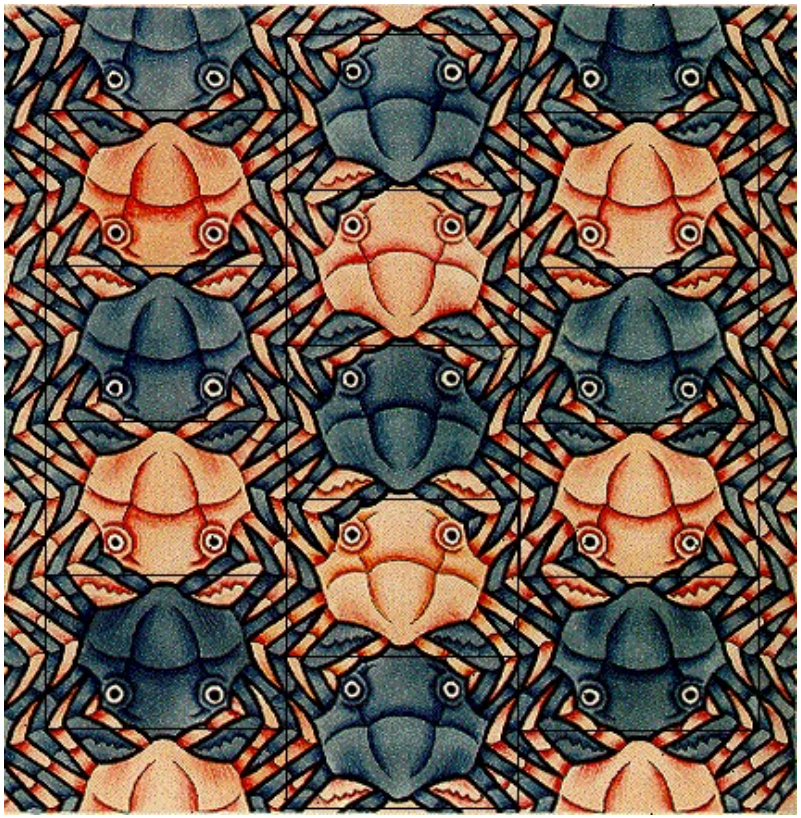
$$\vec{a}_1 = -\frac{a}{2}\hat{x} + \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z}$$

$$\vec{a}_2 = \frac{a}{2}\hat{x} - \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z}$$

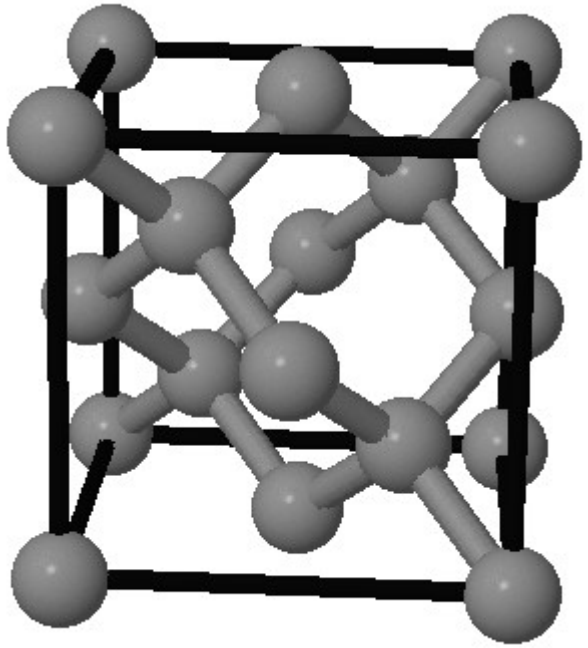
$$\vec{a}_3 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{y} - \frac{a}{2}\hat{z}$$

Basis Vector: $\vec{B}_1 = (0,0,0)$

Inequivalent atoms in the unit cell

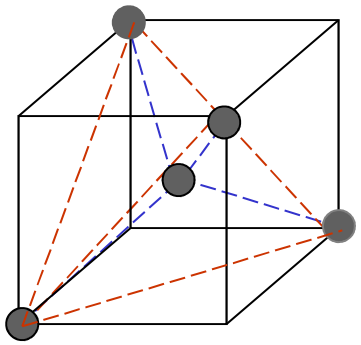


An element can have two distinct positions

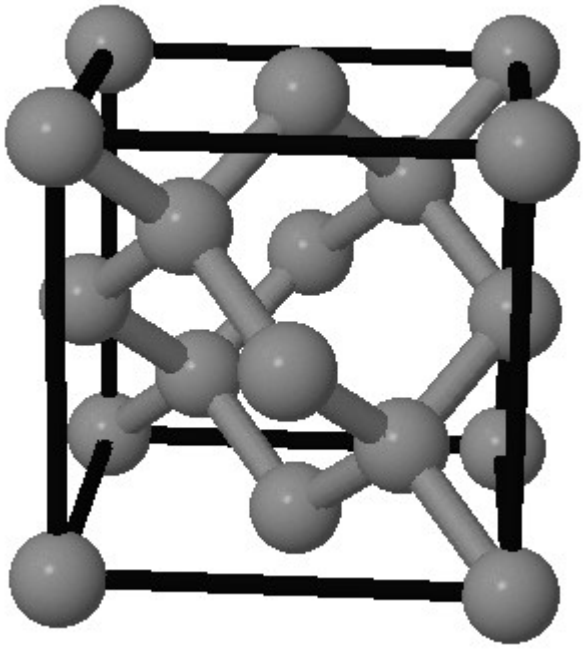


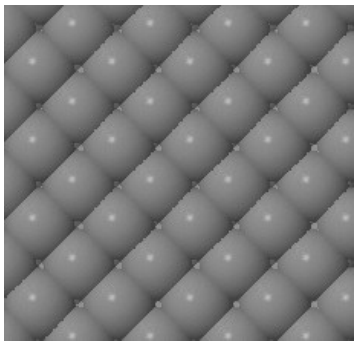
Diamond conventional unit cell

Diamond

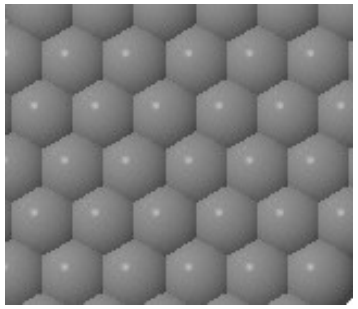


$$a = b = c, \quad \alpha = 90^\circ, \beta = 90^\circ, \gamma = 90^\circ$$





$$(100): \frac{2}{a^2}$$



$$(111): \frac{4}{\sqrt{3}a^2}$$

Space group: 227
point group: m3m

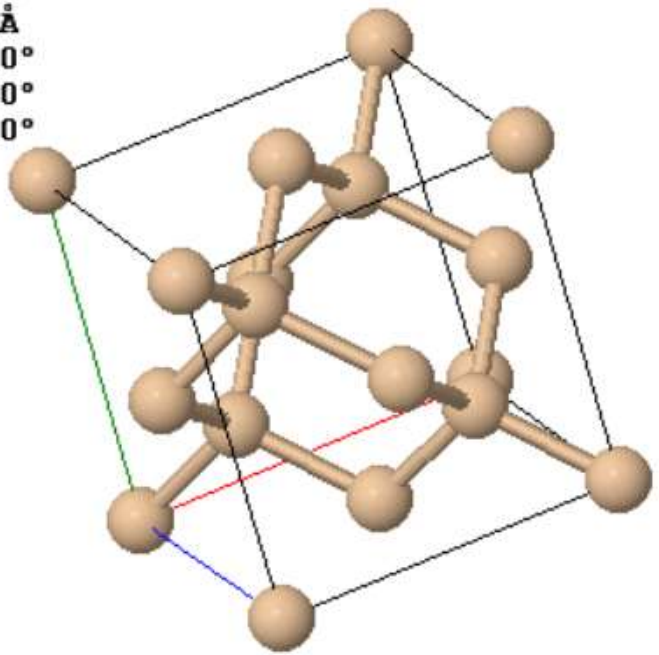
Primitive lattice vectors:

$$\vec{a}_1 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{y}, \qquad \vec{a}_2 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{z}, \qquad \vec{a}_3 = \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z}.$$

Basis: $\vec{B}_1 = (0,0,0), \qquad \vec{B}_2 = (0.25, 0.25, 0.25).$

Silicon

HM:F d -3 m S
a=5.430Å
b=5.430Å
c=5.430Å
α=90.000°
β=90.000°
γ=90.000°



Conventional unit cell | Primitive unit cell | Asymmetric unit

2 x 2 x 2 | 3 x 3 x 3 | 5 x 5 x 5

Ball and Stick | Spacefill

H: 1 K: 0 L: 0

show HKL plane | hide HKL plane

draw atoms in HKL plane

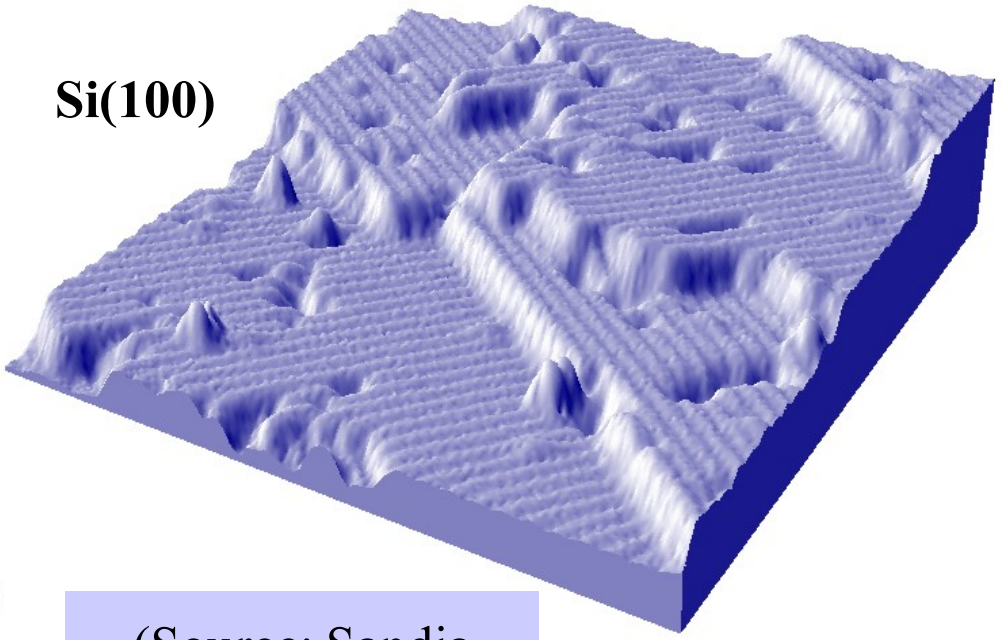
Thickness of HKL planes:

The conventional unit cell is a cube with sides of 0.543 nm. There are 8 atoms atoms in the conventional unit cell. (The image can be rotated with a mouse.)

JSmol

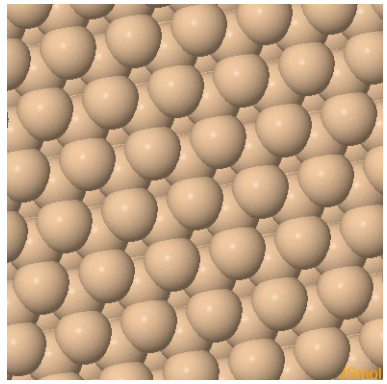
Silicon surfaces

Si(100)

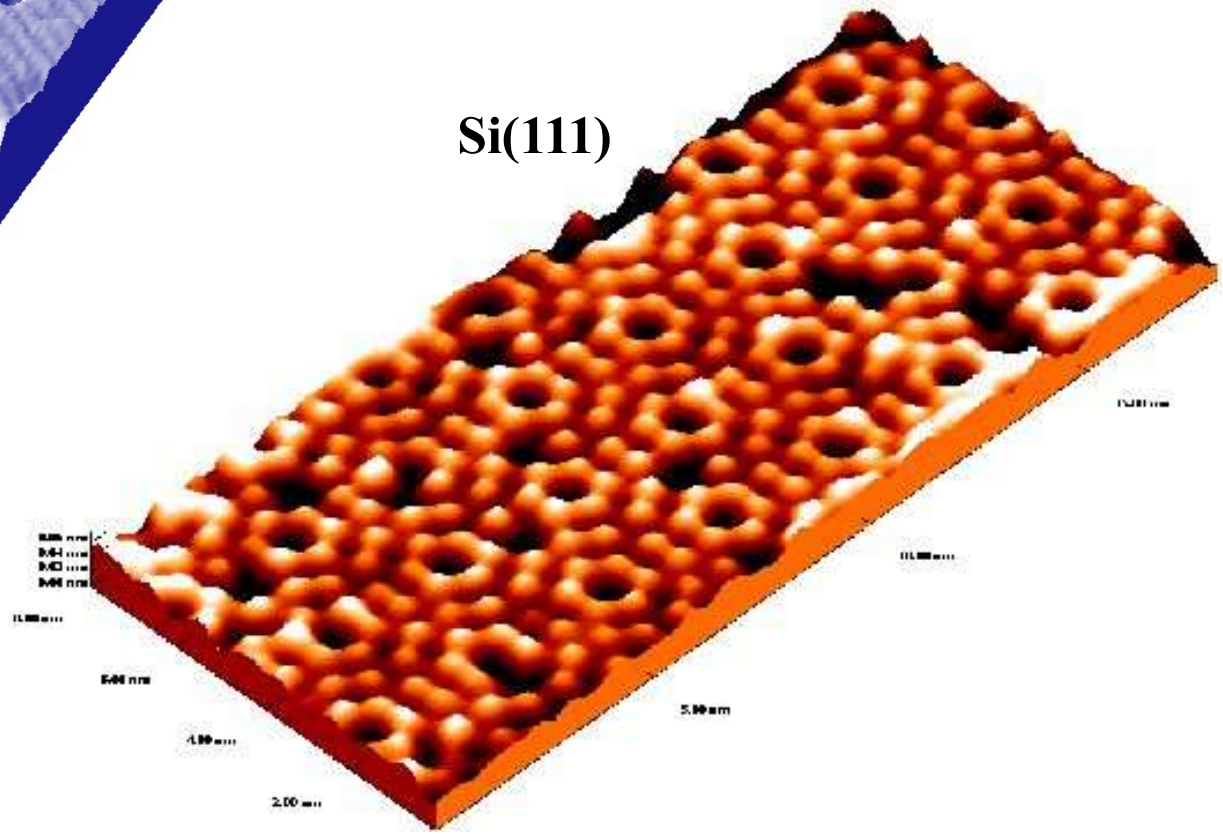


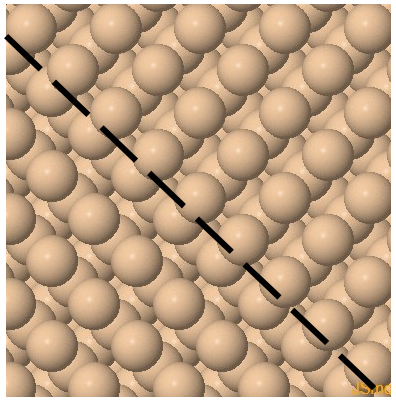
(Source: Sandia Nat.Labs.)

unreconstructed Si(111) →



Si(111)

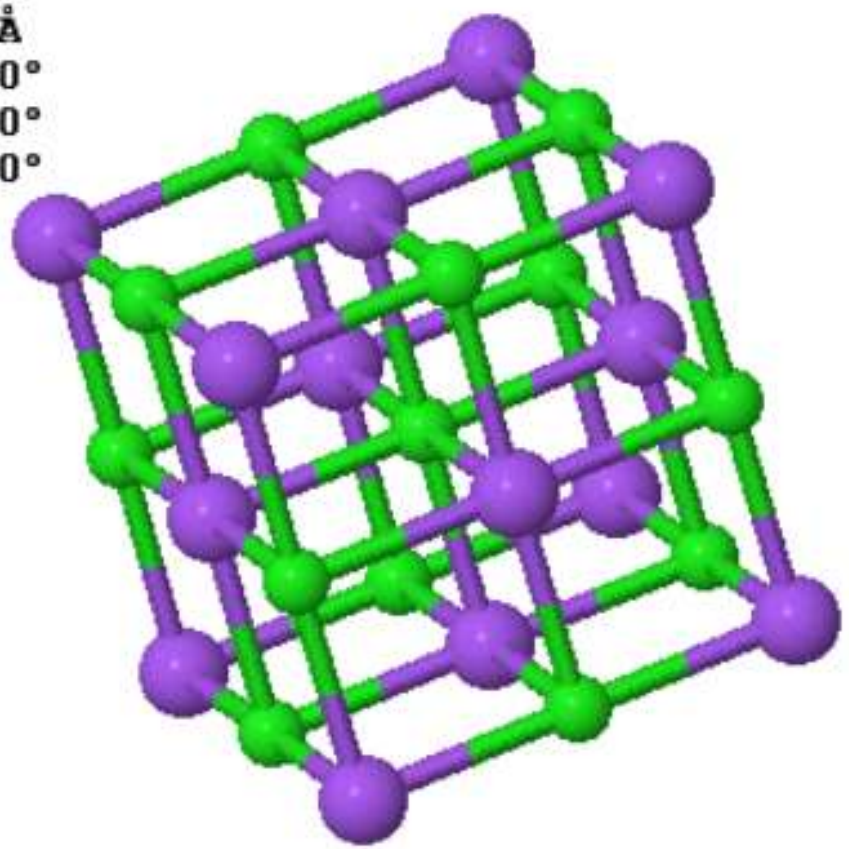




atomic step in Si(100)

NaCl

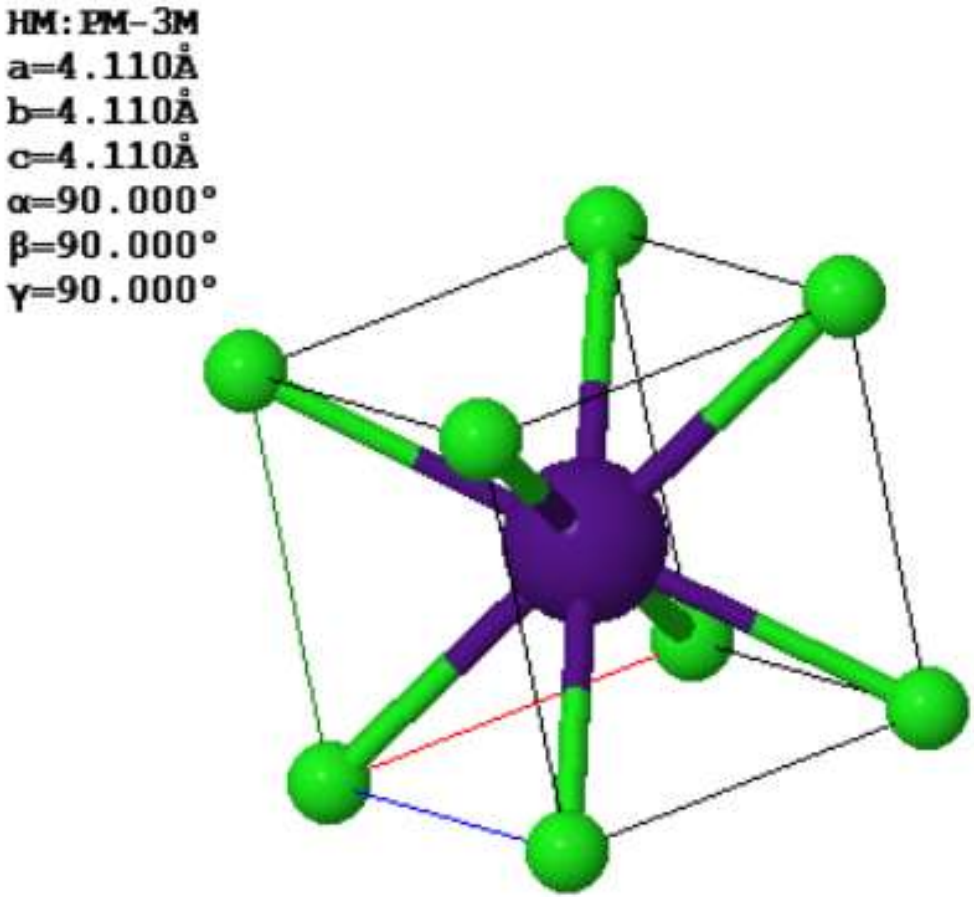
HM:F m -3 m
a=5.639Å
b=5.639Å
c=5.639Å
α=90.000°
β=90.000°
γ=90.000°



Number 225

CsCl

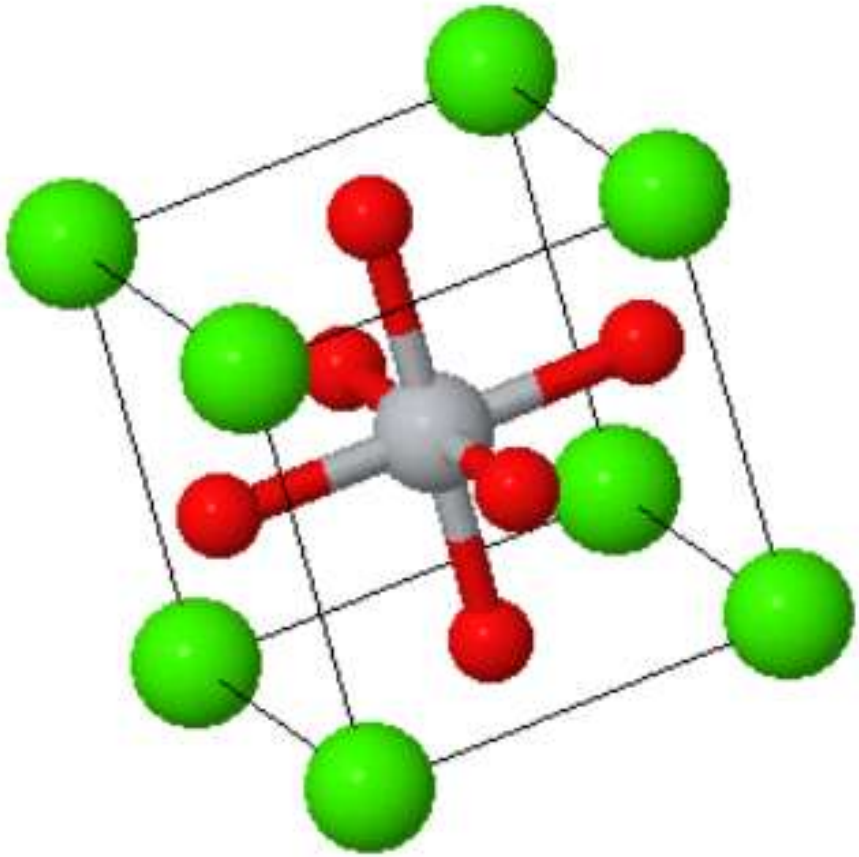
Number 221



perovskite

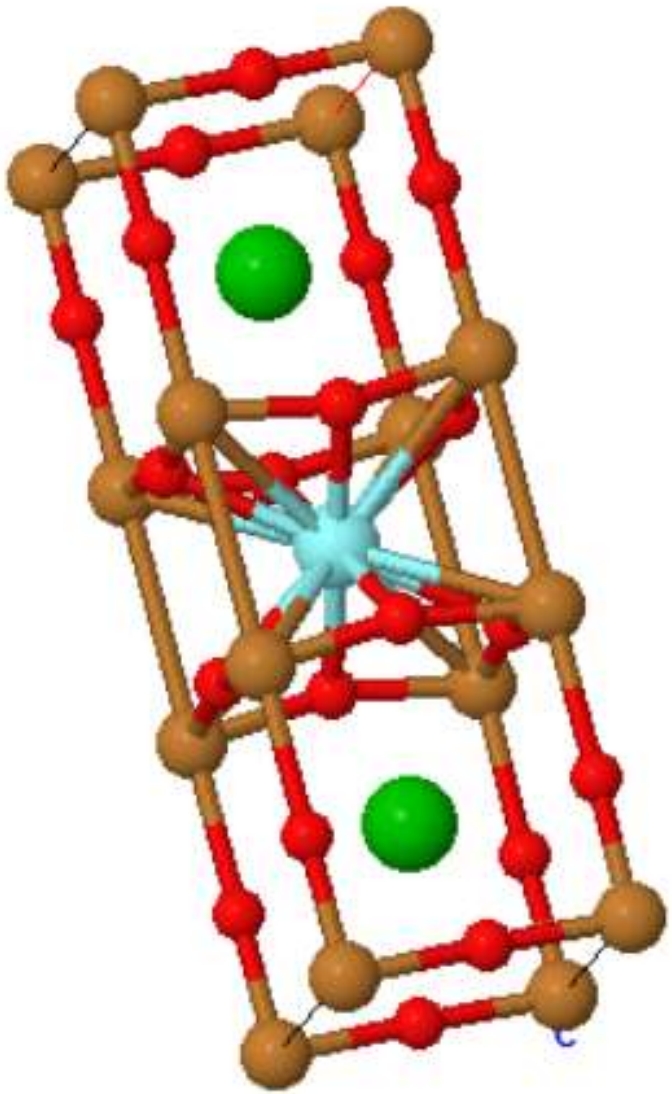
$SrTiO_3$
$LiNbO_3$
$BaTiO_3$
$Pb_xZr_{1-x}TiO_3$

Number 221



$YBa_2Cu_3O_7$

HM:P m m m
a=3.820Å
b=3.885Å
c=11.683Å
α=90.000°
β=90.000°
γ=90.000°

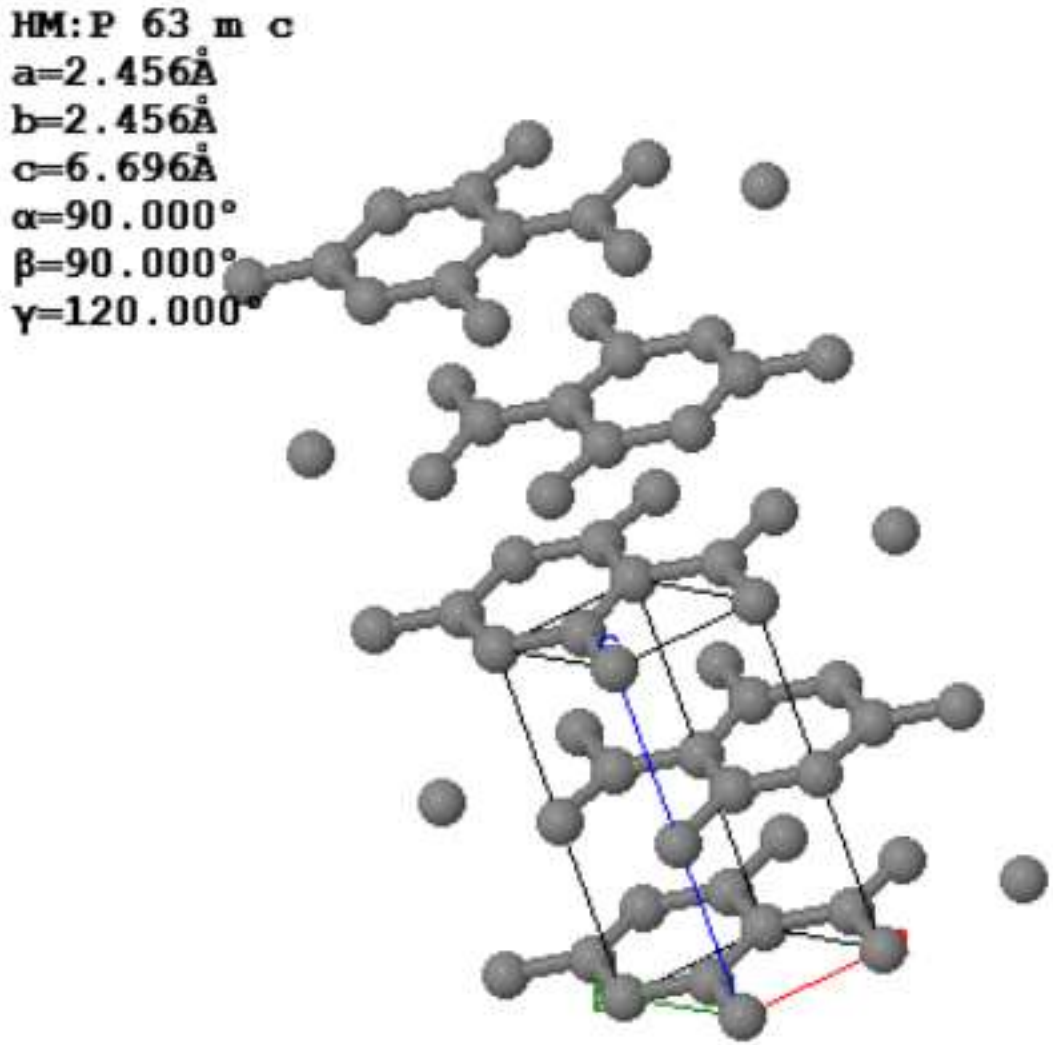


Number 47

graphite

Space group 194

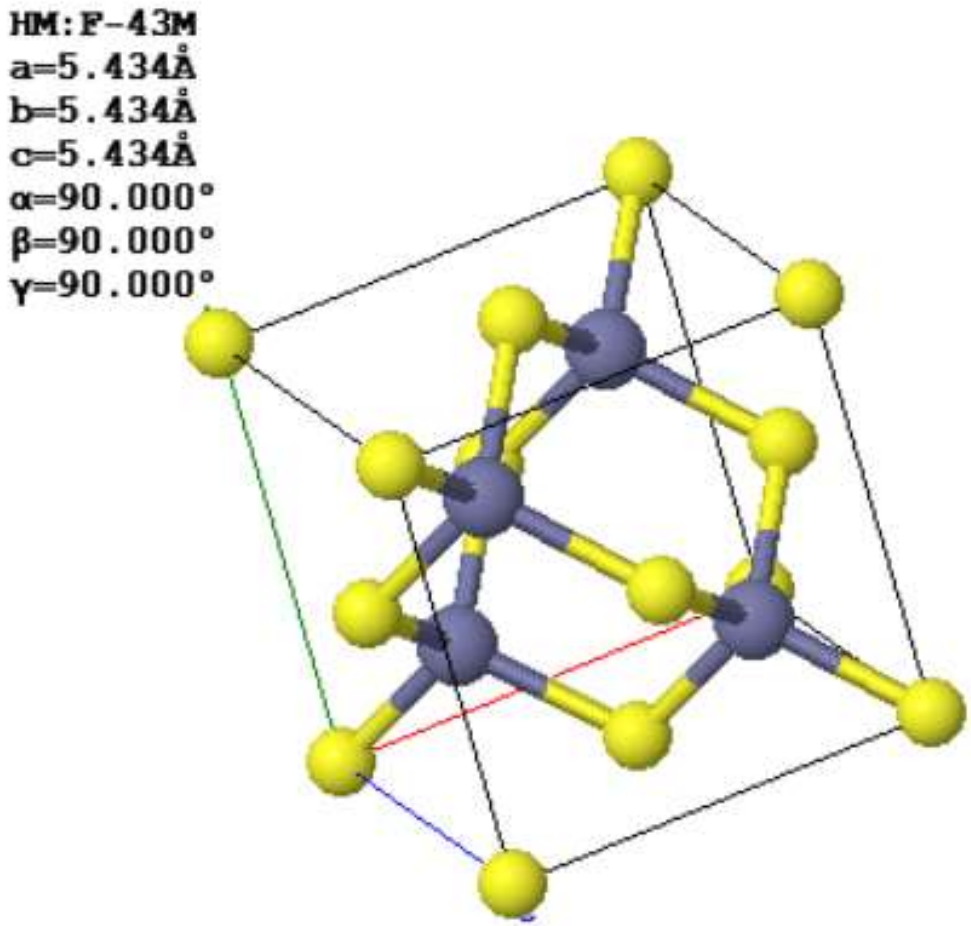
4 inequivalent C atoms in the primitive unit cell



Polytypes of carbon
graphite (hexagonal)
graphene
carbon nanotubes
diamond
rhobohedral graphite
hexagonal diamond

zincblende

ZnS
GaAs
InP

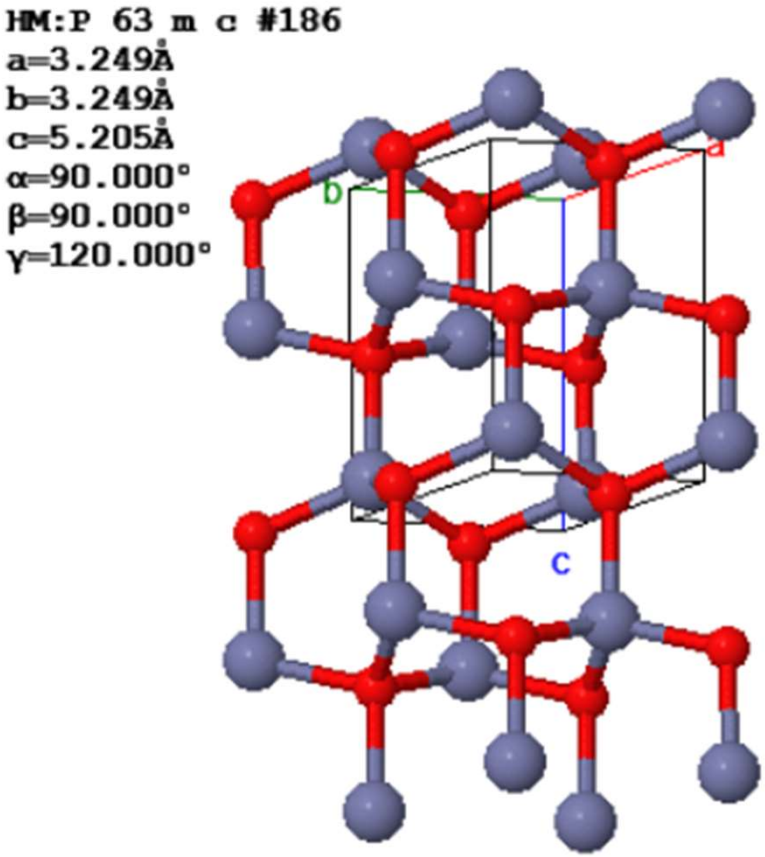


space group 216
F$\bar{4}$3m

wurtzite

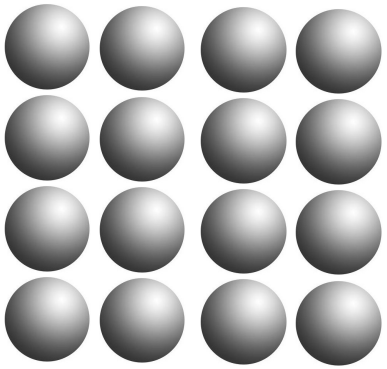
ZnS
ZnO
CdS
CdSe
GaN
AlN

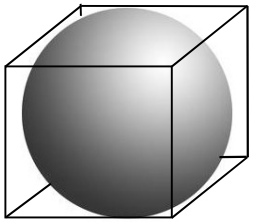
Number 186



There are 2 polytypes of ZnS: zincblende and wurtzite

atomic packing density



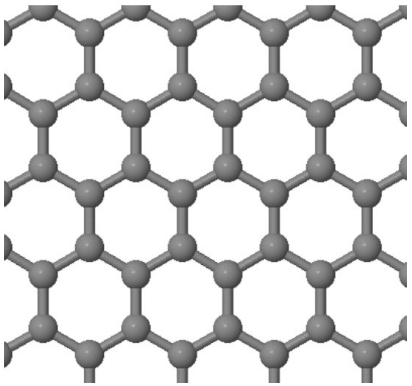


$$\frac{\frac{4}{3}\pi\left(L/2\right)^3}{L^3} = \frac{\pi}{6} \approx 0.52$$

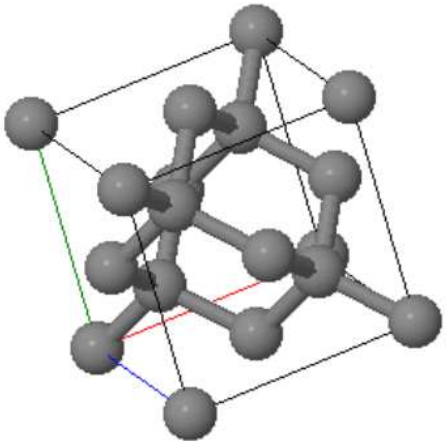
fcc, hcp = 0.74
random close pack = 0.64
simple cubic = 0.52
diamond = 0.34

Coordination number

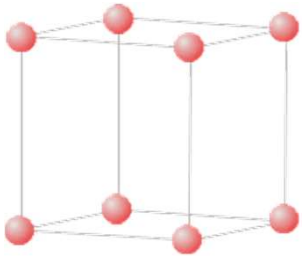
Number of nearest neighbors an atom has in a crystal



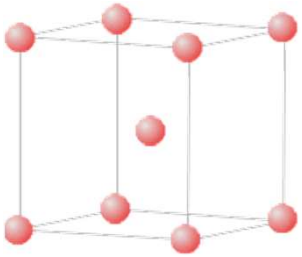
Graphene 3



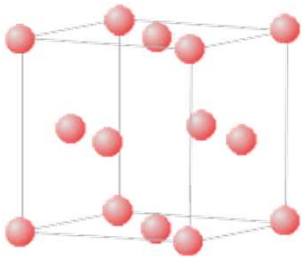
diamond 4



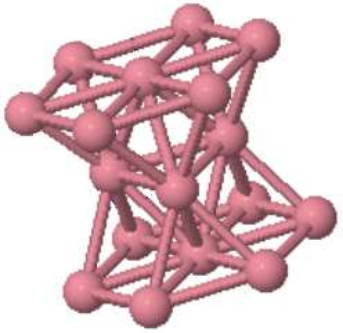
sc 6



bcc 8



fcc 12



hcp 12

CIF files and programs to visualize crystal structures

Crystal structure data is often stored in a CIF file. This is a text file that contains the asymmetric unit of the crystal, the symmetries of the space group, and a reference to the source where the data was first published. It is important to check the publication to see the conditions used during the experiment. Some experiments are performed at high temperatures or high pressures where the crystal structure can be different than at room temperature and ambient pressure. The links below will display a crystal structure and it's corresponding CIF file.

Simple Cubic, Polonium Po $Pm\bar{3}m$ #221
Face-centered Cubic (fcc) $Fm\bar{3}m$ #225
Body-centered Cubic (bcc) $Im\bar{3}m$ #229
Hexagonal, Boron nitride BN #194
Hexagonal Close Packed (hcp) P63/mmc #194
Perovskite, Calcium titanate $CaTiO_3$ (perovskite) $Pm\bar{3}m$ #221
Caesium chloride CsCl $Pm\bar{3}m$ #221
Rocksalt NaCl $Fm\bar{3}m$ #225
Zincblende #216
Wurtzite #186
Diamond (C) #227
β-Sn #141
Graphite C P63mc #186

Sucrose P21 #4
Magnetite Fe_3O_4 Fd3m #227
Cementite Fe_3C #62
Copper oxide CO (Tenorite) #15
Pyrite FeS_2 #205
Rutile TiO_2 #136
Spinel $MgAl_2O_4$ #227
$Sr_2FeMoO6_6$ (double perovskite) I4/mmm #139
$YBa_2Cu_3O_7$ #47
ZIF8 #1
Zinc oxide ZnO (wurtzite) P63mc #186
ZnS (wurtzite) #186

Prototypes | Periodic Table | Semiconductors | Ceramics

ICSD

Inorganic Crystal Structure Database

Materials Project