

적외선 분광법(Infrared spectroscopy) /라만 분광법(Raman spectroscopy)의 이해

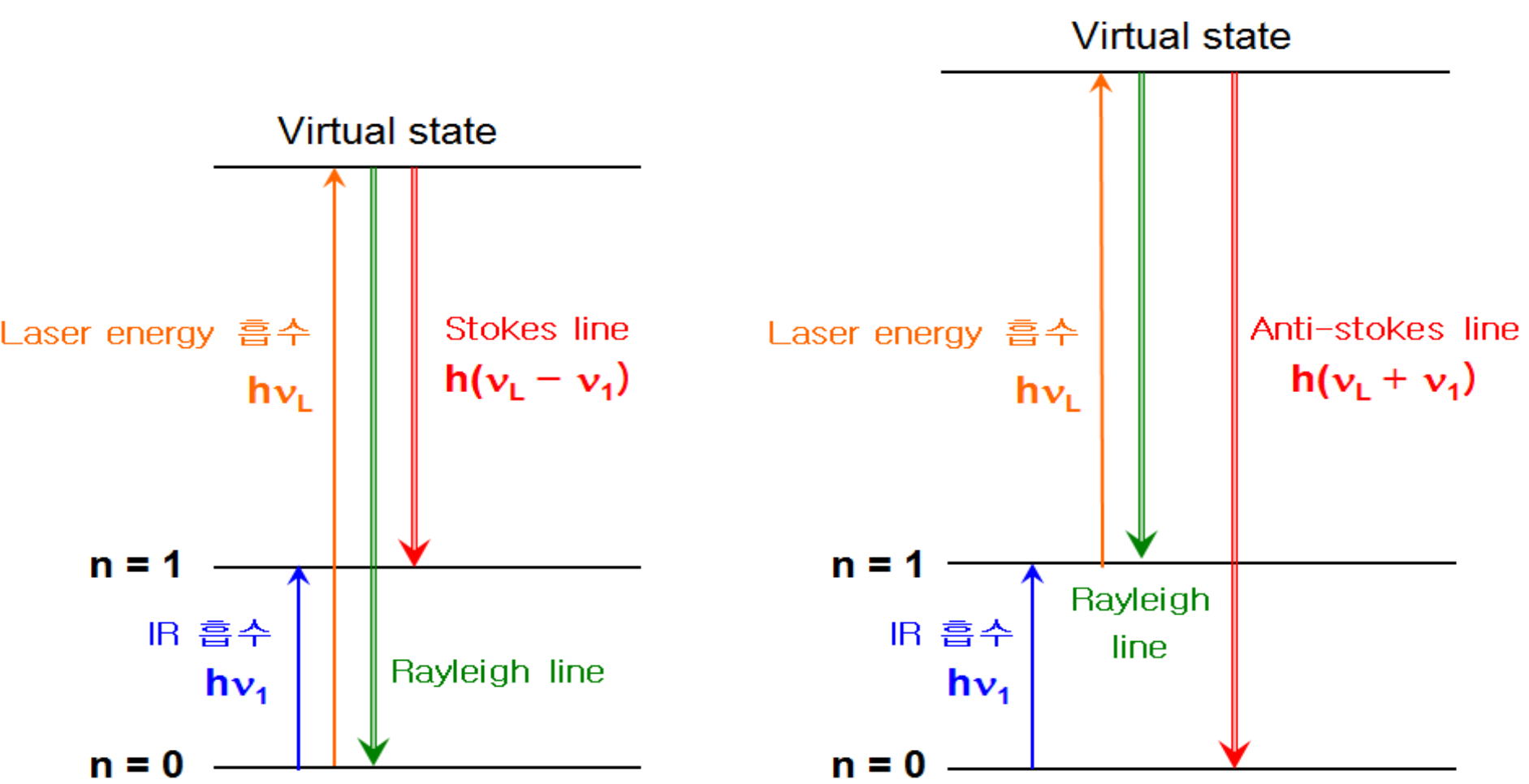
융복합섬유팀



ECO융합섬유연구원
Korea Institute of Convergence Textile

- ★ IR 및 Raman 분광법은 분자분광법으로 원자분광법과 다름 :
분자에너지변화는 전자전이 뿐만 아니라 **분자진동**, 분자회전과 결합세기에 따라서도 변하므로 이들로부터 기하학적 분자구조와 결합에 대한 정보를 제공 받아 해석. 하지만 분자와의 상호작용 메카니즘은 서로 다름.
- ★ IR 분광법은 직접 흡수분광법인 반면 Raman 분광법은 시료분자에 대한 조사광의 두 가지 비탄성적 산란(분자로 에너지 공급을 통한 낮은 에너지로 산란: Stokes선 , 분자로부터 에너지 흡수를 통한 높은 에너지로 산란: Anti-stokes선)복사선의 진동수를 해석하여 분자에너지 준위를 유추하는 분광법.

적외선 분광법(Infrared spectroscopy)/라만 분광법(Raman spectroscopy) (2)

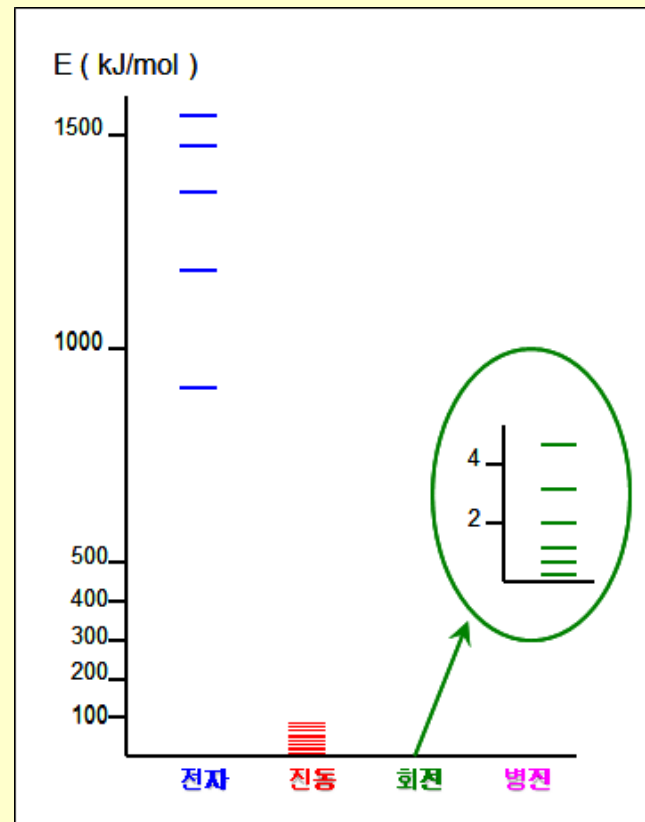


Rayleigh scattering의 진동수(ν_L)에서 Raman shift가 일어난
진동수 차이 ($\pm\nu_1$)가 특정분자의 진동주파수

- ★ IR 및 Raman 둘다 진동주파수에 대한 정보를 제공하지만 전자 전하의 분포와 원자변위의 방향에 따라 IR active와 Raman active가 구분됨. (분자가 대칭중심을 갖는 경우 : IR active인 진동모드는 Raman inactive, Raman active인 진동모드는 IR inactive함)
- ★ IR 분광법 : 분자의 진동모드가 분자의 쌍극자 모멘트를 변화시키면 IR 흡수가 일어남. 광학 이성질체 제외하고 모든 물질 차이.
→ $O=C=O \rightarrow$: IR active, Raman inactive
←
- ★ Raman 분광법 : 복사선과 분자가 에너지전이와 같은 상호작용을 통해 분자의 전자분포가 섭동되어 편극율이 변하는 분자의 진동모드는 Raman active함.
← $O=C=O \rightarrow$: IR inactive, Raman active

- * 격리된 분자의 총 에너지(E_{tot})는 전자 에너지(E_{elec}), 회전 에너지(E_{rot}), 진동 에너지(E_{vib})의 합

$$E_{\text{tot}} = E_{\text{elec}} + E_{\text{rot}} + E_{\text{vib}}$$



적외선 분광법 /라만 분광법 (5)

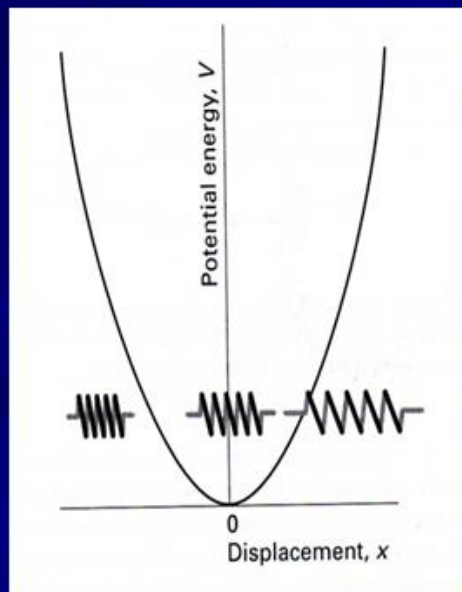
★ 조화진동형 진동운동 조화진동: 평형으로부터 변형에 비례하는 복원력 작용

Hook 법칙 적용됨 $F = ma = m(\partial^2 x / \partial t^2) = -kx$ (k : 힘 상수)

$$v = (\partial x / \partial t) \rightarrow (\partial^2 x / \partial t^2) = (\partial v / \partial t) = (\partial v / \partial x)(\partial x / \partial t) = v(\partial v / \partial x)$$

$$F = mv(\partial v / \partial x) = -kx \rightarrow v(\partial v / \partial x) + (k/m)x = 0$$

$$v^2/2 + (k/2m)x^2 = C_1 \rightarrow v^2 + (k/m)x^2 = C$$



조화진동의 종점 $x = A$ (진폭)에서 운동에너지 및 속력 0

$$(k/m)A^2 = C \rightarrow v^2 + (k/m)x^2 = (k/m)A^2$$

$$v^2 = (k/m)(A^2 - x^2) \rightarrow v = (k/m)^{1/2}(A^2 - x^2)^{1/2} = (\partial x / \partial t)$$

$$(k/m)^{1/2} dt = (A^2 - x^2)^{-1/2} dx \quad \text{적분표} \rightarrow$$

$$\sin^{-1}(x/A) = (k/m)^{1/2}t + C'$$

초기 $t = 0$ 에서 $x = 0$ 이므로 $c' = 0$

$$x = A \sin[(k/m)^{1/2}t] \rightarrow x = A \sin(2\pi vt) = A \sin(\omega t)$$

$$\omega = 2\pi v = (k/m)^{1/2} \rightarrow \text{진동수 } v = (1/2\pi)(k/m)^{1/2}$$

적외선 분광법 /라만 분광법 (6)

★ 조화진동자의 Schrödinger 방정식

$$F = ma = -kx \rightarrow \text{위치에너지 } V = kx^2/2$$

$$(\partial^2 \Psi / \partial x^2) + (2m/\hbar^2)(E - V)\Psi = 0 \rightarrow (\partial^2 \Psi / \partial x^2) + (2m/\hbar^2)(E - kx^2/2)\Psi = 0$$

편의상 매개변수 도입 ① $a^4 = (\hbar^2/km)$

$$\textcircled{2} \varepsilon = (2a^2 m E / \hbar^2) = (2mE/\hbar^2) * (\hbar^2/km)^{1/2} = E / [(1/2)\hbar(k/m)^{1/2}] = E / (\hbar\omega/2)$$

$$(\partial^2 \Psi / \partial x^2) + (2m/\hbar^2)(\hbar\omega\varepsilon/2 - kx^2/2)\Psi = (\partial^2 \Psi / \partial x^2) + (mk/\hbar^2)(\hbar\omega\varepsilon/k - x^2)\Psi = 0$$

$$(\partial^2 \Psi / \partial x^2) + (mk/\hbar^2)(\hbar\varepsilon/(mk)^{1/2} - x^2)\Psi = (\partial^2 \Psi / \partial x^2) + (1/a^4)(a^2\varepsilon - x^2)\Psi = 0$$

$$a^2(\partial^2 \Psi / \partial x^2) + (\varepsilon - x^2/a^2)\Psi = 0 \quad \text{독립변수 } x \text{를 } x = ay \text{로 두면}$$

$$(\partial \Psi / \partial x) = (\partial \Psi / \partial y)(\partial y / \partial x) = a^{-1}(\partial \Psi / \partial y) \rightarrow (\partial^2 \Psi / \partial x^2) = a^{-2}(\partial^2 \Psi / \partial y^2)$$

$$a^2(\partial^2 \Psi / \partial x^2) + (\varepsilon - x^2/a^2)\Psi = 0 \rightarrow (\partial^2 \Psi / \partial y^2) + (\varepsilon - y^2)\Psi = 0$$

점근해법: $(\partial^2 \Psi / \partial y^2) + (1 - y^2)\Psi = 0$ 해인 근사해 $\Psi = A \exp(y^2/2) + B \exp(-y^2/2)$ 변형

y값의 증가에 따라 파동함수가 급격히 증가하는 것은 불가능하므로 $A = 0$

근사해 $\Psi = B \exp(-y^2/2)$ - 변형 $\rightarrow \Psi = \kappa(y) \exp(-y^2/2)$ 진짜 해

$$(\partial \Psi / \partial y) = \exp(-y^2/2)(\partial \kappa / \partial y) - y\kappa(y)\exp(-y^2/2)$$

$$(\partial^2 \Psi / \partial y^2) = \exp(-y^2/2)(\partial^2 \kappa / \partial y^2) - 2y\exp(-y^2/2)(\partial \kappa / \partial y) - \kappa(y)\exp(-y^2/2)$$

$$+ y^2\kappa(y)\exp(-y^2/2) = \exp(-y^2/2)[(\partial^2 \kappa / \partial y^2) - 2y(\partial \kappa / \partial y) + y^2\kappa(y) - \kappa(y)]$$

$$\exp(-y^2/2)[(\partial^2 \kappa / \partial y^2) - 2y(\partial \kappa / \partial y) + y^2\kappa(y) - \kappa(y)] + (\varepsilon - y^2)\kappa(y)\exp(-y^2/2) = 0$$

적외선 분광법 /라만 분광법 (7)

$$\exp(-y^2/2)[(\partial^2 \kappa / \partial y^2) - 2y(\partial \kappa / \partial y) + y^2 \kappa(y) - \kappa(y)] + (\epsilon - y^2) \kappa(y) \exp(-y^2/2) = 0$$

$$\exp(-y^2/2)[(\partial^2 \kappa / \partial y^2) - 2y(\partial \kappa / \partial y) + (\epsilon - 1) \kappa] = 0 \quad \text{Hermite 방정식}$$

$$\kappa(y) = \sum a_n y^n = a_0 + a_1 y + a_2 y^2 + a_3 y^3 + \dots$$

$$(\partial \kappa / \partial y) = a_1 + 2a_2 y + 3a_3 y^2 + 4a_4 y^3 + \dots$$

$$(\partial^2 \kappa / \partial y^2) = (1 \times 2)a_2 + (2 \times 3)a_3 y + (3 \times 4)a_4 y^2 + \dots$$

$$[2a_2 + (\epsilon - 1)a_0] + [(2 \times 3)a_3 + (\epsilon - 3)a_1]y + [(3 \times 4)a_4 + (\epsilon - 5)a_2]y^2 + \dots = 0$$

y 또한 독립변수이므로 식이 성립되기 위해선 모든 계수가 0이어야 함

$$(2 \times 1)a_2 + (\epsilon - 1)a_0 = 0$$

$$(2 \times 3)a_3 + (\epsilon - 3)a_1 = 0$$

$$(3 \times 4)a_4 + (\epsilon - 5)a_2 = 0$$

$$(4 \times 5)a_5 + (\epsilon - 7)a_3 = 0$$

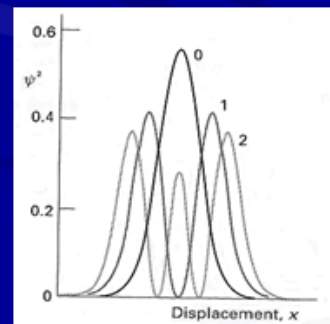
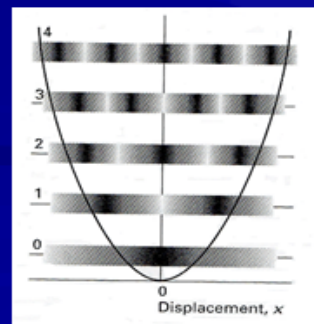
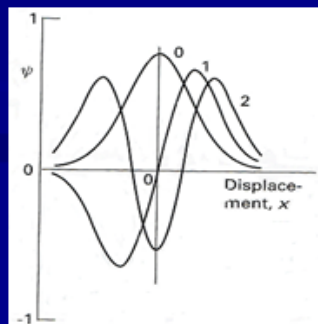
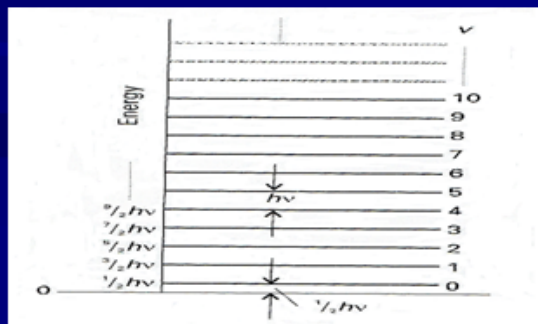
$$\text{일반식 } (n + 1)(n + 2)a_{n+2} + (\epsilon - 1 - 2n)a_n = 0$$

경계조건 $y = \infty$ 에선 $\Psi = 0$ 이어야 하지만 $\Psi(\infty) = \kappa(\infty)\exp(-\infty/2) = \infty$

따라서 $\kappa(y)$ 가 무한급수이어선 안돼요 따라서 $\epsilon = 2n + 1 \quad n = 0, 1, 2, 3, \dots$

$$\epsilon = E/(\hbar\omega/2) \rightarrow E = \epsilon \hbar\omega/2 = (n + \frac{1}{2})\hbar\omega = (n + \frac{1}{2})\hbar(2\pi\nu) = (n + \frac{1}{2})h\nu$$

진동운동에너지 역시 양자화!! $\rightarrow E = (v + \frac{1}{2})h\nu, v = 0, 1, 2, 3, \dots$ (진동 양자수)



적외선 분광법 /라만 분광법 (8)

★ 고리 상 파동/입자의 회전운동 반경 r , 각운동량 $J = pr = \hbar r/\lambda$

$$E = p^2/2m = \hbar^2/2mr^2 = \hbar^2/2I \quad (I : \text{관성모멘트})$$

순환경계조건: 고리 상 파동의 생존 $\rightarrow 2\pi r = n\lambda$ 이어야 함, $n = 0, 1, 2, \dots$

$J = \hbar r/\lambda = nh/2\pi \rightarrow E = n^2\hbar^2/8\pi^2I = n^2\hbar^2/2I$, $n = 0, \pm 1, \pm 2, \dots$ 회전방향

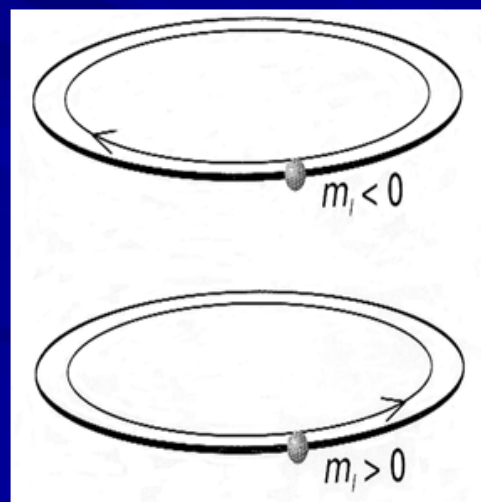
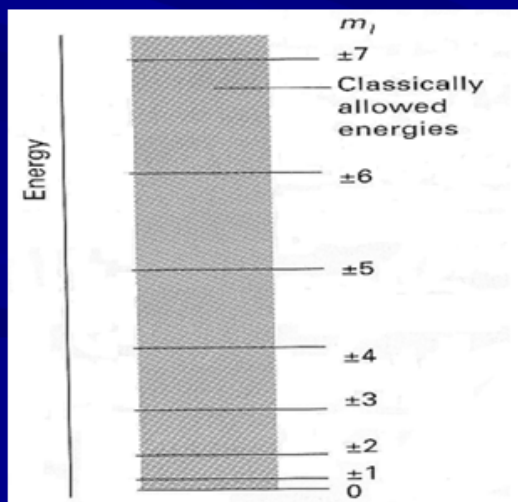
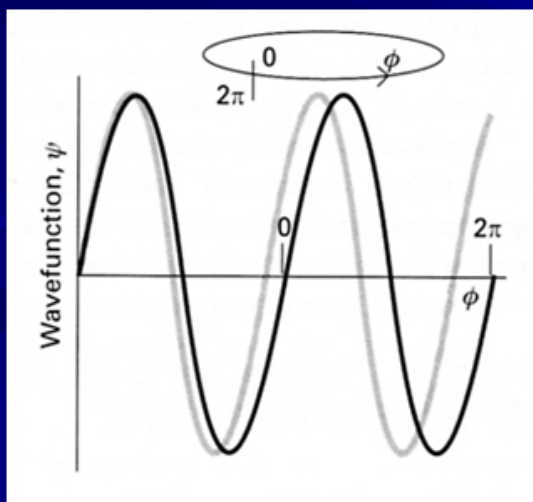
병진운동과 달리 $n = 0$ 가 존재하는 이유? + 와 -가 공존하므로 상쇄

$$E = m_\ell^2\hbar^2/8\pi^2I = m_\ell^2\hbar^2/2I, \quad m_\ell = 0, \pm 1, \pm 2, \dots \quad (\text{자기 양자수})$$

입자의 회전운동 에너지 양자화

축퇴 : $m_\ell = +1$ 또는 -1 어느 쪽이어도 동일 에너지

$$J = m_\ell\hbar/2\pi = m_\ell\hbar, \quad m_\ell = 0, \pm 1, \pm 2, \dots$$



적외선 분광법 /라만 분광법 (9)

★ $r = r_0$ 로 고정된 3차원 회전

$$-(\hbar^2/2m)[(1/r^2)(\partial/\partial r)r^2(\partial R(r)\Theta(\theta)\Phi(\phi)/\partial r) + (1/r^2\sin^2\theta)(\partial^2 R(r)\Theta(\theta)\Phi(\phi)/\partial \phi^2) + (1/r^2\sin\theta)(\partial/\partial \theta)\sin\theta(\partial R(r)\Theta(\theta)\Phi(\phi)/\partial \theta)] = E R(r)\Theta(\theta)\Phi(\phi)$$

$$-(\hbar^2/2mr_0^2)[(1/\sin^2\theta)(\partial^2 \Theta(\theta)\Phi(\phi)/\partial \phi^2) + (1/\sin\theta)(\partial/\partial \theta)\sin\theta(\partial \Theta(\theta)\Phi(\phi)/\partial \theta)] = E \Theta(\theta)\Phi(\phi)$$

$$(1/\sin^2\theta)(\partial^2 \Theta(\theta)\Phi(\phi)/\partial \phi^2) + (1/\sin\theta)(\partial/\partial \theta)\sin\theta(\partial \Theta(\theta)\Phi(\phi)/\partial \theta) = -(2mr_0^2 E/\hbar^2) \Theta(\theta)\Phi(\phi)$$

$$(\partial^2 \Theta(\theta)\Phi(\phi)/\partial \phi^2) + \sin\theta(\partial/\partial \theta)\sin\theta(\partial \Theta(\theta)\Phi(\phi)/\partial \theta) + (2mr_0^2 E/\hbar^2)*\sin^2\theta*\Theta(\theta)\Phi(\phi) = 0$$

$\Theta(\theta)$ 와 $\Phi(\phi)$ 는 독립함수이므로 양변을 $\Theta(\theta)\Phi(\phi)$ 로 나누기

$$\Theta(\theta)*(\partial^2 \Phi(\phi)/\partial \phi^2) + \Phi(\phi)*\sin\theta(\partial/\partial \theta)\sin\theta(\partial \Theta(\theta)/\partial \theta) + (2mr_0^2 E/\hbar^2)*\sin^2\theta*\Theta(\theta)\Phi(\phi) = 0$$

$$(1/\Phi(\phi))*(\partial^2 \Phi(\phi)/\partial \phi^2) + (1/\Theta(\theta))*\sin\theta(\partial/\partial \theta)\sin\theta(\partial \Theta(\theta)/\partial \theta) + (2mr_0^2 E/\hbar^2)*\sin^2\theta = 0$$

$$(1/\Theta(\theta))*\sin\theta(\partial/\partial \theta)\sin\theta(\partial \Theta(\theta)/\partial \theta) + (2mr_0^2 E/\hbar^2)*\sin^2\theta = -[(1/\Phi(\phi))*(\partial^2 \Phi(\phi)/\partial \phi^2)]$$

좌변은 θ 함수로만 구성

우변은 ϕ 함수로만 구성

↓
두 개의 독립변수 함수가 동일할 수 있는 유일한 방법은 동일한 상수

↓

Legendre 함수 $(1/\Theta(\theta))*\sin\theta(\partial/\partial \theta)\sin\theta(\partial \Theta(\theta)/\partial \theta) + (2mr_0^2 E/\hbar^2)*\sin^2\theta = m_\ell^2$

$$(1/\Theta(\theta))*\sin\theta(\partial/\partial \theta)\sin\theta(\partial \Theta(\theta)/\partial \theta) + m_\ell^2*\sin^2\theta = m_\ell^2$$

적외선 분광법 / 라만 분광법 (10)

Legendre 배다함수 $(1/\Theta(\theta)) * \sin\theta(\partial/\partial\theta)\sin\theta(\partial\Theta(\theta)/\partial\theta) + m_\ell^2 * \sin^2\theta = m_\ell^2$
 $\sin\theta(\partial/\partial\theta)\sin\theta(\partial\Theta(\theta)/\partial\theta) + m_\ell^2 * [\sin^2\theta - 1] * \Theta(\theta) = 0$
 $\sin^2\theta * (\partial^2\Theta(\theta)/\partial\theta^2) + \sin\theta * \cos\theta * (\partial\Theta(\theta)/\partial\theta) + m_\ell^2 * [\sin^2\theta - 1] * \Theta(\theta) = 0$
 $(\partial^2\Theta(\theta)/\partial\theta^2) + (\cos\theta/\sin\theta) * (\partial\Theta(\theta)/\partial\theta) + m_\ell^2 * [1 - (1/\sin^2\theta)] * \Theta(\theta) = 0$

↓

Legendre 배다함수의 조건부 해 $(2mr_0^2E/\hbar^2) = \ell(\ell+1)$
 조건 ① $\ell = 0, 1, 2, 3, \dots$ 조건 ② $|m_\ell| \leq \ell$

↓

$E = \ell(\ell+1) * (\hbar^2/2mr_0^2)$, $\ell = 0, 1, 2, 3, \dots$ (궤도 각운동량 양자수, 방위 양자수)

$m_\ell = -\ell, -\ell+1, -\ell+2, \dots, -1, 0, 1, \dots, \ell-2, \ell-1, \ell$ (자기 양자수)

에너지는 ℓ 에 의해서 결정되고 m_ℓ 에는 무관 $\rightarrow m_\ell$ 이 다른 동일한 에너지의 파동함수가
 $2\ell + 1$ 개 존재

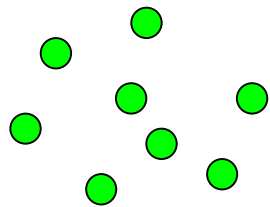
$$-(\hbar^2/2mr_0^2) [(1/\sin^2\theta)(\partial^2\Theta(\theta)\Phi(\phi)/\partial\phi^2) + (1/\sin\theta)(\partial/\partial\theta)\sin\theta(\partial\Theta(\theta)\Phi(\phi)/\partial\theta)] =$$

$$\ell(\ell+1) * (\hbar^2/2mr_0^2) * \Theta(\theta)\Phi(\phi)$$

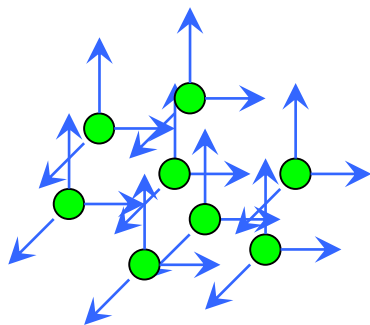
$$(1/\sin^2\theta)(\partial^2\Theta(\theta)\Phi(\phi)/\partial\phi^2) + (1/\sin\theta)(\partial/\partial\theta)\sin\theta(\partial\Theta(\theta)\Phi(\phi)/\partial\theta) = -\ell(\ell+1) * \Theta(\theta)\Phi(\phi)$$

★ $r = r_0$ 로 고정된 2차원 회전の場合 : 1개 양자수 $\rightarrow m_\ell$

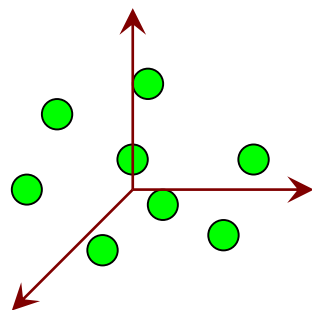
★ $r = r_0$ 로 고정된 3차원 회전の場合 : 2개 양자수 $\rightarrow \ell, m_\ell$



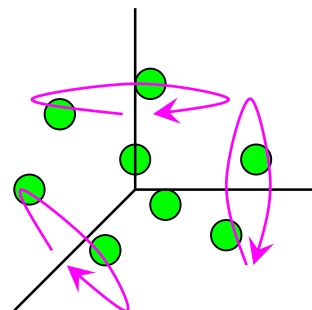
N개의 원자로 구성된
비선형 분자



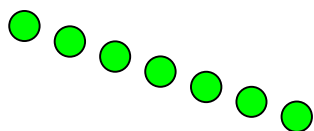
전체자유도 : $3N$ 개



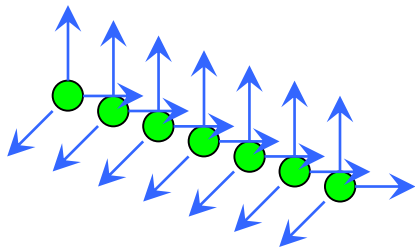
전체 비선형 분자의
병진자유도 : 3 개



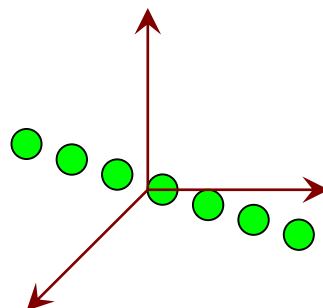
전체 비선형 분자의
회전자유도 : 3 개



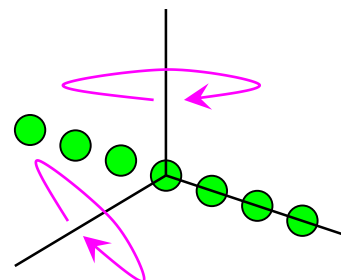
N개의 원자로 구성된
선형 분자



전체자유도 : $3N$ 개



전체 선형 분자의
병진자유도 : 3 개

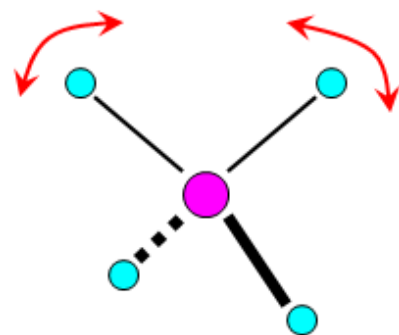


전체 선형 분자의
회전자유도 : 2 개

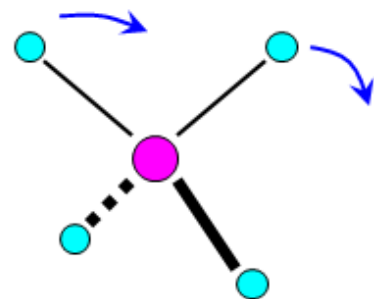
N개의 원자로 구성된 비선형 분자의 진동자유도 : $3N - 3 - 3 = 3N - 6$

N개의 원자로 구성된 선형 분자의 진동자유도 : $3N - 3 - 2 = 3N - 5$

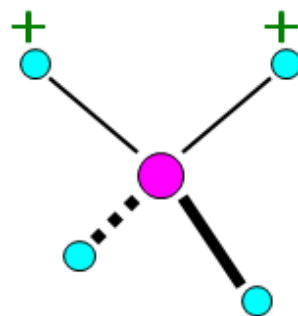
분자진동의 종류 해석 A : [예시 CH₄] $3 \times 5 - 6 = 9$



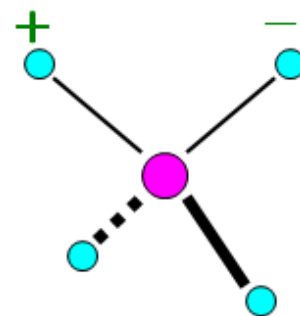
Scissoring



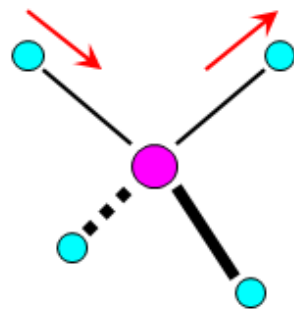
Rocking



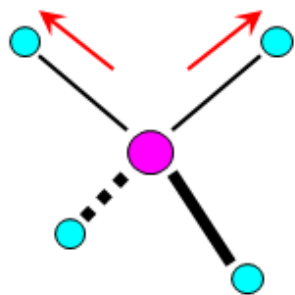
Wagging



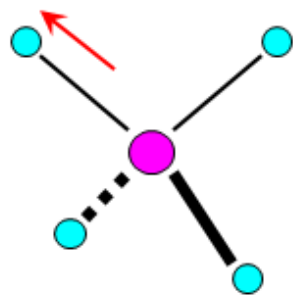
Twisting



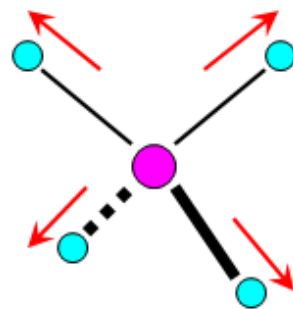
Asymmetric stretching



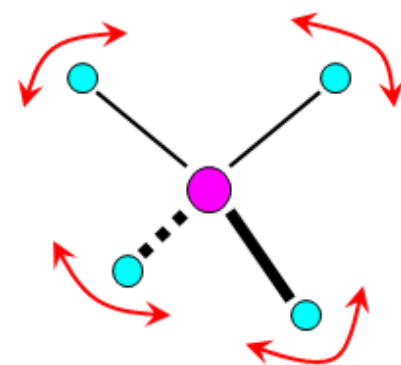
Symmetric stretching



Stretching
1 or 3

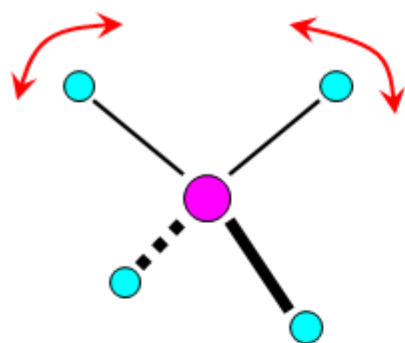


Stretching
4

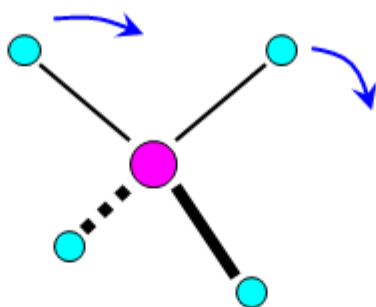


Double
scissoring

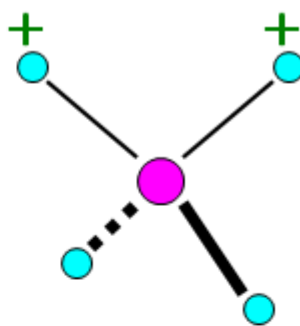
분자진동의 종류 해석 B : [예시 CH_4] $3 \times 4 - 6 = 6$ (자기중심인 C의 부동 처리)



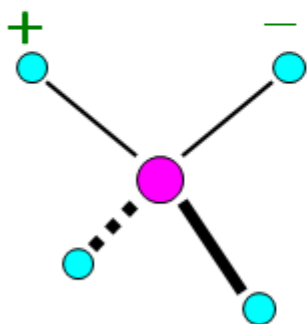
Scissoring



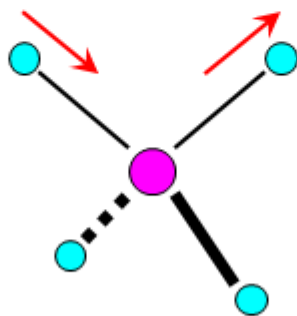
Rocking



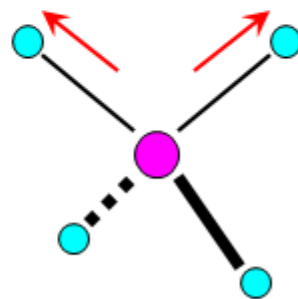
Wagging



Twisting

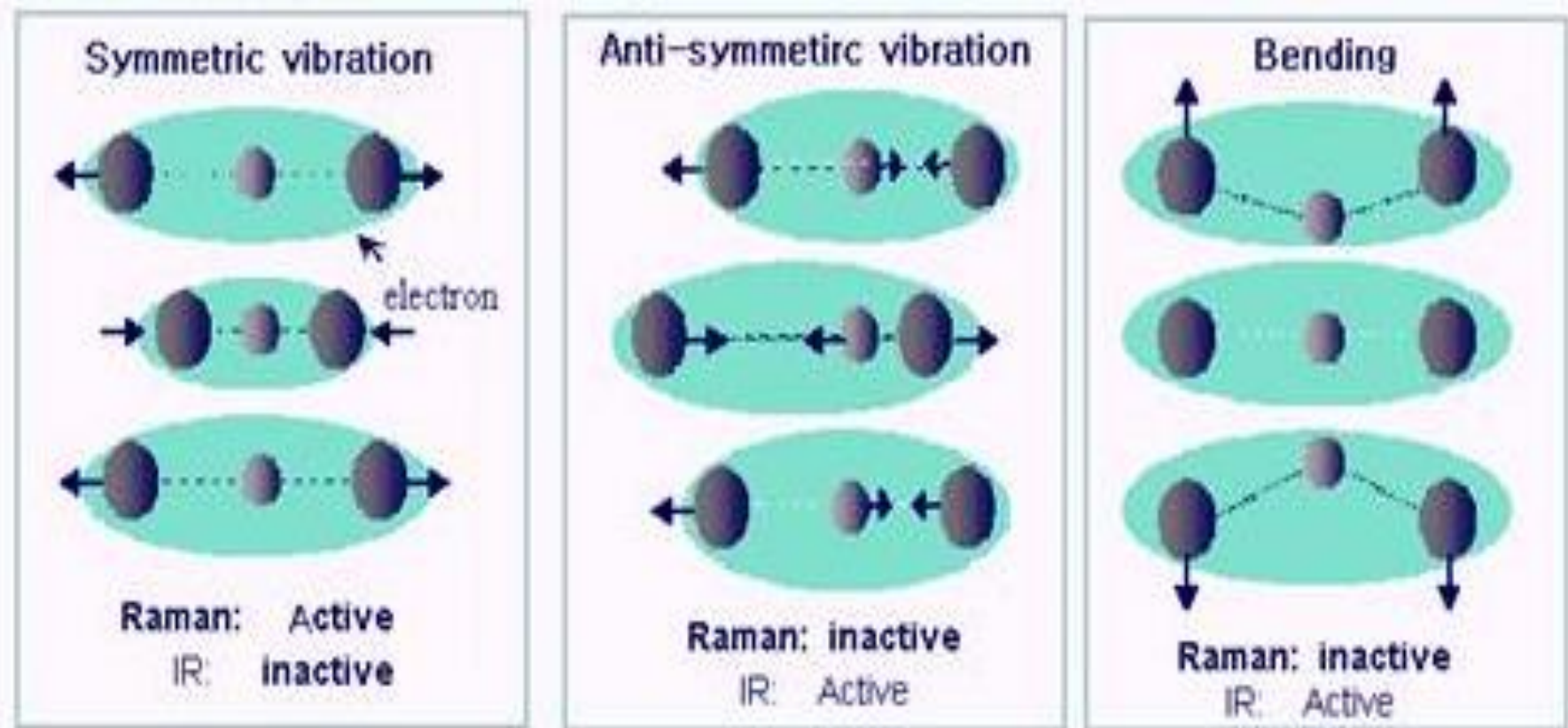


Asymmetric
stretching



Symetric
stretching

적외선 분광법 / 라만 분광법 (11) : CO_2



적외선 분광법 (Infrared spectroscopy) (1)

* **근적외선** ($0.75\sim 3\mu\text{m}$), **적외선** ($3\sim 25\mu\text{m}$), **원적외선** ($25\mu\text{m}$ 이상) 파장을 지닌 전자기 복사선

* **적외선 분광법**: 시료의 분자 진동수와 직결되는 파장의 적외선을 시료가 흡수하는 현상을 이용하여 물질 종류, 물질 구조를 분석하는 방법

시료의 다양한 화학결합 단위에서 한 화학결합 단위의 양끝이 다른 원자일 경우
이 화학결합 단위는 특정 주파수에 진동하는 전기 쌍극자를 형성



비대칭 결합의 기계적 진동수와 동일한 주파수의 전자기 복사선은
그 전기에너지가 화학결합으로 전이되어 화학결합의 진동에너지로 변환
전자기 복사선이 화학결합 단위로 흡수

O_2 , N_2 , Cl_2 와 같이 영구 쌍극자가 없는 비극성 결합은 상호작용 $X = \text{흡수} \times$
진동 동안 분자의 전기 쌍극자 모멘트가 변해야 IR active : 이핵 이원자 분자
흡수 신호의 너비는 들뜬 상태 수명에 반비례 (Heisenberg 불확정성 원리)

적외선 분광법 (Infrared spectroscopy) (2)

- * N개의 원자로 구성된 비선형 분자는 $3N-6$ 개의 진동 모드
- N개의 원자로 구성된 선형 분자는 $3N-5$ 개의 진동 모드

IR inactive

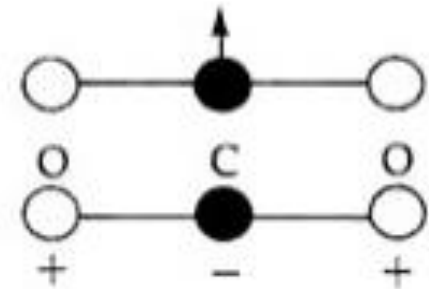


대칭 신축진동

IR active

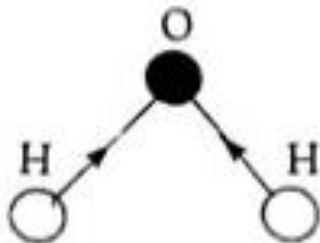


비대칭 신축진동
($2,330\text{cm}^{-1}$)



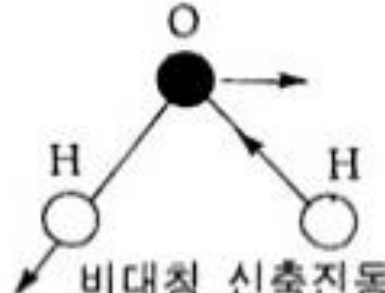
굽힘진동
(667cm^{-1})

IR active



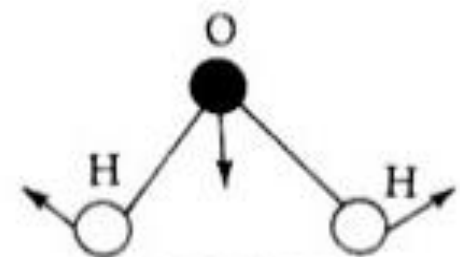
대칭 신축진동
($3,650\text{cm}^{-1}$)

IR active



비대칭 신축진동
($3,760\text{cm}^{-1}$)

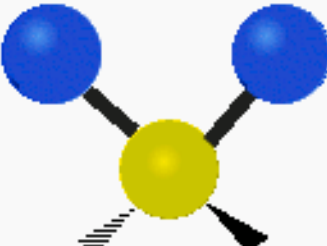
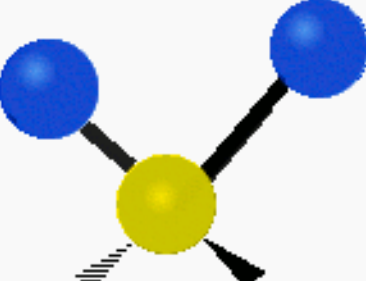
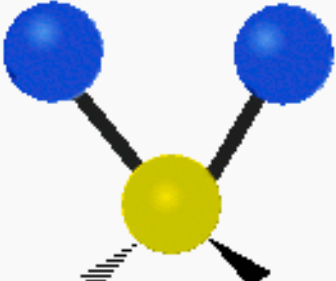
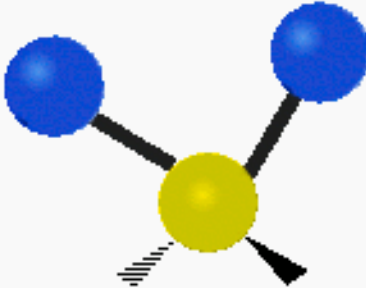
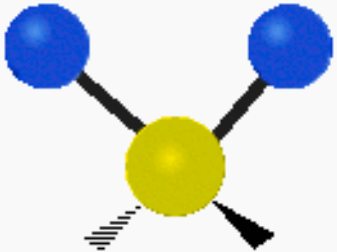
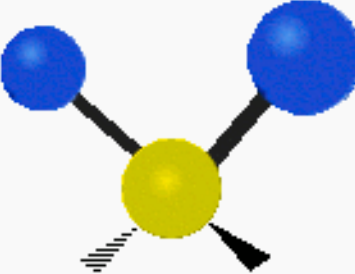
IR active



굽힘진동
($1,595\text{cm}^{-1}$)

적외선 분광법 (Infrared spectroscopy) (3)

$$\text{CH}_2\text{X}_2 : 3 \times 5 - 6 = 9 \rightarrow 3 \times 4 - 6 = 6$$

Symmetrical stretching	Antisymmetrical stretching	Scissoring
		
Rocking	Wagging	Twisting
		

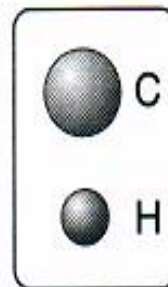
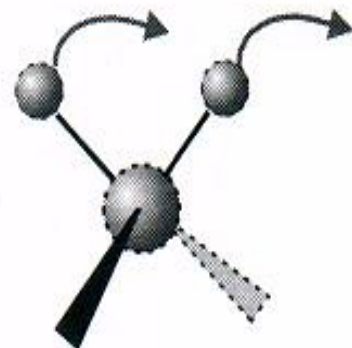
적외선 분광법 (Infrared spectroscopy) (4)



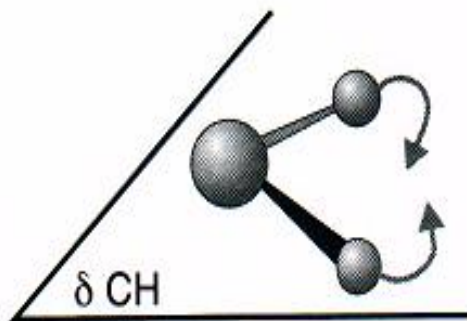
신축 진동 (대칭)



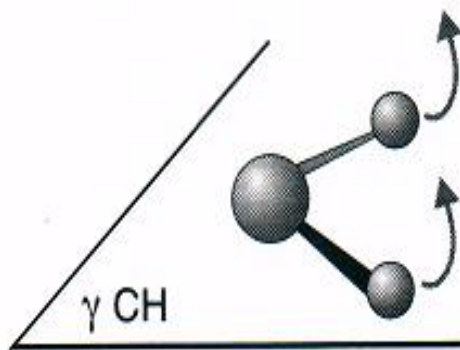
신축 진동 (비대칭)



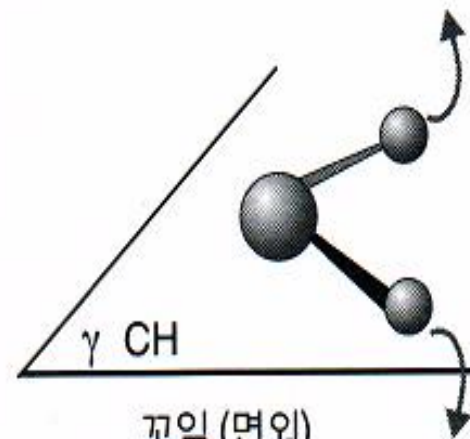
굽힘 진동 : 좌우흔들 (면내)



가위질 (면내)

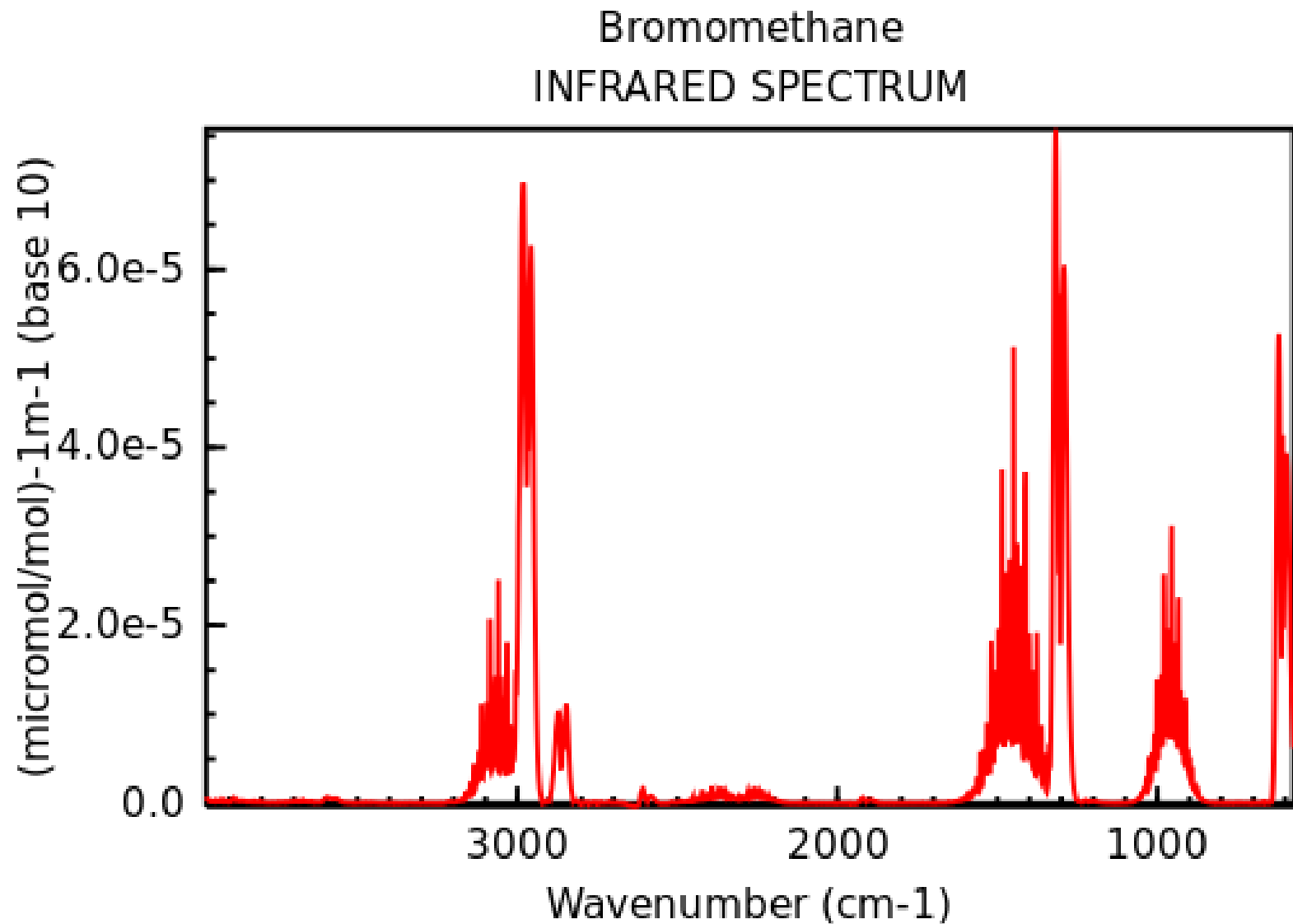


앞뒤흔들 (면외)

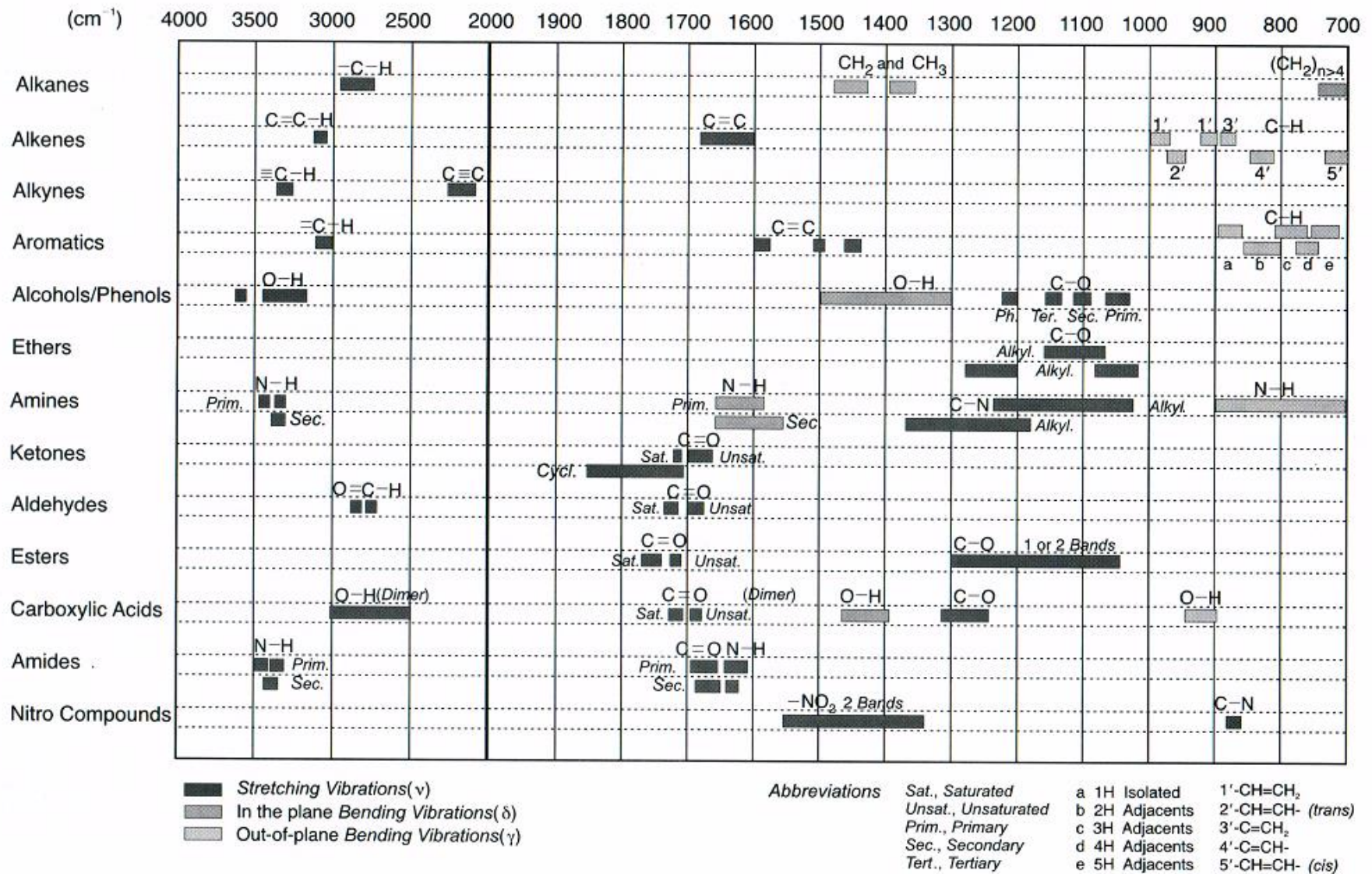


꼬임 (면외)

적외선 분광법 (Infrared spectroscopy) (5)



적외선 분광법 (Infrared spectroscopy) (6)



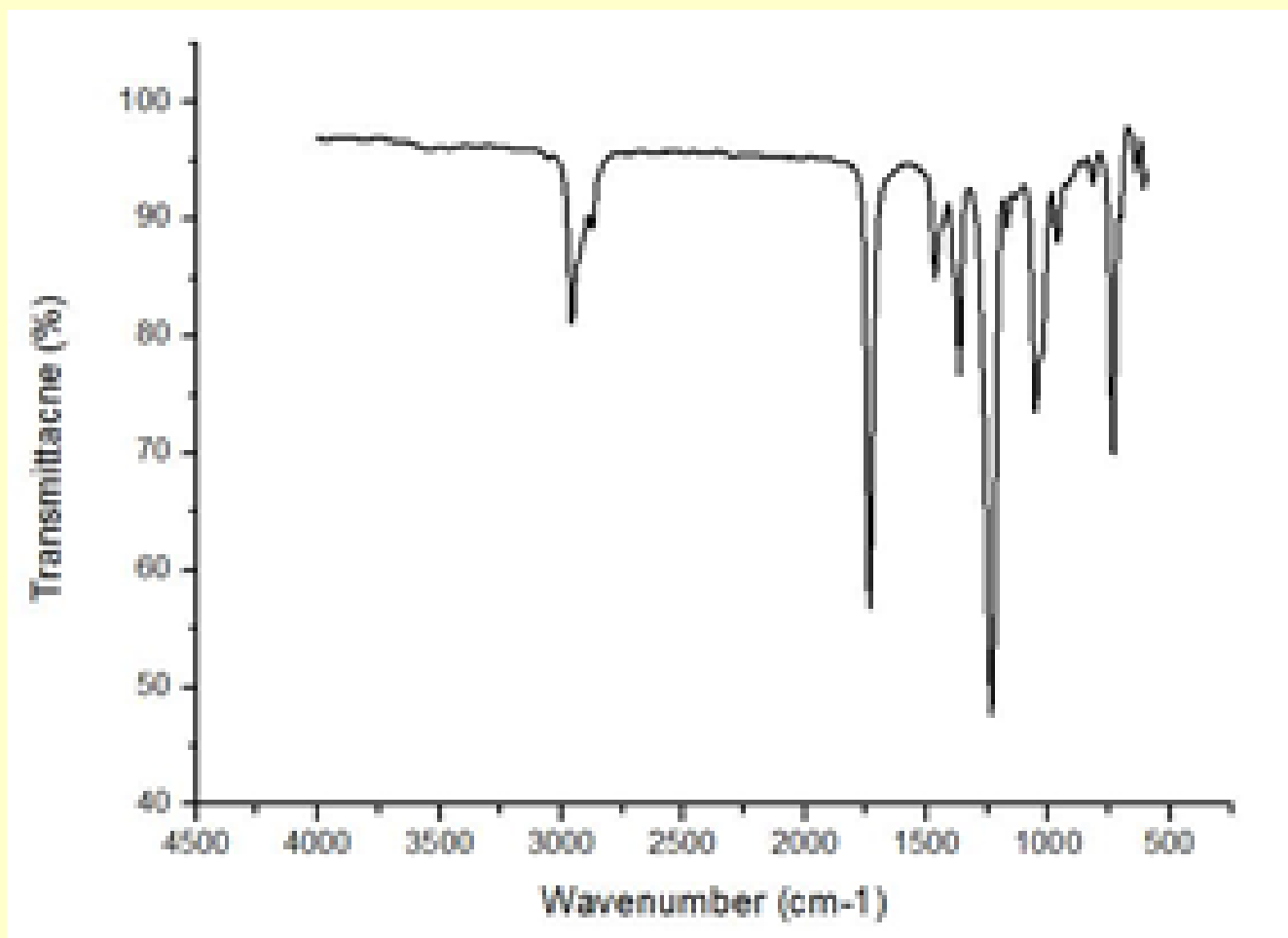
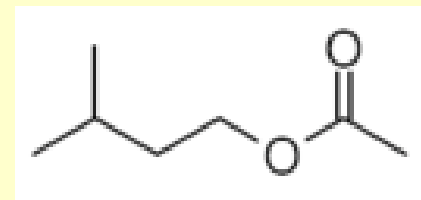
적외선 분광법 (Infrared spectroscopy) (7)

Bond	Type of bond	Specific type of bond	Absorption peak cm^{-1} (nm)	Appearance
C—H	alkyl	methyl	1260 cm^{-1} (7937 nm)	strong
			1380 cm^{-1} (7246 nm)	weak
			2870 cm^{-1} (3484 nm)	medium to strong
		methylene	2980 cm^{-1} (3378 nm)	medium to strong
			1470 cm^{-1} (6803 nm)	strong
			2850 cm^{-1} (3509 nm)	medium to strong
		methine	2925 cm^{-1} (3419 nm)	medium to strong
			2990 cm^{-1} (3460 nm)	weak
			900 cm^{-1} (11111 nm)	strong
	vinyl	C=CH ₂	2975 cm^{-1} (3361 nm)	medium
			3080 cm^{-1} (3247 nm)	medium
			3020 cm^{-1} (3311 nm)	medium
		monosubstituted alkenes	900 cm^{-1} (11111 nm)	strong
			990 cm^{-1} (10101 nm)	strong
			670-700 cm^{-1} (14286-14925 nm)	strong
		trans-disubstituted alkenes	965 cm^{-1} (10363 nm)	strong
			800-840 cm^{-1} (11905-12500 nm)	strong to medium
			3070 cm^{-1} (3257 nm)	weak
	aromatic	benzene / sub-benzene	700-750 cm^{-1} (13333-14286 nm)	strong
			690-710 cm^{-1} (14085-14493 nm)	strong
			750 cm^{-1} (13333 nm)	strong
		ortho-disub. benzene	750-800 cm^{-1} (12500-13333 nm)	strong
			860-900 cm^{-1} (11111-11628 nm)	strong
			800-860 cm^{-1} (11628-12500 nm)	strong
		meta-disub. benzene	750-800 cm^{-1} (12500-13333 nm)	strong
			860-900 cm^{-1} (11111-11628 nm)	strong
			800-860 cm^{-1} (11628-12500 nm)	strong
C—C	alkynes	any	3300 cm^{-1} (3030 nm)	medium
			2720 cm^{-1} (3676 nm)	medium
			2820 cm^{-1} (3546 nm)	medium
	aldehydes	any	1645 cm^{-1} (6079 nm)	medium
			1655 cm^{-1} (6042 nm)	medium
			1660 cm^{-1} (6024 nm)	medium
			1675 cm^{-1} (5970 nm)	medium
			1670 cm^{-1} (5968 nm)	weak
			1600 cm^{-1} (6250 nm)	strong
			1650 cm^{-1} (6061 nm)	strong
			1625 cm^{-1} (6154 nm)	strong
			1600 cm^{-1} (6250 nm)	strong
	acyclic C=C	any	1640-1690 cm^{-1} (5952-6008 nm)	medium
			1450 cm^{-1} (6897 nm)	weak to strong (usually 3 or 4)
			1500 cm^{-1} (6667 nm)	weak to strong (usually 3 or 4)
			1580 cm^{-1} (6329 nm)	weak to strong (usually 3 or 4)
			1600 cm^{-1} (6250 nm)	weak to strong (usually 3 or 4)
			2100-2140 cm^{-1} (4673-4782 nm)	weak
			2190-2260 cm^{-1} (4425-4566 nm)	very weak (often indistinguishable)
			2100-2140 cm^{-1} (4673-4782 nm)	weak
			2190-2260 cm^{-1} (4425-4566 nm)	very weak (often indistinguishable)
			2100-2140 cm^{-1} (4673-4782 nm)	weak
			2190-2260 cm^{-1} (4425-4566 nm)	very weak (often indistinguishable)
	conjugated C=C with benzene ring with C=O	any	1640-1690 cm^{-1} (5952-6008 nm)	medium
			1450 cm^{-1} (6897 nm)	weak to strong (usually 3 or 4)
			1500 cm^{-1} (6667 nm)	weak to strong (usually 3 or 4)
			1580 cm^{-1} (6329 nm)	weak to strong (usually 3 or 4)
			1600 cm^{-1} (6250 nm)	weak to strong (usually 3 or 4)
			2100-2140 cm^{-1} (4673-4782 nm)	weak
			2190-2260 cm^{-1} (4425-4566 nm)	very weak (often indistinguishable)
			2100-2140 cm^{-1} (4673-4782 nm)	weak
			2190-2260 cm^{-1} (4425-4566 nm)	very weak (often indistinguishable)
C=O	aldehyde/ketone	any	1720 cm^{-1} (5814 nm)	strong
			1685 cm^{-1} (5935 nm)	strong
			1665 cm^{-1} (5935 nm)	strong
			1750 cm^{-1} (5714 nm)	strong
			1775 cm^{-1} (5634 nm)	strong
			1720 cm^{-1} (5814 nm)	strong
			1685 cm^{-1} (5935 nm)	strong
			1665 cm^{-1} (5935 nm)	strong
			1750 cm^{-1} (5714 nm)	strong
			1775 cm^{-1} (5634 nm)	strong
			1720 cm^{-1} (5814 nm)	strong
			1685 cm^{-1} (5935 nm)	strong

C—O	aldehydes	1725 cm^{-1} (5797 nm)	influence of conjugation (as with ketones)
		1710 cm^{-1} (5848 nm)	
		1680-1690 cm^{-1} (5917-5952 nm)	
		1735 cm^{-1} (5764 nm)	influenced by conjugation and ring size (as with ketones)
		1760 cm^{-1} (5682 nm)	
		1820 cm^{-1} (5495 nm)	
		1800 cm^{-1} (5556 nm)	
		1650 cm^{-1} (6061 nm)	associated amides
		1550-1610 cm^{-1} (6211-6452 nm)	
		1550-1610 cm^{-1} (6211-6452 nm)	
		1550-1610 cm^{-1} (6211-6452 nm)	
		1550-1610 cm^{-1} (6211-6452 nm)	
	carboxylic acids	1725 cm^{-1} (5797 nm)	
		1710 cm^{-1} (5848 nm)	
		1680-1690 cm^{-1} (5917-5952 nm)	
		1735 cm^{-1} (5764 nm)	
		1760 cm^{-1} (5682 nm)	
		1820 cm^{-1} (5495 nm)	
	alcohols	1040-1060 cm^{-1} (9424-9615 nm)	strong, broad
		~1100 cm^{-1} (~9091 nm)	strong
		1150-1200 cm^{-1} (8333-8696 nm)	medium
		1200 cm^{-1} (8333 nm)	
		1120 cm^{-1} (8929 nm)	
		1220-1260 cm^{-1} (7937-8197 nm)	
	ethers	1250-1300 cm^{-1} (7692-8000 nm)	
		1100-1300 cm^{-1} (7692-9091 nm)	two bands (distinct from ketones, which do not possess a C—O bond)
		1100-1300 cm^{-1} (7692-9091 nm)	
		1100-1300 cm^{-1} (7692-9091 nm)	
		1100-1300 cm^{-1} (7692-9091 nm)	
		1100-1300 cm^{-1} (7692-9091 nm)	

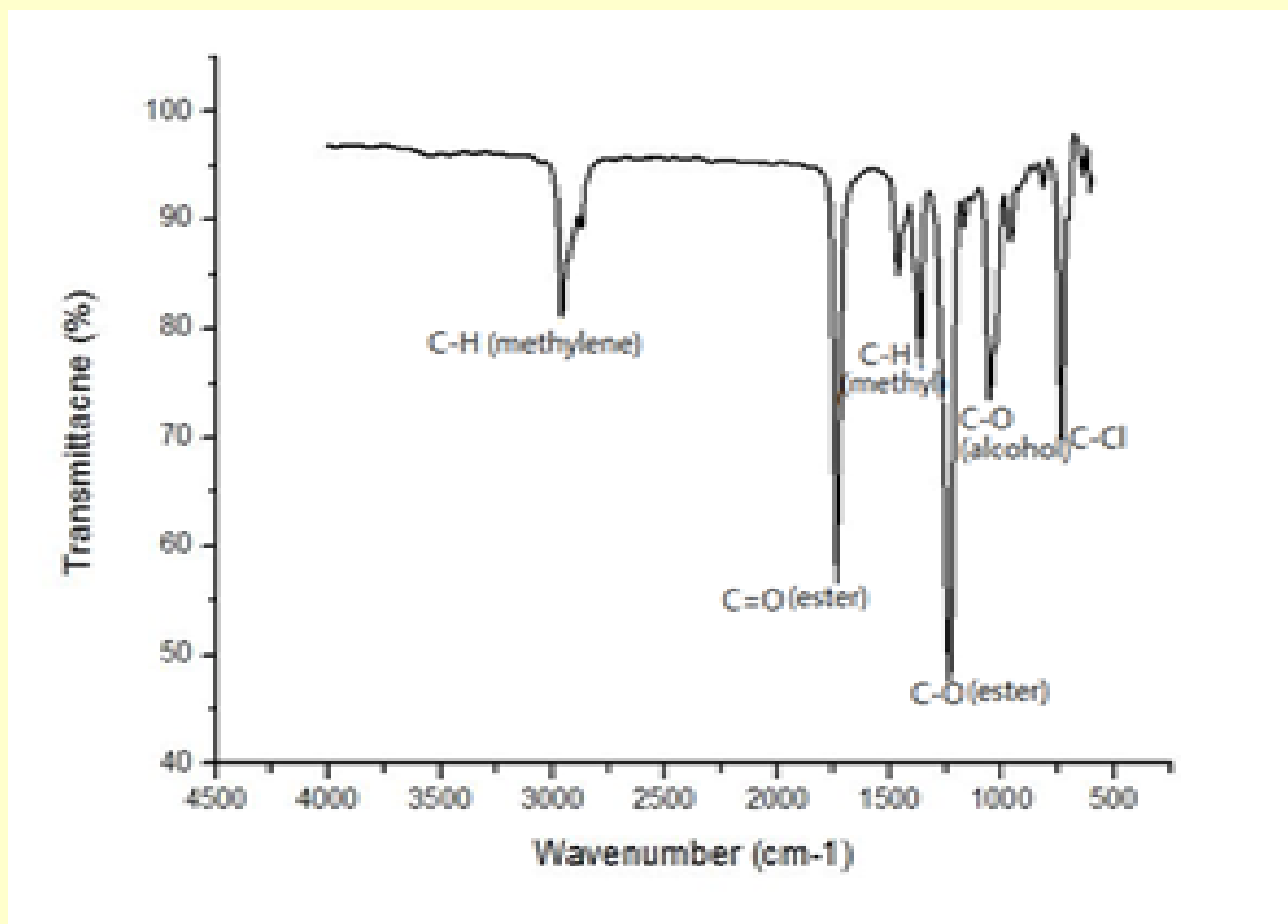
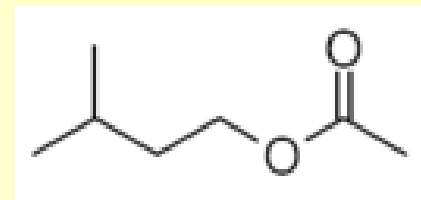
적외선 분광법 (Infrared spectroscopy) (8)

* Isoamyl Acetate : $(\text{CH}_3)_2\text{CH}(\text{CH}_2)_2\text{O}_2\text{CCH}_3$



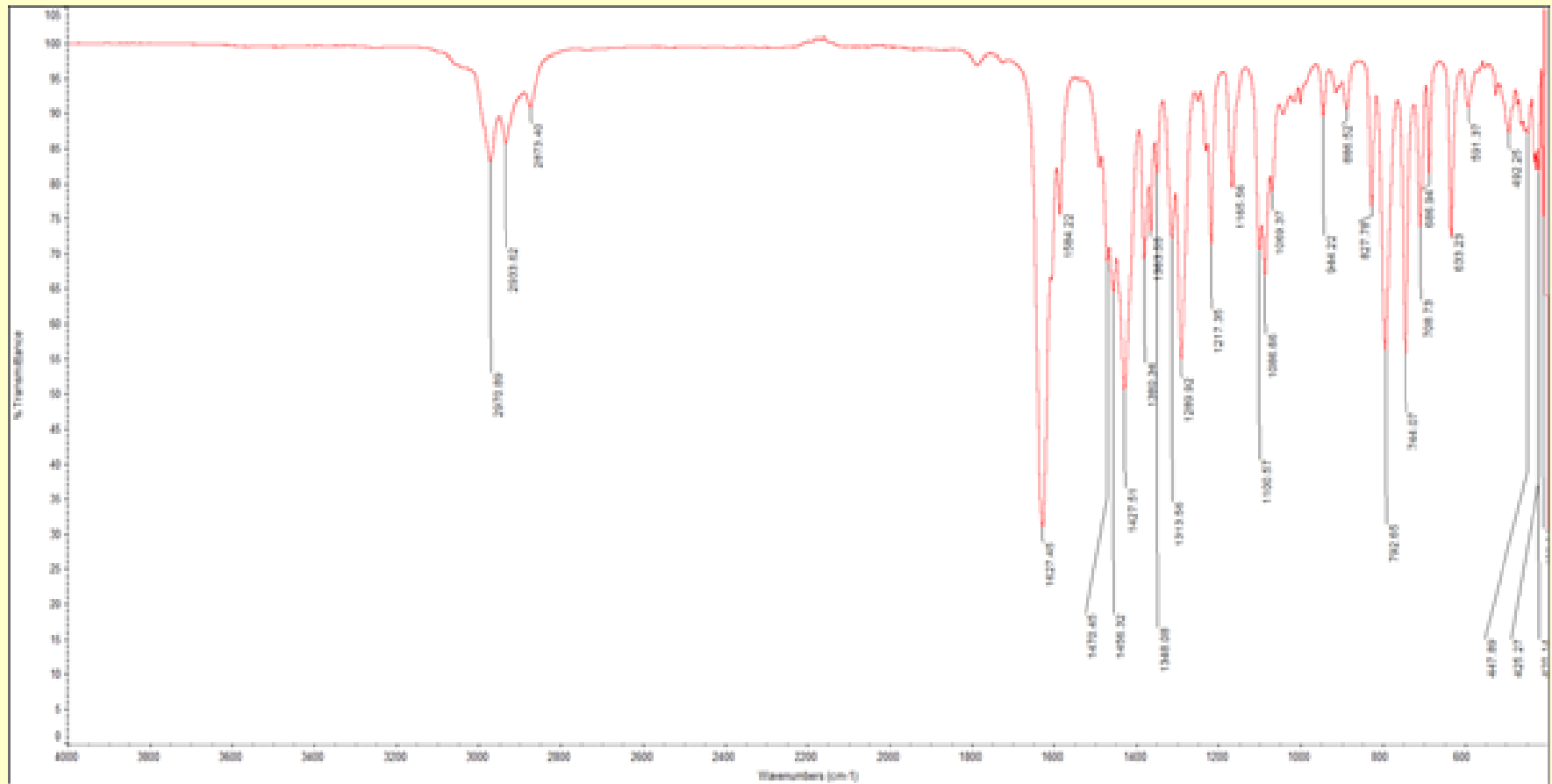
적외선 분광법 (Infrared spectroscopy) (9)

* Isoamyl Acetate : $(\text{CH}_3)_2\text{CH}(\text{CH}_2)_2\text{O}_2\text{CCH}_3$

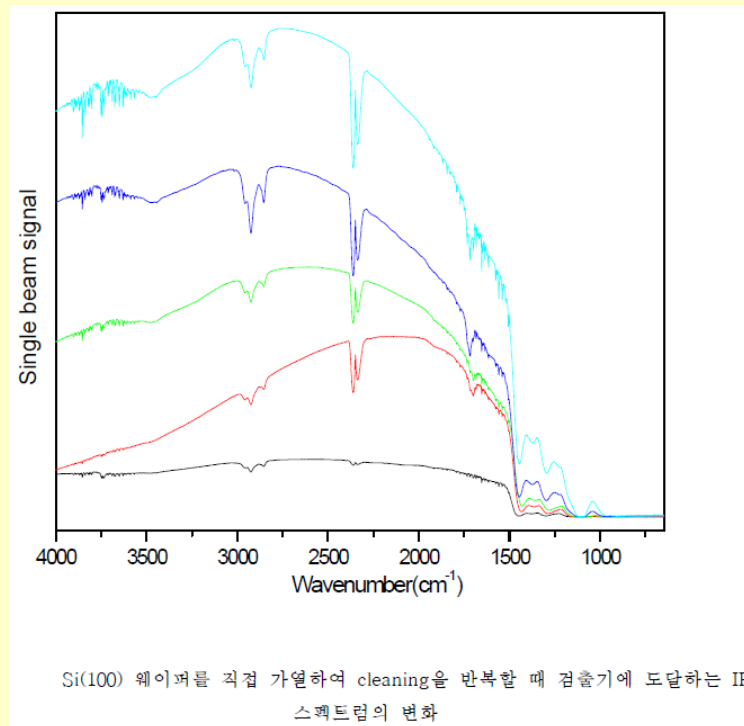
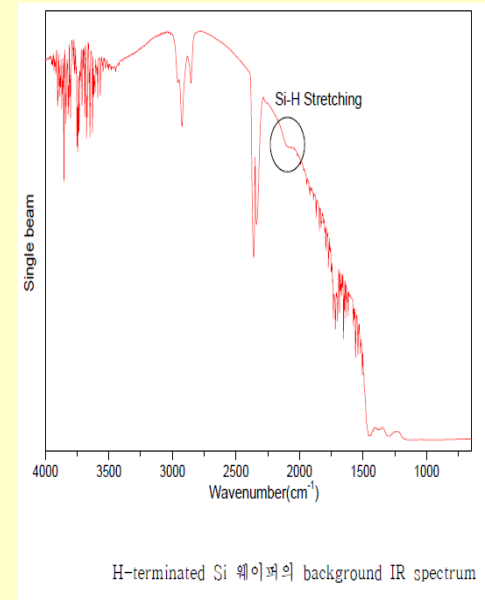
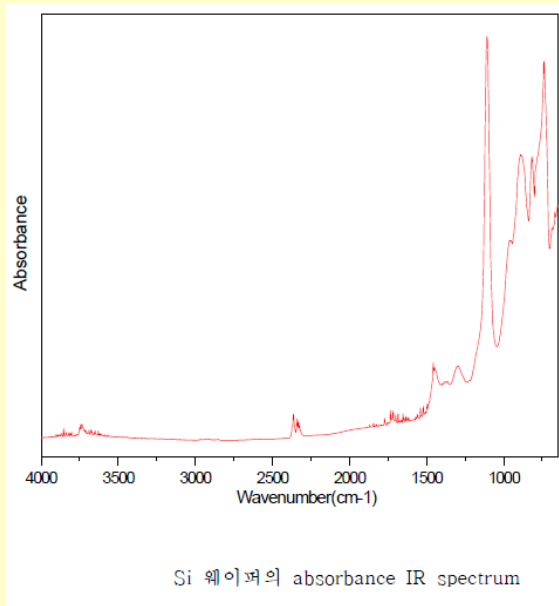


적외선 분광법 (Infrared spectroscopy) (10)

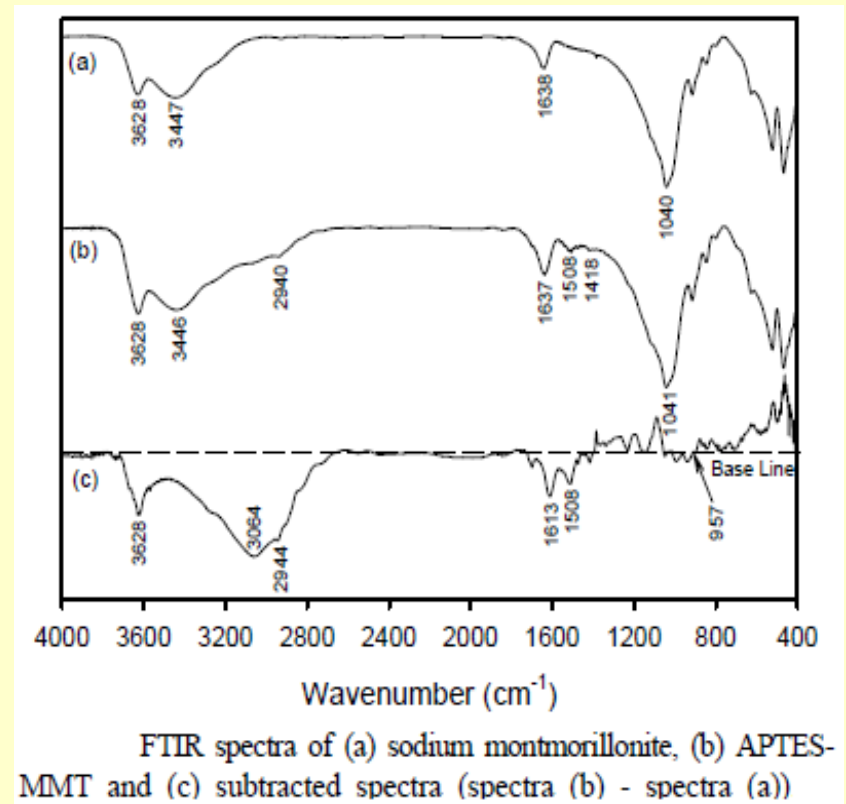
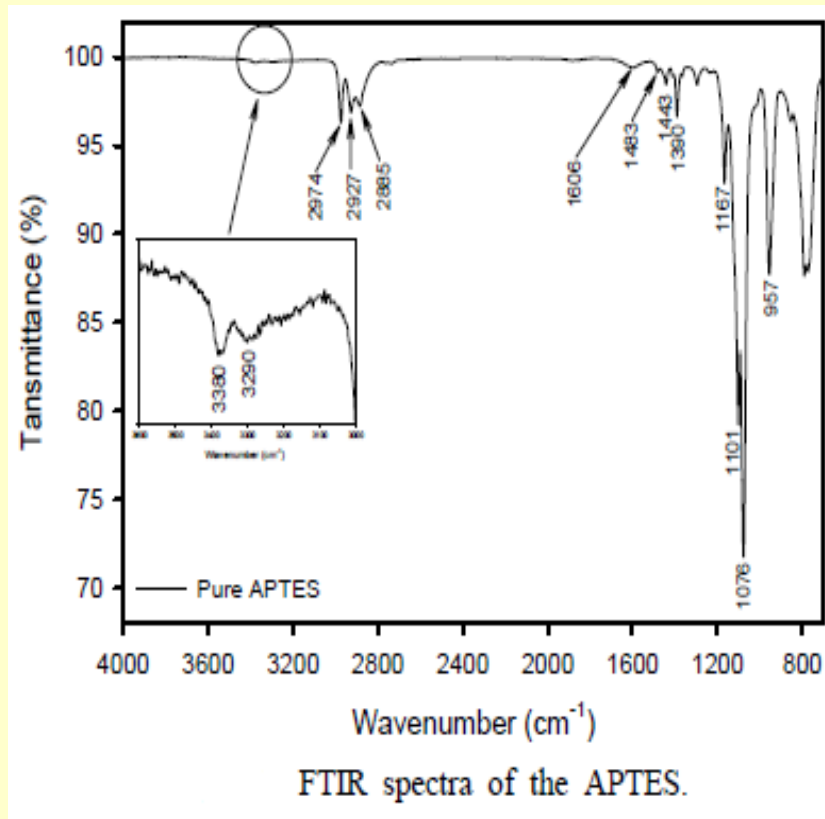
* *N,N*-Diethyl-*m*-Toulamide



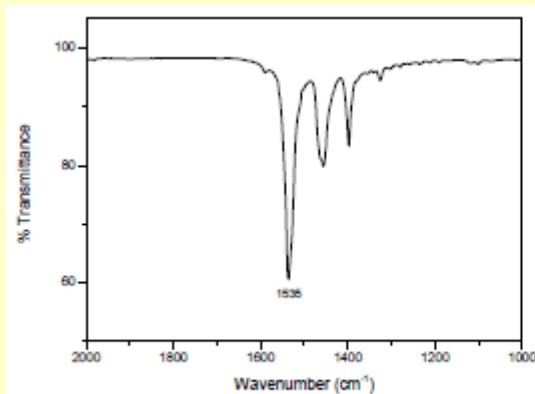
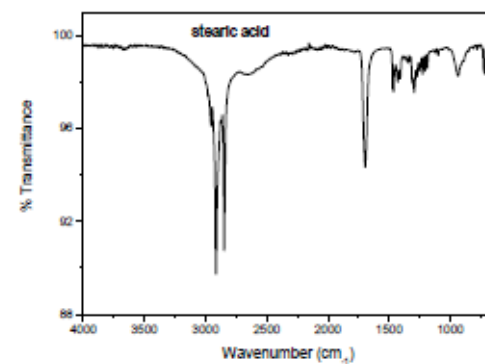
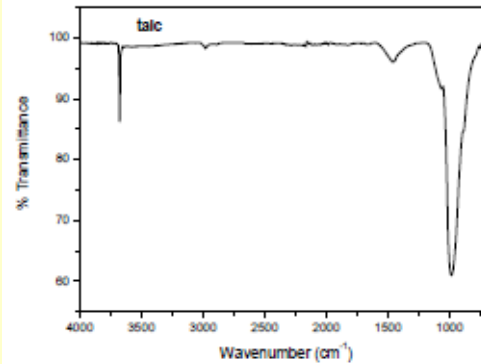
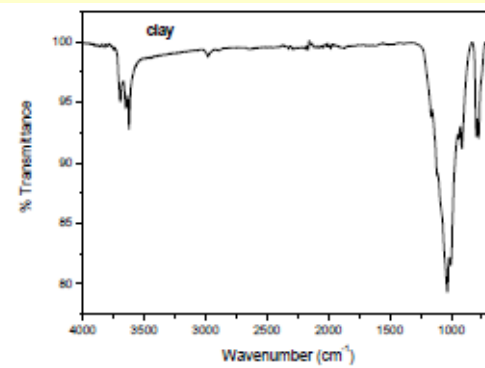
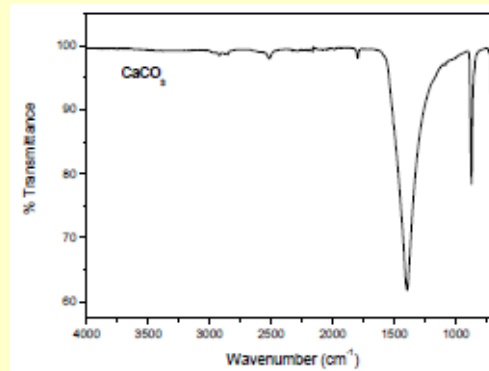
적외선 분광법 (Infrared spectroscopy) (11)



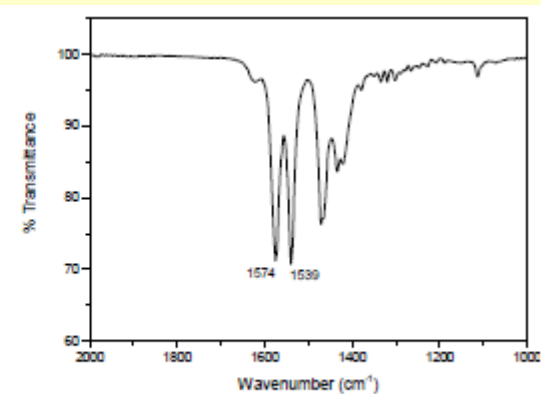
적외선 분광법 (Infrared spectroscopy) (12)



적외선 분광법 (Infrared spectroscopy) (13)

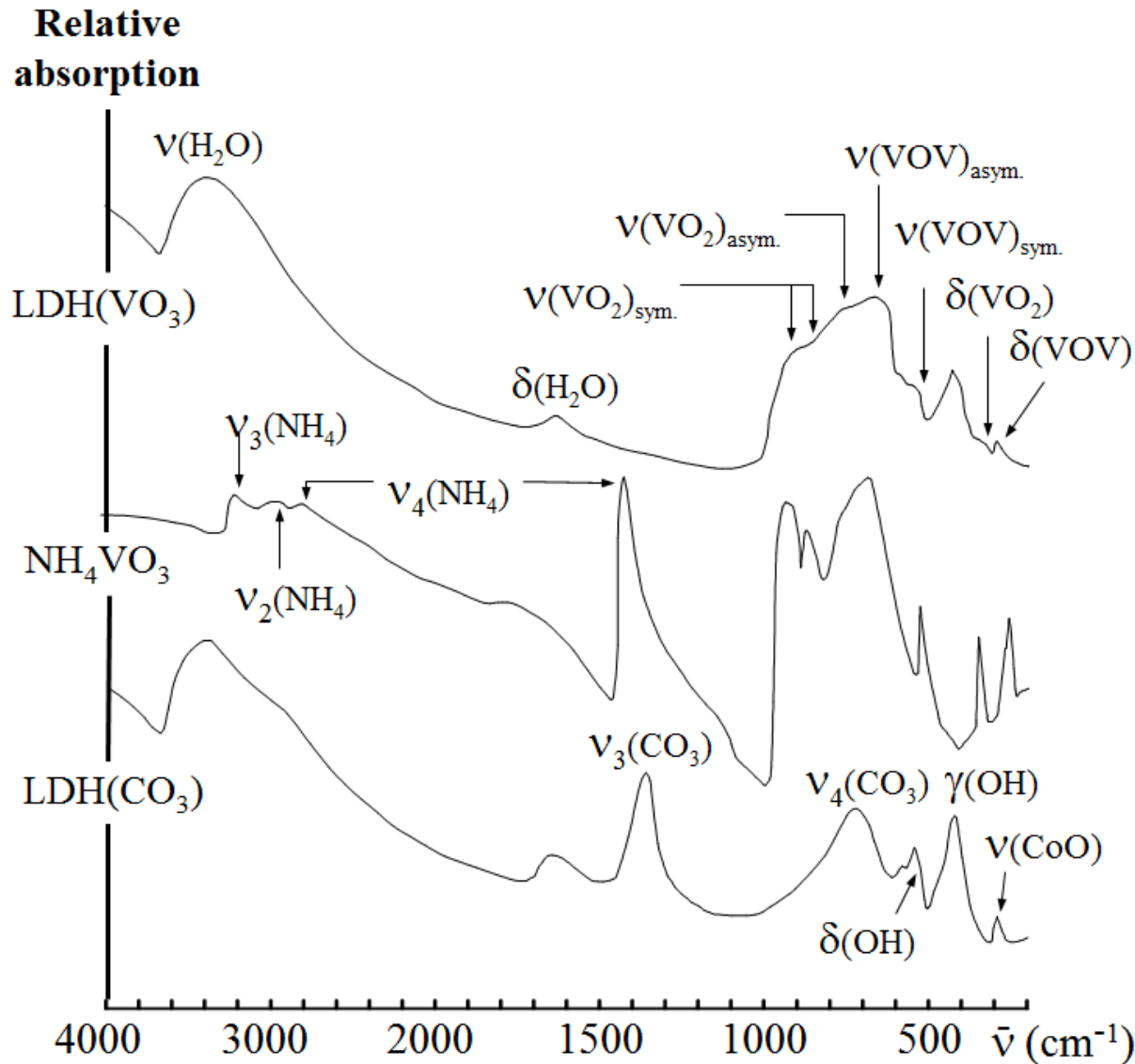


ATR-FTIR spectrum of zinc stearate.



ATR-FTIR spectrum of calcium stearate.

적외선 분광법 (Infrared spectroscopy) (14)

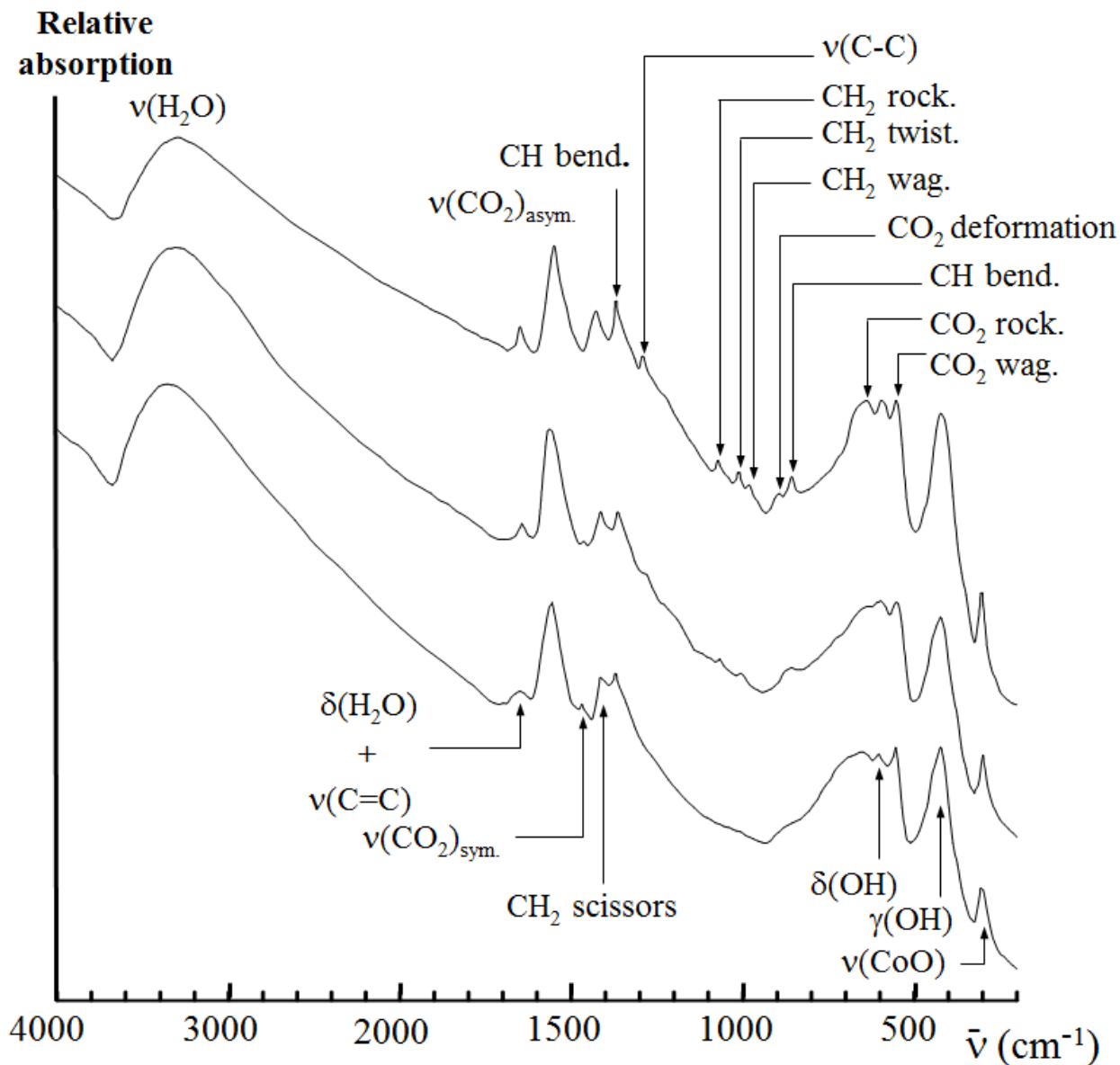


기하학적 안정성 때문에 층상수산화물의 층간 삽입능력이 가장 높은 CO_3^{2-} 의 삽입을 차단하면서 목적기능 확보를 위해 VO_3^{-1} 가 삽입된 소재 개발



층간에 CO_3^{2-} 가 아닌 VO_3^{-1} 가 삽입되었음을 파악할 수 있는 IR spectra

적외선 분광법 (Infrared spectroscopy) (15)

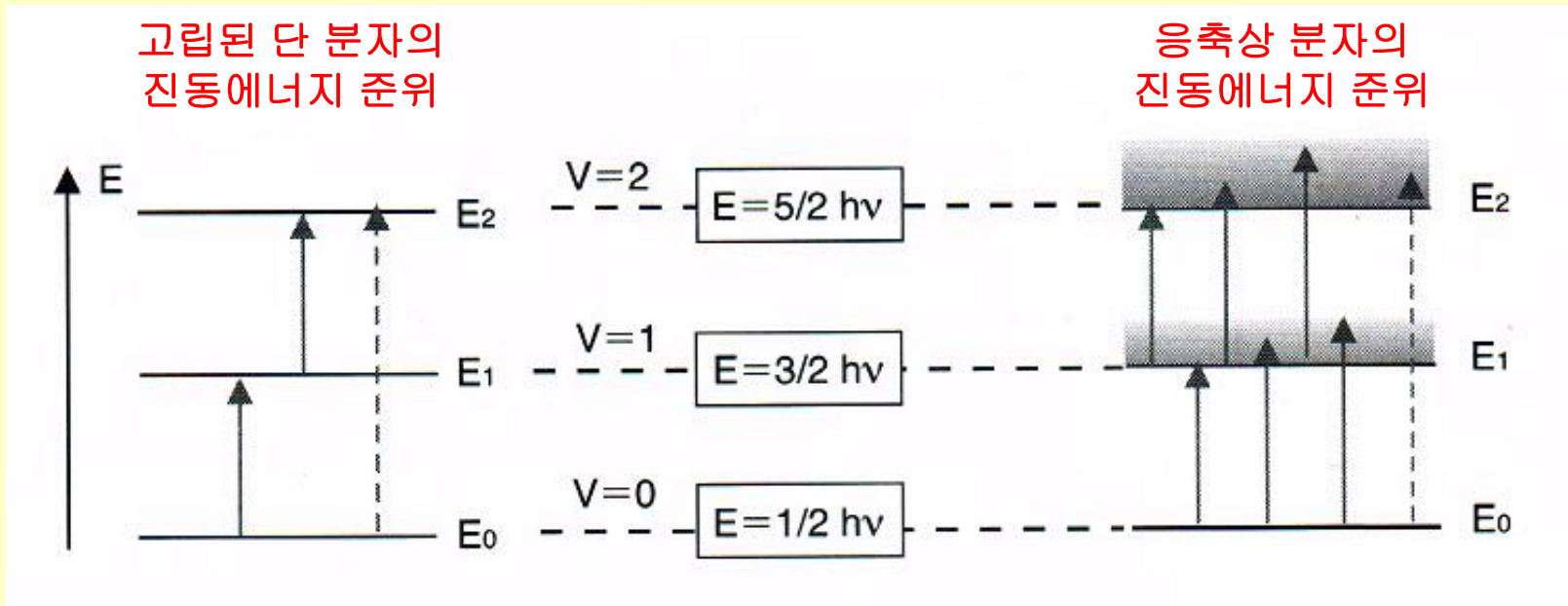


총상수산화물에
monomer를
총간 삽입한 후
polymerization을
통해 Hybrid
Org/Inorg 총상
소재 개발

↓

Polymerization
과정을 보여주는
IR spectra

진동-회전 스펙트럼 (1)

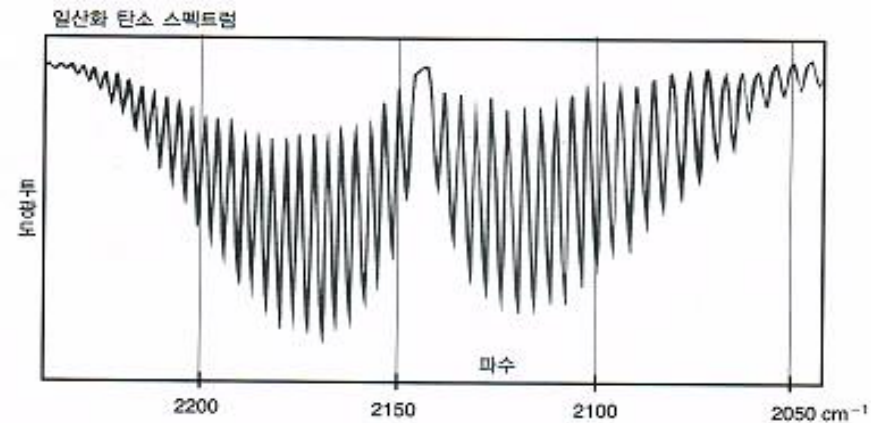
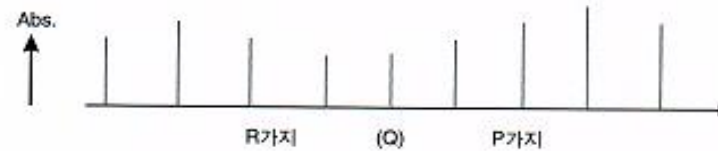
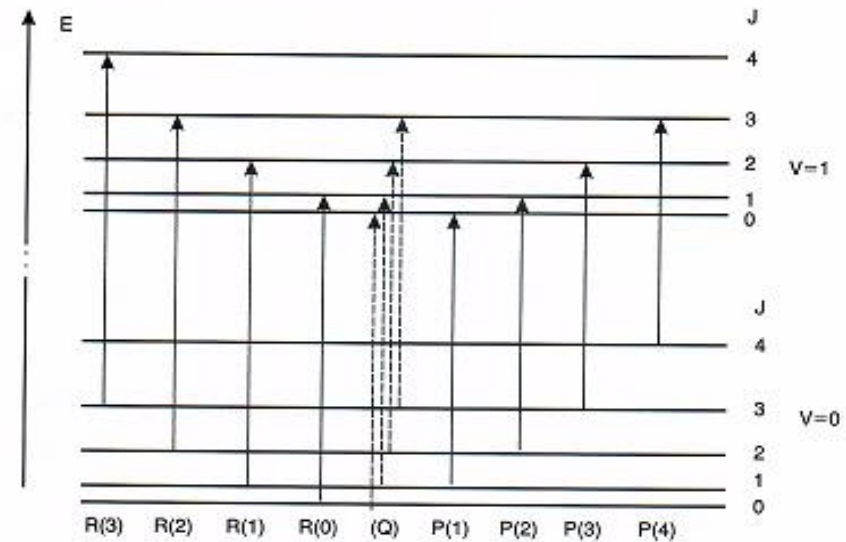


* 적외선의 광자 에너지는 양자화된 E_{vib} 와 E_{rot} 의 준위를 변경하기에 충분하여
진동-회전 스펙트럼 형성



각 진동 전이에 수십 개의 회전 전이가 수반
(V : 진동 양자수 , J : 회전 양자수)

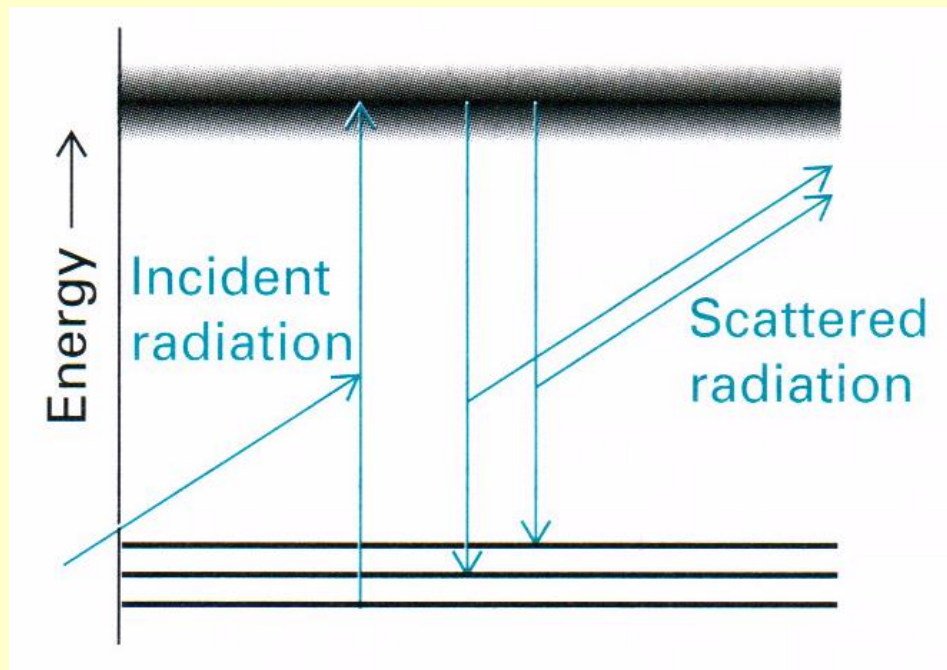
진동-회전 스펙트럼 (2)



라만 분광법 (Raman spectroscopy) (1)

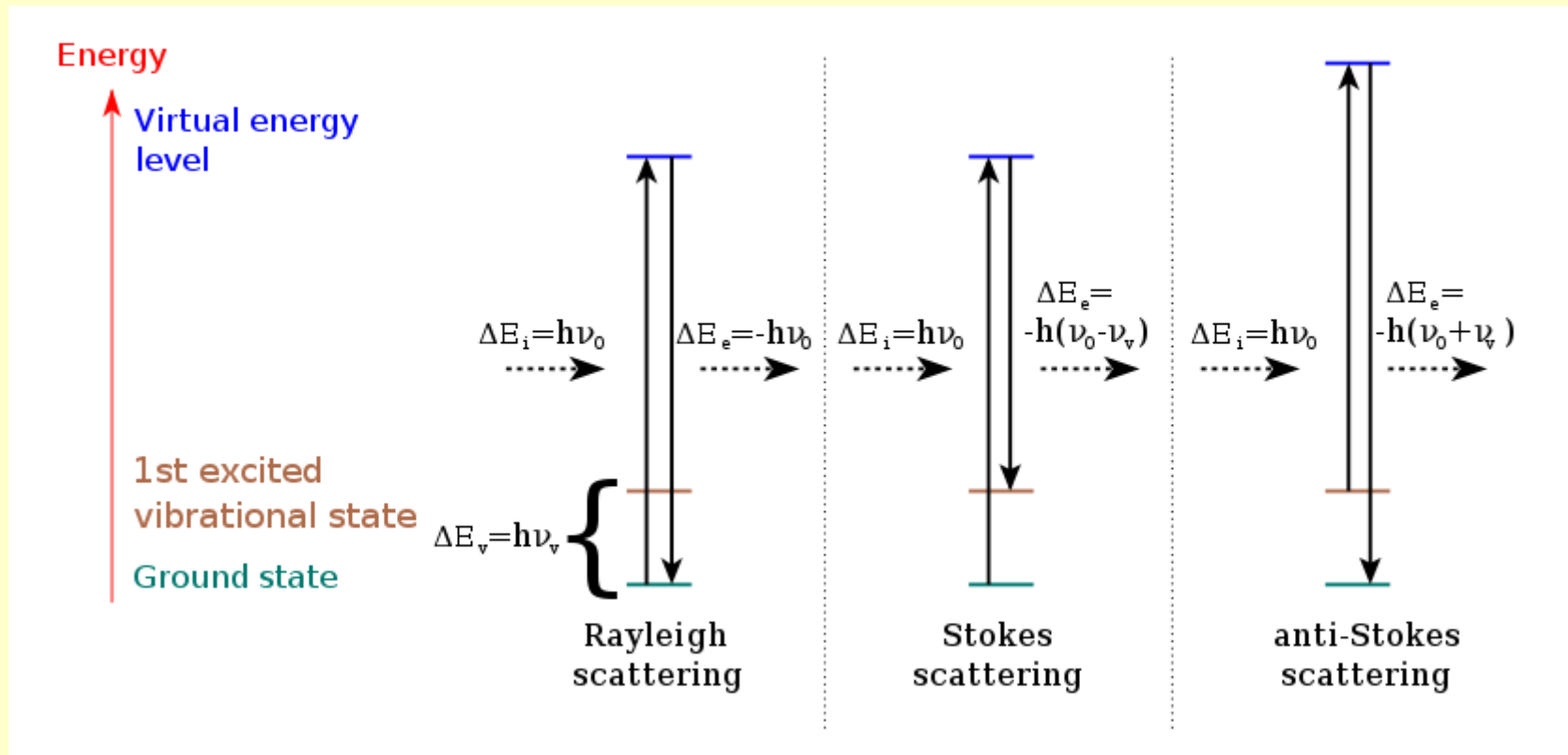
- * 입사 전자기 복사선(가시광선 또는 자외선)의 입사 광자는 분자의 진동수를 증가시키는 과정에서 감소된 에너지(낮은 주파수)의 산란 복사선 및 증가된 에너지(높은 주파수)의 산란 복사선 → 산란된 복사선 진동수 → 분자 에너지 준위 정보

진동 동안 분자의 편극률이 변해야 Raman active : 동핵/이핵 분자

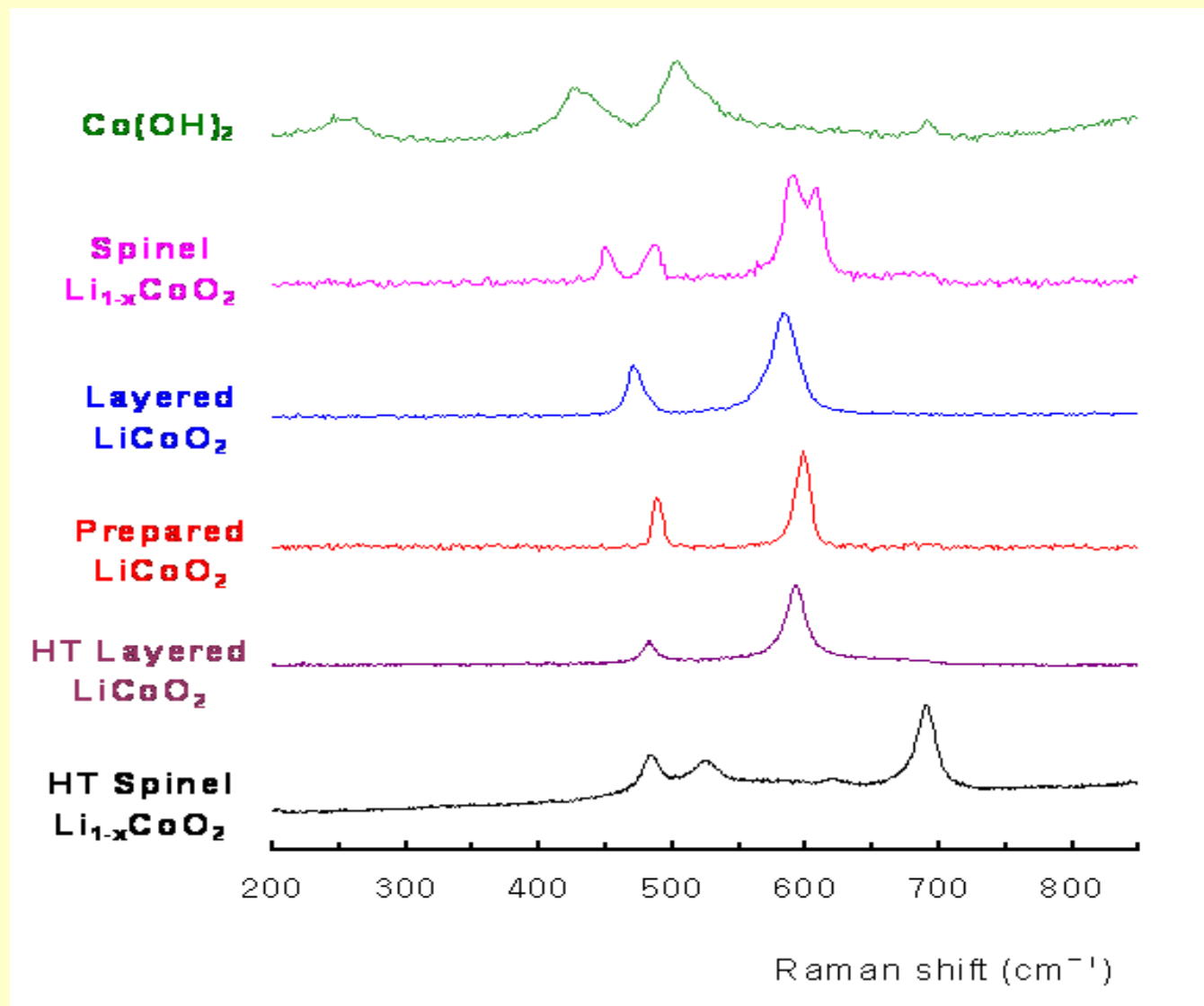


라만 분광법 (Raman spectroscopy) (2)

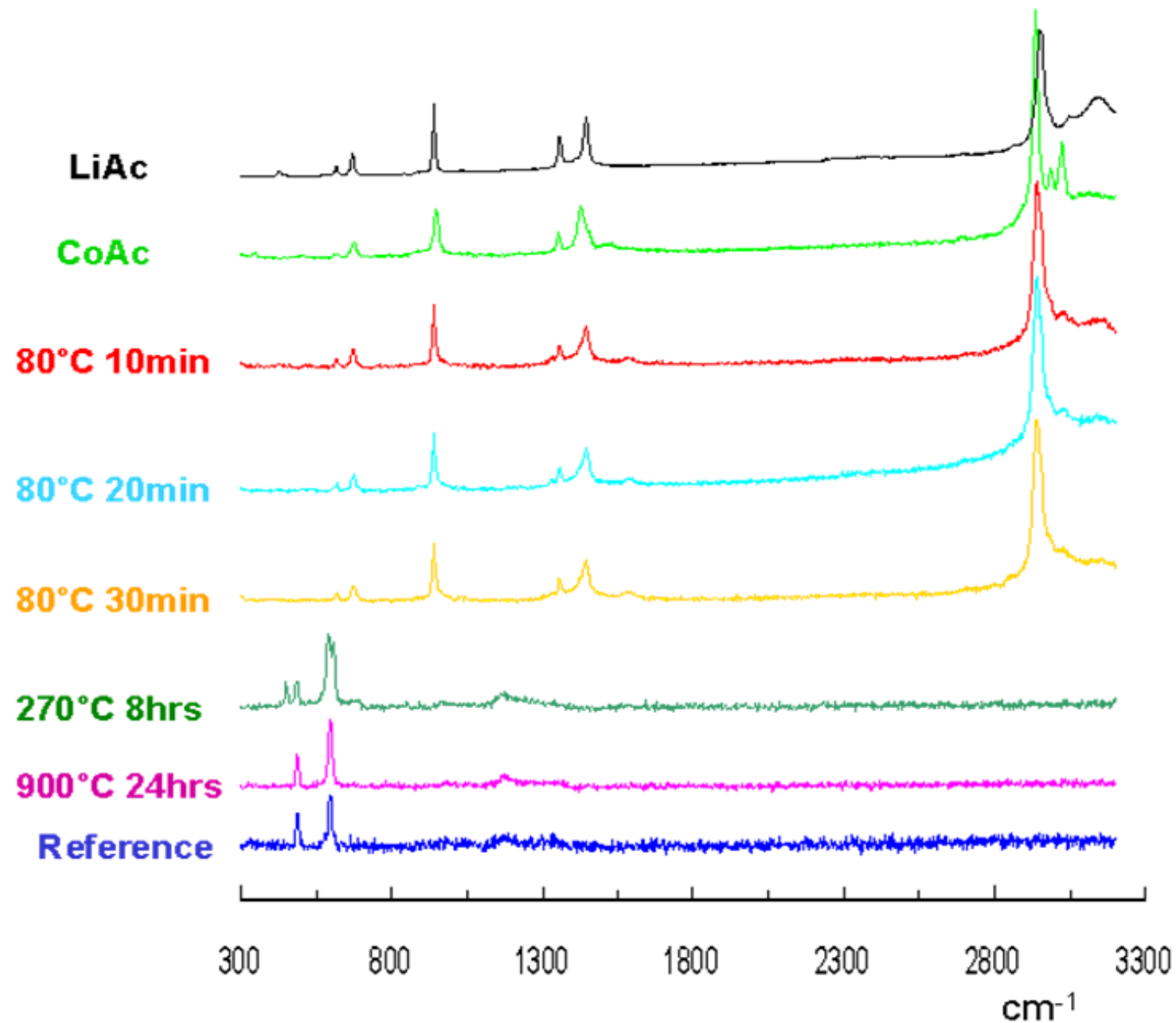
- * 입사파의 광자 에너지보다 작아 낮은 주파수의 산란파 방출 → Stokes 복사선
입사파의 광자 에너지에 여기 상태의 분자가 공급하는 에너지가 추가된 높은 주파수의 산란파도 방출 → Anti-stokes 복사선
주파수 변화 없이 분산된 복사선 → Rayleigh 복사선



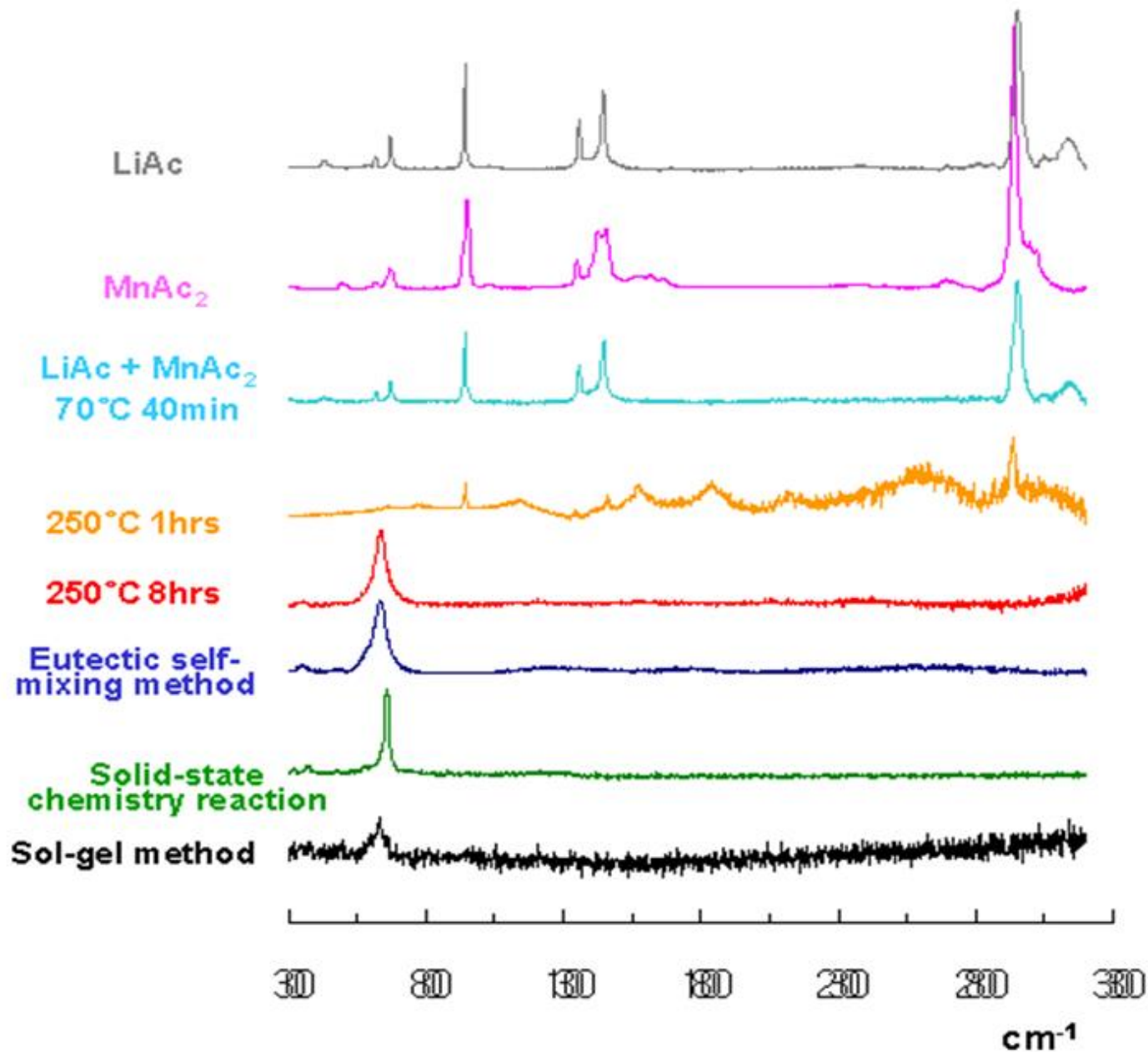
라만 분광법 (Raman spectroscopy) (3)



리튬이온전지 양극활물질인 LiCoO_2 제조에 따른 Raman spectrum 변화

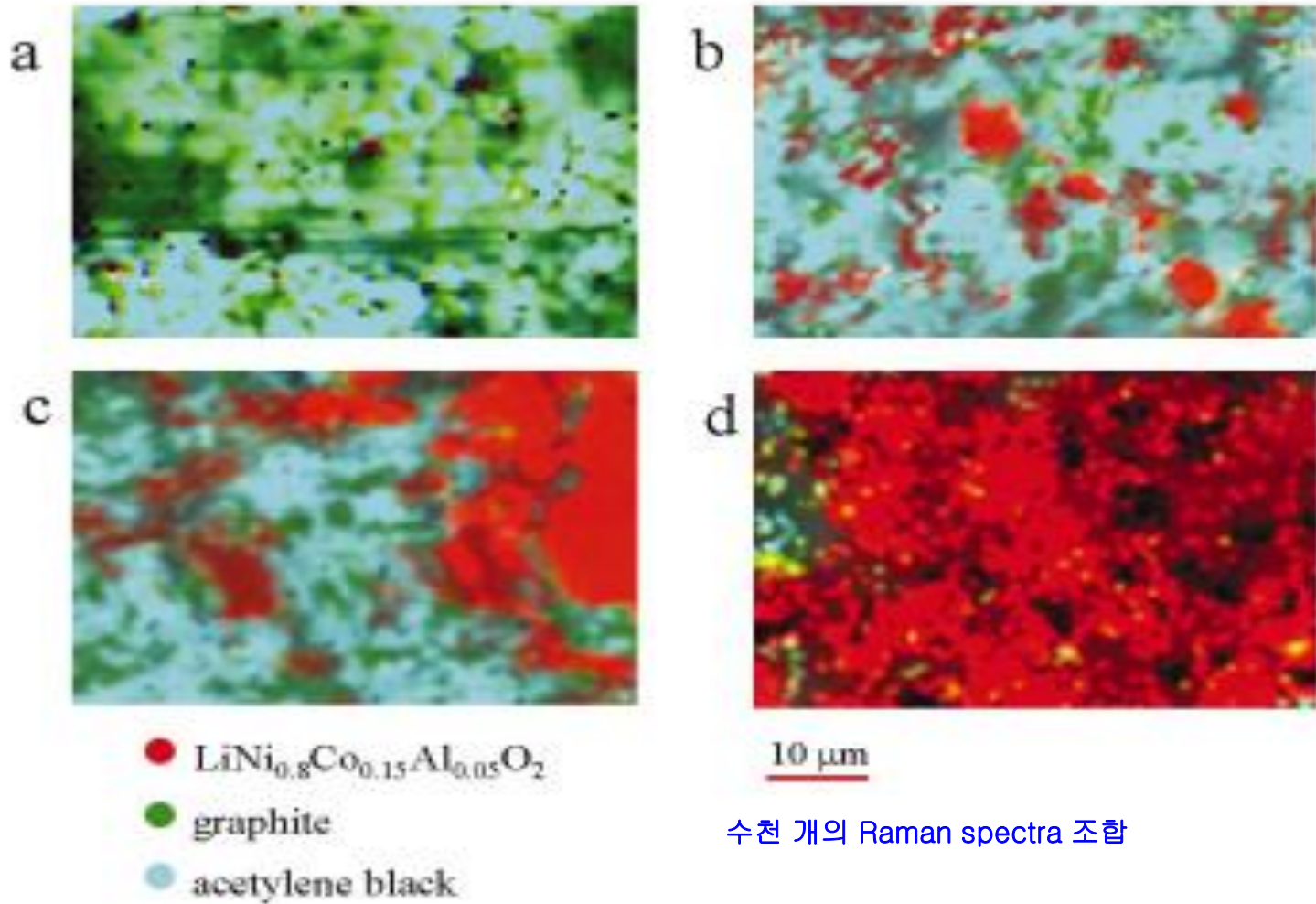


리튬이온전지 양극활물질인 LiMn_2O_4 제조에 따른 Raman spectrum 변화



라만 분광법 (Raman spectroscopy) (6)

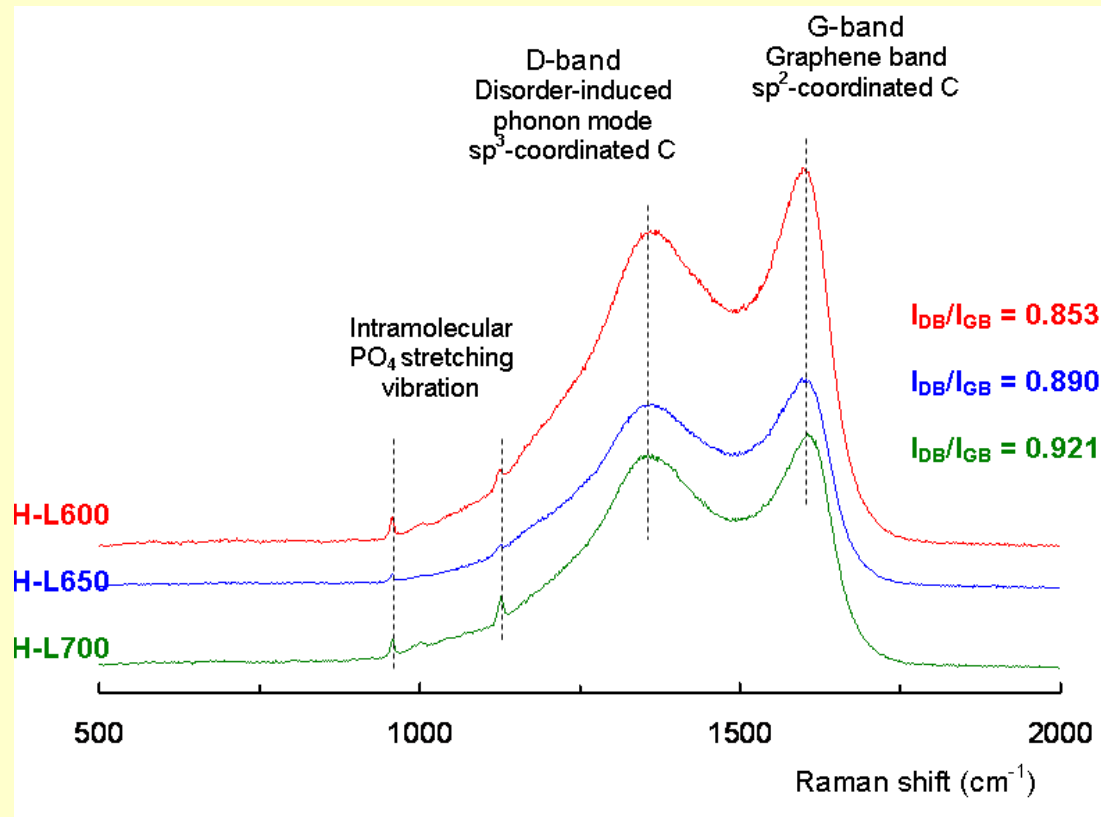
고차원분광 Raman microscope image



수천 개의 Raman spectra 조합

라만 분광법 (Raman spectroscopy) (7)

Raman spectroscopy for LiFePO_4/C : carbon



$I_{\text{DB}}/I_{\text{GB}} \downarrow$ Electric conductivity \uparrow

Temperature dependence of LFP/C (500~800°C, >800°C Fe_2O_3 $\text{Li}_3\text{Fe}_2(\text{PO}_4)_3$)

① Particle size, ② Agglomeration, ③ $I_{\text{DB}}/I_{\text{GB}}$??