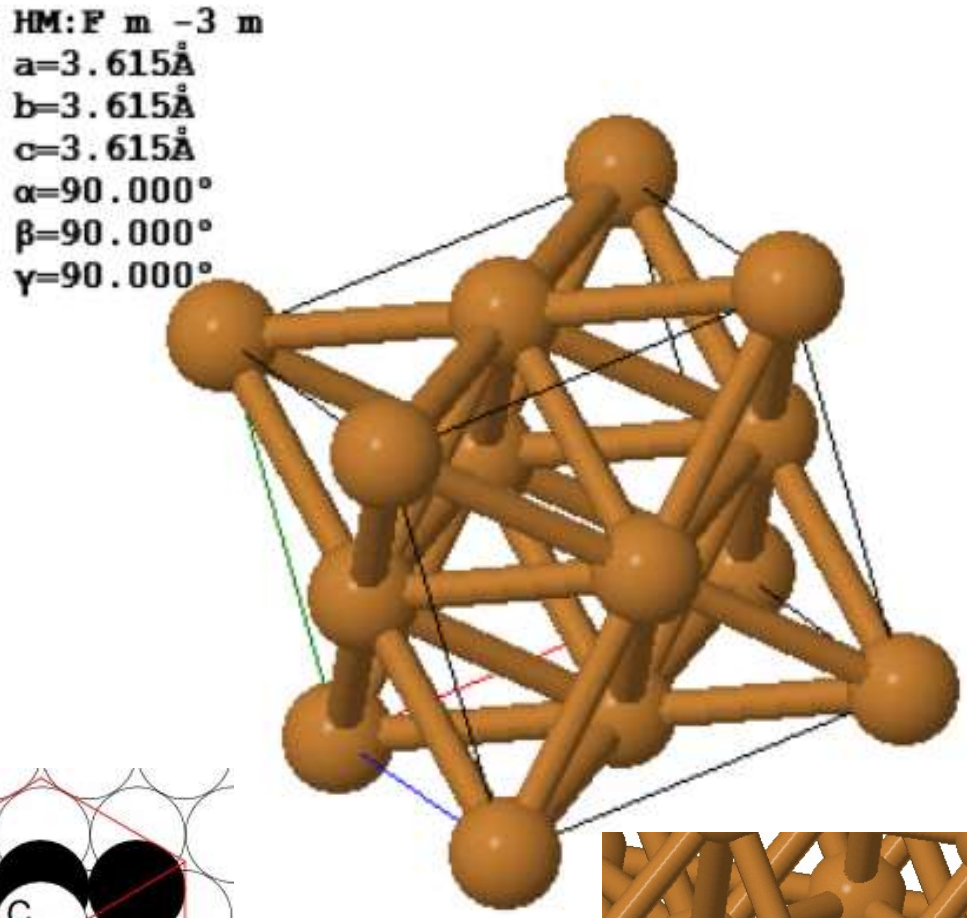
Crystal structure

fcc

Number 225

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



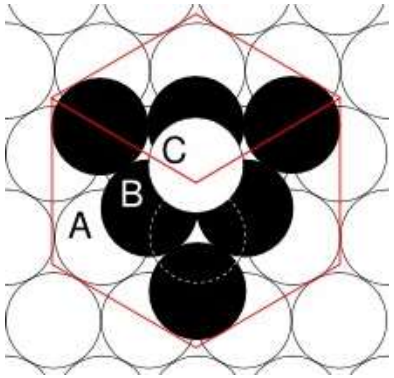
[111]

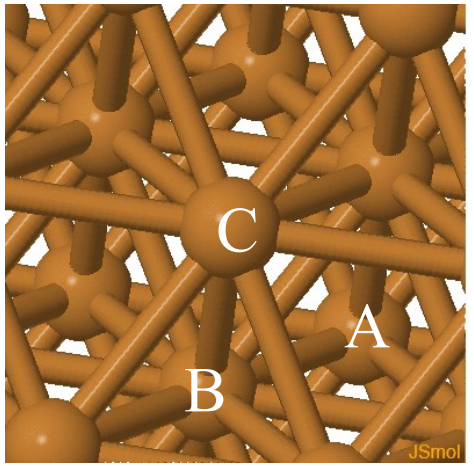
Primitive Vectors:

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

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

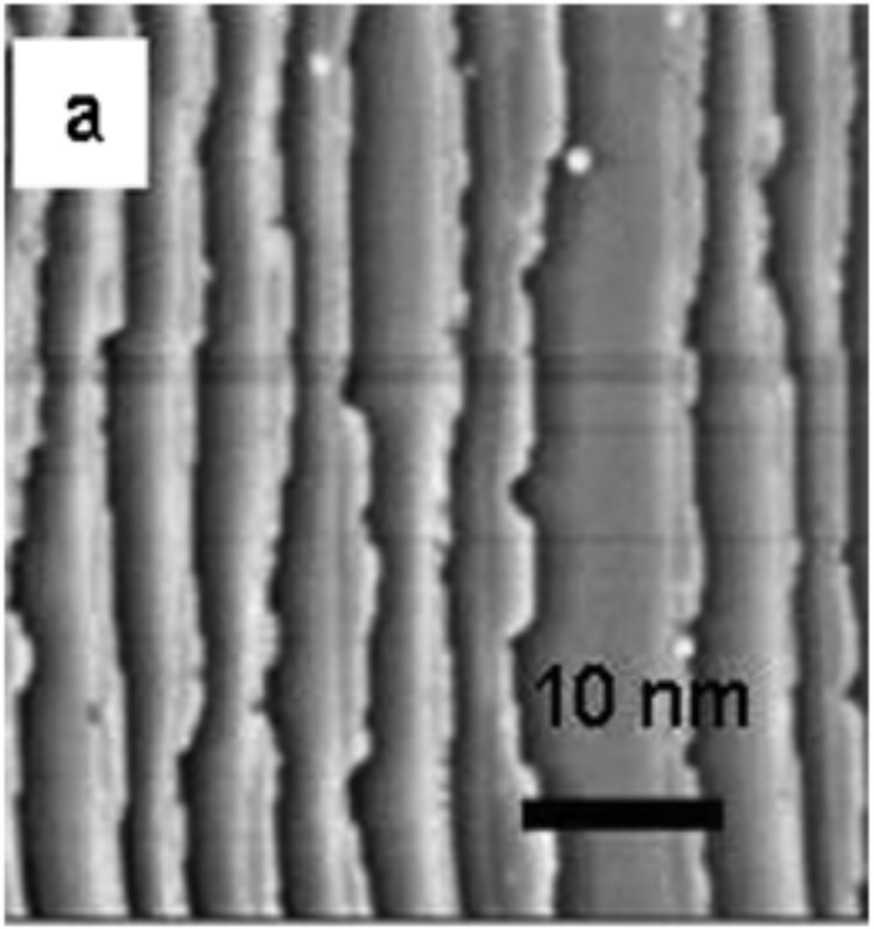
$$\vec{a}_3 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{y}$$



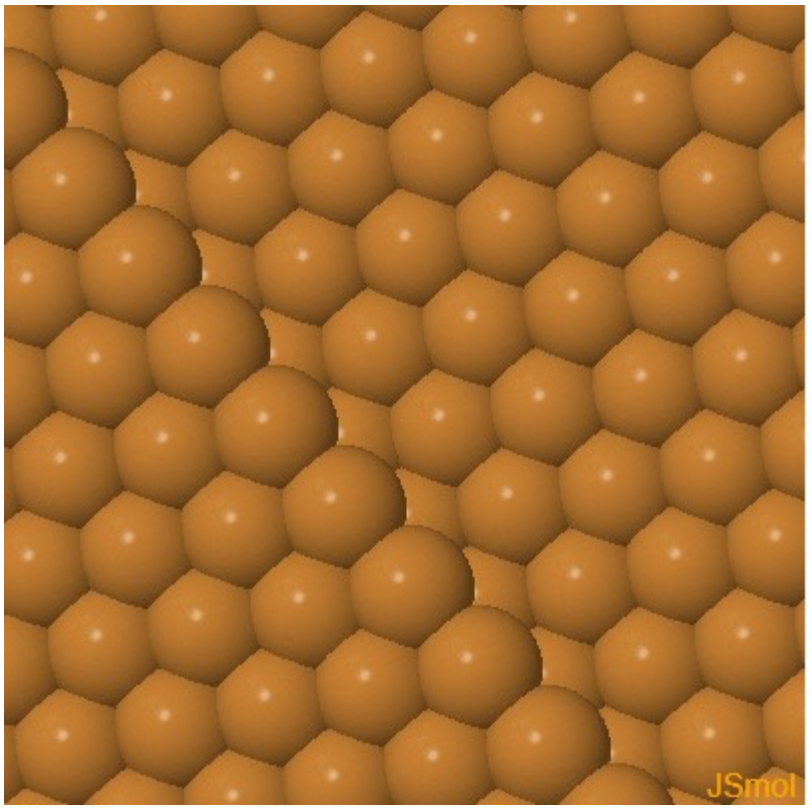


Basis Vector: $\vec{B}_1 = (0,0,0)$

Crystal planes: Miller indices



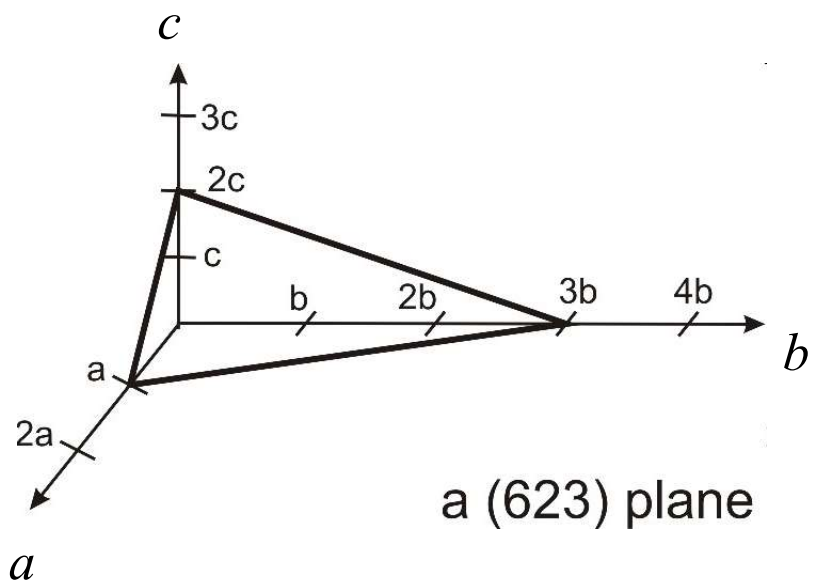
Rh(15,15,13) fcc



(15,15,13) fcc

Reaction studies on nanostructured surfaces, Adolf Winkler, in *The Oxford Handbook of Nanoscience and Technology*, A. V. Narlikar and Y. Y. Fu ed., 2009.

Miller indices: Crystal planes



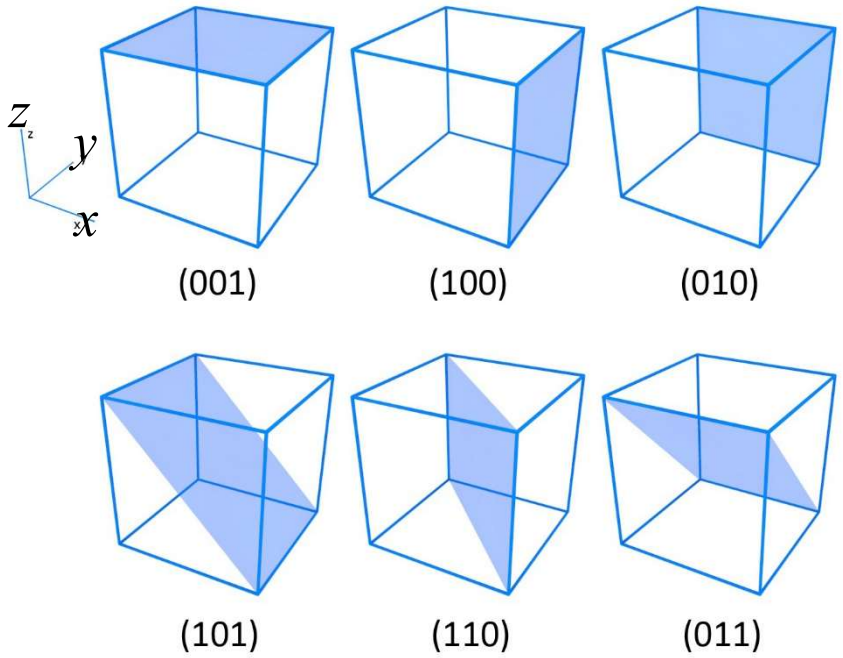
A plane with the intercepts $1/h, 1/k, 1/l$ is the (h,k,l) plane.

always use integers for h,k,l

( ) specific plane

{ } family of equivalent planes

MOSFETs are made on {100} wafers

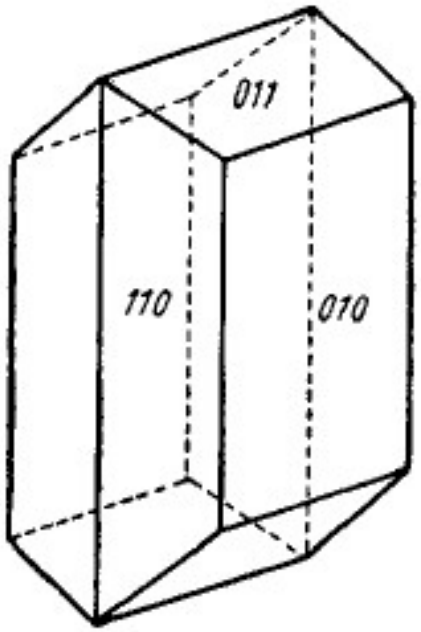


Crystals

rule of rationality

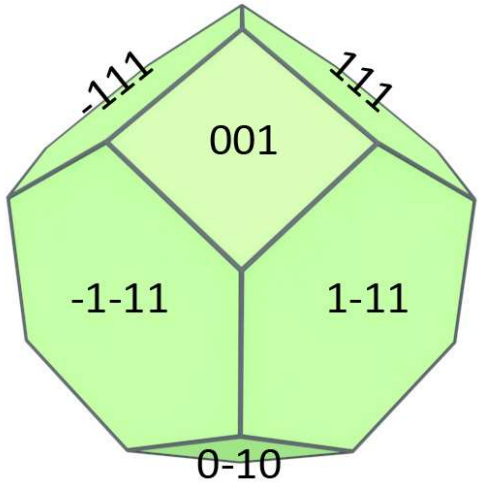
R. J. Haüy (1743-1822):

the indices of external planes of crystals are generally simple full numbers



orthorhombic

Aragonit $CaCO_3$



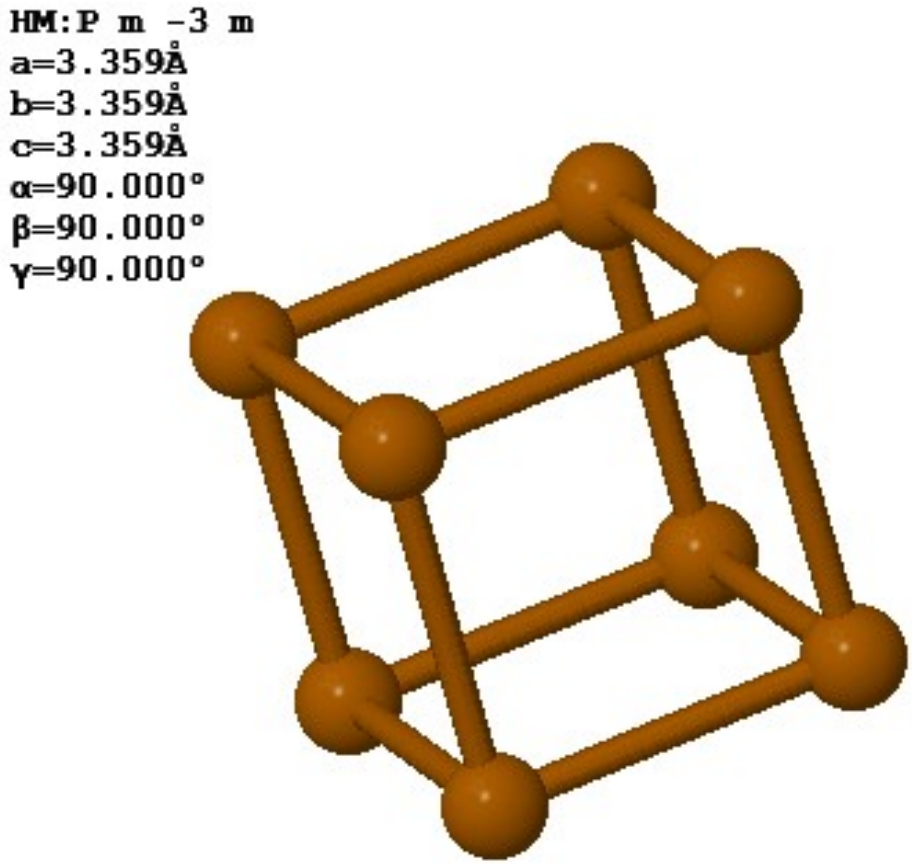
one possible morphology
of a crystal with cubic structure

Bravais:

Planes with high atomic densities tend to dominate

simple cubic

Po



Number: 221

Primitive Vectors:

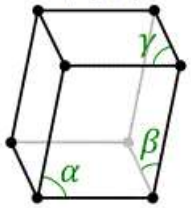
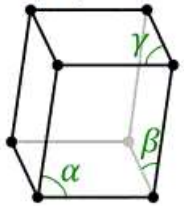
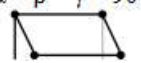
$$\vec{a}_1 = a\hat{x}$$

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

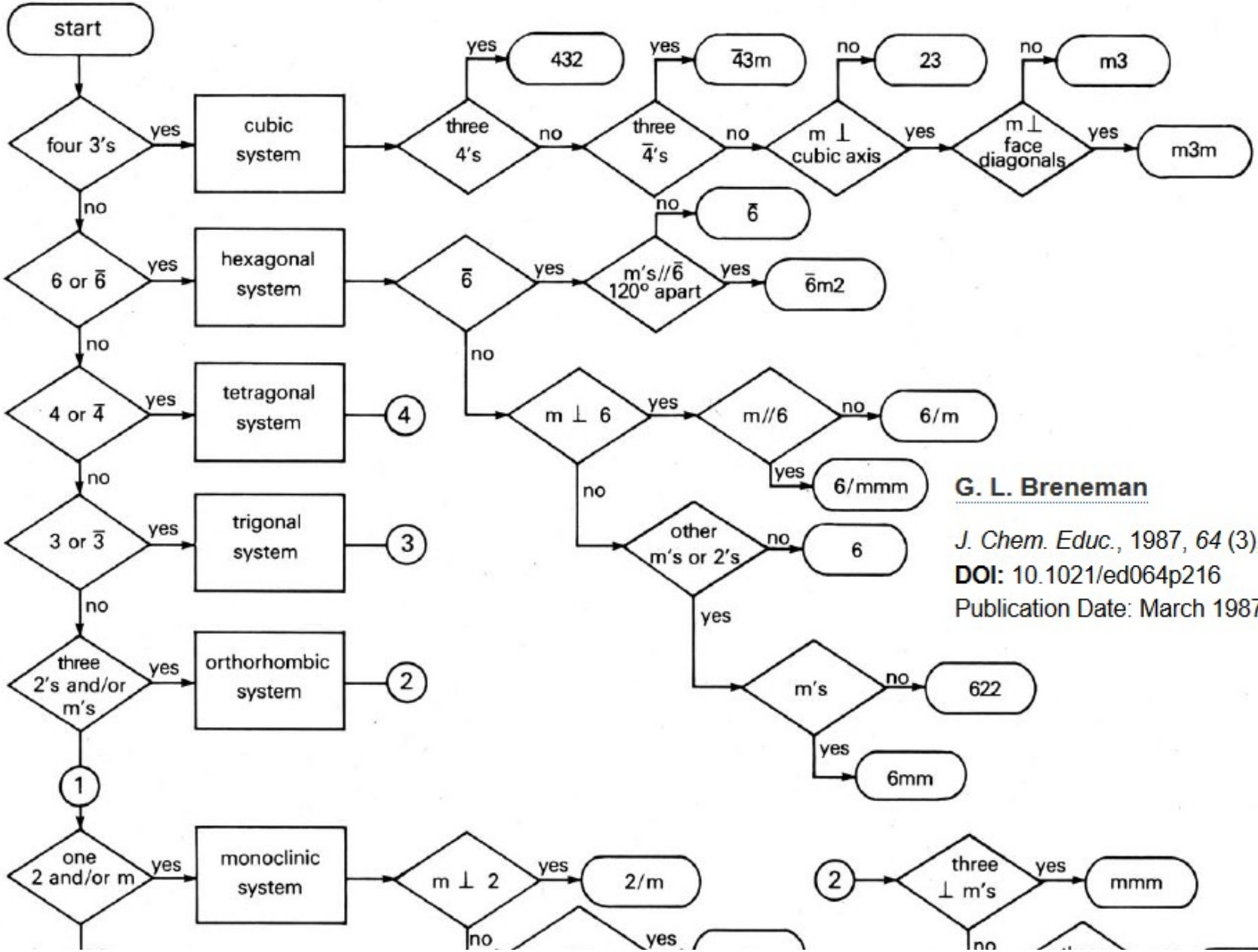
$$\vec{a}_3 = a\hat{z}$$

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

The 32 Crystal Classes

Crystal system	Crystal Class	International symbol	Schoenflies symbol	Space groups	2-fold axes	3-fold axes	4-fold axes	6-fold axes	mirror planes	inversion	Examples	Number of symmetry elements
Triclinic $a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$ 	triclinic-pedial	1	C_1	1: P1	-	-	-	-	-	n		1
	triclinic-pinacoidal	$\bar{1}$	$S_2 = C_i$	2: P$\bar{1}$	-	-	-	-	-	y		2
Monoclinic $a \neq b \neq c$ $\alpha \neq 90°$, $\beta = \gamma = 90°$ 	monoclinic-sphenoidal	2	C_2	3: P2, 4: P2$_1$, 5: C2	1	-	-	-	-	n		2
	monoclinic-domatic	m	$C_{1h} = C_s$	6: Pm, 7: Pc, 8: Cm, 9: Cc	-	-	-	-	1	n		2
	monoclinic-prismatic	$2/m$	C_{2h}	10: P2/m, 11: P2$_1$/m, 12: C2/m, 13: P2/c, 14: P2$_1$/c, 15: C2/c	1	-	-	-	1	y		4
Orthorhombic $a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$ 	orthorhombic-disphenoidal	222	$V = D_2$	16: P222, 17: P222$_1$, 18: P2$_1$2$_1$2, 19: P2$_1$2$_1$2$_1$, 20: C222$_1$, 21: C222, 22: F222, 23: I222, 24: I2$_1$2$_1$2$_1$	3	-	-	-	-	n		4

Crystallographic symmetry point group notation flow chart



G. L. Breneman

J. Chem. Educ., 1987, *64* (3), p 216
DOI: 10.1021/ed064p216
Publication Date: March 1987

http://it.iucr.org/A/

International Tables for Crystallography
Volume A: Space-group symmetry

First online edition (2006) ISBN: 978-0-7923-6590-7 eISBN: 978-1-4020-5406-8 doi: 10.1107/97809553602060000100

Edited by Th. Hahn

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| contributors | editors |

| sample pages | purchase |

| explanation of the space-group data |

Go to space group No. 1 (P 1) Go

1 (P 1)
2 (P -1)
3 (P 2)
4 (P 21)
5 (C 2)
6 (P m)
7 (P c)
8 (C m)
9 (C c)
10 (P 2/m)
11 (P 21/m)
12 (C 2/m)
13 (P 2/c)
14 (P 21/c)
15 (C 2/c)
16 (P 2 2 2)
17 (P 2 2 21)
18 (P 21 21 2)
19 (P 21 21 21)
20 (C 2 2 21)

Volume A treats crystallographic symmetry in direct or physical space. It contains extensi rations of the 17 plane groups, the 230 space groups and the 32 crystallographic point groups.

The first five parts of the volume contain introductory material: lists of symbols and terms; e space-group tables; the determination of space groups; synoptic tables of space-grou symbols; and unit-cell (coordinate) transformations. These are followed by the plane-grou les (Parts 6 and 7). For each group type, the following information is presented:

- headline with the relevant group symbols;
- diagrams of the symmetry elements and of the general position;
- specification of the origin and the asymmetric unit;
- list of symmetry operations;
- generators;
- general and special positions with multiplicities, site symmetries, coordinates and re
- symmetries of special projections;
- extensive subgroup and supergroup data.

Parts 8 to 15 deal with the following aspects of symmetry theory: the mathematical approach to space groups; crystal lattices; point groups and crystal classes; symbols for symmetry operations; symbols for space groups; isomorphic subgroups of space groups; lattice complexes; and normalizers of space groups.

Sodalite

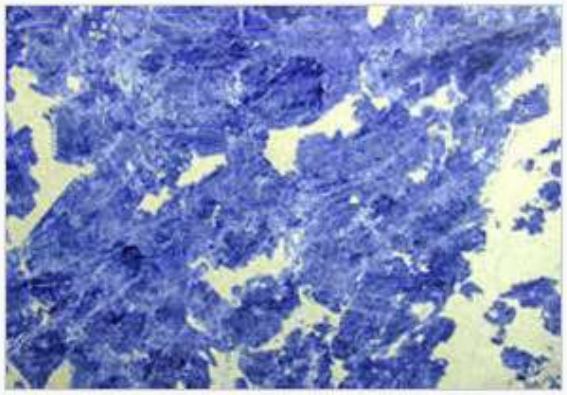
From Wikipedia, the free encyclopedia

Sodalite is a rich royal blue mineral widely enjoyed as an ornamental gemstone. Although massive sodalite samples are opaque, crystals are usually transparent to translucent. Sodalite is a member of the sodalite group with hauyne, nosean, lazurite and tugtupite.

Discovered in 1811 in the Ilimaussaq intrusive complex in Greenland, sodalite did not become important as an ornamental stone until 1891 when vast deposits of fine material were discovered in Ontario, Canada.

Contents [hide]

Properties [edit]



A sample of **sodalite**-carbonate pegmatite from Bolivia, with a polished rock

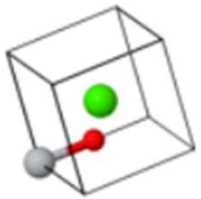
A light, relatively hard yet fragile mineral, sodalite is named after its sodium content; in mineralogy it may be classed as a feldspathoid. Well known for its blue color, sodalite may also be grey, yellow, green, or pink and is often mottled with white veins or patches. The more uniformly blue material is used in jewellery, where it is fashioned into cabochons and beads. Lesser material is more often seen as facing or inlay in

Sodalite

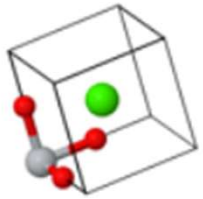
A sample of sodalite

General	
Category	Tectosilicates without zeolitic H_2O
Formula (repeating unit)	$Na_8(Al_6Si_6O_{24})Cl_2$
Strunz classification	09.FB.10
Crystal symmetry	Isometric hextetrahedral H-M symbol: $\bar{4}3m$ Space group: $P\bar{4}3n$
Unit cell	a = 8.876(6) Å; Z = 1
Identification	

Asymmetric unit

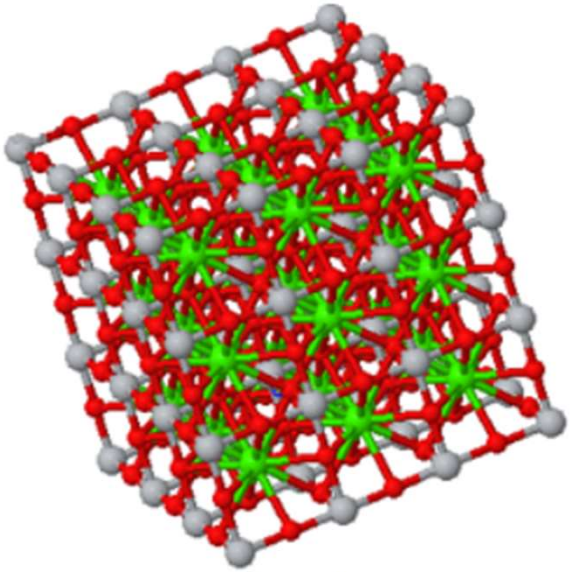


Asymmetric unit



Primitive unit cell

Conventional unit cell

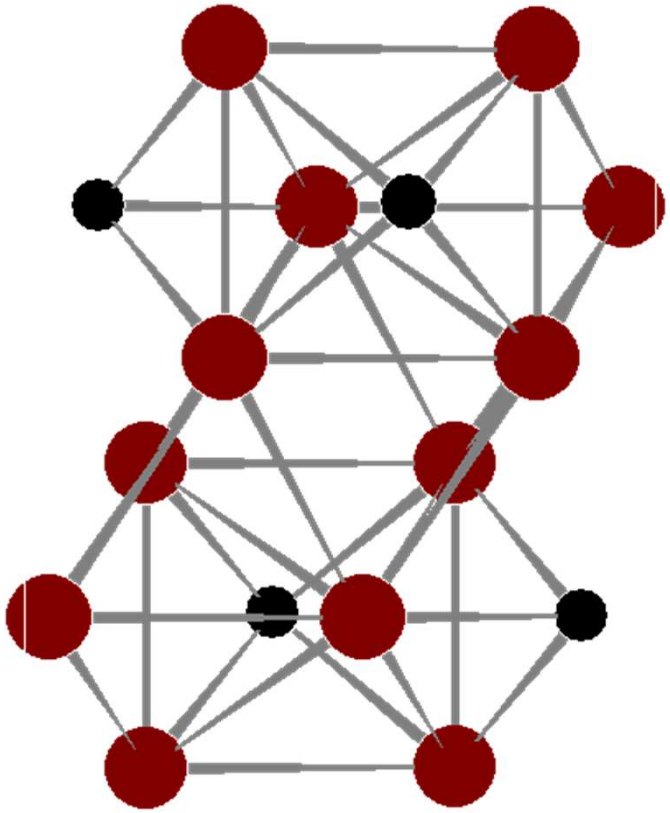


Crystal

Asymmetric unit

cell 5.09000 6.74800 4.52300 90.000 90.000 90.000
natom 3
Fe1 26 0.18600 0.06300 0.32800
Fe2 26 0.03600 0.25000 0.85200
C 6 0.89000 0.25000 0.45000
rgnr 62
Cohenite (Cementite) Fe3 C

Unit cell



Asymmetric unit

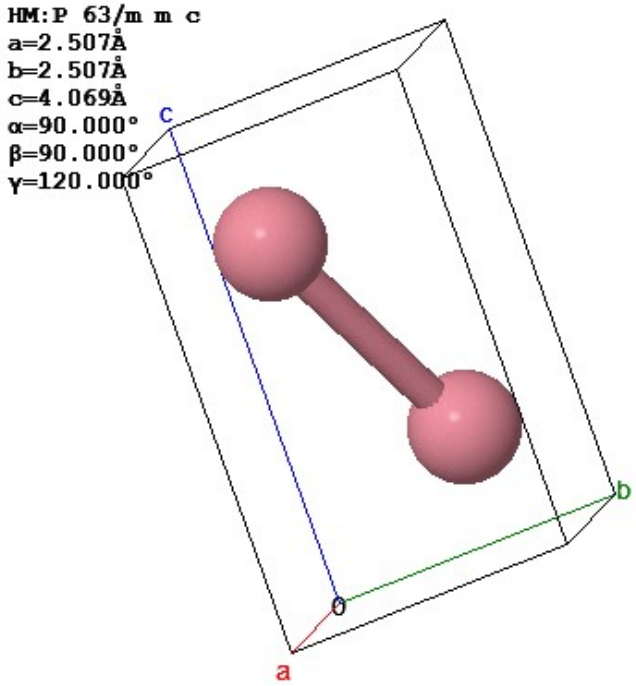
Generated by PowderCell

hcp

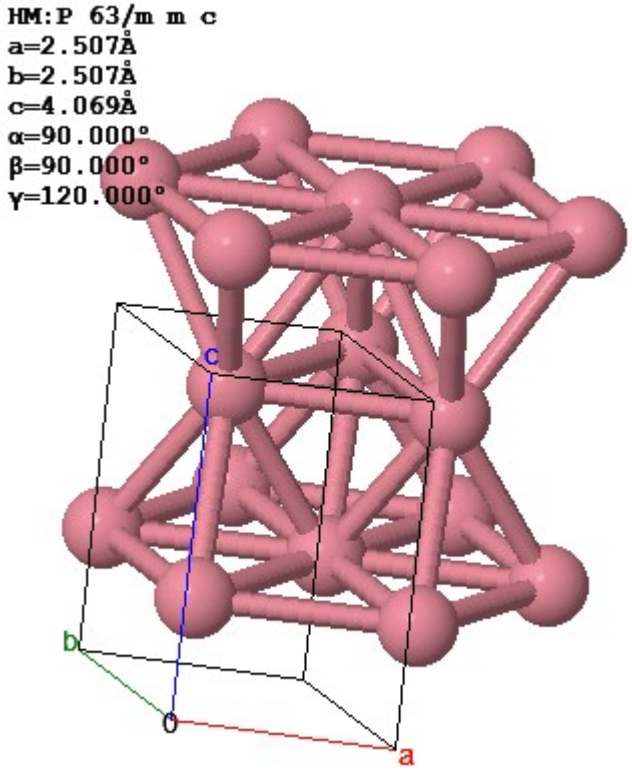
Space group 194

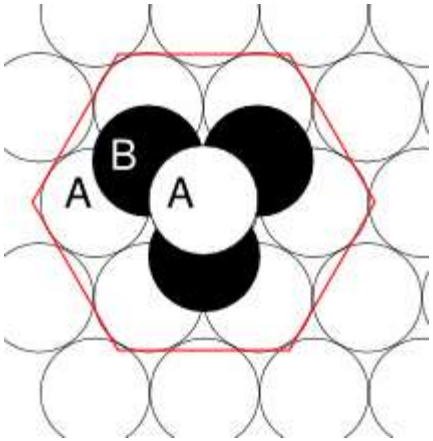
Mg, Be,
Sc, Ti,
Co, Zn,
Y, Zr, Tc,
Ru, Cd,
Gd, Tb,
Dy, Ho,
Er, Tm,
Lu, Hf,
Re, Os,
Tl

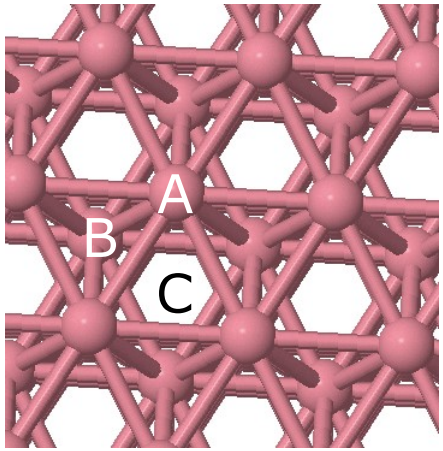
Crystallographic unit cell



Hexagonal unit cell







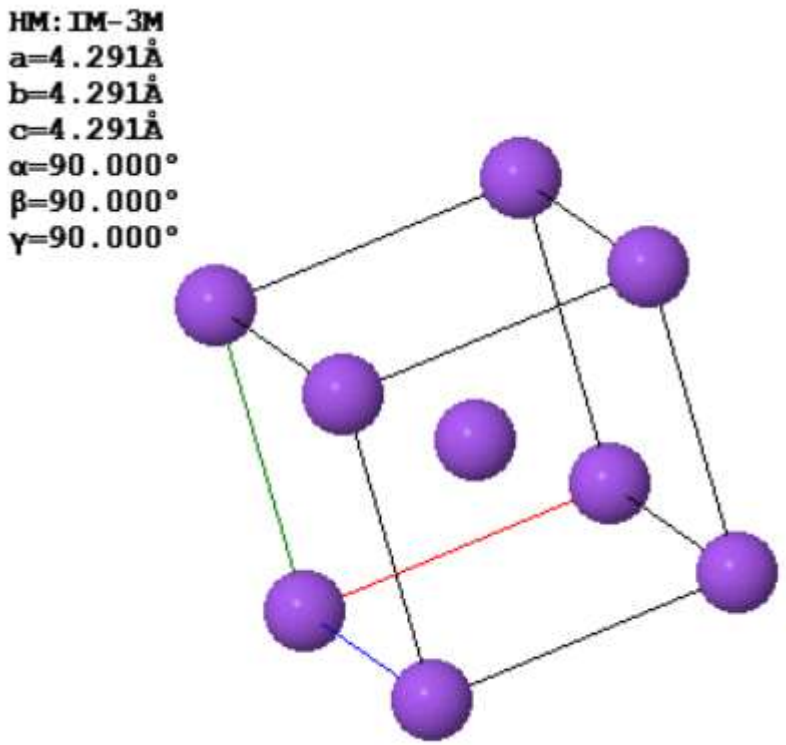
Hexagonal Bravais lattice
Basis vectors:

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

bcc

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

Number 229



Primitive Vectors:

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

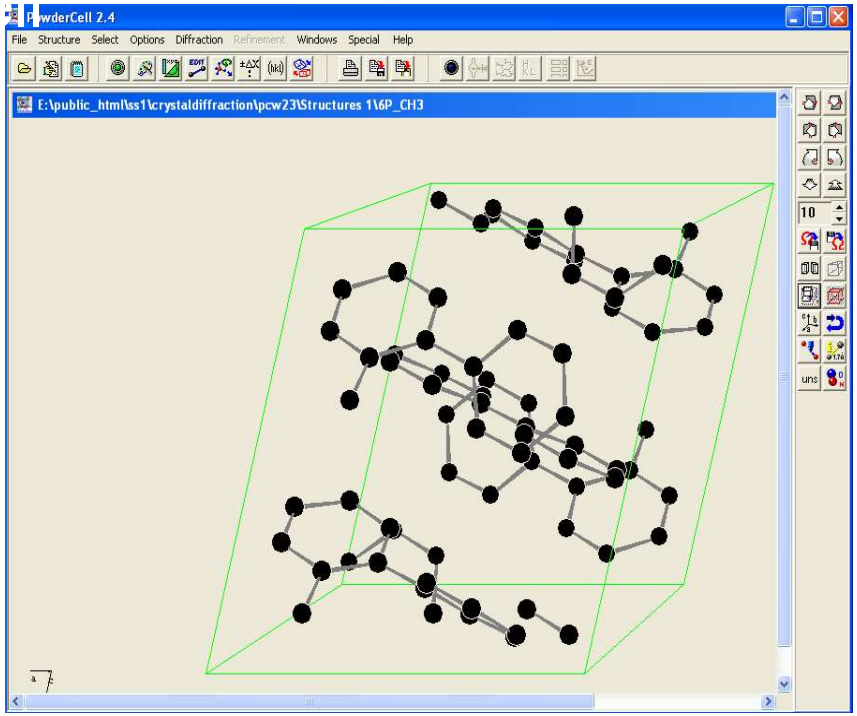
$$\vec{a}_2 = \frac{a}{2}\hat{x} - \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z}$$

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

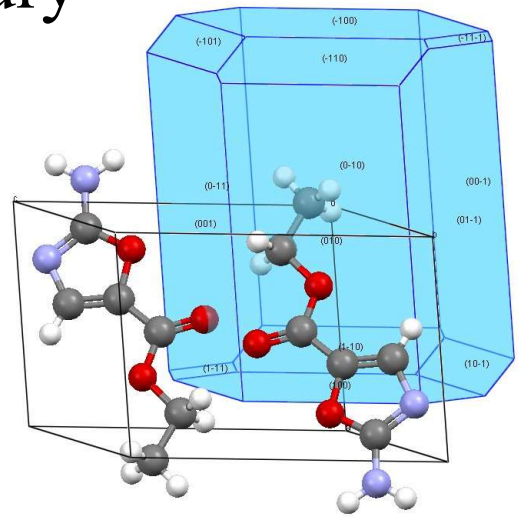
Basis Vector: $\vec{B}_1 = (0,0,0)$

BAM
Bundesanstalt für Materialforschung und -prüfung

PowderCell



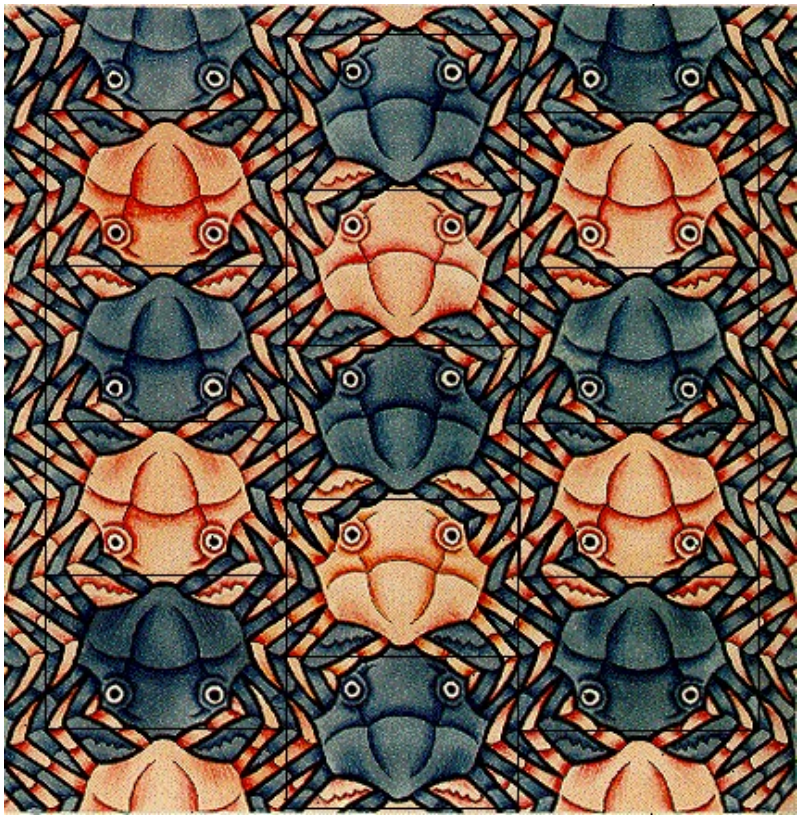
Mercury



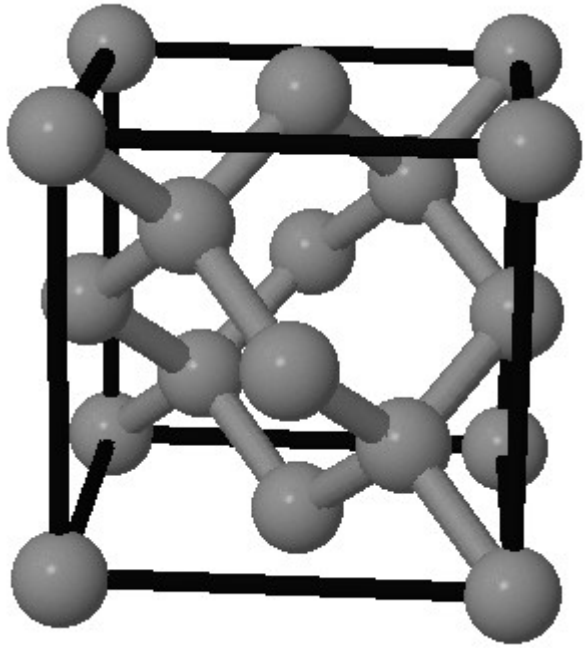
Standard data file: *.cif

http://www.bam.de/de/service/publikationen/powder_cell.htm
https://www.ccdc.cam.ac.uk/Community/csd-community/freemercury/

Inequivalent atoms in the unit cell

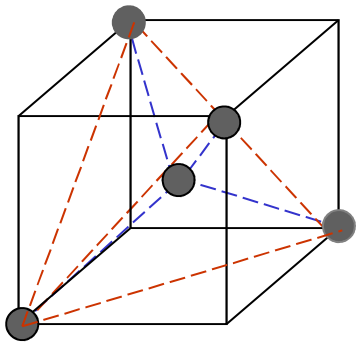


An element can have two distinct positions

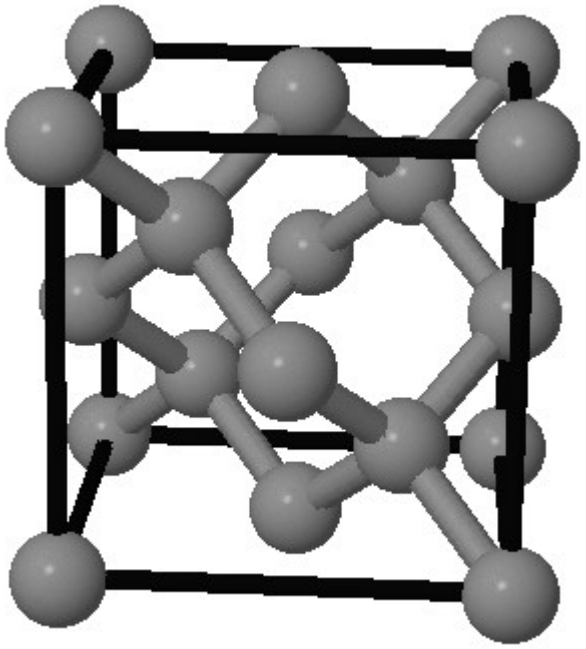


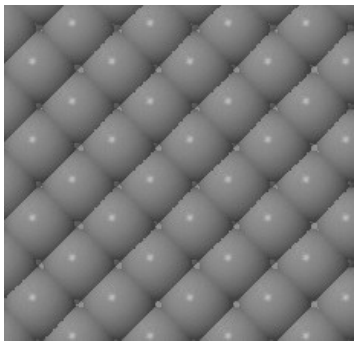
Diamond conventional unit cell

Diamond

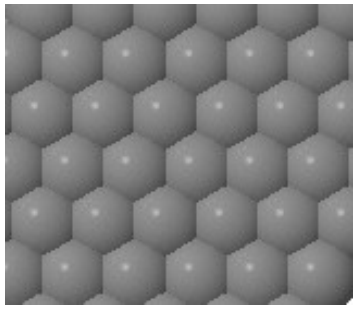


$$a = b = c, \quad \alpha = 90^\circ, \beta = 90^\circ, \gamma = 90^\circ$$





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



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

Space group: 227
point group: m3m

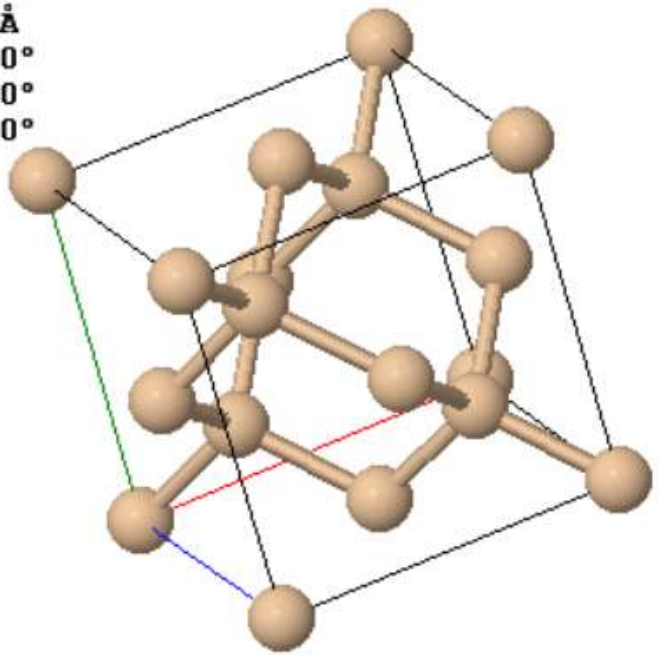
Primitive lattice vectors:

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

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

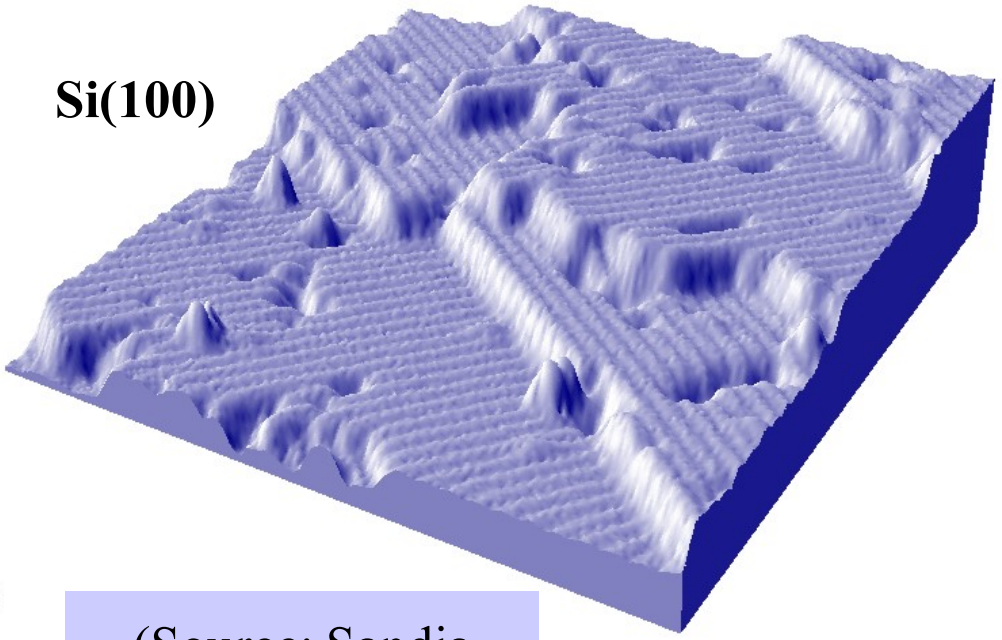
Thickness of HKL planes:

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

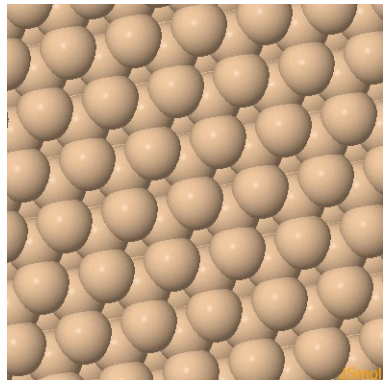
Silicon surfaces

Si(100)

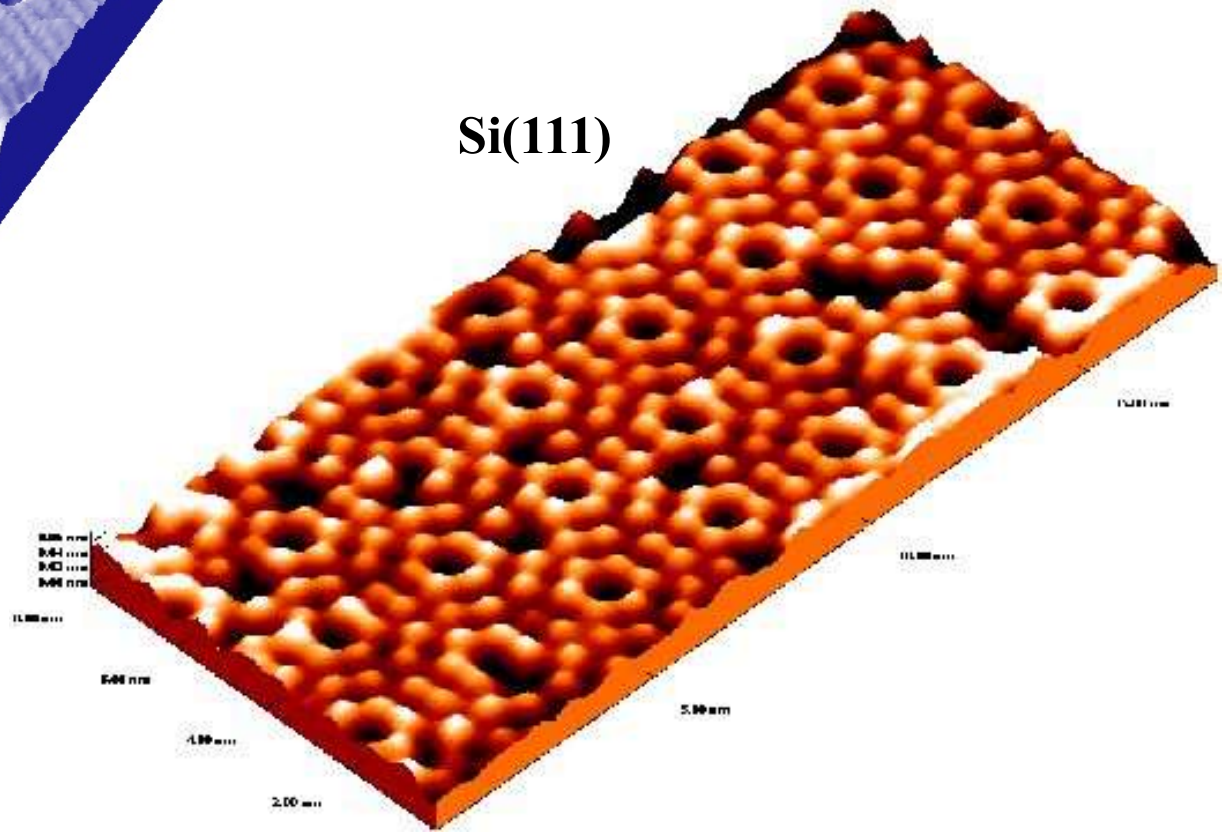


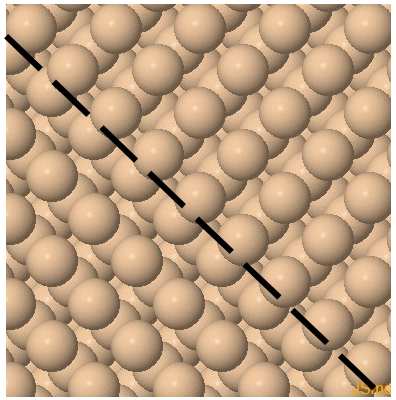
(Source: Sandia Nat.Labs.)

unreconstructed Si(111) →



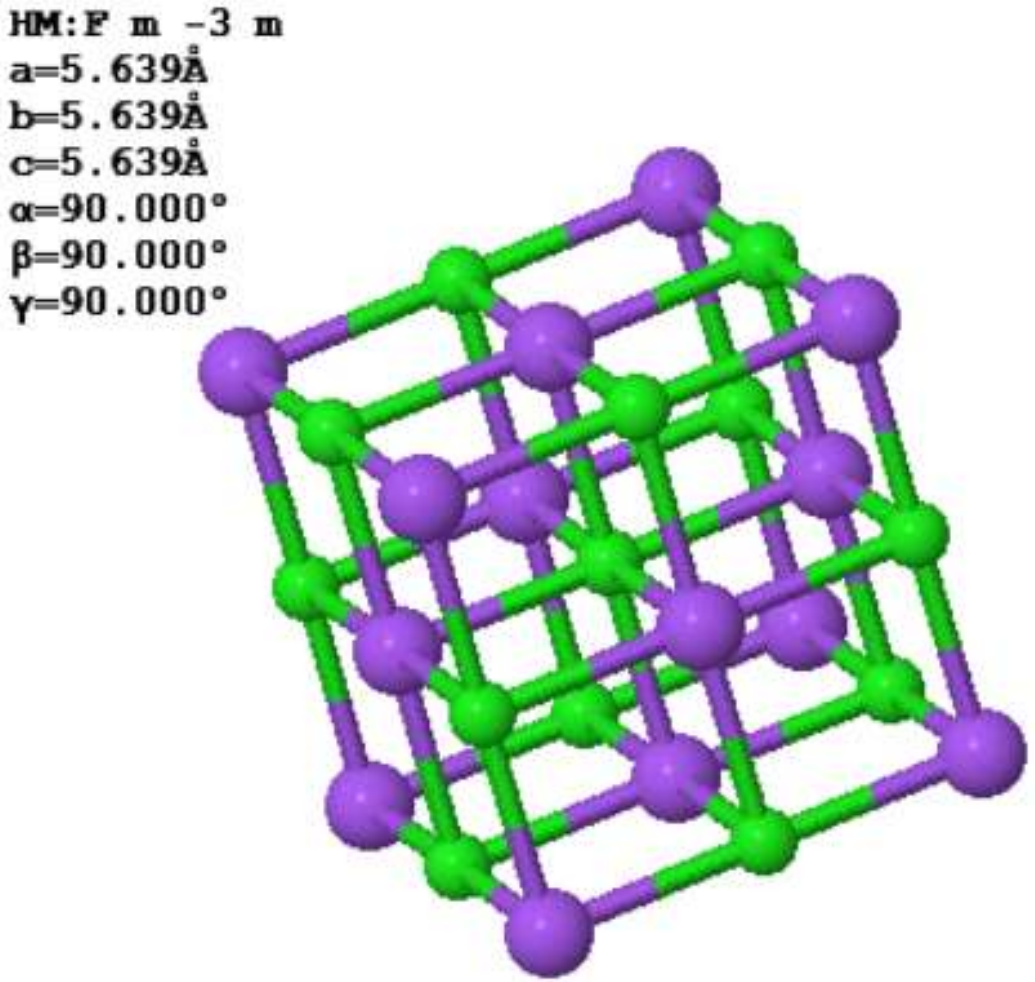
Si(111)





atomic step in Si(100)

NaCl

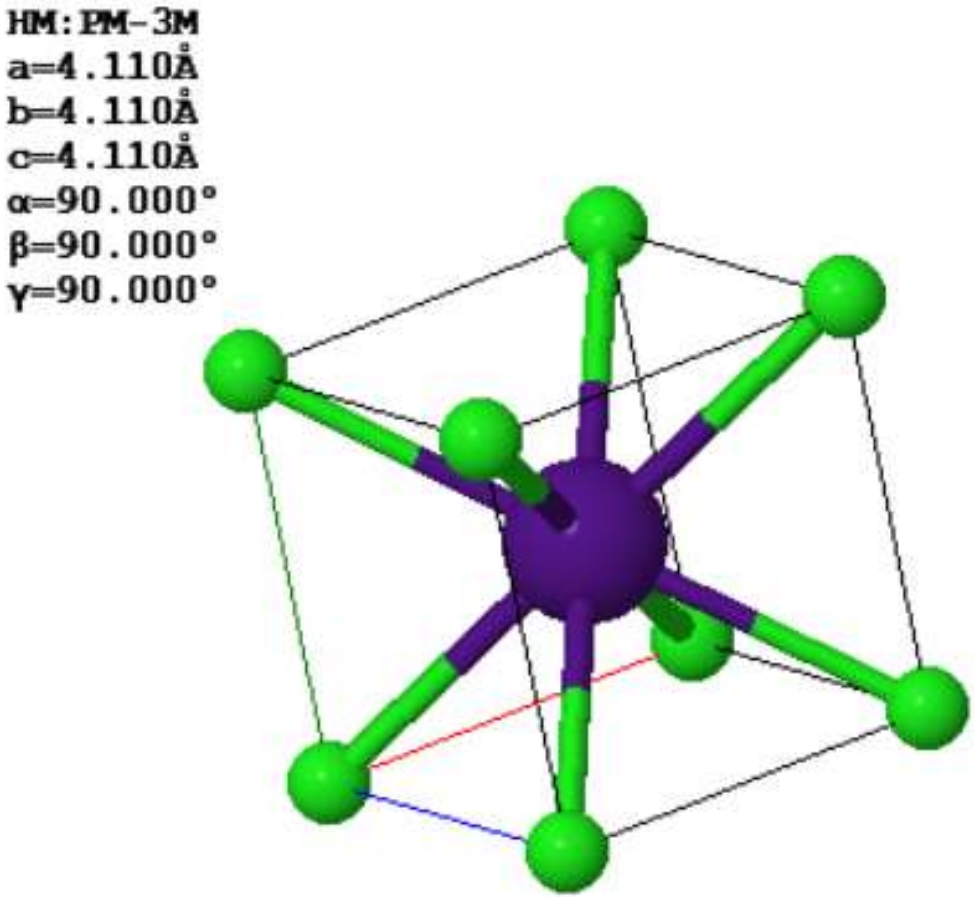


Number 225

Bravais: fcc

CsCl

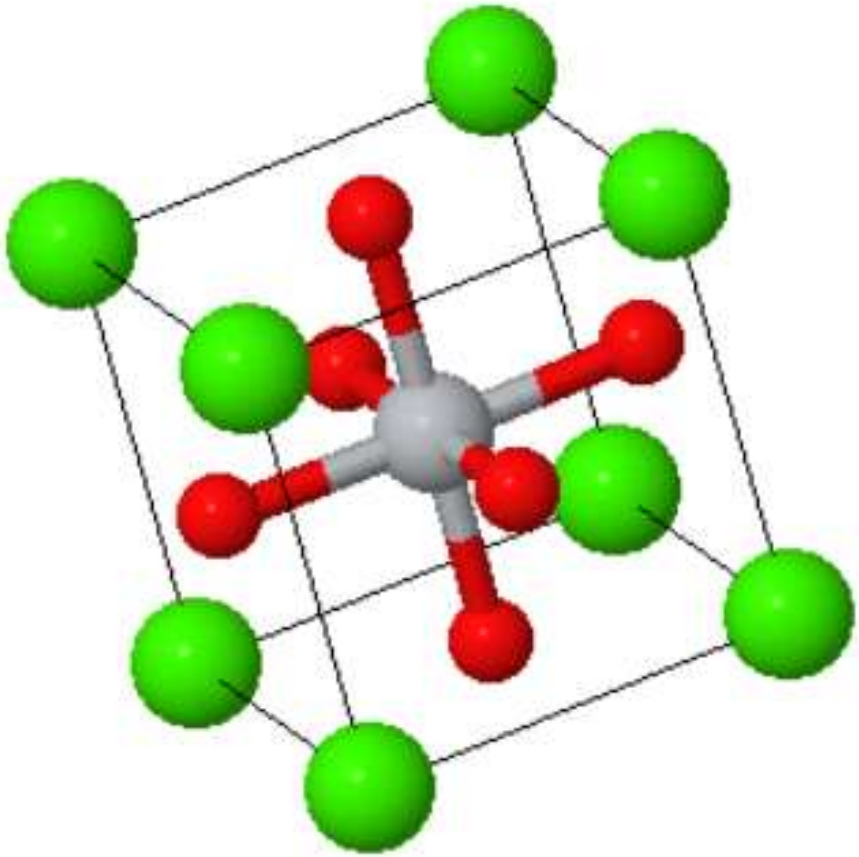
Number 221



perovskite

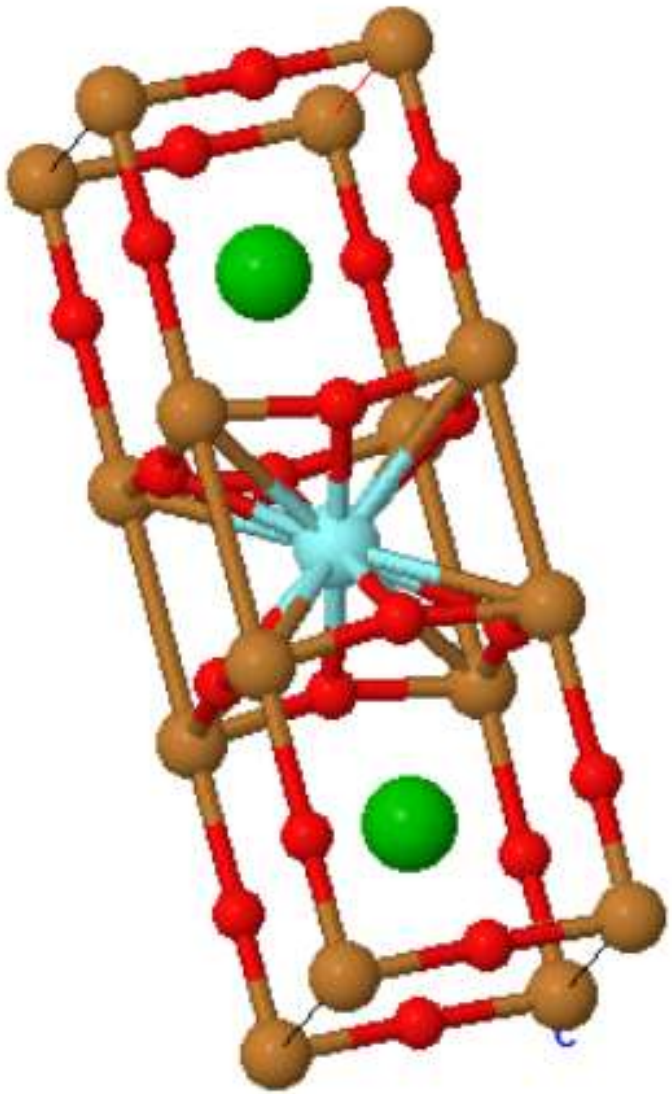
$SrTiO_3$
$LiNbO_3$
$BaTiO_3$
$Pb_xZr_{1-x}TiO_3$

Number 221
simple cubic



$YBa_2Cu_3O_7$

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