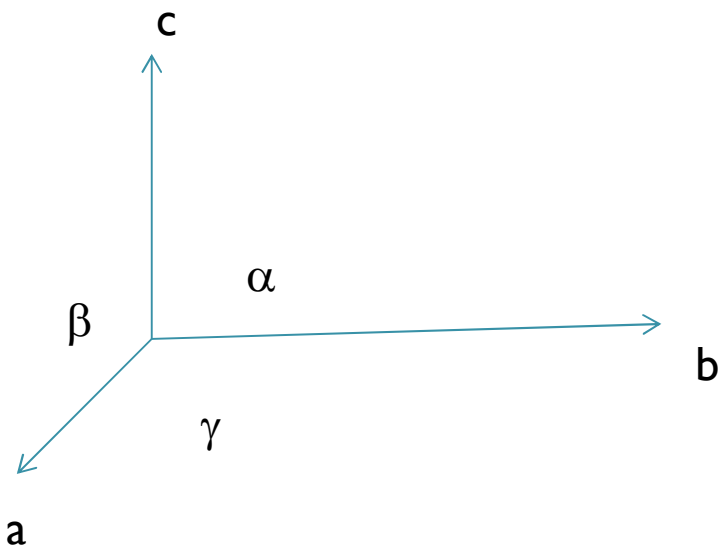
2.6 결정계

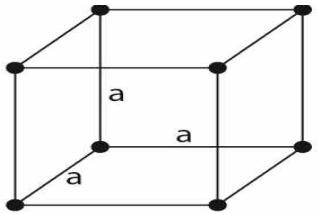
- 결정 (crystal) : 3차원 공간에서 원자가 주기적으로 같은 모양으로 배열을 하고 있는 고체
- 비결정(amorphous): 원자의 규칙 배열이 없다. (예: 유리)

- 단위세포, 단위격자(unit cell) : 결정을 만들 수 있는 점들의 가장 간단한 배열.

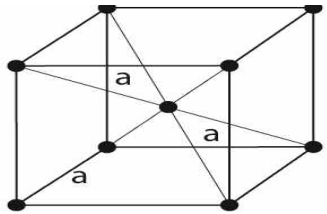
- 격자상수(lattice parameter, lattice constant) : 축의 길이 a, b, c
  축사이의 각 α, β, γ



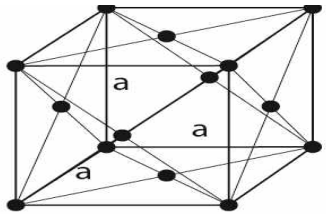
System	Axial lengths and angles	Bravais lattice	Lattice symbol
Cubic 입방	Three equal axes at right angles $a = b = c, \quad \alpha = \beta = \gamma = 90°$	Simple 단순 Body-centered 체심 Face-centered 면심	P I F
Tetragonal 정방	Three axes at right angles, two equal $a = b \neq c, \quad \alpha = \beta = \gamma = 90°$	Simple Body-centered	P I
Orthorhombic 사방	Three unequal axes at right angles $a \neq b \neq c, \quad \alpha = \beta = \gamma = 90°$	Simple Body-centered Base-centered 저심 Face-centered	P I C F
Rhombohedral* 능면체 마름모	Three equal axes, equally inclined $a = b = c, \quad \alpha = \beta = \gamma \neq 90°$	Simple	R
Hexagonal 육방	Two equal coplanar axes at 120°, third axis at right angles $a = b \neq c, \quad \alpha = \beta = 90° \quad \gamma = 120°)$	Simple	P
Monoclinic 단사	Three unequal axes, one pair not at right angles $a \neq b \neq c, \quad \alpha = \gamma = 90° \neq \beta$	Simple Base-centered	P C
Triclinic 삼사	Three unequal axes, unequally inclined and none at right angles $a \neq b \neq c, \quad \alpha \neq \beta \neq \gamma \neq 90°)$	Simple	P



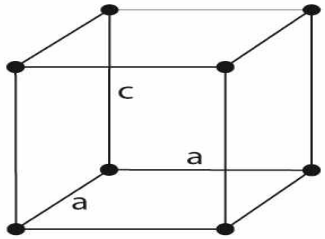
단순입방 (P)



체심입방(I)



면심입방 (F)



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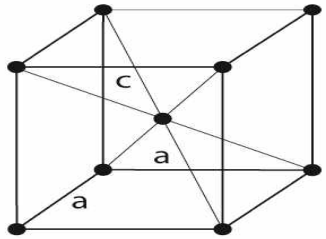

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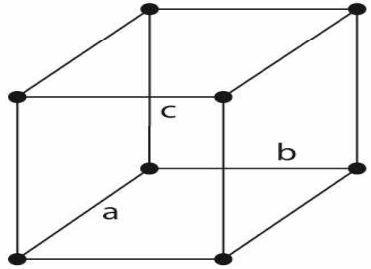

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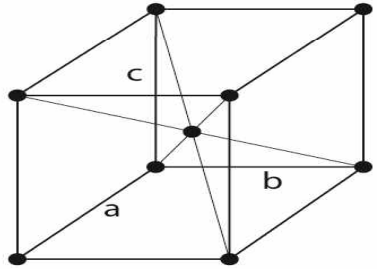
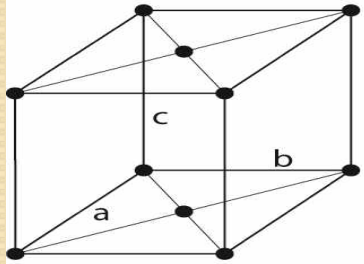
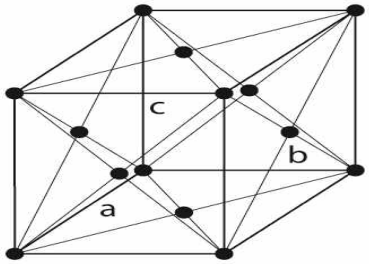


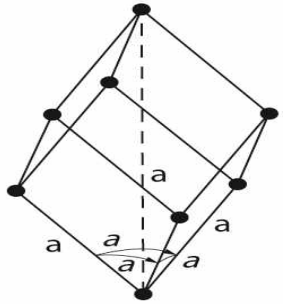
체심사방(I)



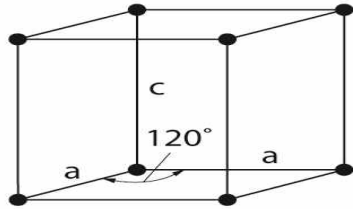
저심사방 (C)



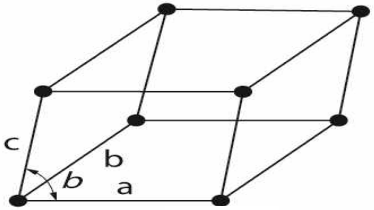
면심사방 (F)



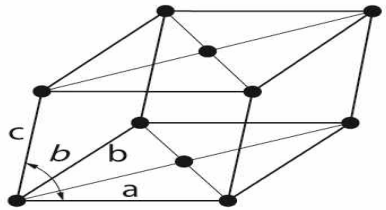
능면체 (R)



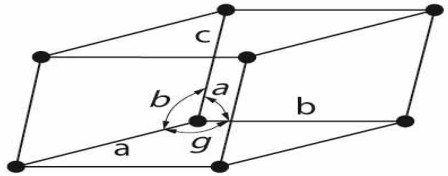
육방 (P)



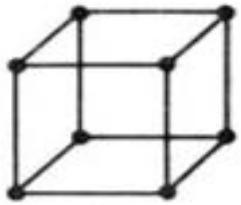
단순, 단사



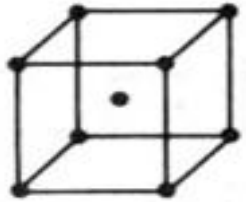
저심단사 (C)



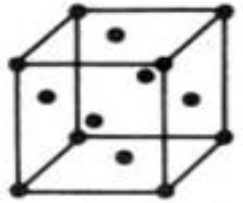
삼사 (P)



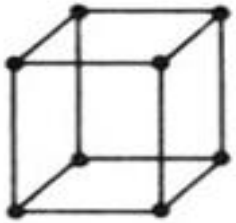
Simple cubic



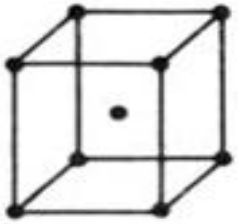
Body-centered cubic



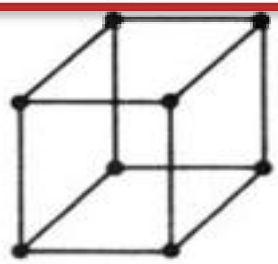
Face-centered cubic



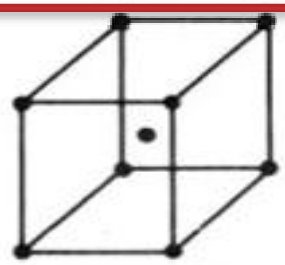
Simple tetragonal



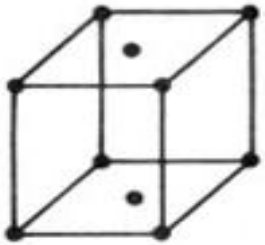
Body-centered tetragonal



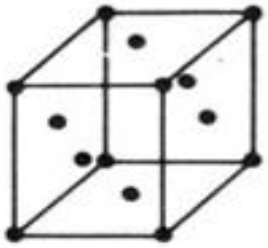
Simple orthorhombic



Body-centered orthorhombic

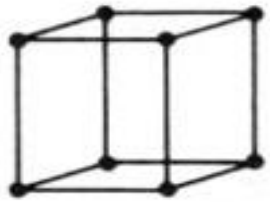


Base-centered orthorhombic

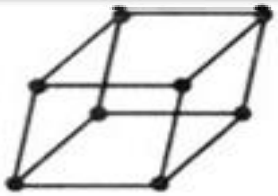


Face-centered orthorhombic

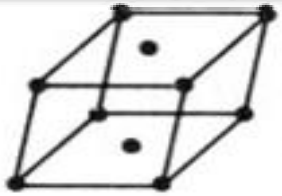
Rhombohedral



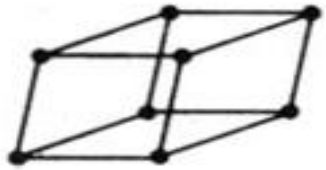
Hexagonal



Simple monoclinic



Base-centered monoclinic

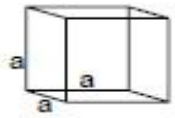


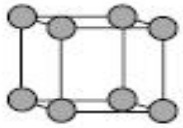
Triclinic

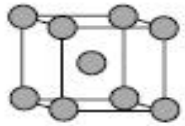
7 Crystal systems

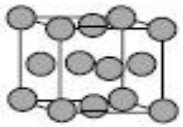
14 Bravais Lattices

cubic
a=b=c
α=β=γ=90°

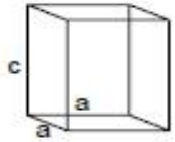


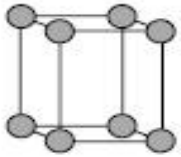


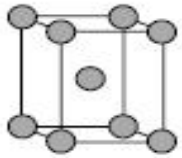




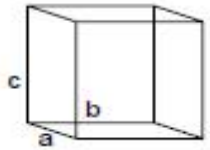
tetragonal
a=b≠c
α=β=γ=90°

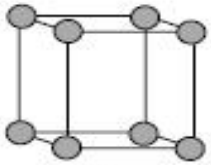


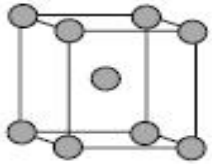


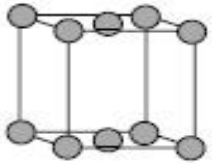


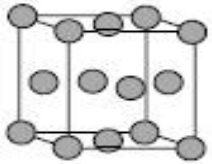
orthorhombic
a≠b≠c
α=β=γ=90°



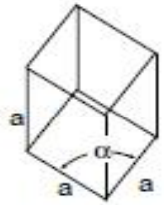


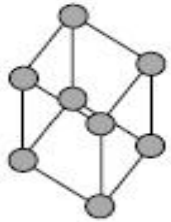




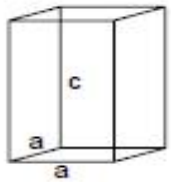


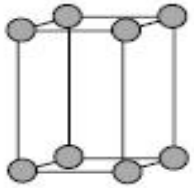
rhombohedral
a=b=c
α=β=γ≠90°



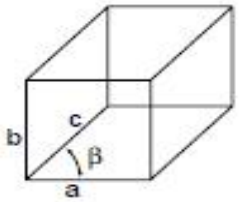


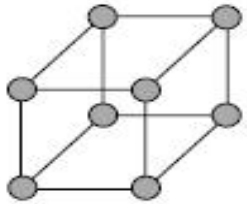
hexagonal
a=b≠c
α=β=90°
γ=120°

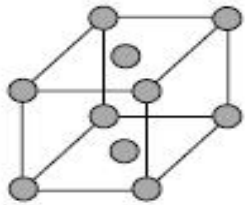




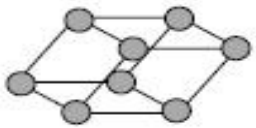
monoclinic
a≠b≠c
α=γ=90° ≠ β







triclinic
a≠b≠c
α≠β≠γ≠90°



대칭요소(symmetry elements)

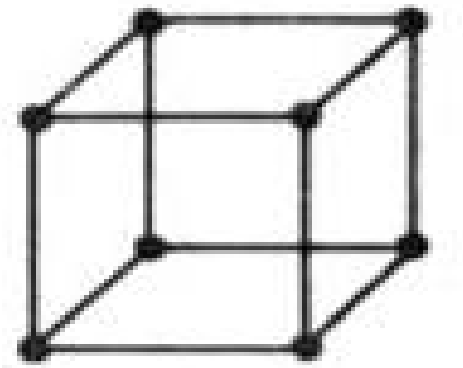
System	Minimum symmetry elements
Cubic	Four 3-fold rotation axes
Tetragonal	One 4-fold rotation (or rotation-inversion) axis
Orthorhombic	Three perpendicular 2-fold rotation (or rotation-inversion) axes
Rhombohedral	One 3-fold rotation (or rotation-inversion) axis
Hexagonal	One 6-fold rotation (or rotation-inversion) axis
Monoclinic	One 2-fold rotation (or rotation-inversion) axis
Triclinic	None

Simple or Primitive

-P – 000

- multiplicity = 1 [8 x (1/8) =1]

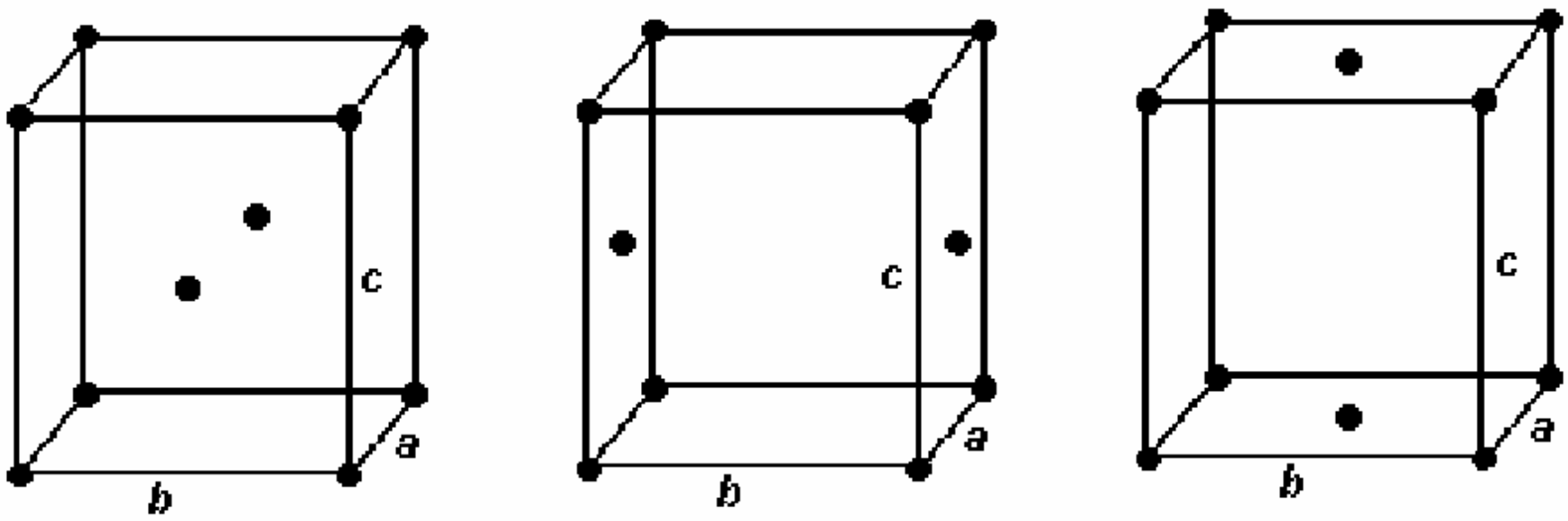
(Atoms/Unit Cell or Lattice point per cell)



Base Centering

– C - Lattice Points at 000 and 0½½
- Lattice Points at 000 and ½0½
-Lattice Points at 000 and ½½0

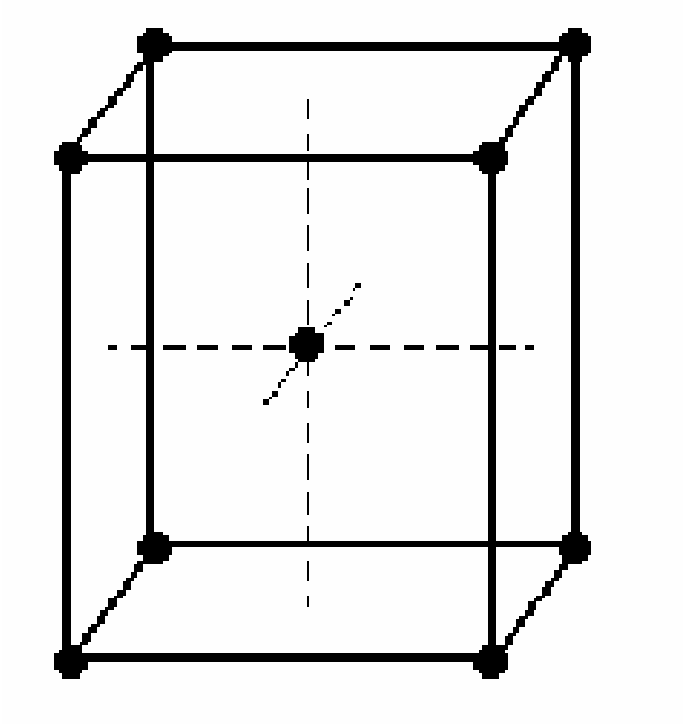
• multiplicity = 2 [8 x (1/8) + 2 x (1/2) =2]



Body Centering

- I - 000 and ½½½

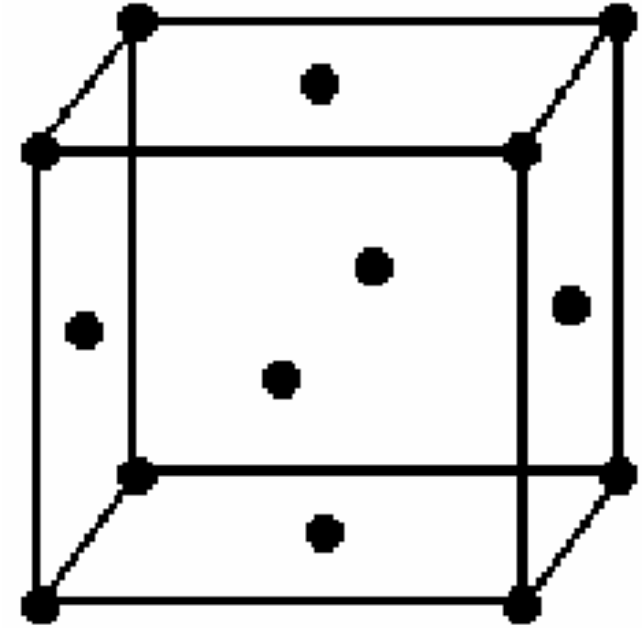
• multiplicity = 2 [8 x (1/8) +1 =2]



Face Centering

– F - 000, ½½0, ½0½ and 0½½

• multiplicity = 4 [8 x (1/8) + 6 x (1/2) =4]

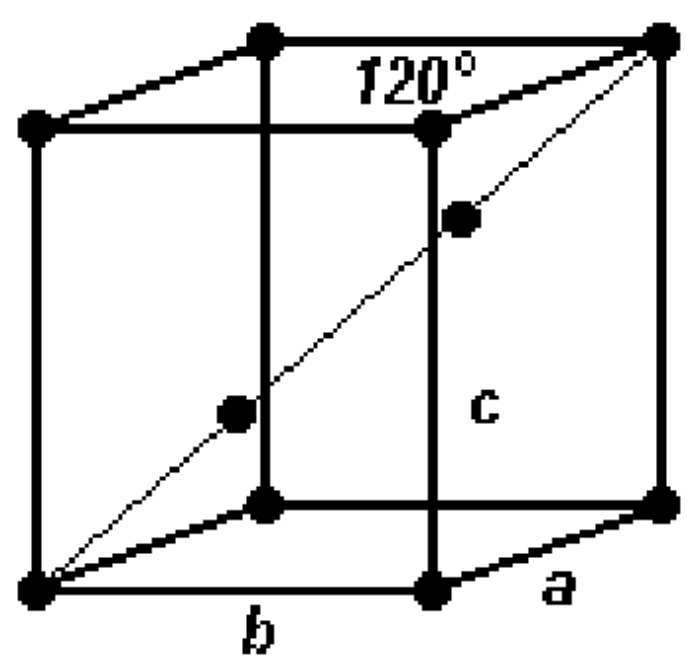


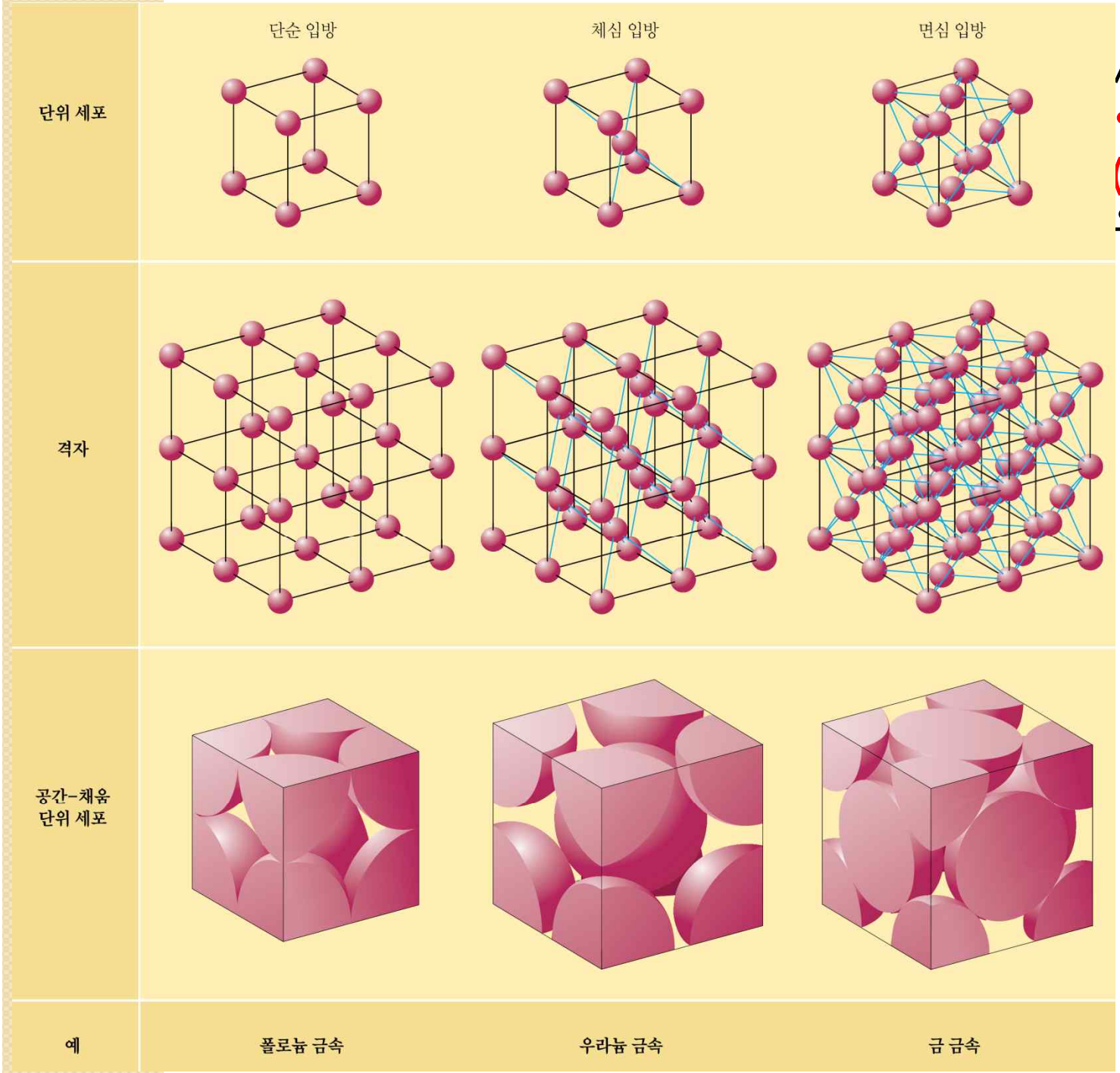
Rhombohedral Centering

– R - 000, 2/31/31/3, and 1/32/32/3

– multiplicity = 3 [8 x (1/8) + 1 + 1 =3]

–Trigonal

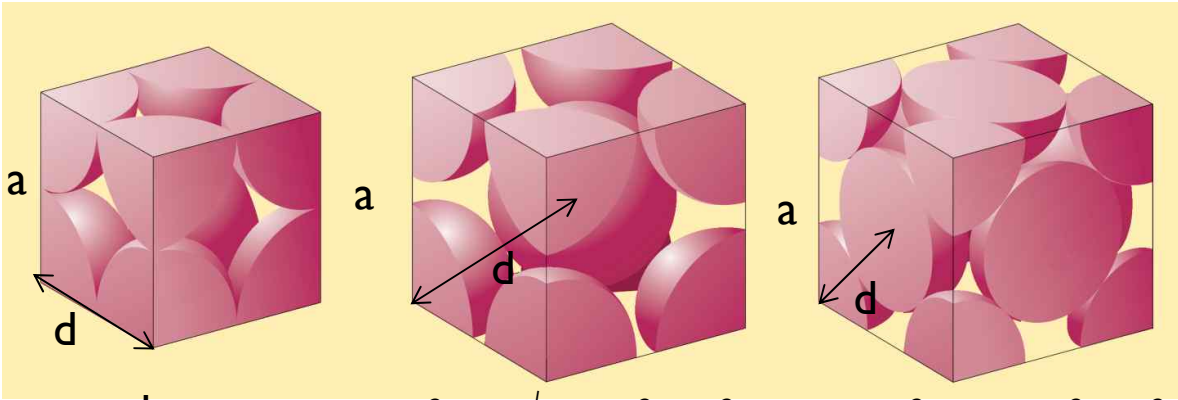




세 개의
입방 결정계
(cubic) 단위 세포
와 그 격자

Characteristics of Cubic Lattices

	Simple	Body-Centered	Face-Centered
Unit Cell Volume	V		
Lattice Points Per Cell	Multiplicity		
Nearest Neighbor Distance	d (2r)		
Number of Nearest Neighbors	CN		



$a = d$

$(a/2)^2 + (\sqrt{2}a/2)^2 = d^2$

$a^2 + (\sqrt{2}a)^2 = (2d)^2$

$(a/2)^2 + (a/2)^2 = d^2$

Determine the density of lead given that it has a face centered cubic structure and an atomic radius of 175 pm.

$D = m/V$

$D = g/cm^3$

m → 4 atoms (face centered)

MW = 207.20g Pb/1mol Pb

Avogadro's number = 1molPb/(6.02×10^{23}Pb atoms)

$V = a^3$ (cubic)

$r = \sqrt{2}a/4$ (face centered)

Determine the density of lead given that it has a face centered cubic structure and an atomic radius of 175 pm.

$D = m/V$

$m = 4\ \cancel{\text{Pb atoms}} \times 207.20\ \text{g Pb}/1\ \cancel{\text{mol Pb}} \times 1\ \cancel{\text{mol Pb}}\ /(6.02 \times 10^{23}\ \cancel{\text{Pb atoms}})$

$m = 1.38 \times 10^{-21}\ \text{g Pb}$

$r = \sqrt{2}\, a/4$

$a = 4 \times 175\ \cancel{\text{pm}} \times 10^{-10}\ \text{cm}/\cancel{\text{pm}}\ /\sqrt{2} = 4.95 \times 10^{-8}\ \text{cm}$

$D = (1.38 \times 10^{-21}\ \text{g})/(4.95 \times 10^{-8}\ \text{cm})^3 = 11.4\ \text{g/cm}^3$

This is in excellent agreement with the listed density of lead, 11.35 g/cm^3.

부록
A3-2
단위포 부피

입방 $V = a^3$

정방 $V = a^2c$

사방 $V = abc$

능면체 $V = a^3\sqrt{1 - 3\cos^2\alpha + 2\cos^2\alpha}$

육방 $V = \frac{\sqrt{3}a^2c}{2} = 0.866a^2c$

단사 $V = abc\sin\beta$

삼사 $V = abc\sqrt{1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\ \cos\beta\ \cos\gamma}$

PDF # 461212, Wavelength = 1.540562 (A)

46-1212 Quality: *

CAS Number:

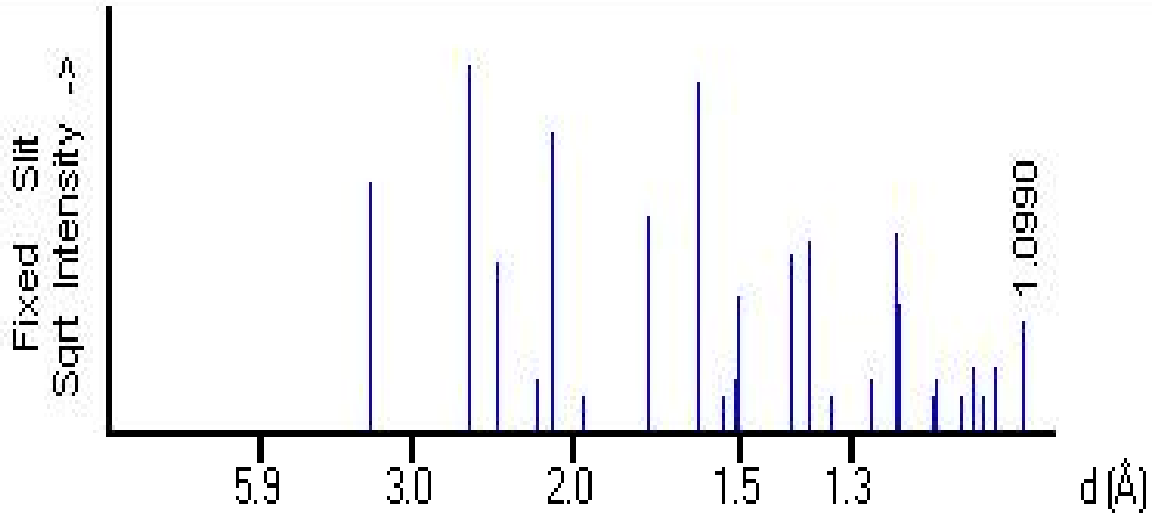
Molecular Weight: 101.96
Volume[CD]: 254.81
Dx: 3.987 Dm:

Sys: Hexagonal
Lattice: Rhomb-centered
S.G.: R3̄c (167)
Cell Parameters:
a 4.758 b c 12.99
α β γ

SS/FOM: F25=358(.0028, 25)
I/Icor:
Rad: CuKa1
Lambda: 1.540562
Filter:
d-sp: diffractometer

Mineral Name:
Corundum, syn

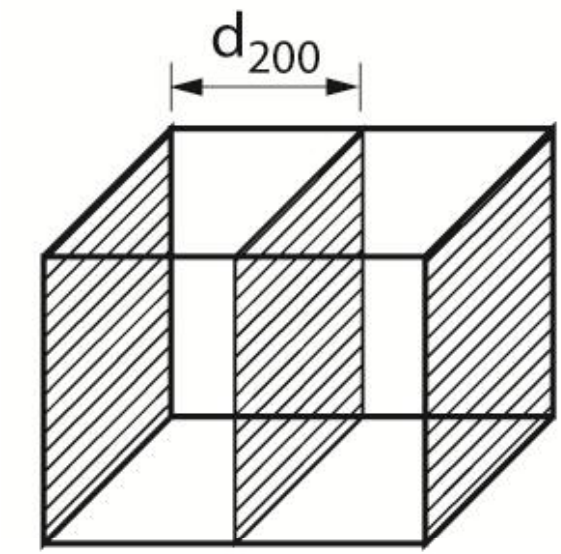
α-Al2 O3
Aluminum Oxide
Ref: Huang, T et al., Adv. X-Ray Anal., 33, 295 (1990)



d(A)	Int-f	h	k	l
3.4797	45	0	1	2
2.5508	100	1	0	4
2.3794	21	1	1	0
2.1654	2	0	0	6
2.0853	66	1	1	3
1.9643	1	2	0	2
1.7400	34	0	2	4
1.6015	89	1	1	6
1.5466	1	2	1	1

d(A)	Int-f	h	k	l
1.5150	2	1	2	2
1.5110	14	0	1	8
1.4045	23	2	1	4
1.3737	27	3	0	0
1.3359	1	1	2	5
1.2755	2	2	0	8
1.2391	29	1	0	10
1.2343	12	1	1	9
1.1931	1	2	1	7

d(A)	Int-f	h	k	l
1.1897	2	2	2	0
1.1600	1	3	0	6
1.1472	3	2	2	3
1.1386	<1	1	3	1
1.1256	2	3	1	2
1.1241	3	1	2	8
1.0990	9	0	2	10



계산 d_{006} =

부록
A3-1
면간거리

입방 $$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2}$$

정방 $$\frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}$$

사방 $$\frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

능면체 $$\frac{1}{d^2} = \frac{(h^2 + k^2 + l^2)\sin^2\alpha + 2(hk + kl + hl)(\cos^2\alpha - \cos\alpha)}{a^2(1 - 3\cos^2\alpha + 2\cos^3\alpha)}$$

육방 $$\frac{1}{d^2} = \frac{4}{3}\left(\frac{h^2 + hk + k^2}{a^2}\right) + \frac{l^2}{c^2}$$

단사 $$\frac{1}{d^2} = \frac{1}{\sin^2\beta}\left(\frac{h^2}{a^2} + \frac{k^2\sin^2\beta}{b^2} + \frac{l^2}{c^2} - \frac{2hl\cos\beta}{ac}\right)$$

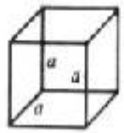
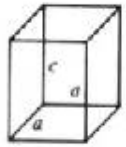
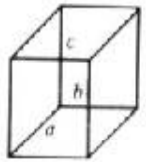
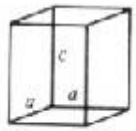
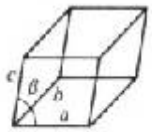
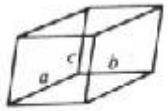
삼사 $$\frac{1}{d^2} = \frac{1}{V^2}(S_{11}h^2 + S_{22}k^2 + S_{33}l^2 + 2S_{12}hk + 2S_{23}kl + 2S_{13}hl)$$

V = volume of unit cell (see below), $S_{11} = b^2c^2\sin^2\alpha$ $S_{22} = a^2c^2\sin^2\beta$ $S_{33} = a^2b^2\sin^2\gamma$

$S_{12} = abc^2(\cos\alpha\cos\beta - \cos\gamma)$ $S_{23} = a^2bc(\cos\beta\cos\gamma - \cos\alpha)$

$S_{13} = ab^2c(\cos\gamma\cos\alpha - \cos\beta)$

7 결정계 :
결정의 대칭성에 따라 정의.
단위 세포의 모서리와 각 사이에 관련성에 따라 결정.

Cubic	$a = b = c,\ \alpha = \beta = \gamma = 90°$		P(Simple, Primitive) I(Body-Centered) F(Face-Centered)
Tetragonal	$a = b \neq c,\ \alpha = \beta = \gamma = 90°$		P(Simple, Primitive) I(Body-Centered)
Orthorhombic	$a \neq b \neq c,\ \alpha = \beta = \gamma = 90°$		P(Simple, Primitive) I(Body-Centered) F(Face-Centered) C(Base-Centered)
Rhombohedral	$a = b = c,\ \alpha = \beta = \gamma \neq 90°$		R(Rhombohedral Centered)
Hexagonal	$a = b \neq c,\ \alpha = \beta = 90°,\ \gamma = 120°$		P(Simple, Primitive)
Monoclinic	$a \neq b \neq c,\ \alpha = \gamma = 90° \neq \beta$		P(Simple, Primitive) C(Base-Centered)
Triclinic	$a \neq b \neq c,\ \alpha \neq \beta \neq \gamma \neq 90°$		P(Simple, Primitive)

14 Bravais Lattice
(동일환경 격자점 조건)

32 Point Group
(한점에 대한 대칭조작)

대칭요소
Reflection
Rotation
Inversion

Schoenflies Symbol
쉔플리스
C_{3v}
$(E, C_3 3\sigma_v)$
&
Hermann-Mauguin Symbol
3m

73 Space Group

32 Point Group
+
14 Bravais Lattice

230 Space Group

230 Unique Combi-nation

73 Space Group
+
11 Screw Axis
+
5 Glide Plane

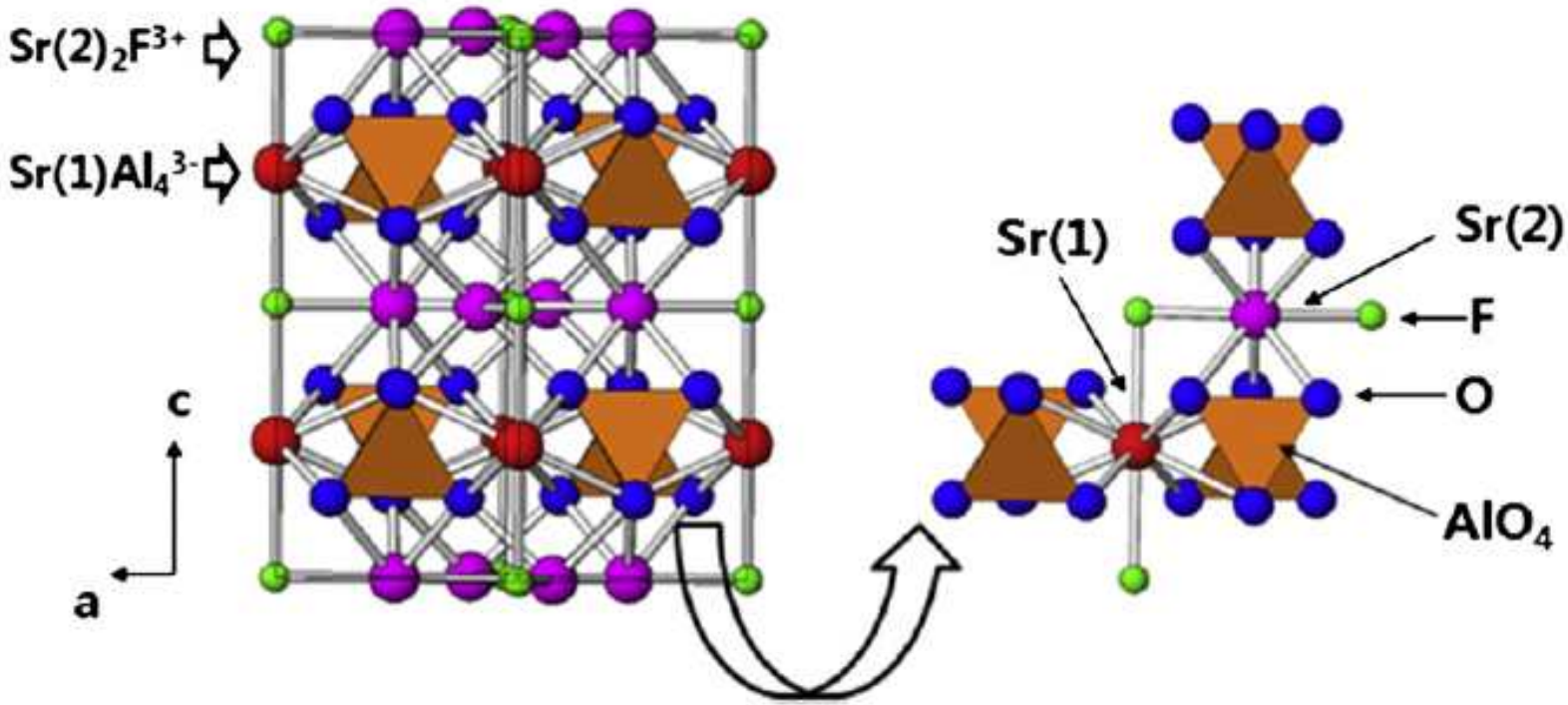
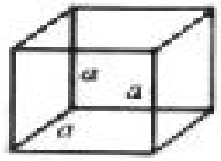
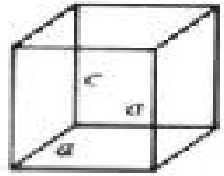
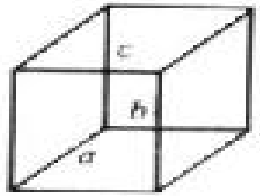
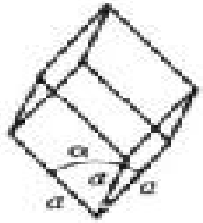
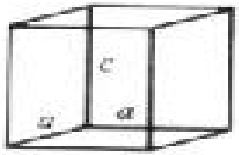
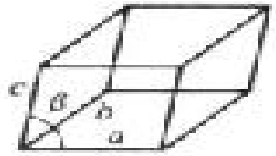
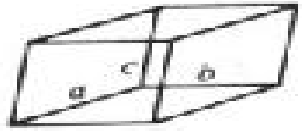


Fig. 1. Crystallographic structure of Sr_3AlO_4F oxyfluoride host lattice [8].

As reported previously, Fig. 1 shows the anion-ordered Sr_3AlO_4F oxyfluoride structure, which is a tetragonal phase with space group I4/mcm; it is arranged by stacking alternating $Sr(2)_2F^{3+}$ and $Sr(1)AlO_4^{3-}$ layers along the c axis [8]. There are 10-fold-coordinated Sr(1), 8-foldcoordinated Sr(2), and 4-fold-coordinated Al^{3+} cation sites in the host structure.

Cubic	$a = b = c, \quad \alpha = \beta = \gamma = 90°$	
Tetragonal	$a = b \neq c, \quad \alpha = \beta = \gamma = 90°$	
Orthorhombic	$a \neq b \neq c, \quad \alpha = \beta = \gamma = 90°$	
Rhombohedral	$a = b = c, \quad \alpha = \beta = \gamma \neq 90°$	
Hexagonal	$a = b \neq c, \quad \alpha = \beta = 90°, \gamma = 120°$	
Monoclinic	$a \neq b \neq c, \quad \alpha = \gamma = 90° \neq \beta$	
Triclinic	$a \neq b \neq c, \quad \alpha \neq \beta \neq \gamma \neq 90°$	

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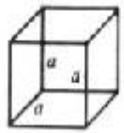
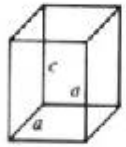
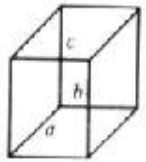
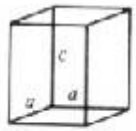
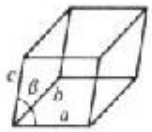
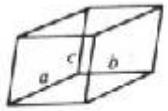
Cubic	$a = b = c,\ \alpha = \beta = \gamma = 90°$		P(Simple, Primitive) I(Body-Centered) F(Face-Centered)
Tetragonal	$a = b \neq c,\ \alpha = \beta = \gamma = 90°$		P(Simple, Primitive) I(Body-Centered)
Orthorhombic	$a \neq b \neq c,\ \alpha = \beta = \gamma = 90°$		P(Simple, Primitive) I(Body-Centered) F(Face-Centered) C(Base-Centered)
Rhombohedral	$a = b = c,\ \alpha = \beta = \gamma \neq 90°$		R(Rhombohedral Centered)
Hexagonal	$a = b \neq c,\ \alpha = \beta = 90°,\ \gamma = 120°$		P(Simple, Primitive)
Monoclinic	$a \neq b \neq c,\ \alpha = \gamma = 90° \neq \beta$		P(Simple, Primitive) C(Base-Centered)
Triclinic	$a \neq b \neq c,\ \alpha \neq \beta \neq \gamma \neq 90°$		P(Simple, Primitive)

14 Bravais Lattice
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32 Point Group
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Reflection
Rotation
Inversion

Schoenflies Symbol
쉔플리스
C_{3v}
$(E, C_3 3\sigma_v)$
&
Hermann-Mauguin Symbol
3m

73 Space Group

32 Point Group
+
14 Bravais Lattice

230 Space Group

230 Unique Combi-nation

73 Space Group
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11 Screw Axis
+
5 Glide Plane