

제2장 결정 기하학

2-1 서언

결정의 X선 회절 → 결정기하학과 구조

2-2 격자

Crystal (결정)

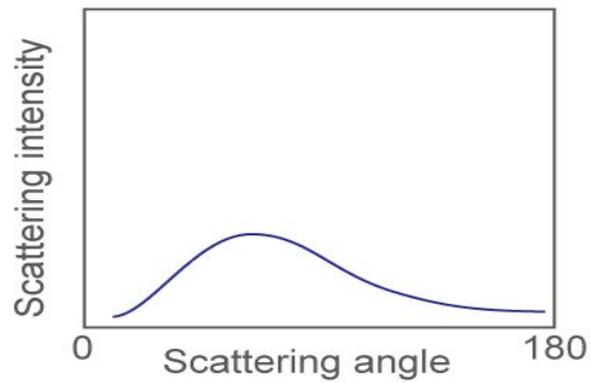
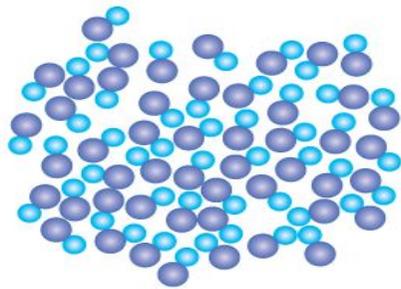
원자, 이온, 또는 분자가 주기적인 방식으로 3차원 공간에서 배열하고 있는 것.

:단결정(singlecrystalline)

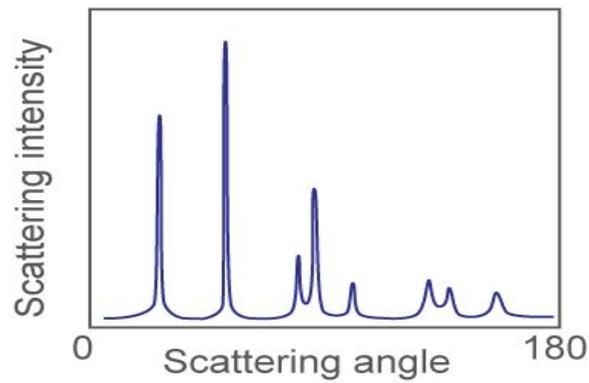
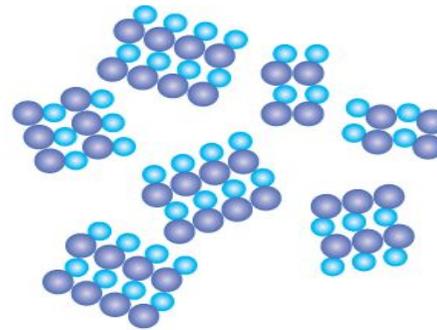
다결정(polycrystalline)-접촉면이 많은 결정

모든 고체는 다 결정질이 아니다 : (예)유리 (비정질, amorphous)

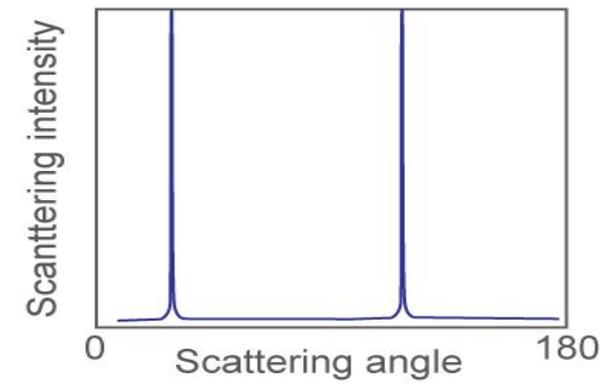
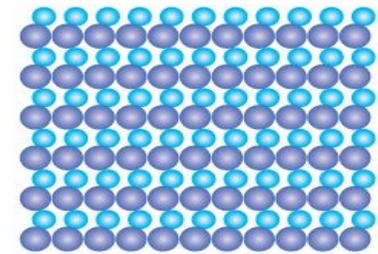
X-ray Diffraction Patterns



amorphous



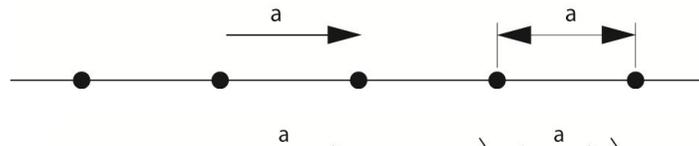
Powder / polycrystalline



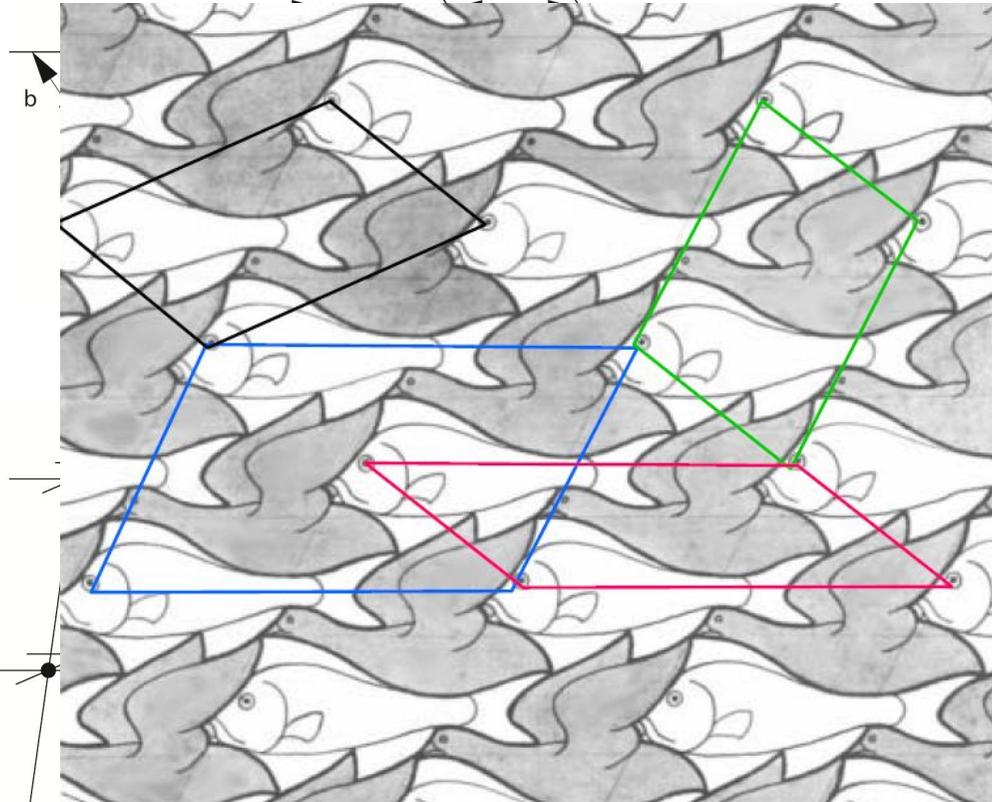
Single crystal

결정 격자(crystal lattice)- 점(lattice point)의 3 차원적인 배열

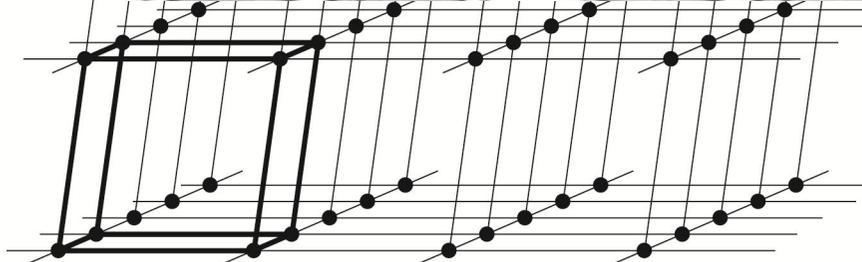
1차원 격자
: 결정모양이 아님



2차원 격자
: 두 개의 격자 병진벡터
평면 망

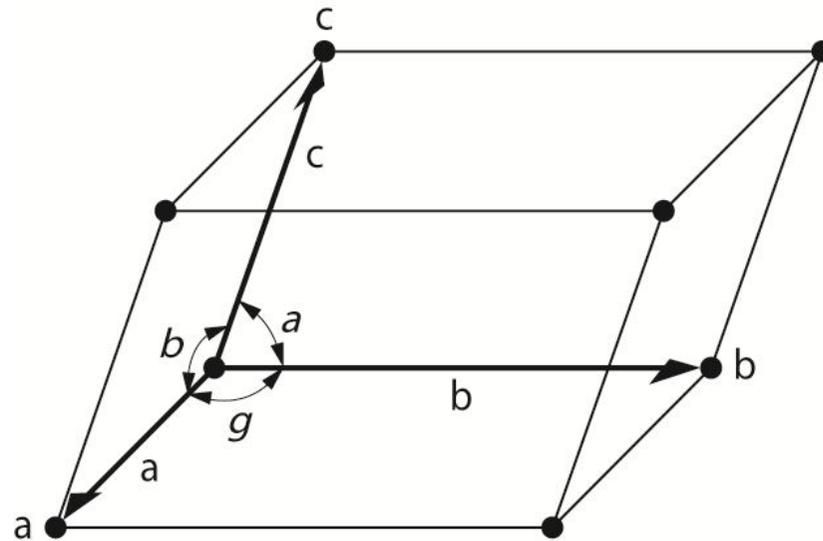


3차원 격자
: 세 개의 격자 병진벡터
공간 격자



- Unit Cell (단위세포)

- Space lattice를 구성하는 가장 해석이 용이한 최소 repeating unit.
- Unit cell은 세 crystallographic axes로 정의되며, 이 세 vector들의 길이(a, b, c)와 이들이 서로 이루는 각(α, β, γ)을 unit cell의 lattice parameter(격자계수)라 한다.





PDF # 461212, Wavelength = 1.540562 (Å)



46-1212 Quality: *

CAS Number:

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

Sys: Hexagonal
Lattice: Rhomb-centered
S.G.: $R\bar{3}c$ (167)
Cell Parameters:
a 4.758 b c 12.99
 α β γ

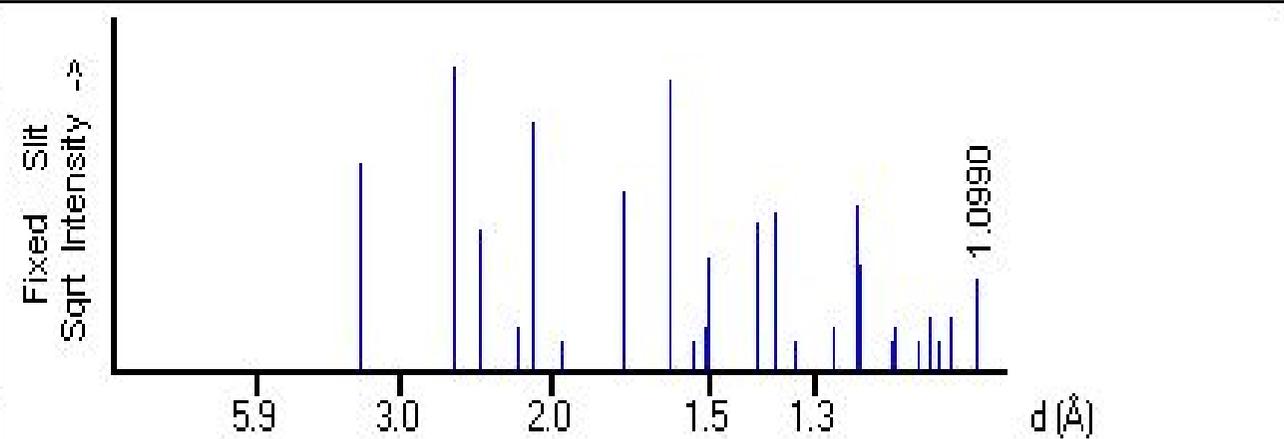
SS/FOM: F25=358(.0028, 25)
I/|cor:
Rad: CuK α 1
Lambda: 1.540562
Filter:
d-sp: diffractometer

Mineral Name:
Corundum, syn

α -Al₂O₃

Aluminum Oxide

Ref: Huang, T et al., Adv. X-Ray Anal., 33, 295 (1990)



d(Å)	Int-f	h	k	l	d(Å)	Int-f	h	k	l	d(Å)	Int-f	h	k	l
3.4797	45	0	1	2	1.5150	2	1	2	2	1.1897	2	2	2	0
2.5508	100	1	0	4	1.5110	14	0	1	8	1.1600	1	3	0	6
2.3794	21	1	1	0	1.4045	23	2	1	4	1.1472	3	2	2	3
2.1654	2	0	0	6	1.3737	27	3	0	0	1.1386	<1	1	3	1
2.0853	66	1	1	3	1.3359	1	1	2	5	1.1256	2	3	1	2
1.9643	1	2	0	2	1.2755	2	2	0	8	1.1241	3	1	2	8
1.7400	34	0	2	4	1.2391	29	1	0	10	1.0990	9	0	2	10
1.6015	89	1	1	6	1.2343	12	1	1	9					
1.5466	1	2	1	1	1.1931	1	2	1	7					

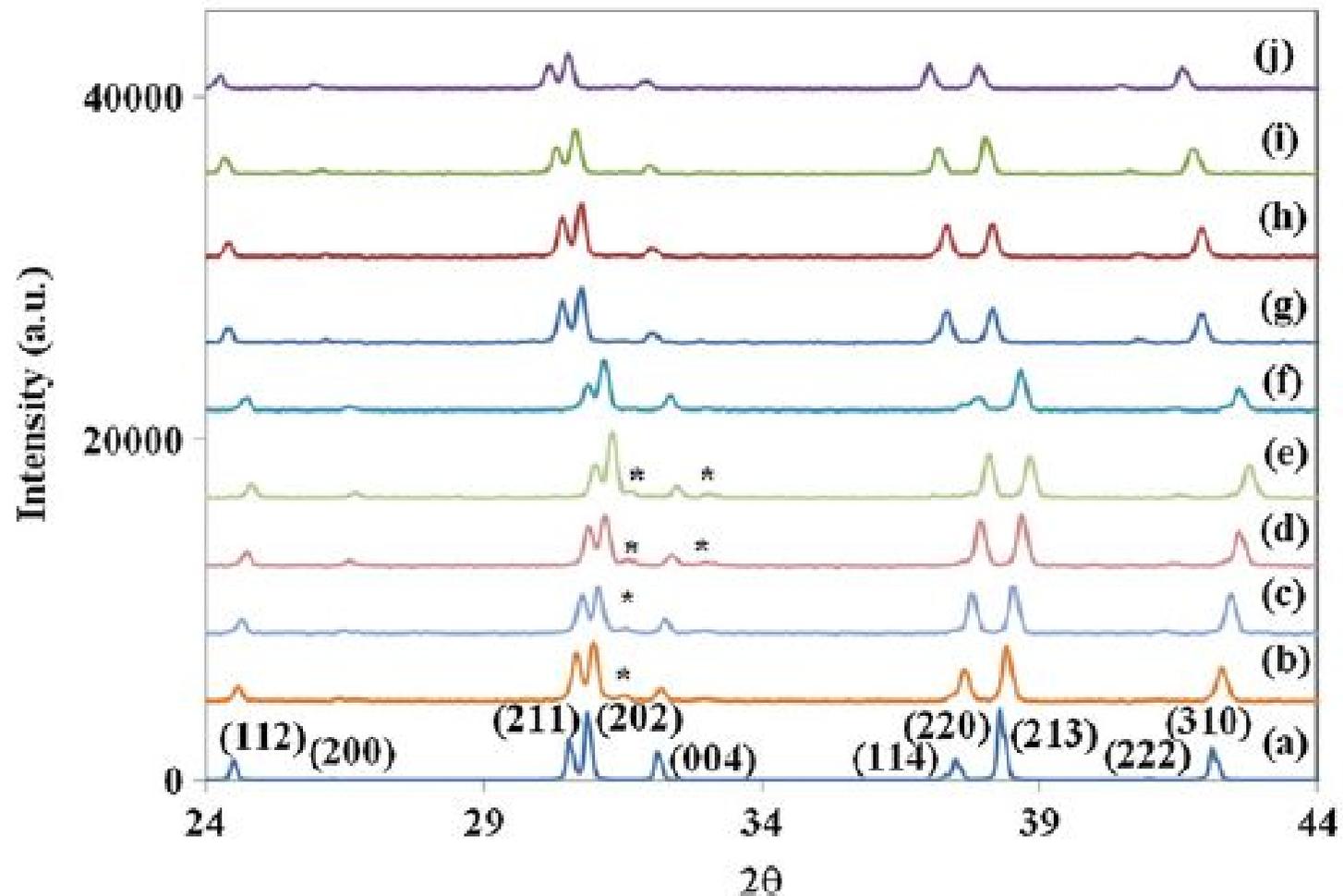


Fig. 2. X-ray diffraction patterns of (a) calculated $\text{Sr}_3\text{AlO}_4\text{F}$ host lattice, experimentally observed (b)–(e) $\text{Sr}_{3-x}\text{Ca}_x\text{Al}_{0.9}\text{In}_{0.1}\text{O}_4\text{F}$ ($x = 0.1, 0.3, 0.5, 0.7$), (f) $\text{Sr}_{2.5}\text{Ca}_{0.5}\text{Al}_{0.9}\text{In}_{0.1}\text{O}_{4-\alpha}\text{F}_{1-\delta}$, and (g)–(j) $\text{Sr}_{3-x}\text{Ba}_x\text{Al}_{0.9}\text{In}_{0.1}\text{O}_4\text{F}$ ($x = 0.1, 0.3, 0.5, 0.7$) oxyfluorides.

2-3 점, 선, 평면의 표기

$(h\ k\ l)$: 괄호, 면이 결정축과 만드는 분율 절편(fractional intercept)의

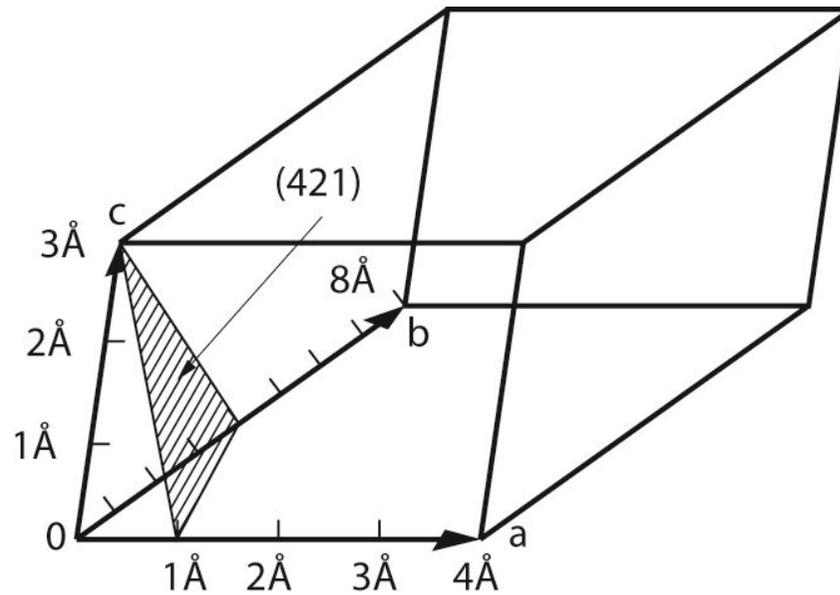
역수로 정의

: Miller 지수

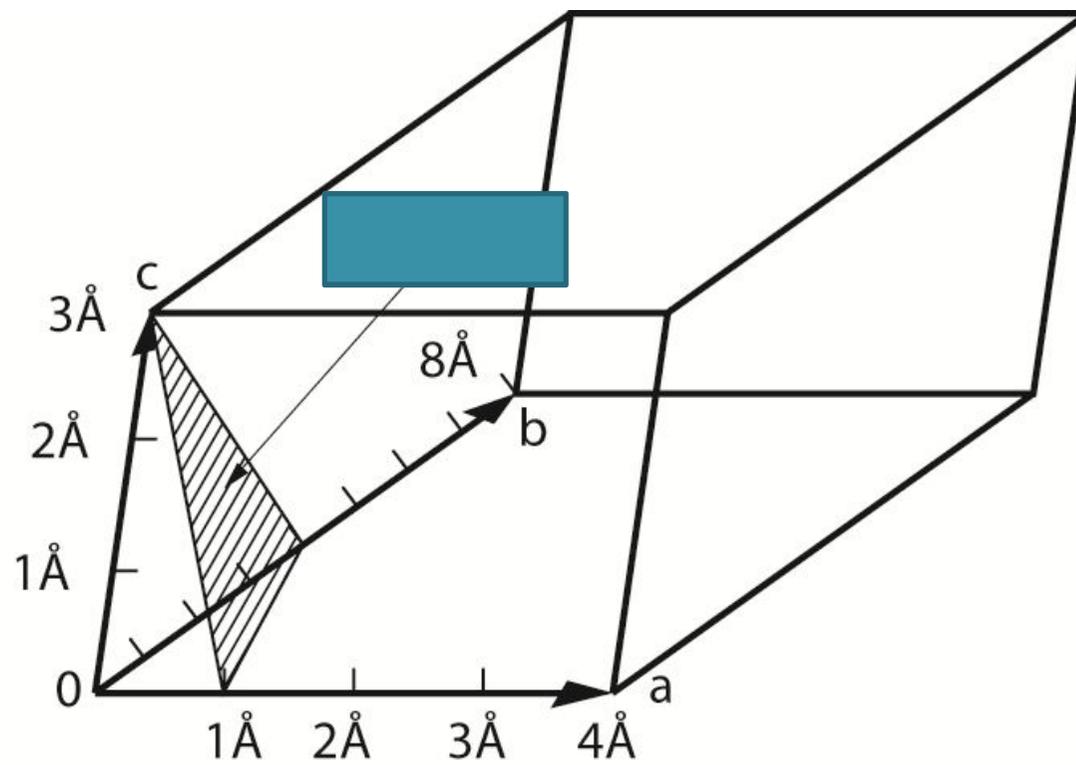
(hkl) → 면은 축과 분율절편이 $1/h, 1/k, 1/l$ 절편

축 길이가 a, b, c → 실제절편 $a/h, b/k, c/l$

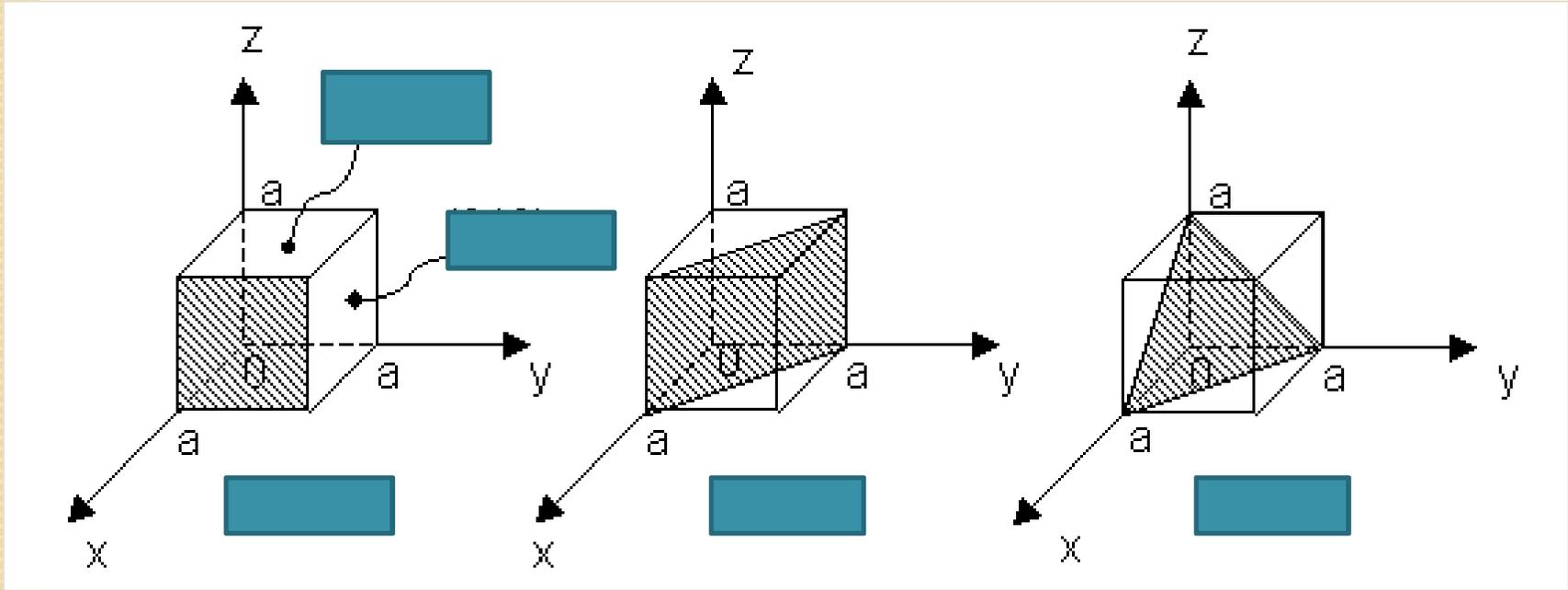
축 길이	4 Å	8 Å	3 Å
절편 길이	1 Å	4 Å	3 Å
분율절편	$\frac{1}{4}$	$(4/8) \rightarrow \frac{1}{2}$	1
Miller 지수	4	2	1



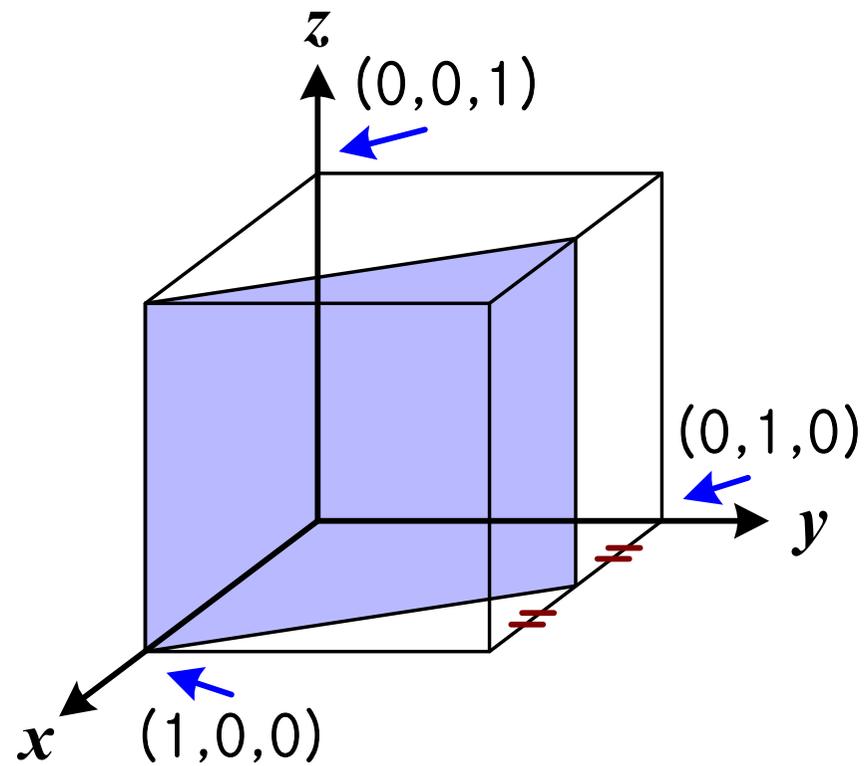
(b)



(b)

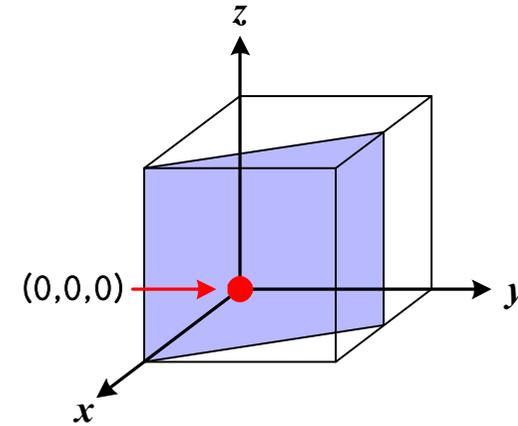


Example : 다음 면의 Miller Index를 구하라.



Solution

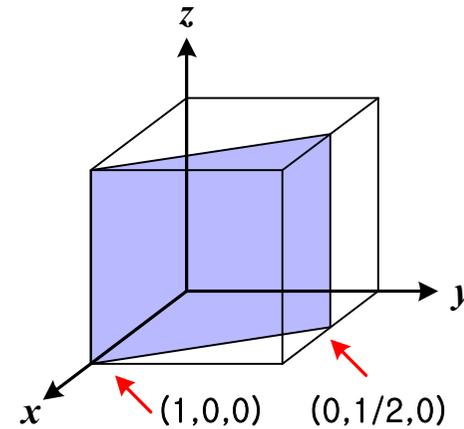
1. 원점인 $(0,0,0)$ 을 정한다.



2. 결정면이 x, y, z 축과 만나는 접점을 조사한다.

즉, $x=1, y=2, z=\infty$ 이다.

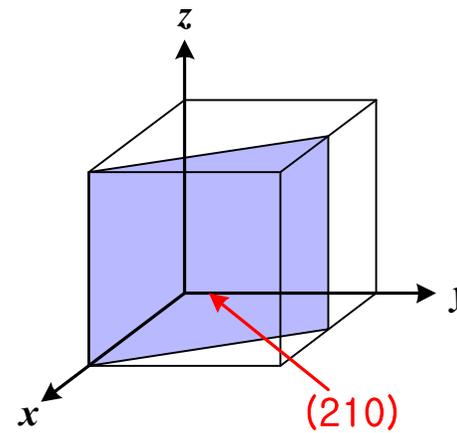
z 축은 만나는 점이 없다.



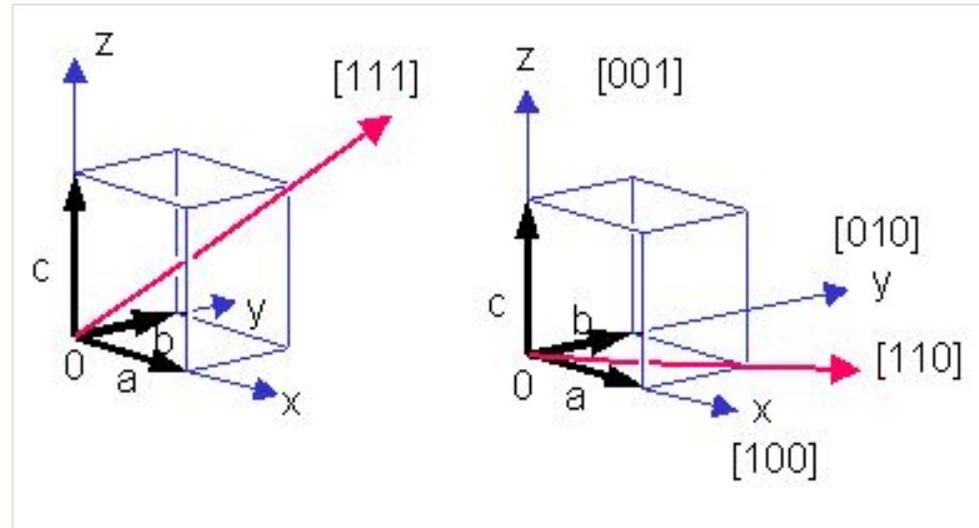
Solution

3. 역수를 취한다.
 $x=1, y=1/2, z=0$

4. Miller index 결정면은 (210)



[h k l] : 꺾쇠괄호안, 선의 방향지수 **one direction**

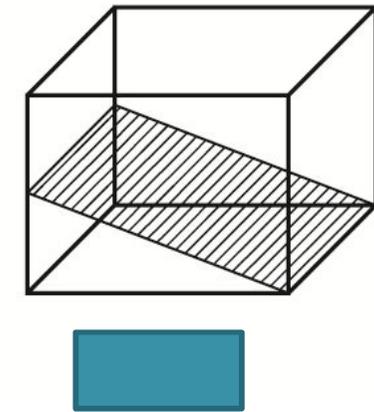
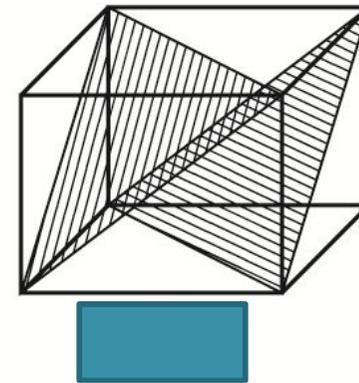
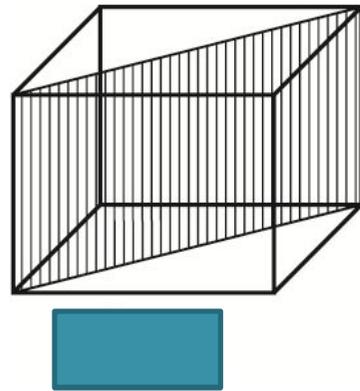
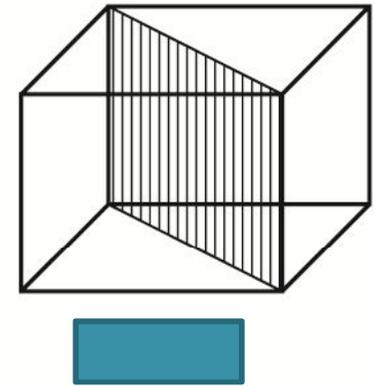
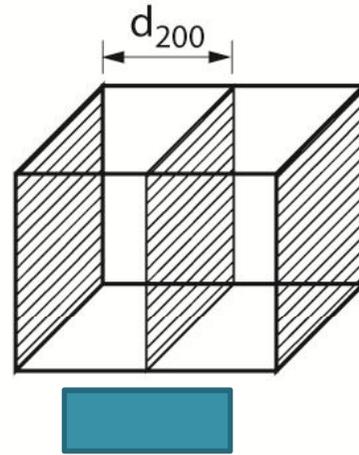
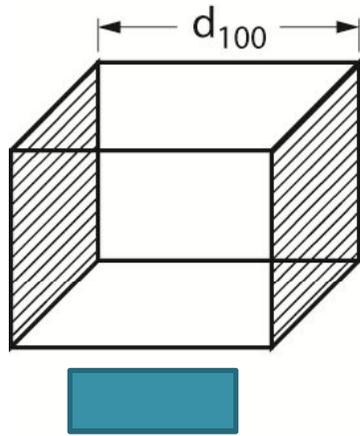
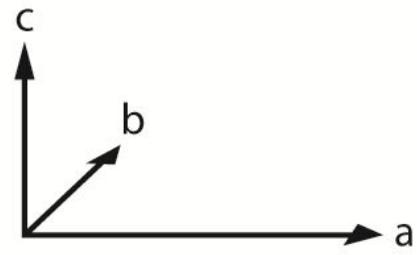


<h k l> : 모난괄호안, 결정형의 방향

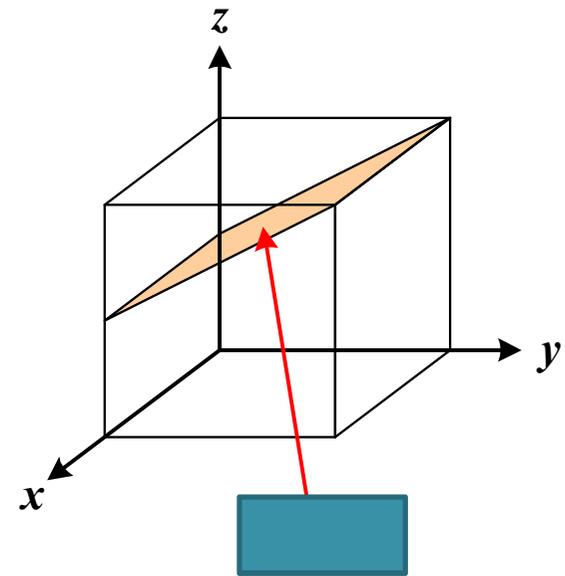
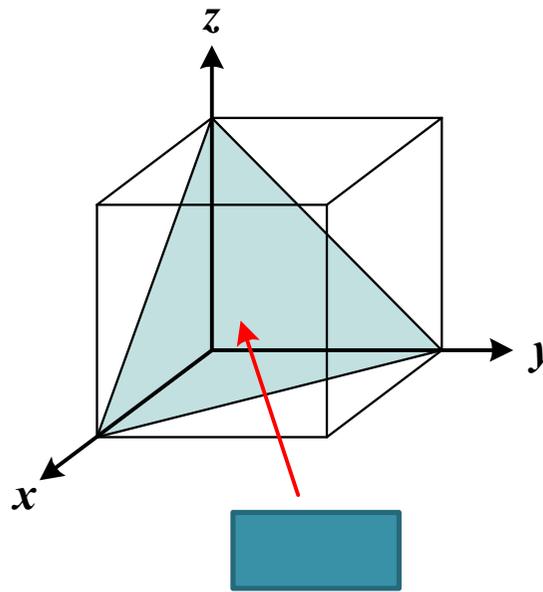
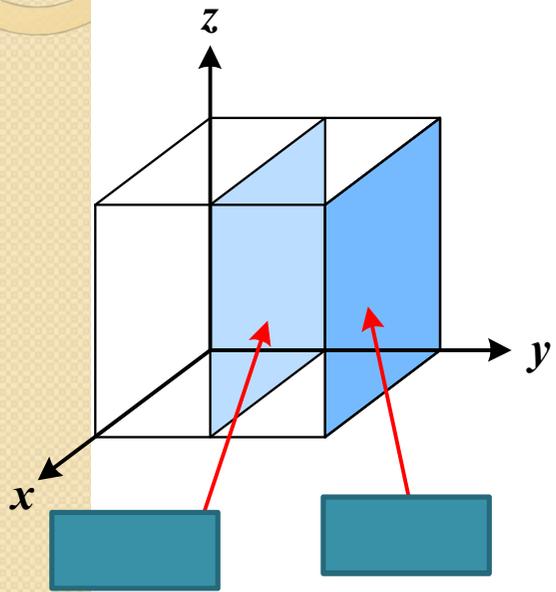
$$\langle 100 \rangle \equiv [100], [010], [001], [\bar{1}00], [0\bar{1}0], [00\bar{1}]$$

음의 지수는 숫자위에 가로줄(bar)을 그어 반대방향

(예) $[\bar{1}\bar{2}0]$



Examples



- **$\{h k l\}$: planes of a form**

(ex) equivalent planes for cubic symmetry

$$\{100\} = (100) + (010) + (001) + (\bar{1}00) + (0\bar{1}0) + (00\bar{1})$$

- Hexagonal의 경우 : $(h k \overline{h+k} l)$ 로 표시 가능함.

예) $(11\bar{2}0) = (110)$ Miller plane

2-5 대칭

대칭요소와 대칭조작

대칭요소(symmetry element) :

거울면 (mirror plane)

반전중심(inversion axis)

회전축(rotation axis)

대칭조작(symmetry operation) :

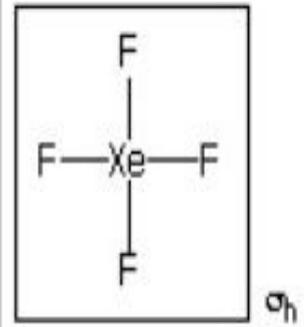
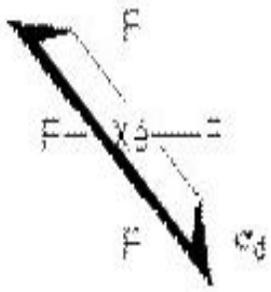
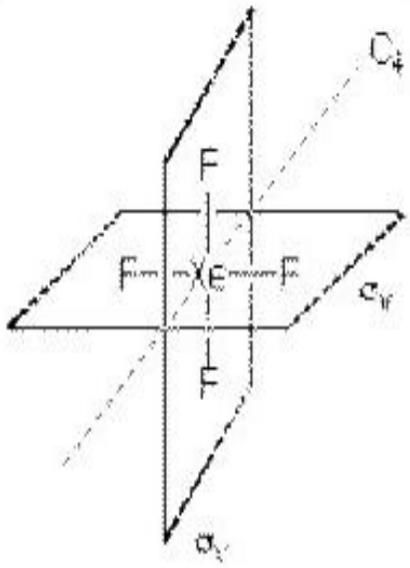
실질적인 거울면, 반사, 축과 점을 중심으로 한 움직임.

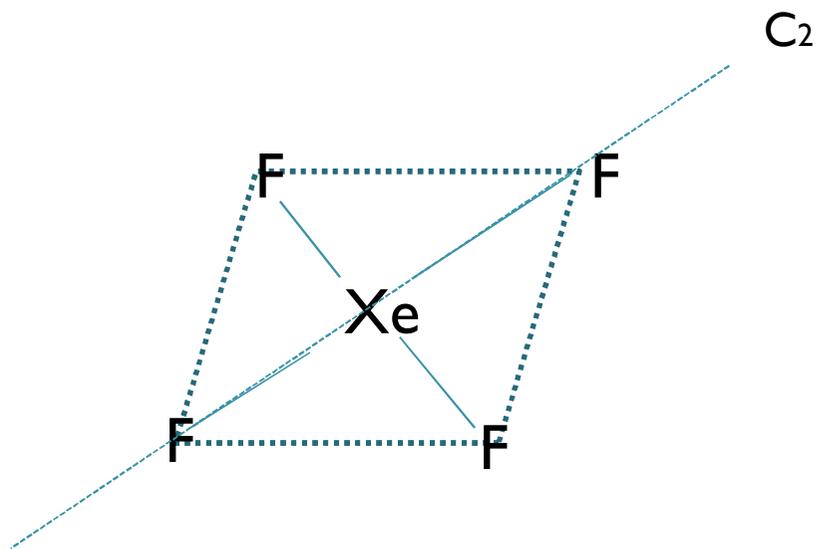
Mirror Plane, σ 거울면

σ_h : horizontal 수평면, 거울면이 주축에 대하여 수직이다.

σ_v : vertical 수직면, 거울면이 주축을 포함한다.

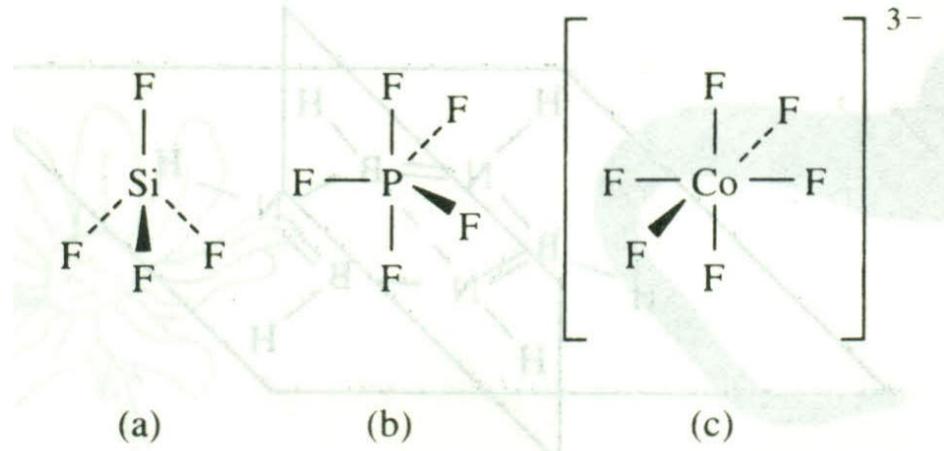
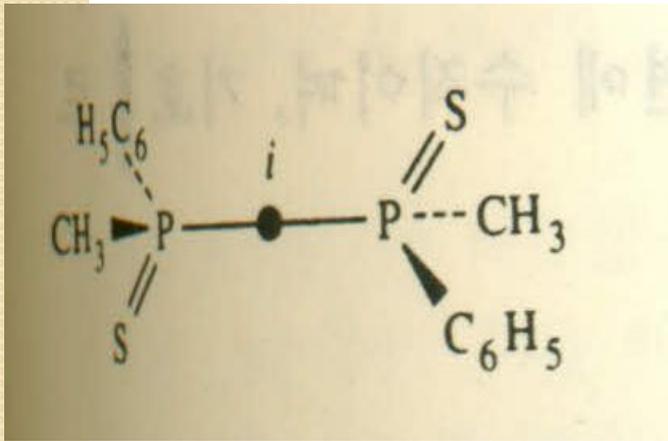
σ_d : 주축에 수직인 C_2 축 사이의 각을 반으로 나누는 반사면.



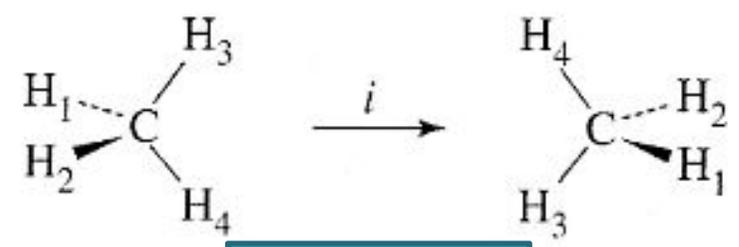
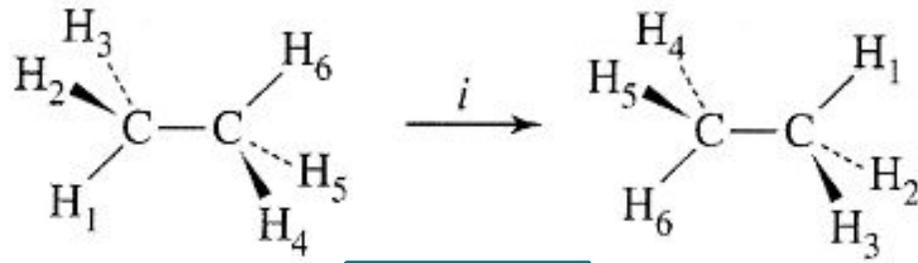


대칭중심, i 반전중심(inversion center)

: 각 점은 분장의 중심점에 대하여 시작점이 반대 방향의 같은 거리로 이동된다.



(c)에만 대칭중심

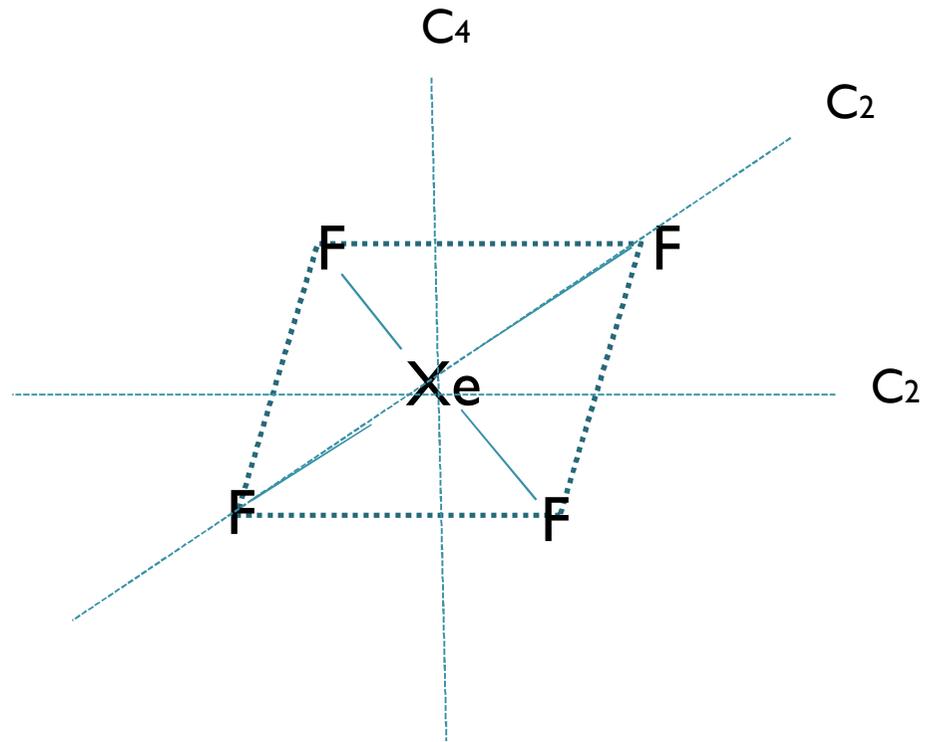


회전축, C_n (rotation operation, proper rotation)

: 분자를 $360^\circ/n$ 만큼 회전시켜, 그 전과 구별이 불가능한

원자의 배열이 되는 경우, 그 분자는 n 겹(n -fold) 회전축을 갖는다.

n 의 order가 제일 높은 것을 z 축의 잡는다.



C₄축을 principal axis로 잡음!

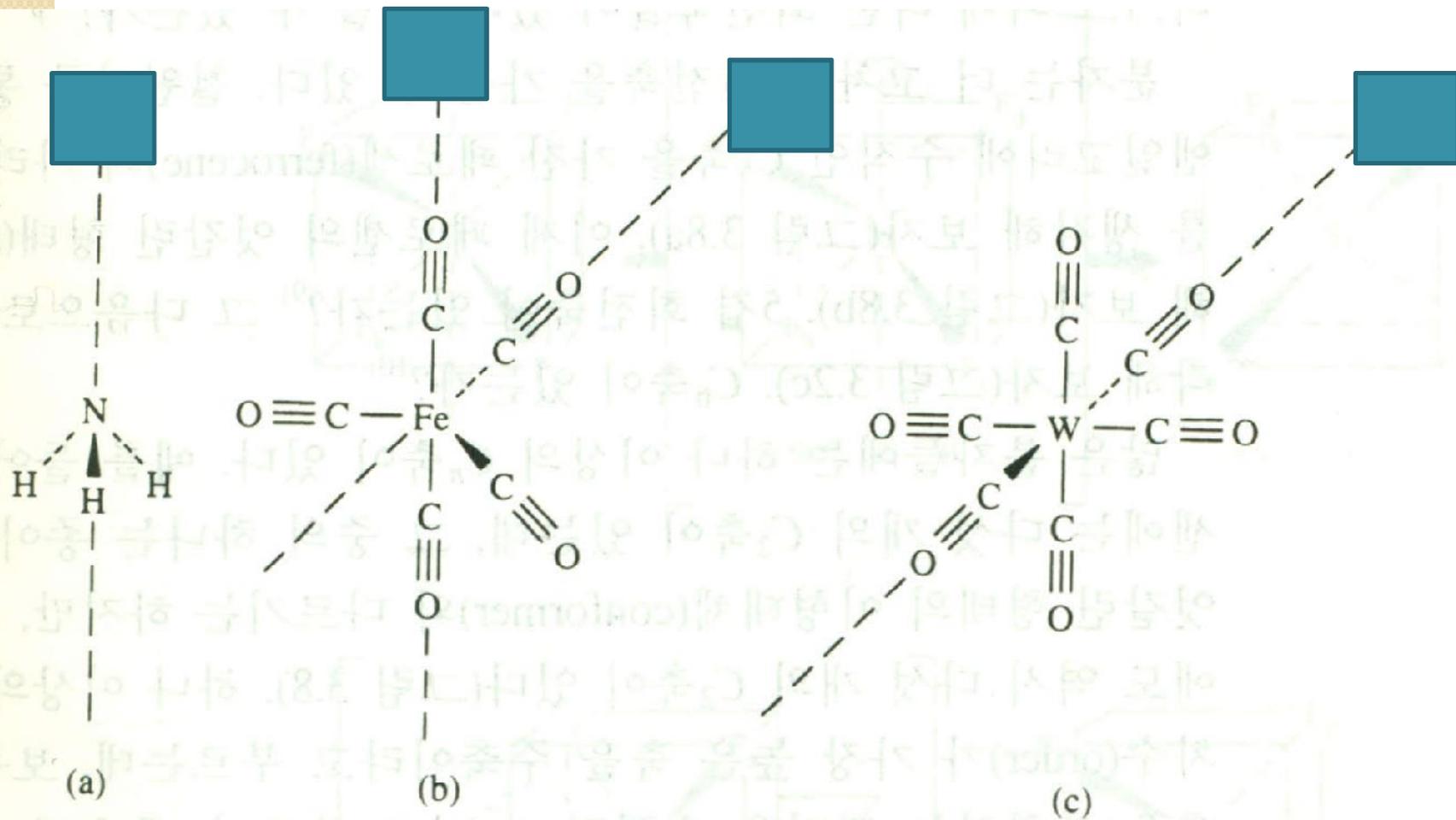
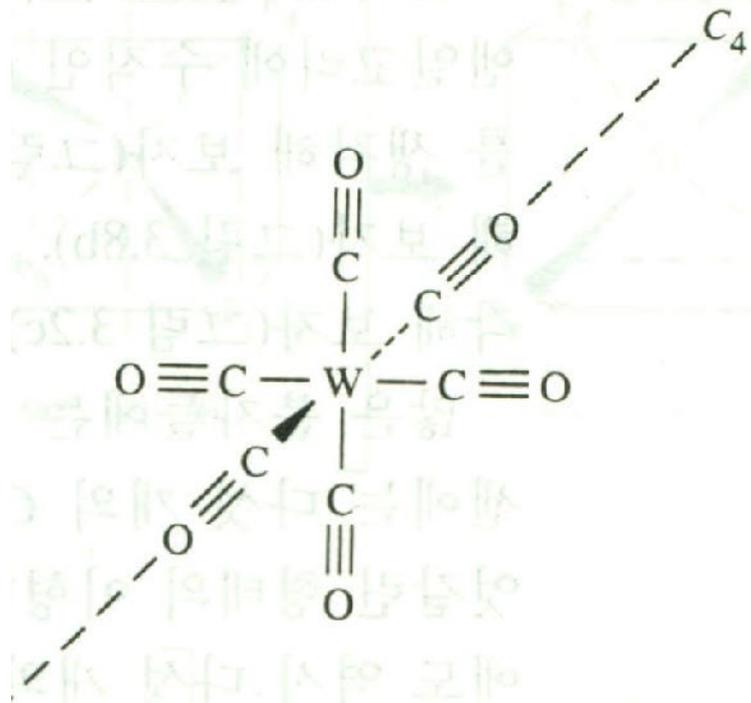


그림 3.7 n 접축이 있는 또 다른 분자들 : (a) 암모니아, (b) pentacarbonyliron, (c) hexacarbonyltungsten.



- 7H C₄
- 7H C₃
- 7H C₂