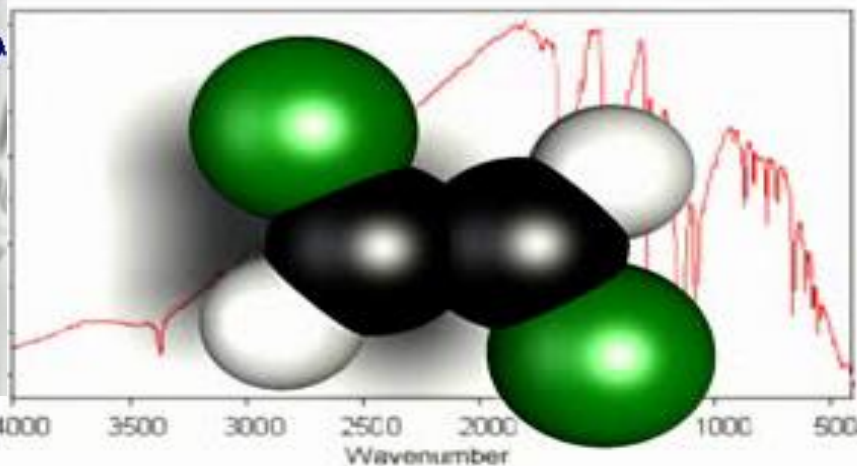
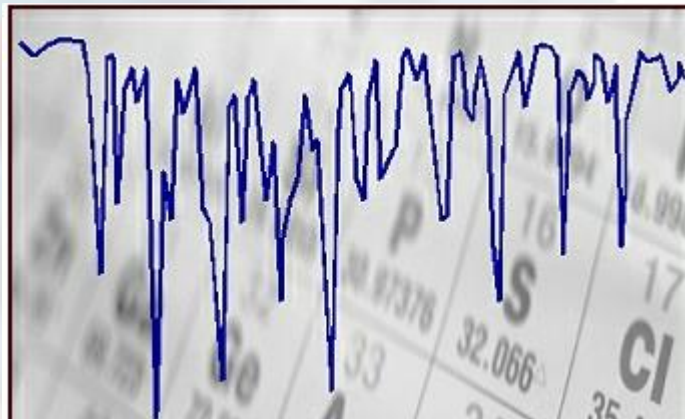
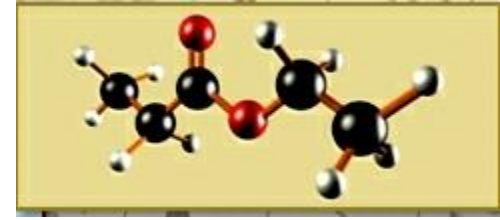


KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

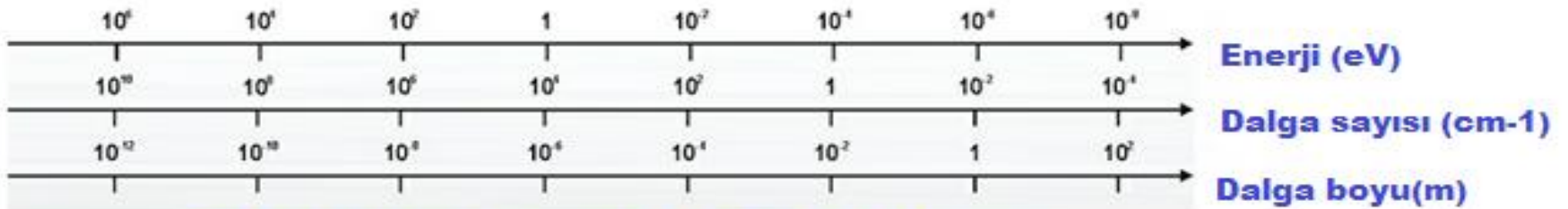
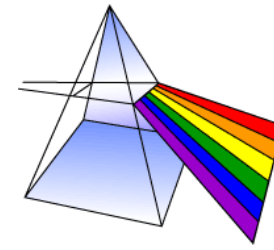


Spektroskopi

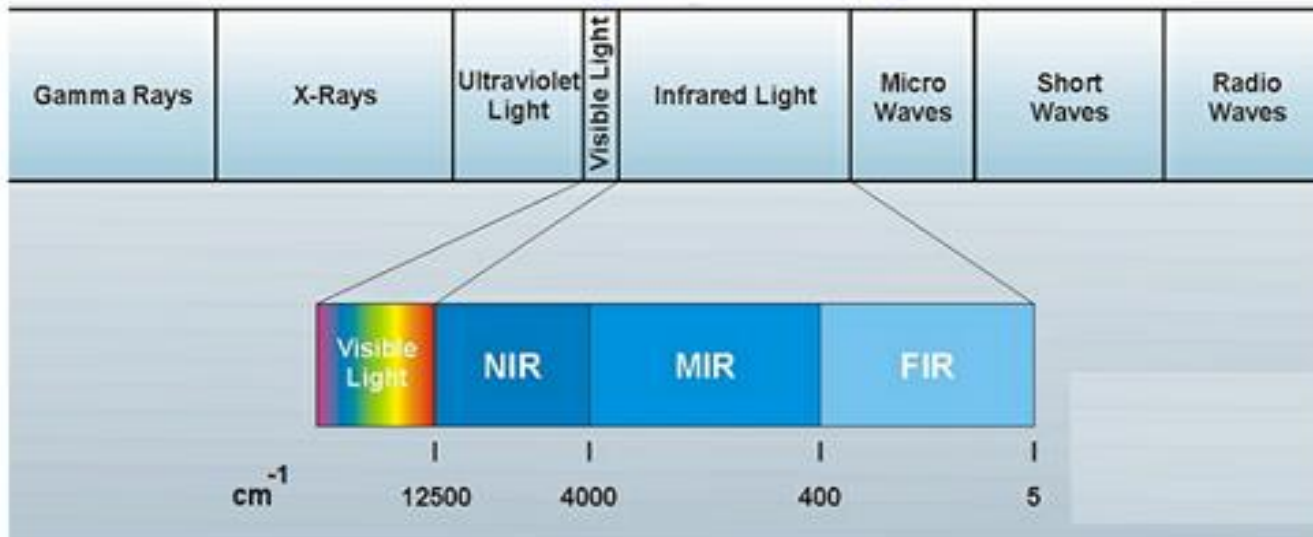


- Elektromagnetik ışının madde ile etkileşimini konu alan bilim dalına **spektroskopi** denir.
- Elektromagnetik ışının organik moleküller tarafından absorpsiyonu (soğurulması), **moleküldeki atomların türüne, düzenlenmesine, moleküllerin şekline, büyüklüğüne** bağlı olduğundan organik kimyada spektroskopik yöntemler,
 - ❖ Organik maddelerin kalitatif ve kantitatif analizi,
 - ❖ Yapıların aydınlatılması
 - ❖ **Saflık kontrolü** gibi çok geniş bir alanda uygulanmaktadır.

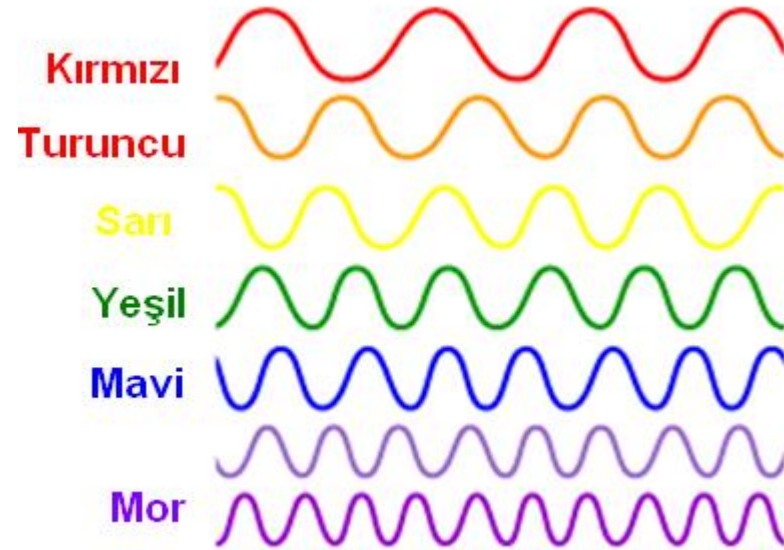
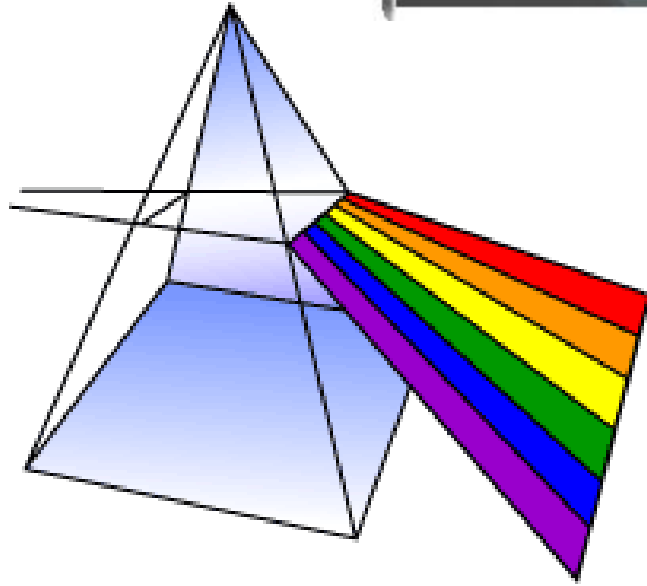
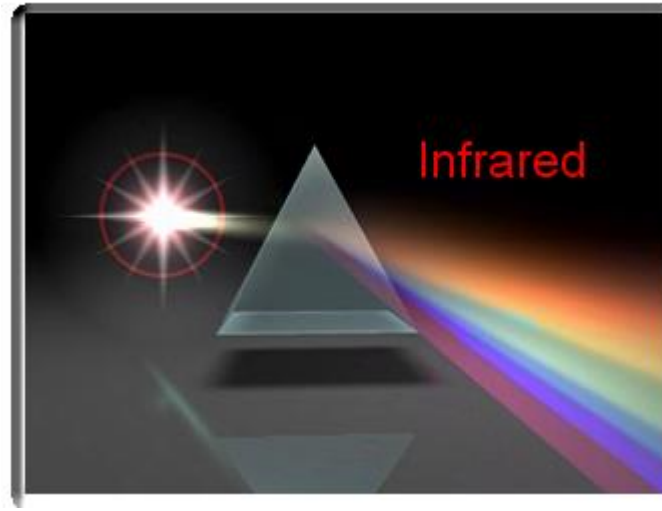
Elektromanyetik Spektrum



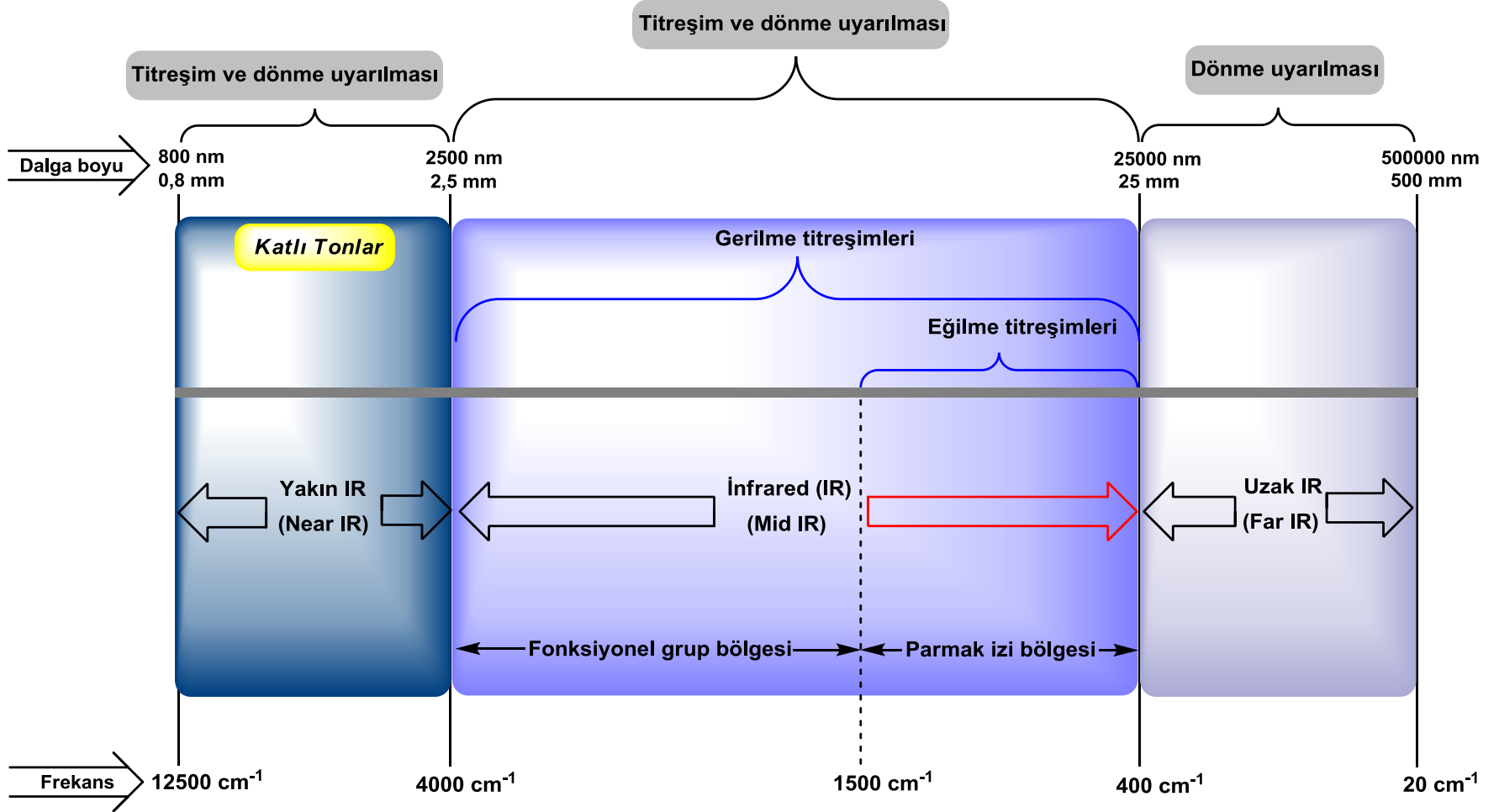
Elektromagnetik Spektrum



KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

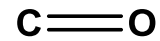
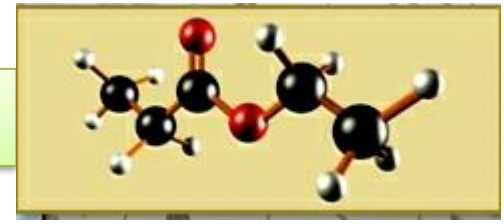


KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ



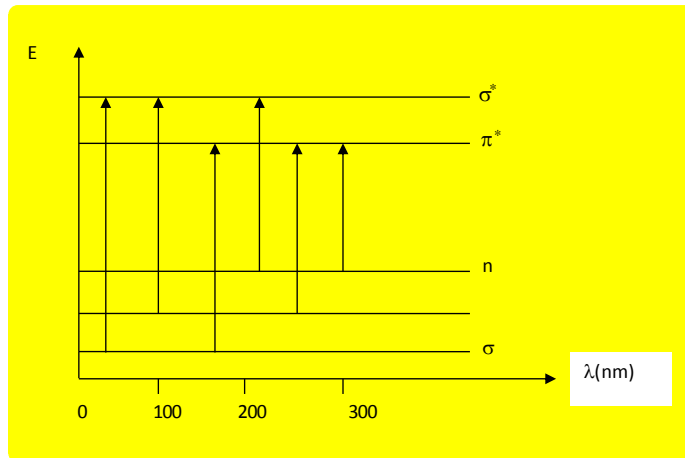
KIRMIZI ÖTESİ (İNFRARED, IR) SPEKTROSKOPİSİ

2. Kırmızı Ötesi (IR) Işıma ile Madde Etkileşimi



Kırmızı Ötesi Işınları

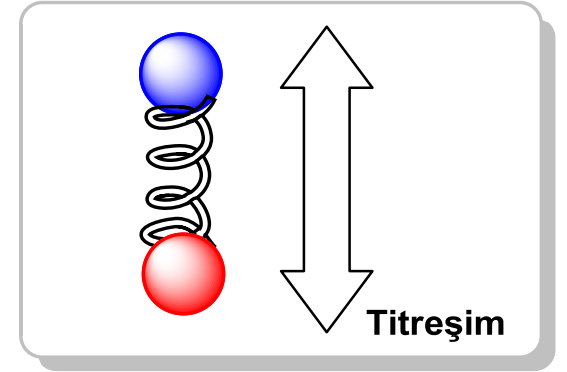
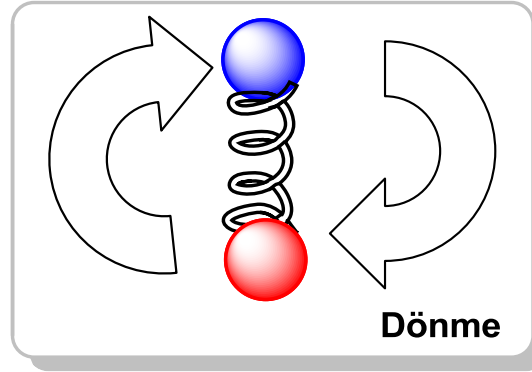
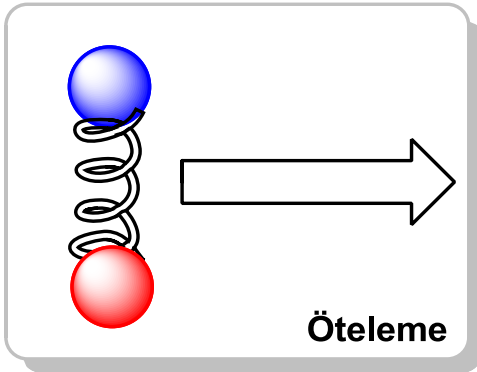
- Titreşim
- Dönme enerji düzeylerini uyarabilir



KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

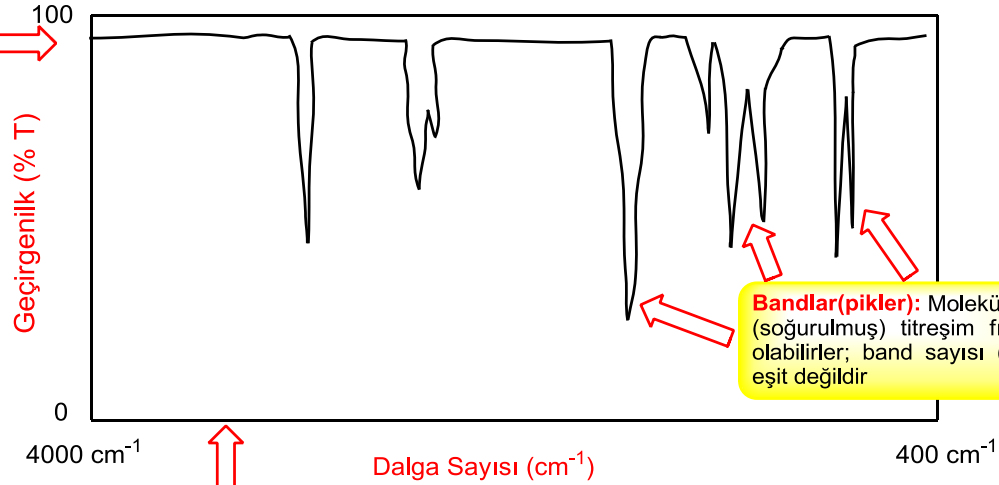
Kırmızı Ötesi (IR) bölgede absorbsiyon yapan organik moleküller

- 1) Titreşim hareketleri
- 2) Dönme (rotasyon) hareketleri
- 3) Ötelenme hareketleri olmak üzere üç tür hareket yaparlar.



3. Genel Kırmızı Ötesi (IR) Spektrumu

Baseline (Temel çizgi)



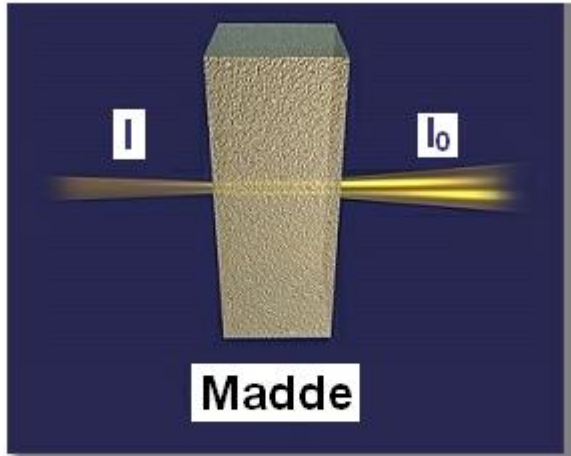
Geçirgenlik (%T):

$$\%T = \frac{I}{I_0} \quad A = \log \left(\frac{I}{I_0} \right) = \epsilon bc$$

I_0 : Madde üzerine gelen ışımının şiddeti

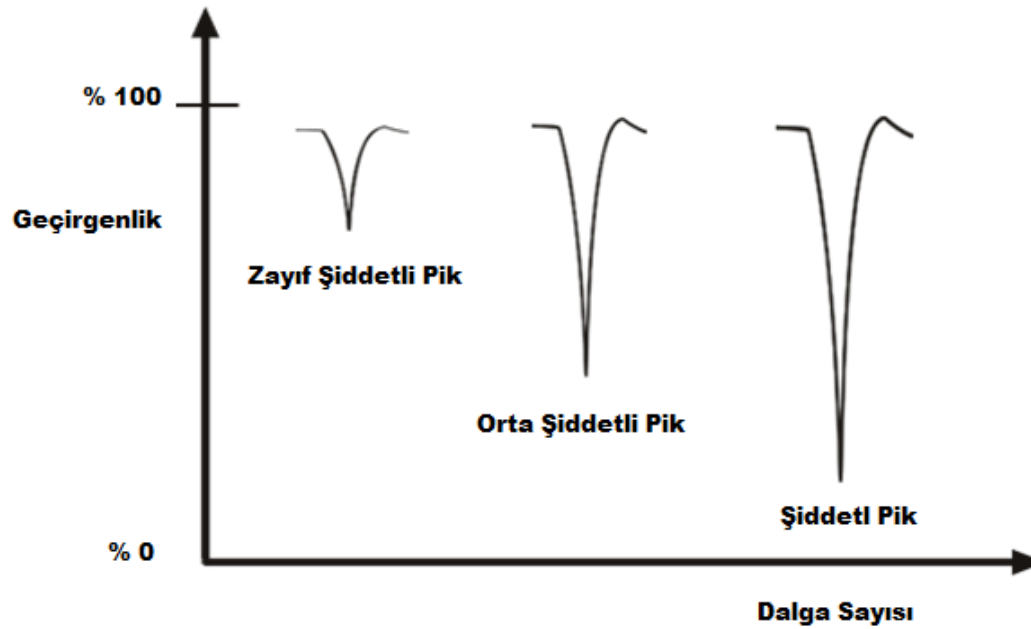
I : Madde üzerinden geçen ışımının şiddeti

Frekans: Genel olarak dalgasayısı (cm⁻¹) cinsinden ifade edilir



←
Işın yolu

KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ



Pikin Şiddeti : Bağıın dipol momenti (μ) ile ilgilidir. Bir sistemde dipol moment değışikliğı ne kadar fazla ise, yani sistem ne kadar polarsa IR piki o kadar şiddetlidir (C=O, C=N gibi).

4. Molekülde Gözlenebilecek Titreşimler

➤ Gerilme Titreşimi

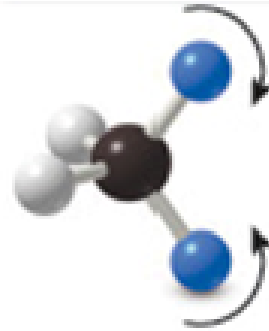
➤ Eğilme Titreşimi

Gerilme



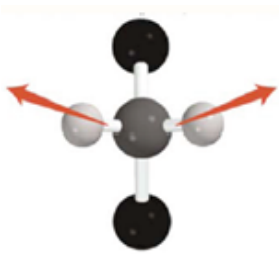
Bir bağ gerilebilir

Eğilme

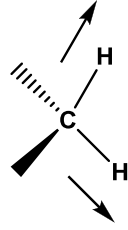


İki bağ eğilebilir

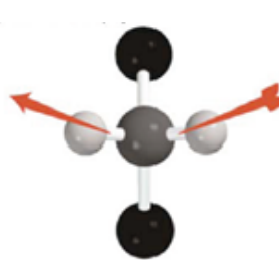
Gerilme Titreşimleri



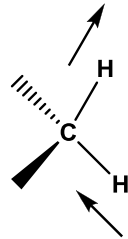
Simetrik gerilme



Simetrik gerilme (ν_s)
(~2853 cm^{-1})



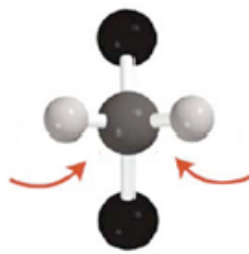
Asimetrik gerilme



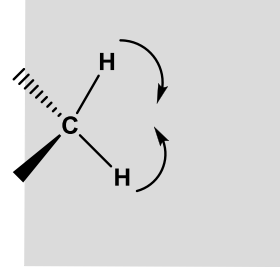
Asimetrik gerilme (ν_{as})
(~2926 cm^{-1})

Eğilme Titreşimleri

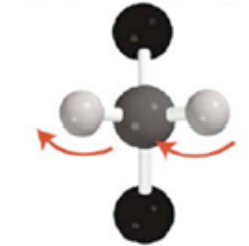
Düzlem içi



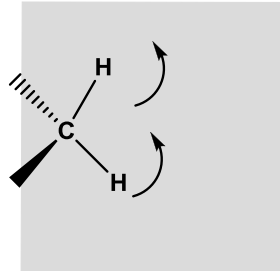
Makaslama



Makaslama (δ)
(~1450 cm^{-1})

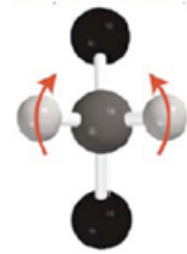


Sallanma

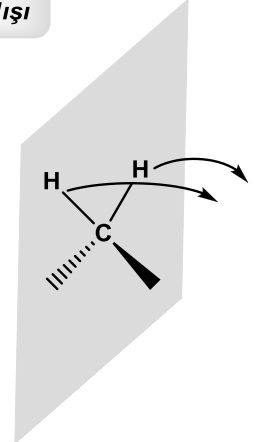


Sallanma (ρ)
(~720 cm^{-1})

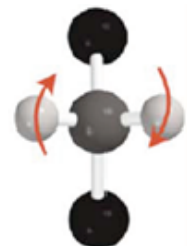
Düzlem dışı



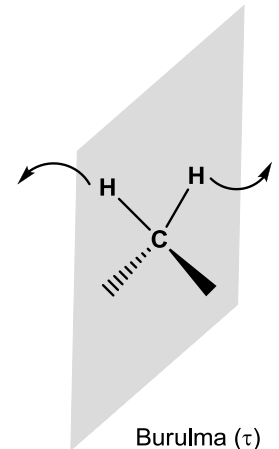
Dalgalanma



Dalgalanma (ω)
(~1250 cm^{-1})

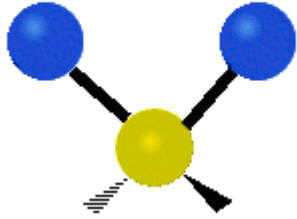
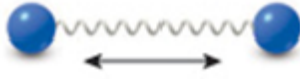


Burulma

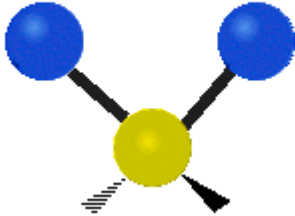


Burulma (τ)
(~1250 cm^{-1})

➤ Gerilme Titreşimi

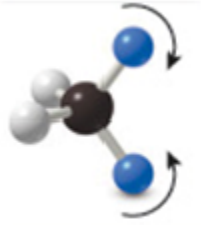


Simetrik Gerilme

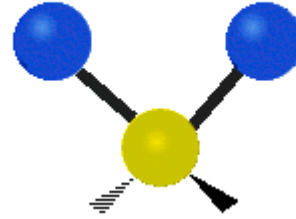


Asimetrik Gerilme

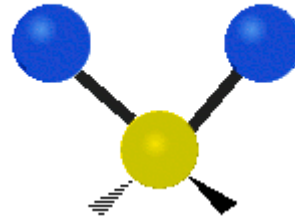
➤ Eğilme Titreşimi



Düzlem içi

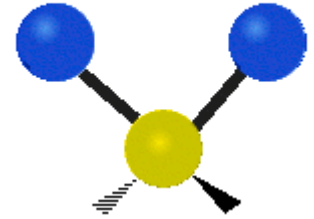


Makaslama

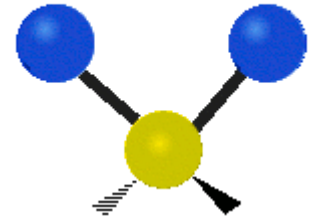


Sallanma

Düzlem dışı



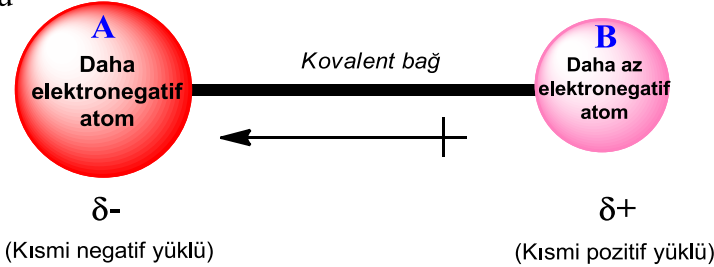
Dalgalanma



Burulma

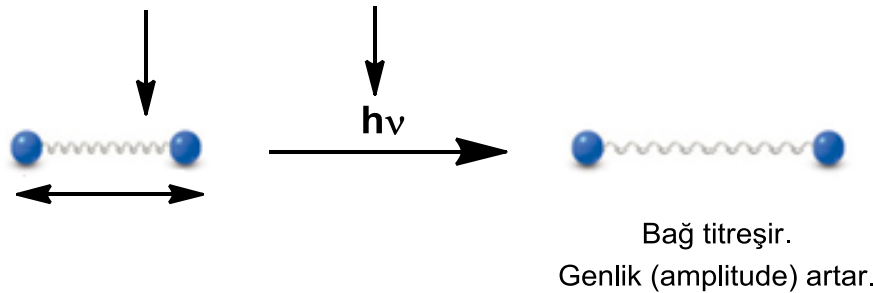
5. Hangi Moleküller IR Spektroskopisiyle incelenebilir

A-B molekülü

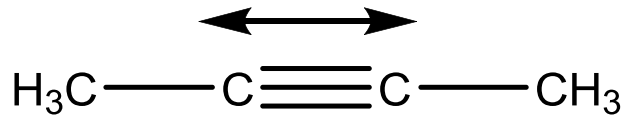


Bir kovalent bağın gerilme ve eğilme frekanslarını ölçmek için, kovalent bağ bir **dipol momente** sahip olmalıdır (μ)

IR ışığının frekansı (ν) = bağ titreşim frekansına (ν) eşit olduğunda, IR ışıması absorblanır



1 Farklı bağ tipleri, farklı frekansta titreşir. Bu sebeple IR ışımının farklı frekanslarını absorblarlar.

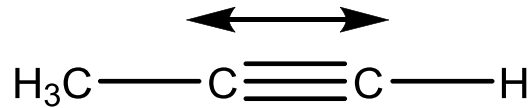


2-Bütün

Simetrik

Dipol momente sahip değil

IR inaktif

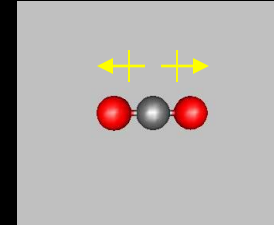
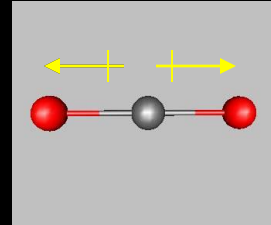


Propin

Asimetrik

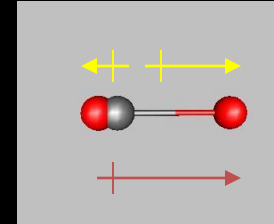
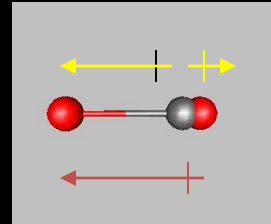
Dipol momente sahip

IR aktif



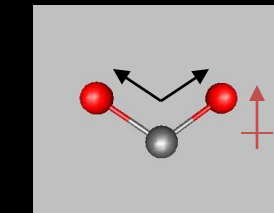
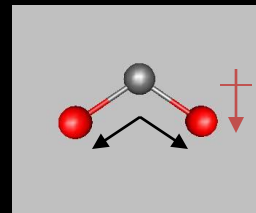
*Simetrik
gerilme*

Dipolde değişim yok



*Asimetrik
gerilme*

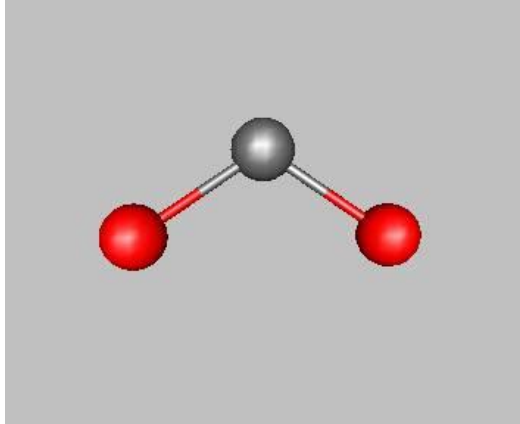
Dipolde değişim var - **IR aktif**



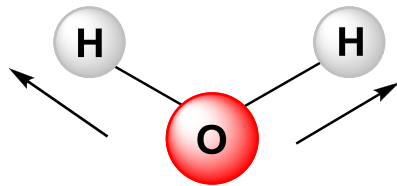
Eğilme

Dipolde değişim var - **IR aktif**

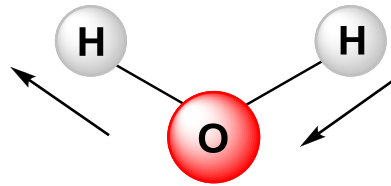
6. Molekölün Titreşim Sayısının (Pik Sayısının) Bulunması



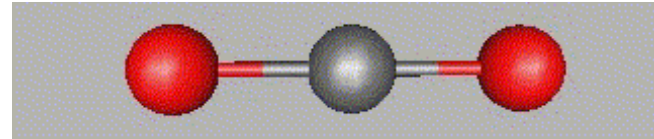
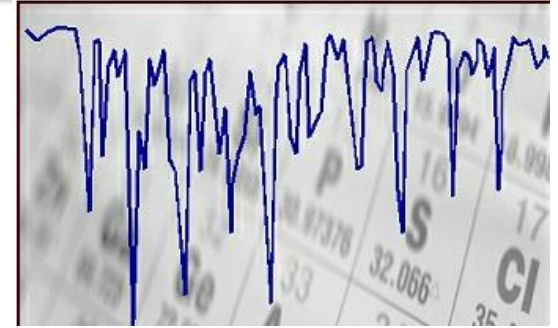
3N-6



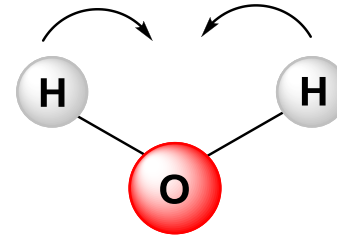
Simetrik gerilme
3625 cm⁻¹



Asimetrik gerilme
3756 cm⁻¹



3N-5

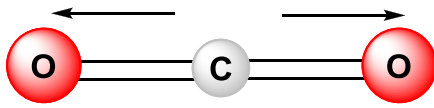


Eğilme
1595 cm⁻¹

$$\text{Pik sayısı} = 3N - 6 = 3 \cdot 3 - 6 = 3$$

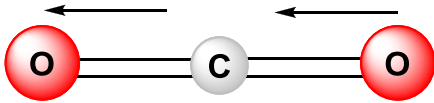
H₂O molekülünün temel titreşim hareketleri

KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

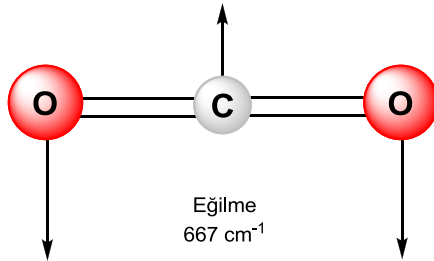


*Simetrik gerilme
1337 cm^{-1}

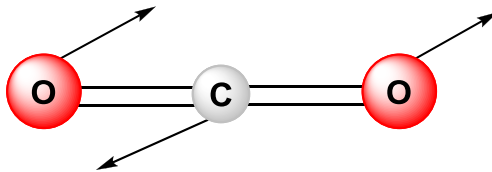
* Raman spektrumunda gözlenir.



Asimetrik gerilme
2349 cm^{-1}
(IR absorpsiyonu gözlenir)



Eğilme
667 cm^{-1}

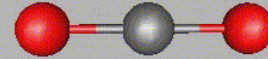


Eğilme
667 cm^{-1}

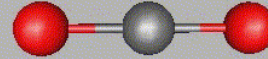
$$\text{Pik sayısı} = 3N - 5 = 3 \cdot 3 - 5 = 4$$

CO₂ molekülünün temel titreşim hareketleri

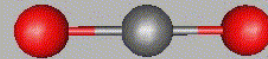
CO₂



*Simetrik
gerilme*



*Asimetrik
gerilme*



Eğilme

KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

7. Titreşim Modeli ve Bir Kimyasal Bağın Frekansının Hesaplanması



$$\nu = \frac{1}{2\pi} \sqrt{\frac{k}{m_{ind.}}}$$

ν = Titreşim Frekansı

k = N/m olarak bağın kuvveti

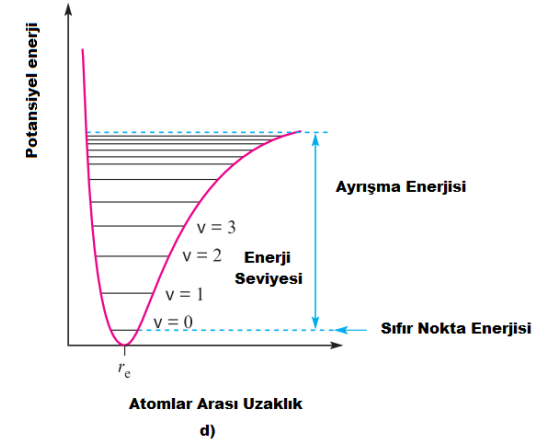
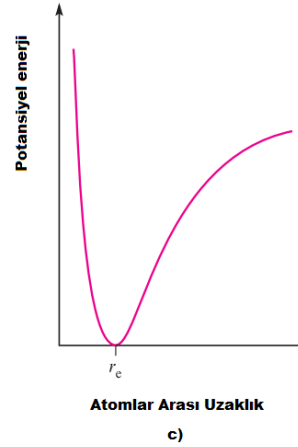
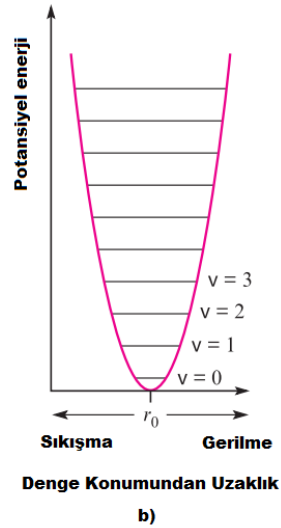
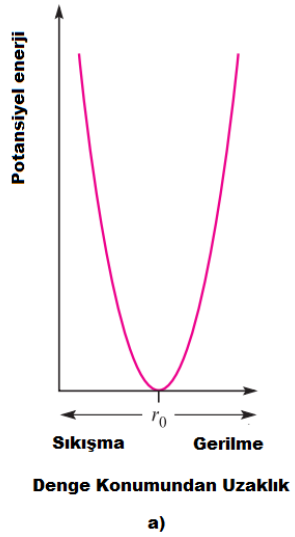
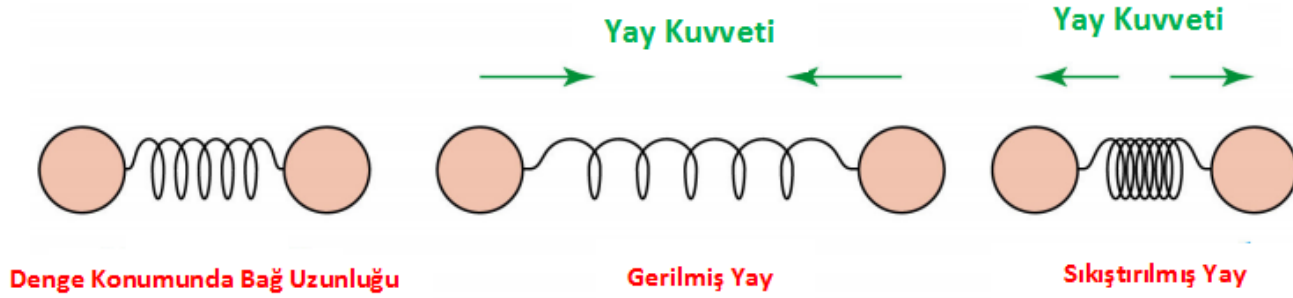
$m_{ind.}$ = İndirgenmiş kütle

[7-1]

$$m_{ind.} = \frac{m_A \times m_B}{m_A + m_B}$$

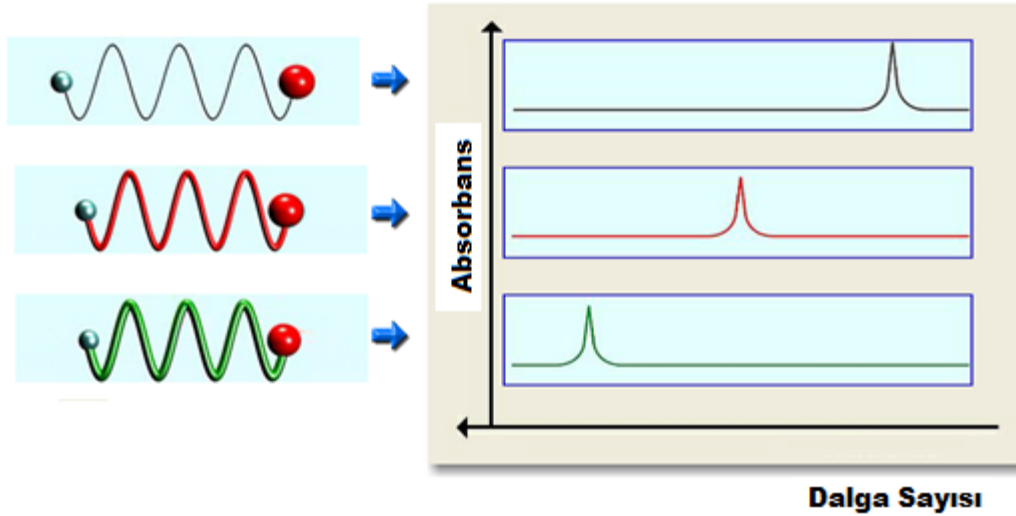
m_A, m_B : Atomların kütlesi (Moleküler ağırlıkları değil)

İndirgenmiş kütle hesabında birim olarak kg ($1 \text{ akb} : 1,66 \cdot 10^{-27} \text{ kg}$) kullanılır



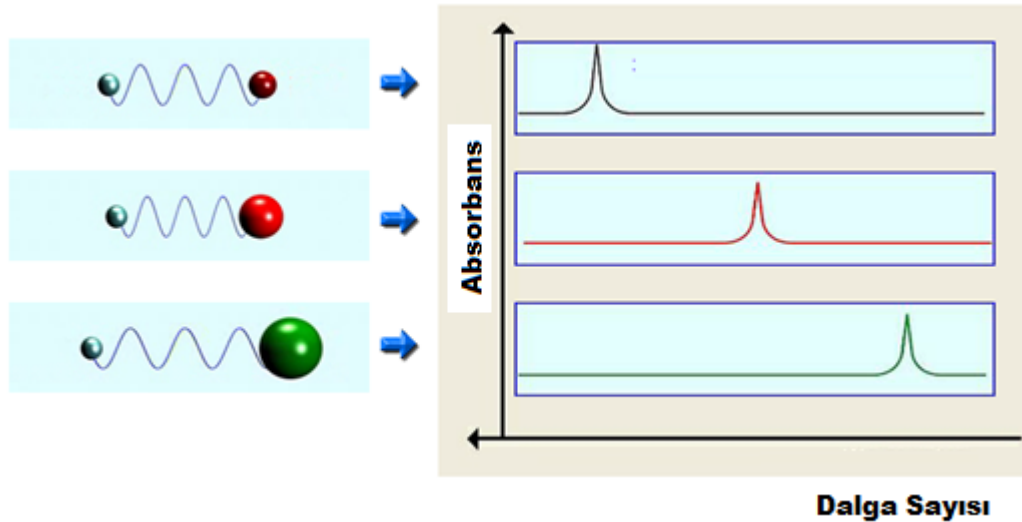
KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

Bağın kuvvet sabiti (k)



Kuvvet sabitini etkileyen faktörler

- ❖ Atomların kütlesi
- ❖ Bağın uzunluğu ve gücü
- ❖ Atomların elektronegatifliği



KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

Bir bağıın kuvvet sabiti ve bağıın iki yanındaki atomlar bilinirse, bağıın frekansı hesaplanabilir.

$$\nu = \frac{1}{2\pi} \sqrt{\frac{k}{m_{ind.}}}$$

ν = Titreşim Frekans

k = N/m olarak bağıın kuvveti

$m_{ind.}$ = İndirgenmiş kütle

$$m_{ind.} = \frac{m_A \times m_B}{m_A + m_B}$$

m_A, m_B : Atomların kütlesi (Moleküler ağırlıkları değil)

İndirgenmiş kütle hesabında birim olarak kg (1 akb : $1,66 \cdot 10^{-27}$ kg) kullanılır

$$\nu = \frac{c}{\lambda} \quad \lambda = \frac{1}{\bar{\nu}} \quad \nu = c \bar{\nu}$$

$$\bar{\nu} = \frac{1}{2\pi c} \sqrt{\frac{k}{m_{ind.}}}$$

c = Işık hızı, $3 \cdot 10^{10}$ cm/s

$\bar{\nu}$ = Dalga sayısı, cm^{-1}

Titreşim frekansı
(enerjisi),
hem
bağıın gücüne
(yay kuvvet sabiti)
hemde
bağ yapan
atomların
kütlelerine
bağılıdır

Örnek: Karbonil grubunun, C=O, gerilme titreşimi sebebiyle meydana gelen temel absorpsiyon pikinin yaklaşık, ***dalga sayısını*** hesaplayınız.

Karbon için

6,02.10²³ tane Karbon (C) atomu 12.10⁻³ kg/mol ise
1 tane Karbon (C) atomu x kg/mol

$$x = 2.10^{-26} \text{ kg/mol}$$

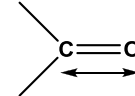
Oksijen için

6,02.10²³ tane Oksijen (O) atomu 16.10⁻³ kg/mol ise
1 tane Oksijen (O) atomu x kg/mol

$$x = 2,7.10^{-26} \text{ kg/mol}$$

İndirgenmiş kütle $m_{ind.} = \frac{m_O \times m_C}{m_O + m_C} = \frac{2.10^{-26} \text{ kg/mol} \times 2,7.10^{-26} \text{ kg/mol}}{(2 + 2,7).10^{-26} \text{ kg/mol}} = 1,1.10^{-26} \text{ kg/mol}$

$$\bar{\nu} = \frac{1}{2\pi c} \sqrt{\frac{k}{m_{ind.}}} = \frac{1}{2,3,14.3.10^{10} \text{ cm/s}} \sqrt{\frac{1.10^3 \text{ N/m}}{1,1.10^{-26} \text{ kg/mol}}} = 1600 \text{ cm}^{-1}$$

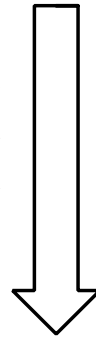


c = Işık hızı, 3.10^{10} cm/s

k = 1.10^3 N/m (Çift bağ için)

Karbonil grubunun gerilme pikinin deneysel olarak $1600\text{-}1800 \text{ cm}^{-1}$ ($6,3\text{-}5,6 \mu\text{m}$) bölgesinde olduğu bulunmuştur.

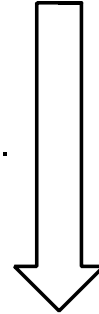
Hibritleşmede **s karakteri** aşağıya doğru artmaktadır. s Karakteri artıkça bağ elektronları çekirdek tarafından daha sıkı tutulduğundan üçlü bağ daha kuvvetli olacaktır.



sp^3 C—C	bağı için	1300 - 800 cm^{-1}
sp^2 C=C	bağı için	1700 - 1500 cm^{-1}
sp C≡C	bağı için	2300 - 2100 cm^{-1}

sp^3 C—O	bağı için	~1100 cm^{-1}
sp^2 C=O	bağı için	~1700 cm^{-1}
sp C≡O	bağı için	2143 cm^{-1} (Serbest CO)

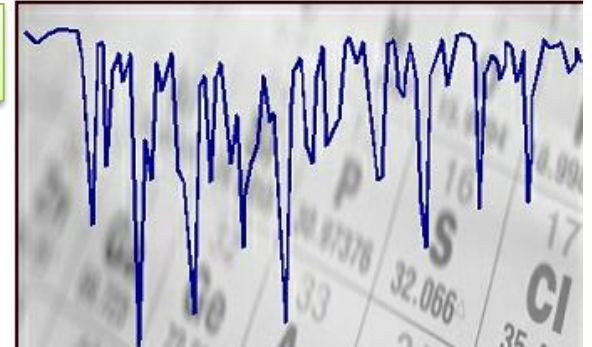
Kütle artışıyla frekansın azaltığı görülmektedir.
 Kütle artışıyla dalgasayısının azaltığı görülmektedir.
 Kütle artışıyla titreşim hareketi zorlaşır.



C—H	bağı için	3000 cm ⁻¹
C—C	bağı için	1200 cm ⁻¹
C—O	bağı için	1100 cm ⁻¹
C—Cl	bağı için	800 cm ⁻¹
C—Br	bağı için	550 cm ⁻¹
C—I	bağı için	500 cm ⁻¹

sp³ C—C—H	bağı için gerilme frekansı	3000 cm ⁻¹
sp² C=C—H	bağı için gerilme frekansı	3100 cm ⁻¹
sp C≡C—H	bağı için gerilme frekansı	3300 cm ⁻¹

8. IR Spektrumuna Etki Eden Etkenler



❖ Dış Etkenler

❖ İç Etkenler (Molekül Yapısına Bağlı Olan Yapısal Etkenler)

1) Hidrojen Bağı

2) Elektronik Etkiler (İndüktif ve Mezomerik Etki)

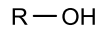
3) Konjügasyon

4) Halka Büyüklüğü

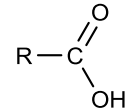
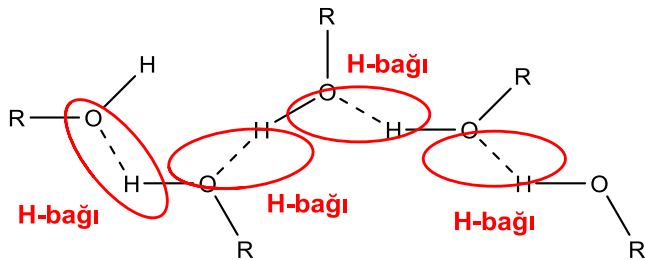
5) Alan Etkieri

1) Hidrojen Bağı

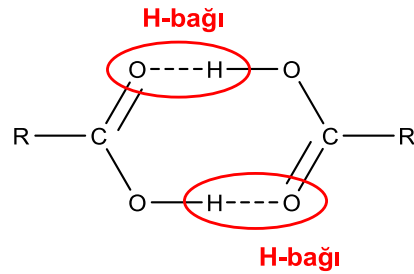
Moleküller arası H-bağı



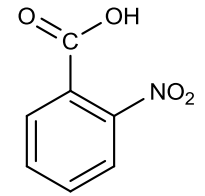
Alkol



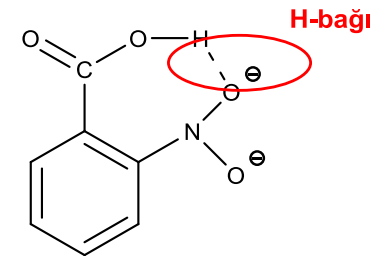
Karboksilli Asit



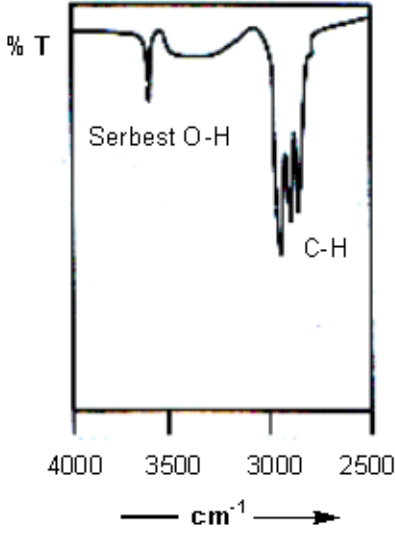
Molekül içi H-bağı



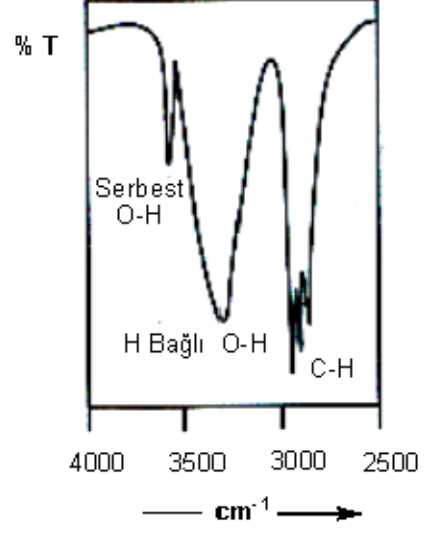
o-Nitrobenzoik asit



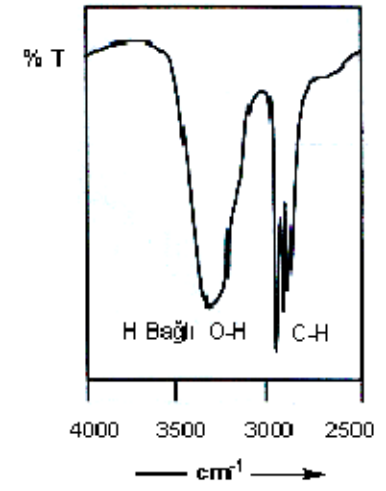
KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ



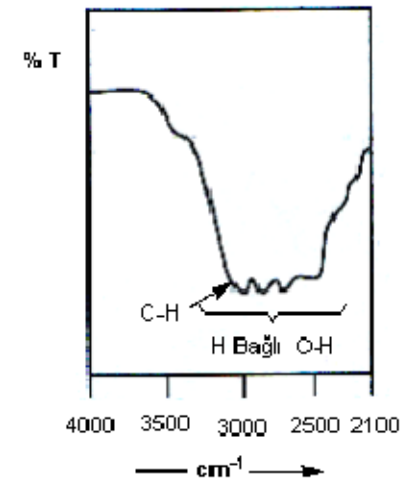
1



2



3



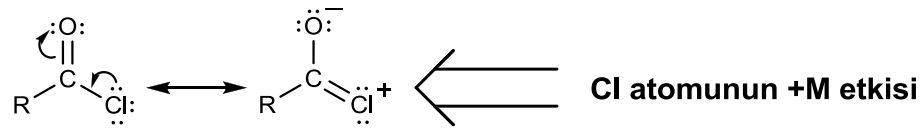
4

2) Elektronik Etkiler (İndüktif ve Mezomerik Etki)

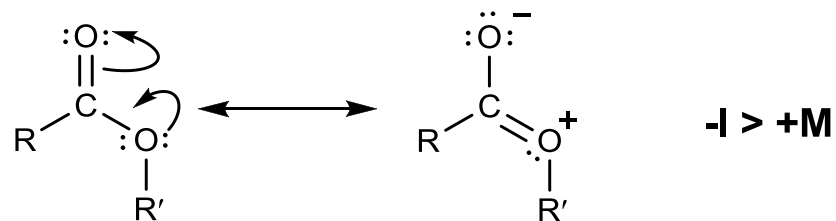
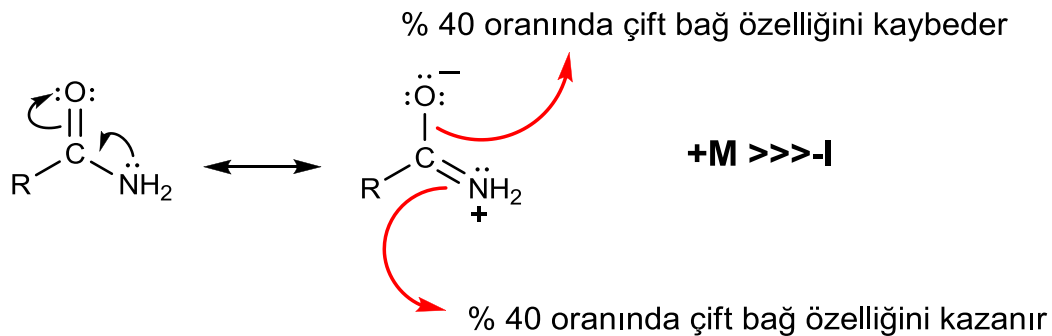
İndüktif etki: Bağlı grup ya da atomların σ -bağları aracılığı ile elektron itmesi veya çekmesi indüktif etkiyi (+I, -I) oluşturur.

Mezomerik etki: Bağlı grup ya da atomların n elektronları ya da π -bağlarının elektron vermesi veya alması mezomerik etkiyi (+M, -M) oluşturur. Bağ kuvvetini azaltan etkiler bu bağa ait absorpsiyon frekanslarının küçülmesine sebep olurken, tersi bir etki absorpsiyonun daha büyük frekanslarda gözlenmesi sonucunu doğurur.

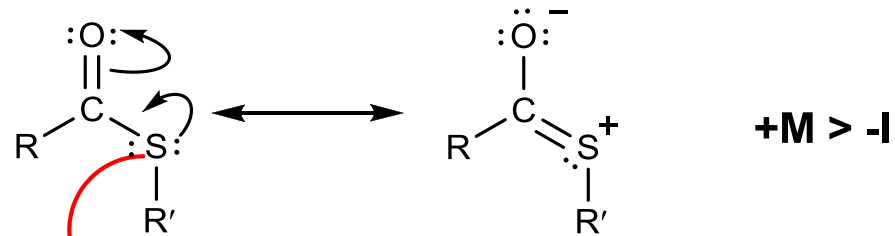
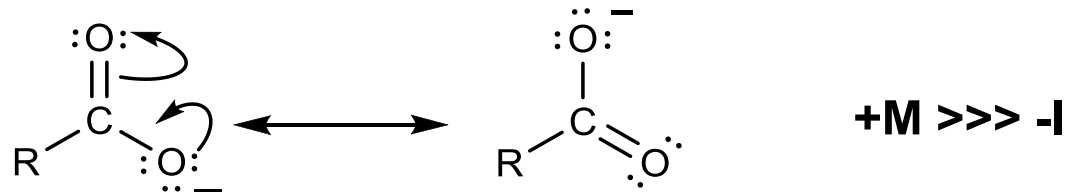
	Aldehit	Keton	Karboksilli asit	Ester	Açıl klorür	Amit	Anhidrit
Foksiyonel Grup	$\begin{array}{c} \text{O} \\ \\ \text{R}-\text{C}-\text{H} \end{array}$	$\begin{array}{c} \text{O} \\ \\ \text{R}-\text{C}-\text{R}' \end{array}$	$\begin{array}{c} \text{O} \\ \\ \text{R}-\text{C}-\text{OH} \end{array}$	$\begin{array}{c} \text{O} \\ \\ \text{R}-\text{C}-\text{OR}' \end{array}$	$\begin{array}{c} \text{O} \\ \\ \text{R}-\text{C}-\text{Cl} \end{array}$	$\begin{array}{c} \text{O} \\ \\ \text{R}-\text{C}-\text{NH}_2 \end{array}$	$\begin{array}{c} \text{O} \quad \text{O} \\ \quad \\ \text{R}-\text{C}-\text{O}-\text{C}-\text{R}' \end{array}$
Karbonil bileşiklerinin IR absorpsiyonları (cm^{-1})	1720	1710	1700 dimer 1760 monomer	1740	1800	1660-1600	1820-1760 (iki band)



* Cl atomunun +M etkisi -I etkisinden küçüktür

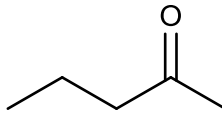


KIRMIZI ÖTESİ (İNFRARED, IR) SPEKTROSKOPİSİ

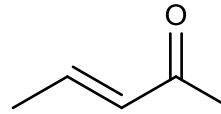


Elektronlarını daha kolay verir

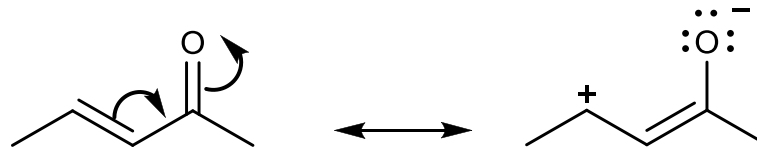
3) Konjügasyon



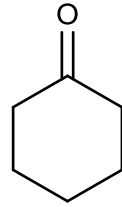
1710 cm⁻¹



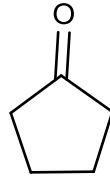
1680 cm⁻¹



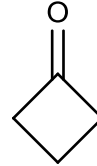
4) Halka Büyüklüğü



1710 cm⁻¹



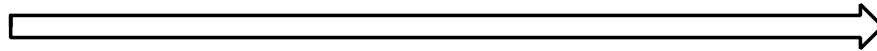
1751 cm⁻¹



1775 cm⁻¹



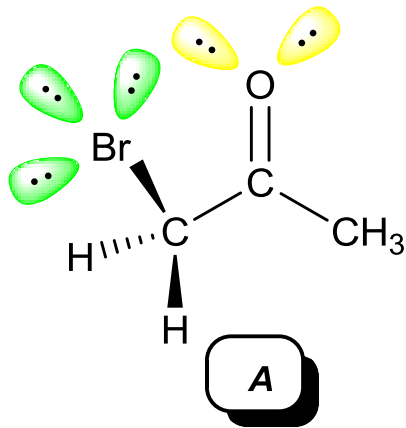
1815 cm⁻¹



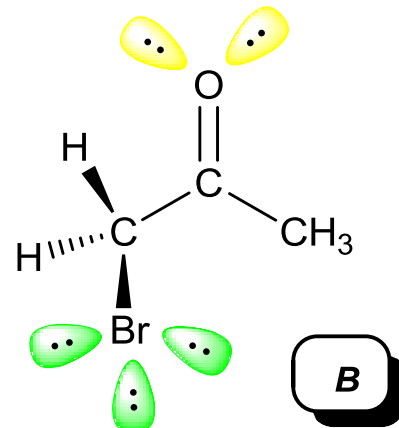
Küçülen halkada artan halka gerginliğinin hibritleşmeyi **sp²** den **sp** ye zorlaması C=O bağınyı kuvvetlendirir.

Ve C=O absorpsiyonu yüksek frekansa kayar.

5) Alan Etkileri



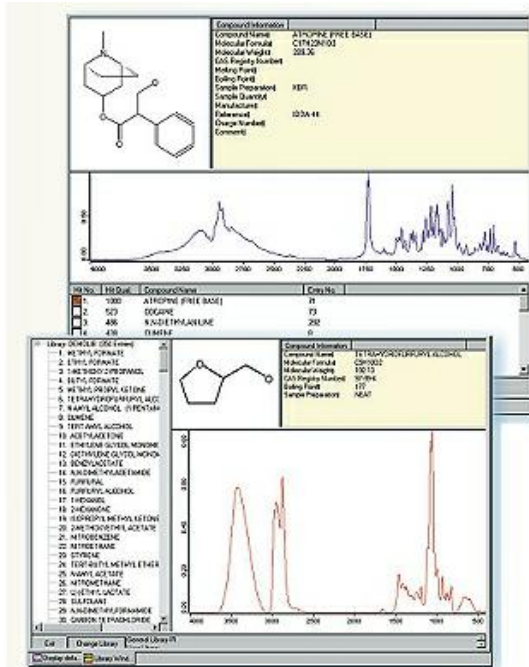
1745 cm^{-1}



1725 cm^{-1}

9. Kırmızı Ötesi (IR) Spektroskopisinin Uygulamaları

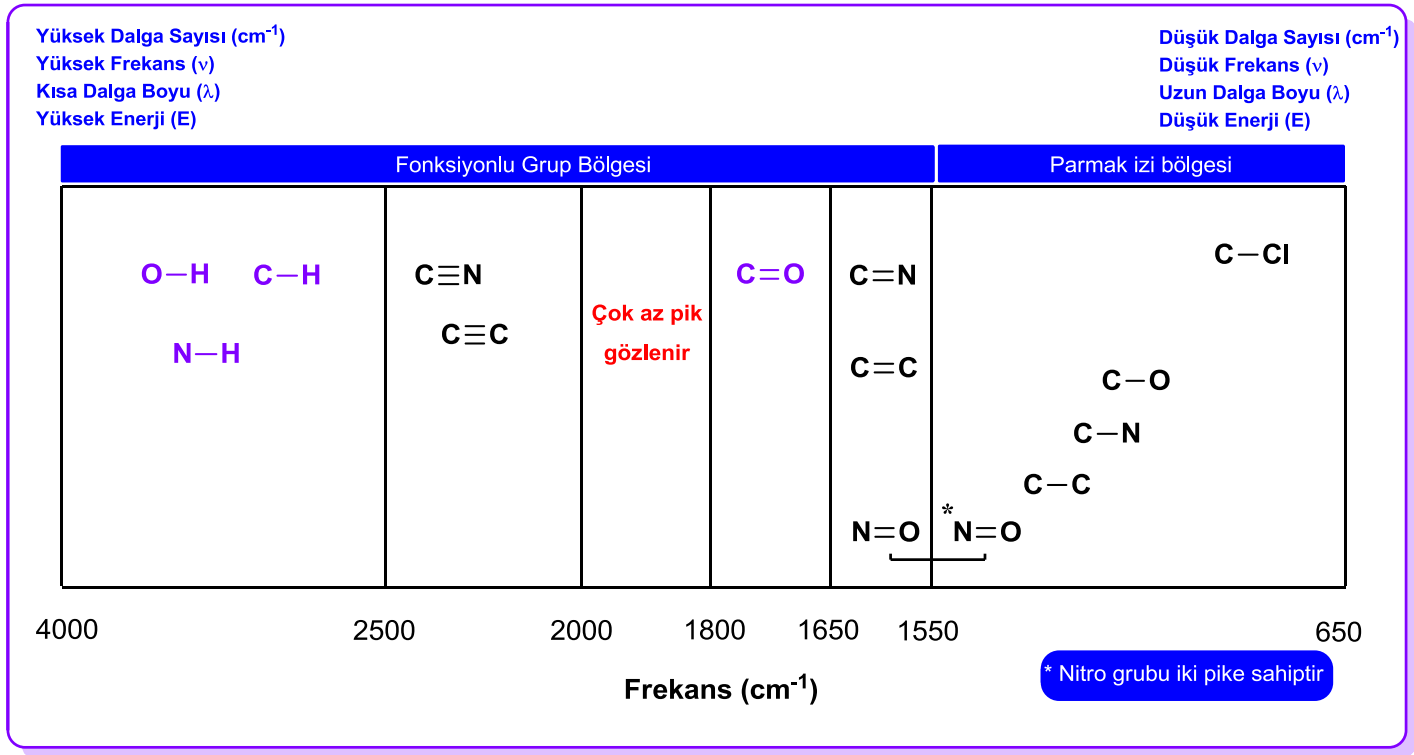
- Yapı tayini
- Kalitatif Analiz
- Saflık kontrolünde ve Endüstride Kullanılması



KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

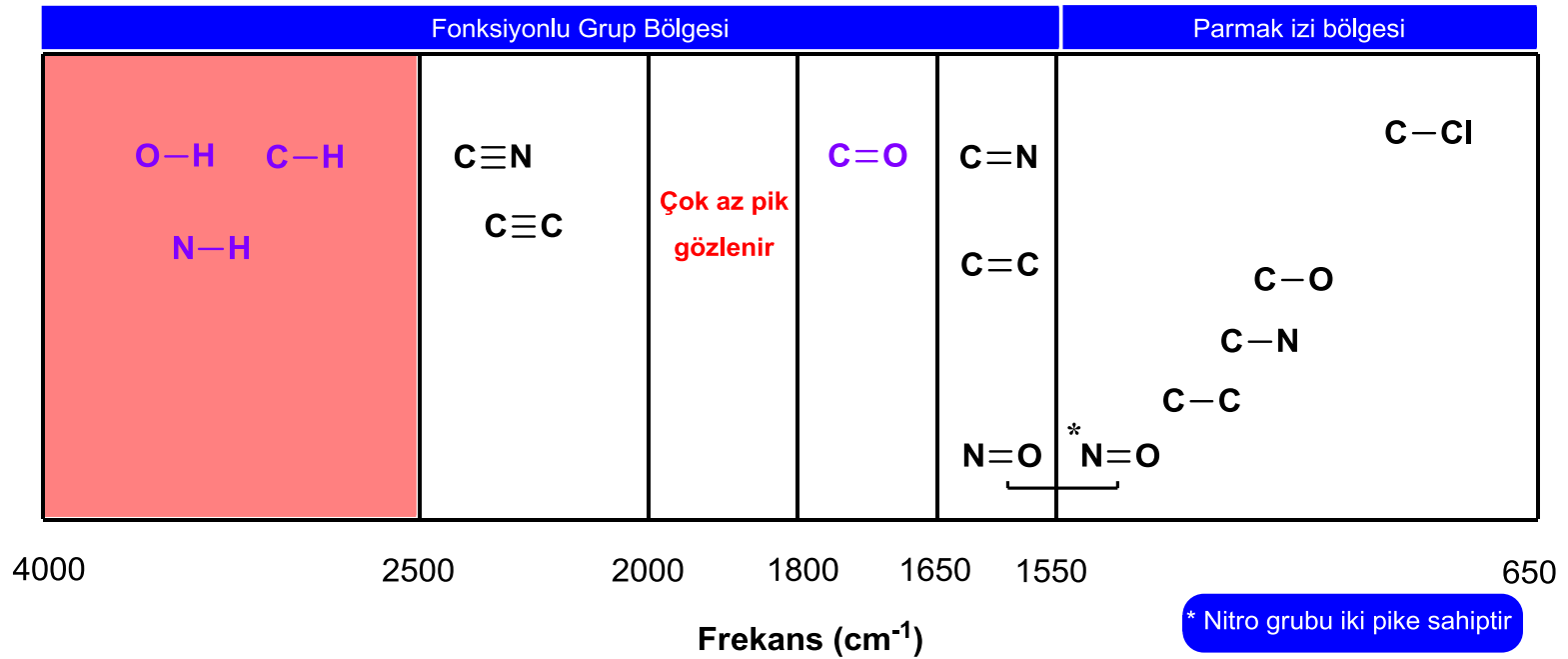
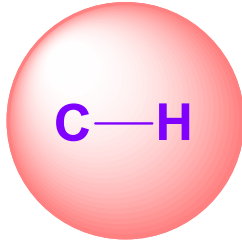
10. Kırmızı Ötesi (IR) Spektrumu-Yapı Değerlendirmesi

10.1. Kırmızı Ötesi (IR) Soğurma Bölgeleri



10.2. Kırmızı Ötesi (IR) Soğurma Bölgeleri (Tablolar)

10.4. Fonksiyonel Gruplara Sahip Bileşikler İçin Kırmızı Ötesi (IR) Spektrum Örnekleri



C-H Gerilme Bölgesi

Temel Değer = 3000 cm^{-1}

•C-H sp gerilme $\sim 3300 \text{ cm}^{-1}$

DOYMAMIŞ

•C-H sp^2 gerilme $> 3000 \text{ cm}^{-1}$

3000

•C-H sp^3 stretch $< 3000 \text{ cm}^{-1}$

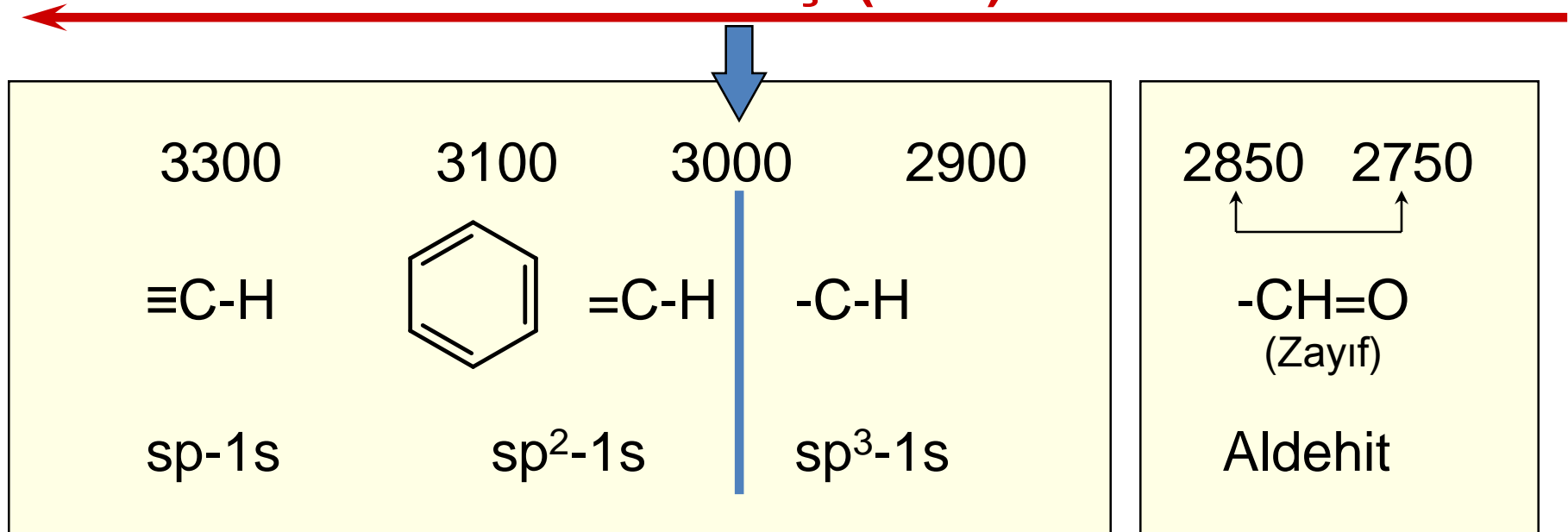
DOYMUŞ

•C-H aldehit, iki pik (ikiside zayıf)

~ 2850 and 2750 cm^{-1}

Güçlü Bağlar Büyük Kuvvet Sabitine Sahiptir ve Yüksek Frekansta IR Işınını Soğururlar (Absorplarlar)

Frekans artışı (cm^{-1})



s Karakterinde artma

CH Bağ Titreşim Frekansında Artma

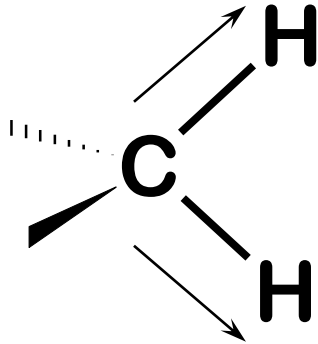
K, Kuvvet Sabitinde Artış

KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

METİLEN GRUBU GERİLME TİTREŞİMİ

İki C-H Bağı Merkezi Bir Karbonu Paylaşırlar
(Hidrojenler Aynı C Bağlıdır)

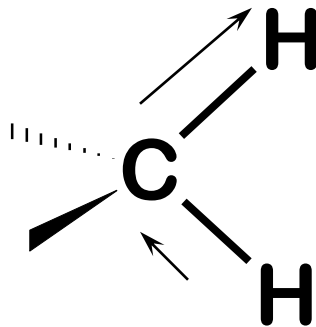
Düzlem içi



Simetrik Gerilme

$\sim 2853 \text{ cm}^{-1}$

Düzlem dışı



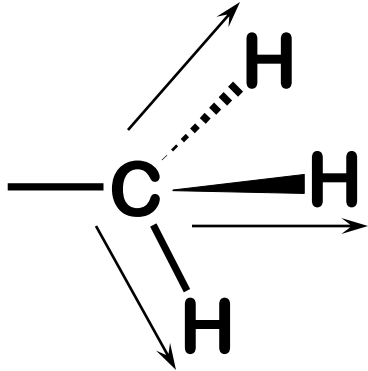
Asimetrik Gerilme

$\sim 2926 \text{ cm}^{-1}$

METİL GRUBU GERİLME TİTREŞİMLERİ

Üç C-H bağı Merkezi bir karbonu paylaşır

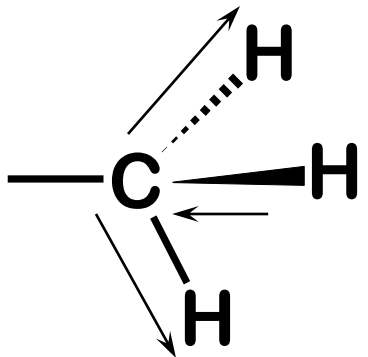
Düzlem içi



Simetrik Gerilme

$\sim 2872 \text{ cm}^{-1}$

Düzlem dışı

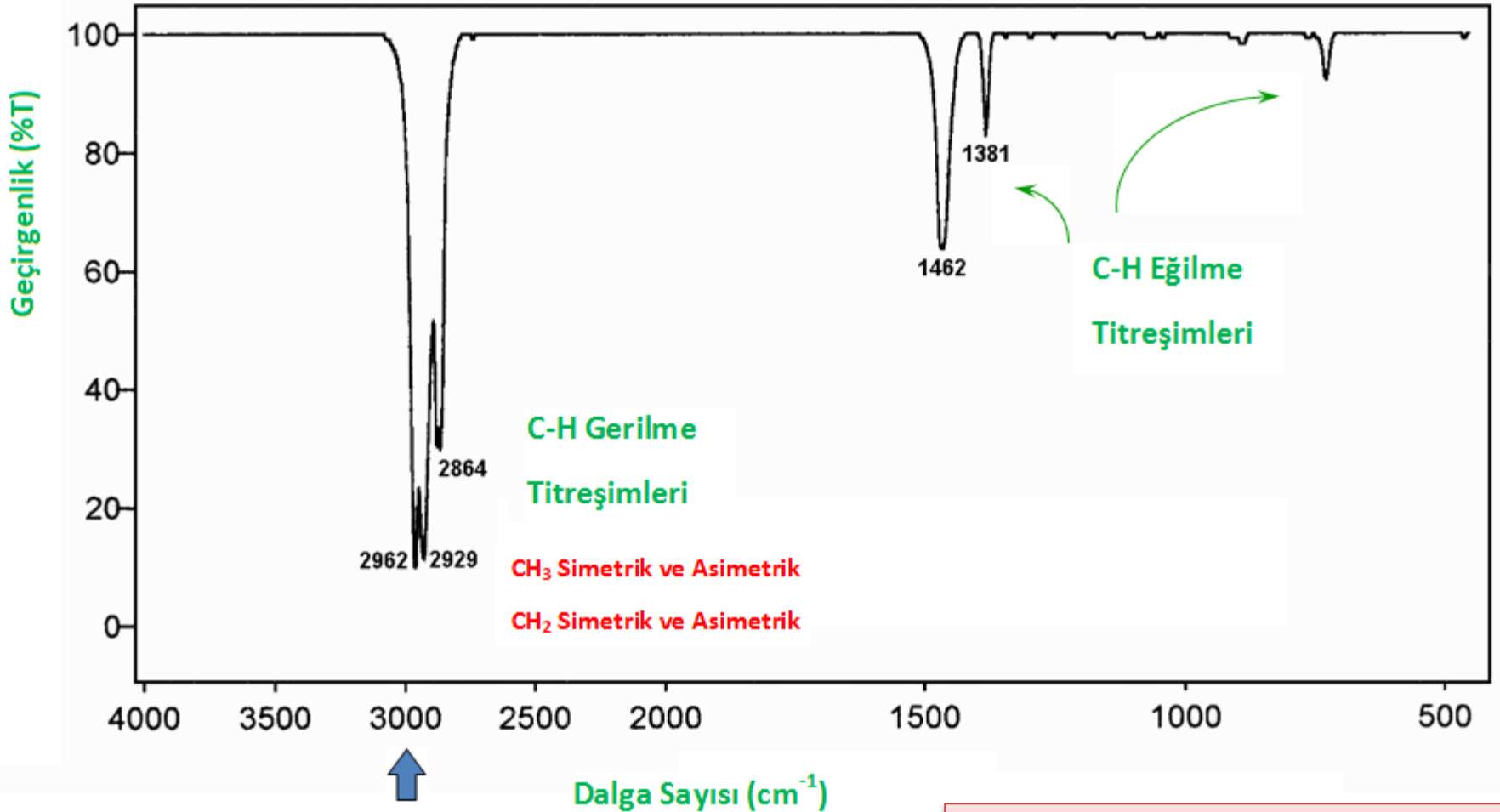
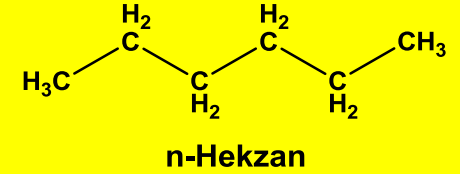


Asimetrik Gerilme

$\sim 2962 \text{ cm}^{-1}$

ALKANLAR

n-Hekzan



KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

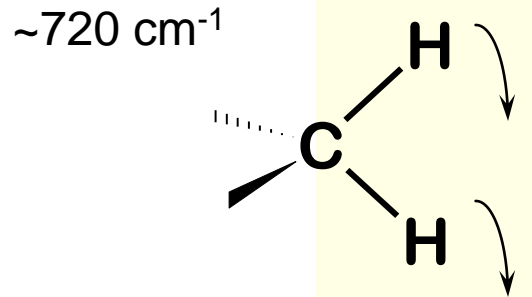
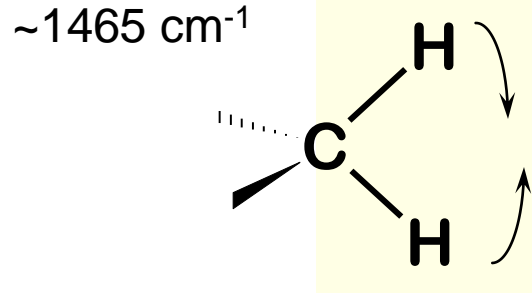
C-H EĞİLME BÖLGESİ

- CH_2 eğilme $\sim 1465 \text{ cm}^{-1}$

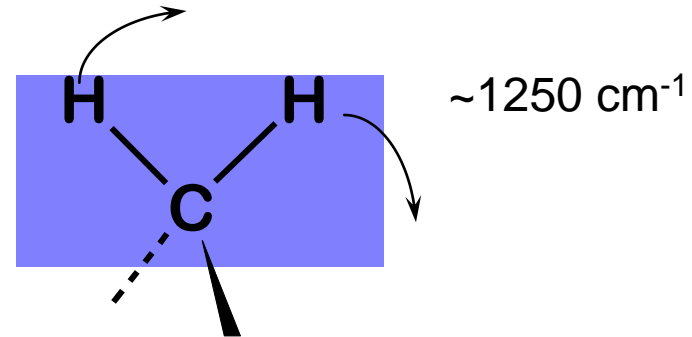
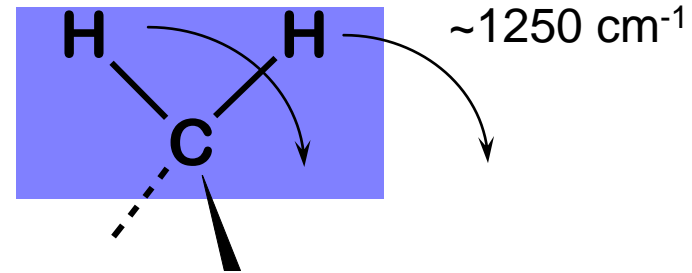
- CH_3 eğilme (asim.) CH_2 ile aynı yerde $\sim 1460 \text{ cm}^{-1}$ görülür
- CH_3 eğilme (sim.) $\sim 1375 \text{ cm}^{-1}$

METİLEN GRUBU EĞİLME TİTREŞİMLERİ

Makaslama



Dalgalanma



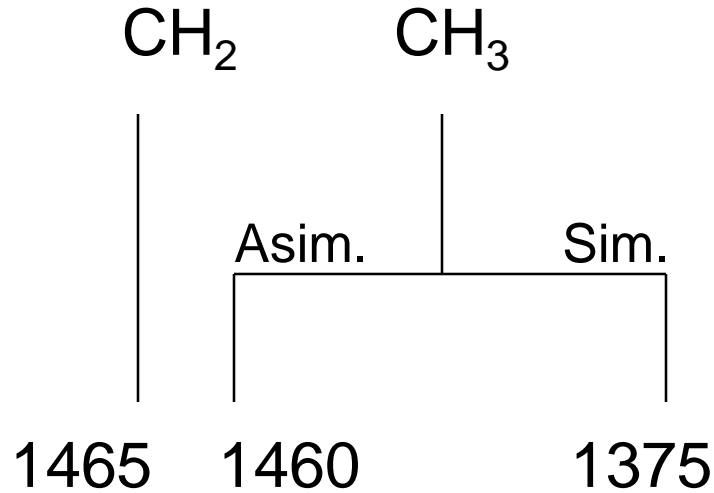
Sallanma

Burulma

— Düzlem içi — — Düzlem dışı —
Eğilme titreşimleri

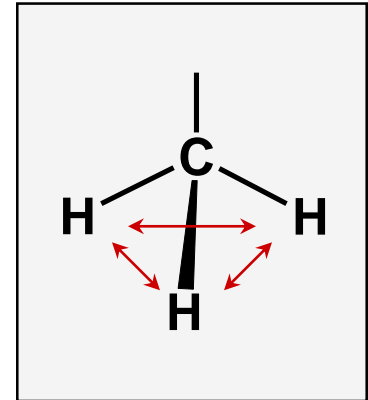
KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

METİLEN ve METİL EĞİLME TİTREŞİMLERİ



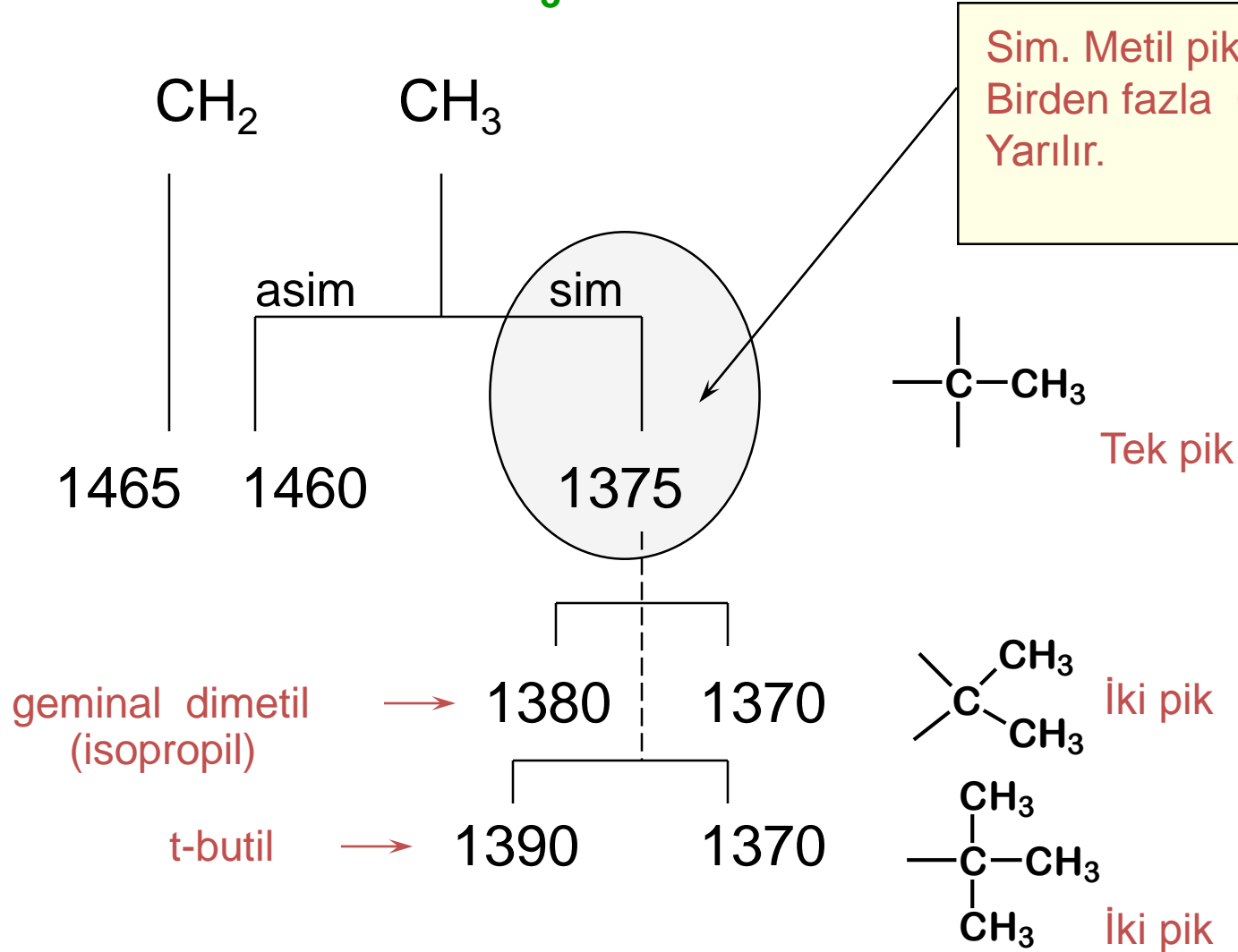
Bu iki pik üst üste örtüşürler
ve ayırt edilemezler

C-H eğilme, yaklaşık
1465 ve 1375 cm⁻¹ gözlenir



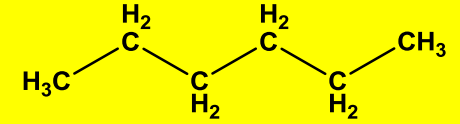
METİLEN ve METİL EĞİLME TİTREŞİMLERİ

İÇİN EK DETAYLAR SİM. CH_3

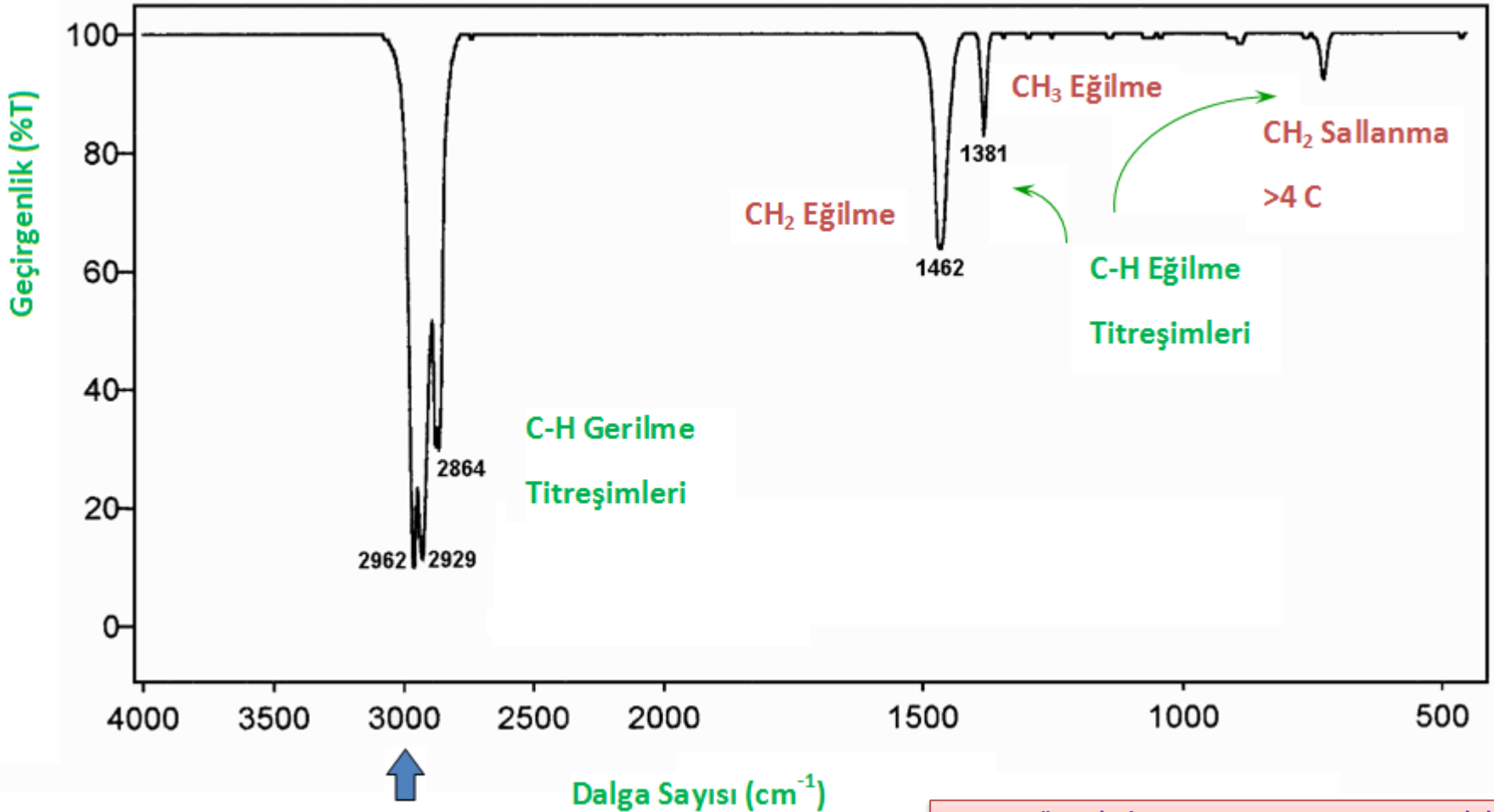


KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

n-Hekzan



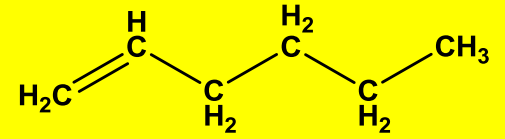
n-Hekzan



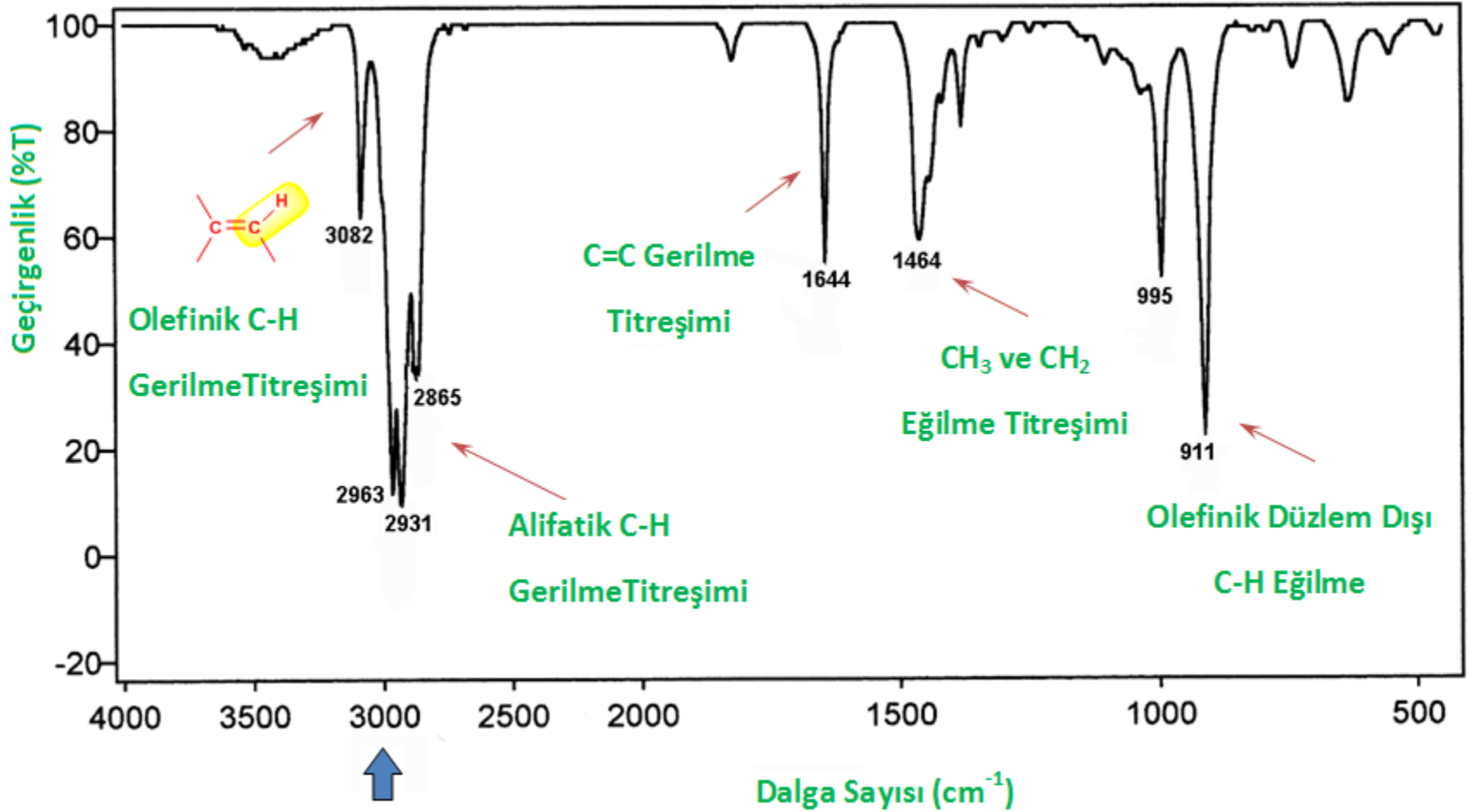
KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

ALKENLER

1-Hekzen



1-Hekzen

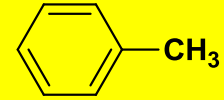


KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

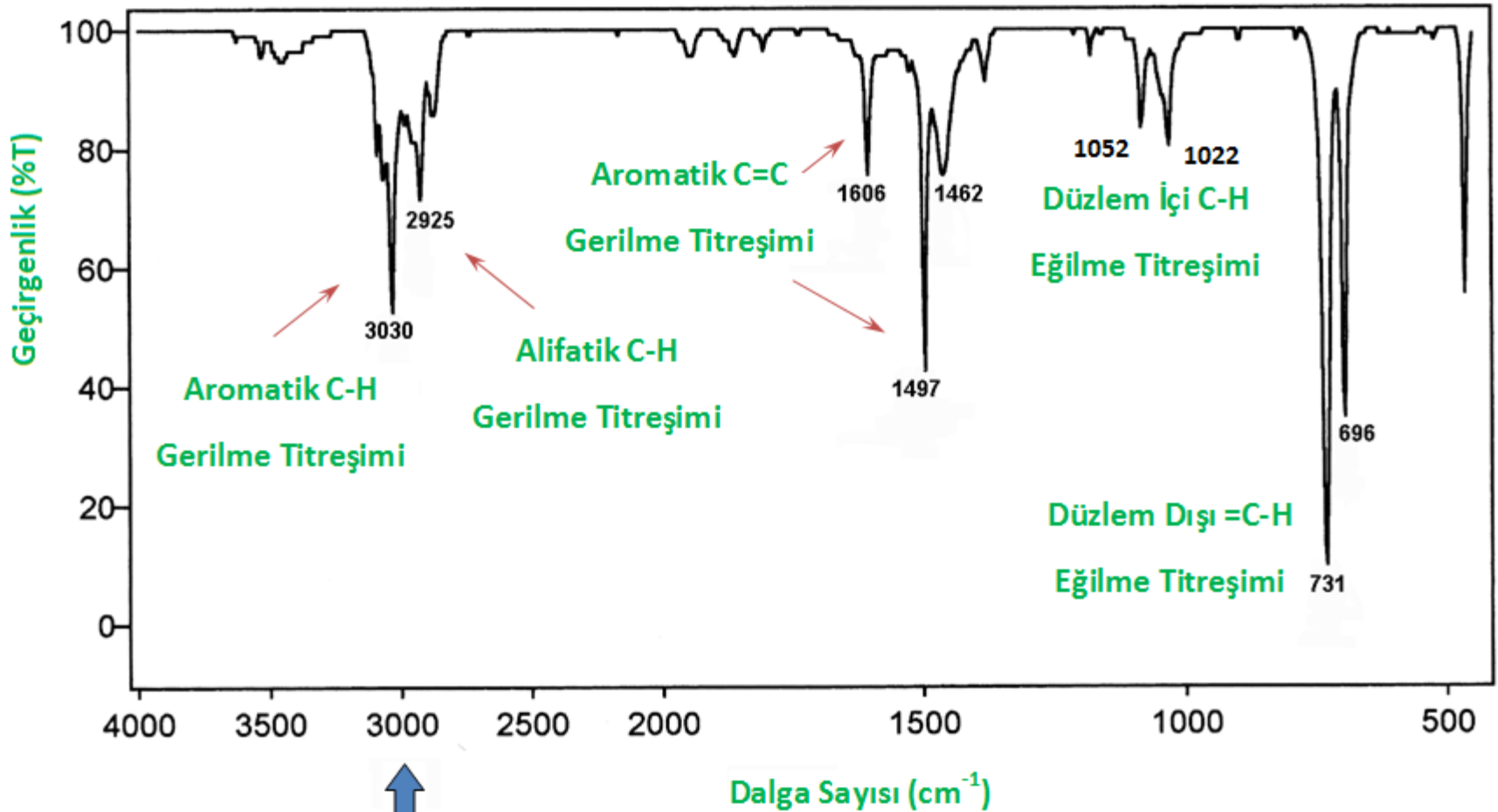
AROMATİK YAPILAR

Katlı ton veya Kombinasyon bandları;

2000-1667 cm^{-1}

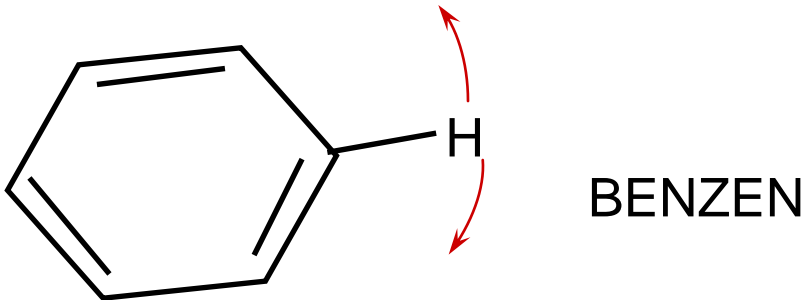
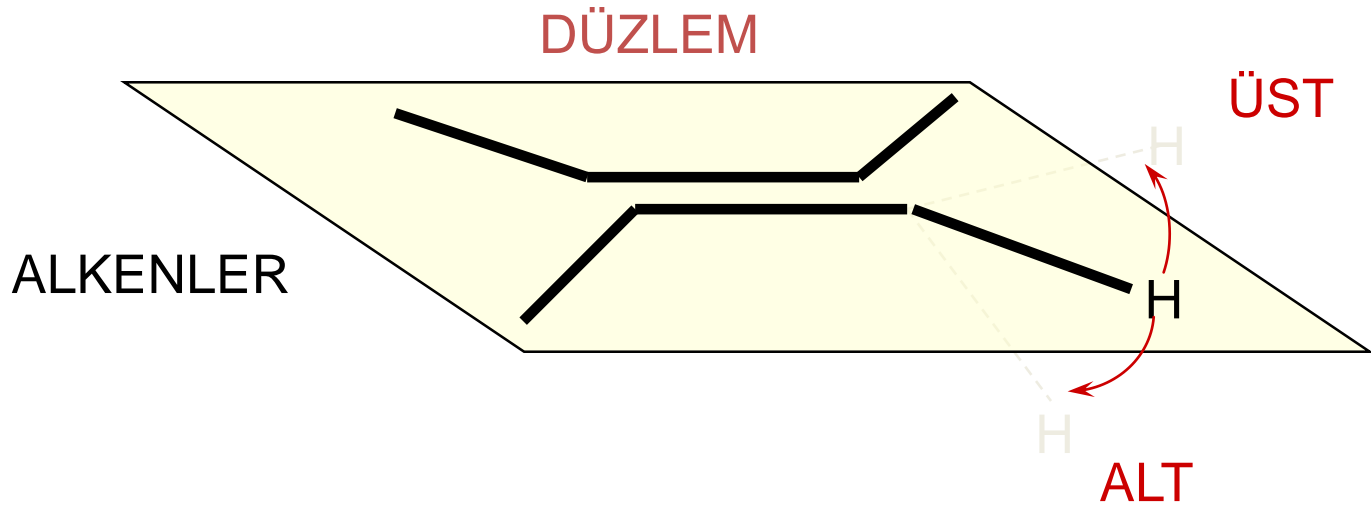


Toluen



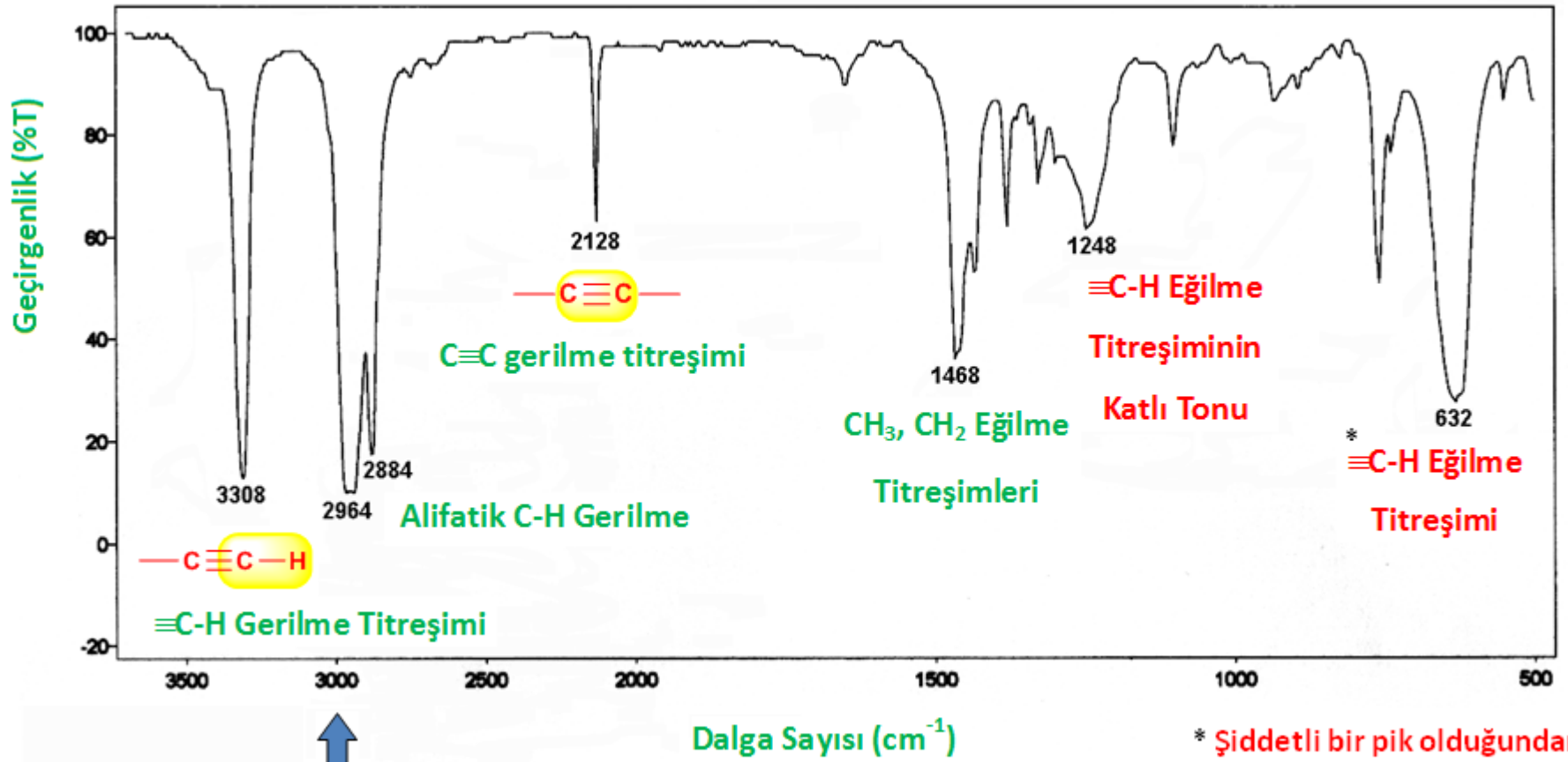
KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

DÜZLEM DIŐI EĞİLMELER



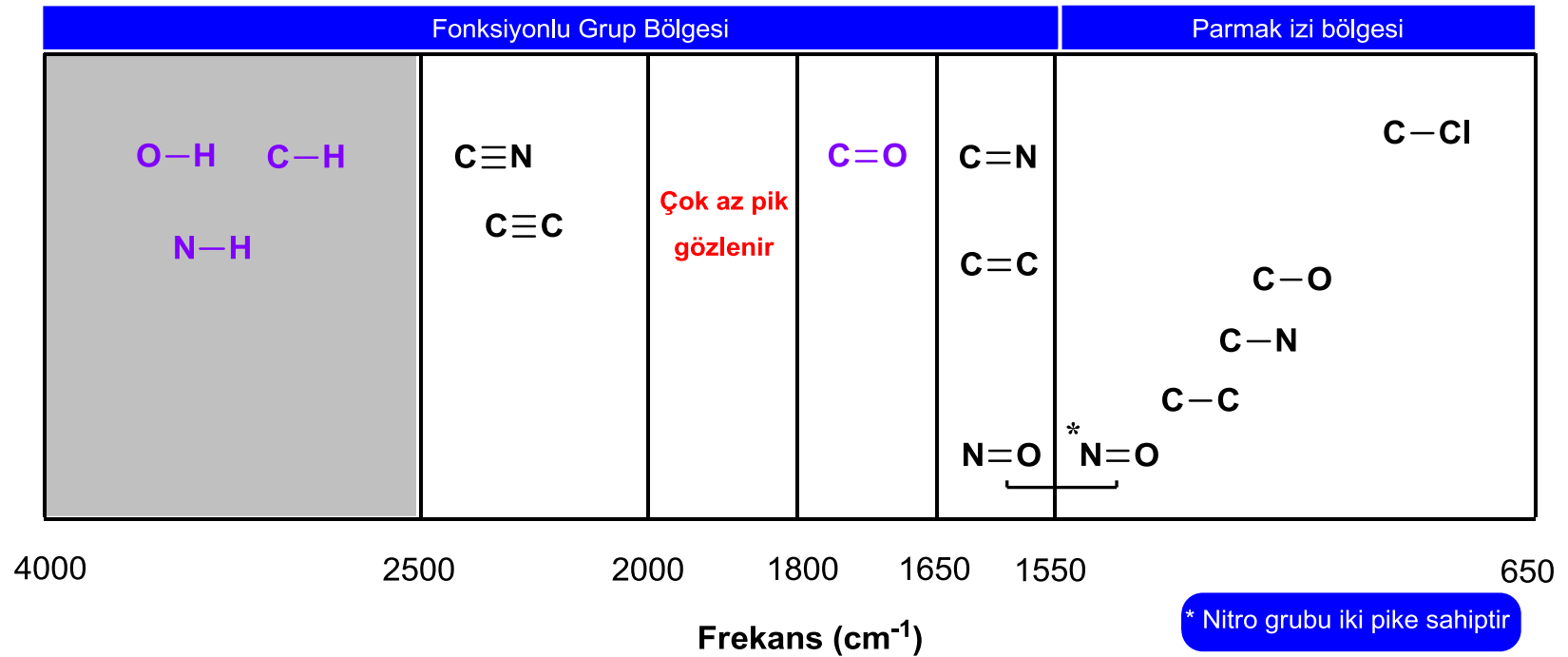
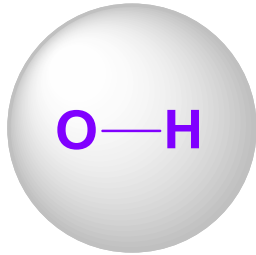
ALKİNLER

1-Hekzin



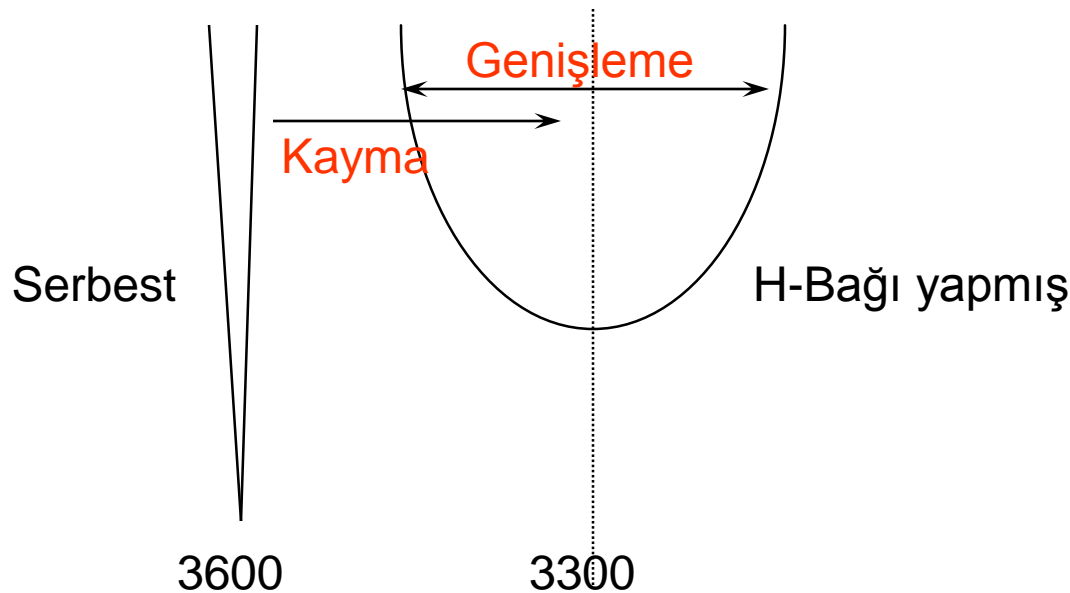
* Şiddetli bir pik olduğundan Overtonu (katlıtonu) gözlenir

KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ



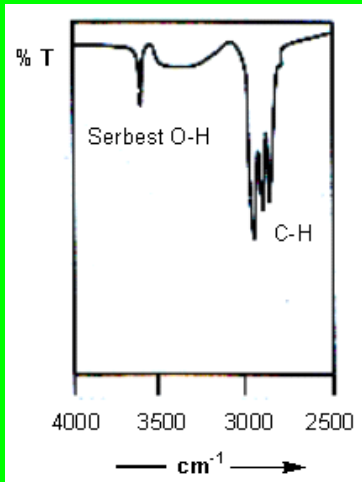
O-H Gerilme Bölgesi

- O-H 3600 cm^{-1} (alkol, serbest)
- O-H 3300 cm^{-1} (alkoller & k.asitler, H-bağı yapmış)

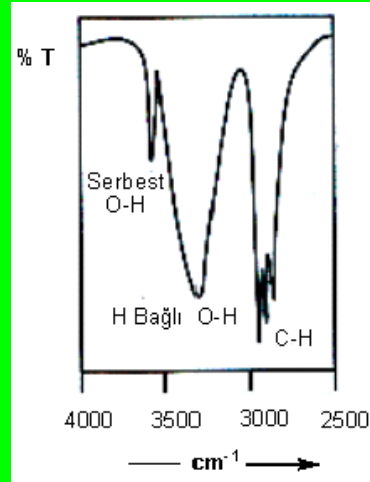


➤ Bu titreşimlerden ileri gelen absorpsiyonlar hidrojen bağına karşı hassastırlar.

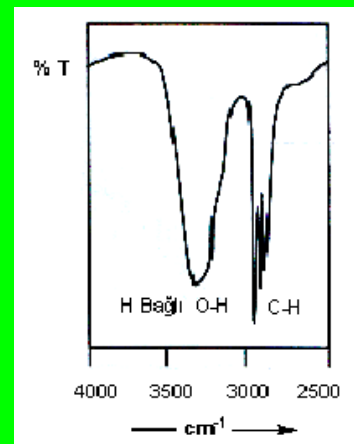
O-H Gerilmesine Hidrojen Baęının Etkisi



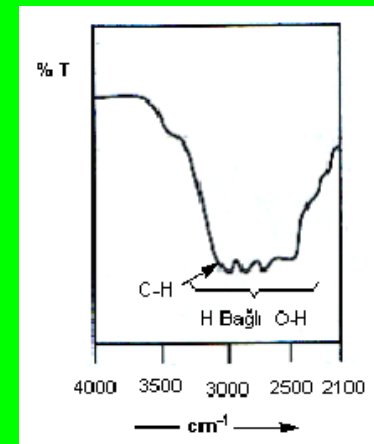
1



2



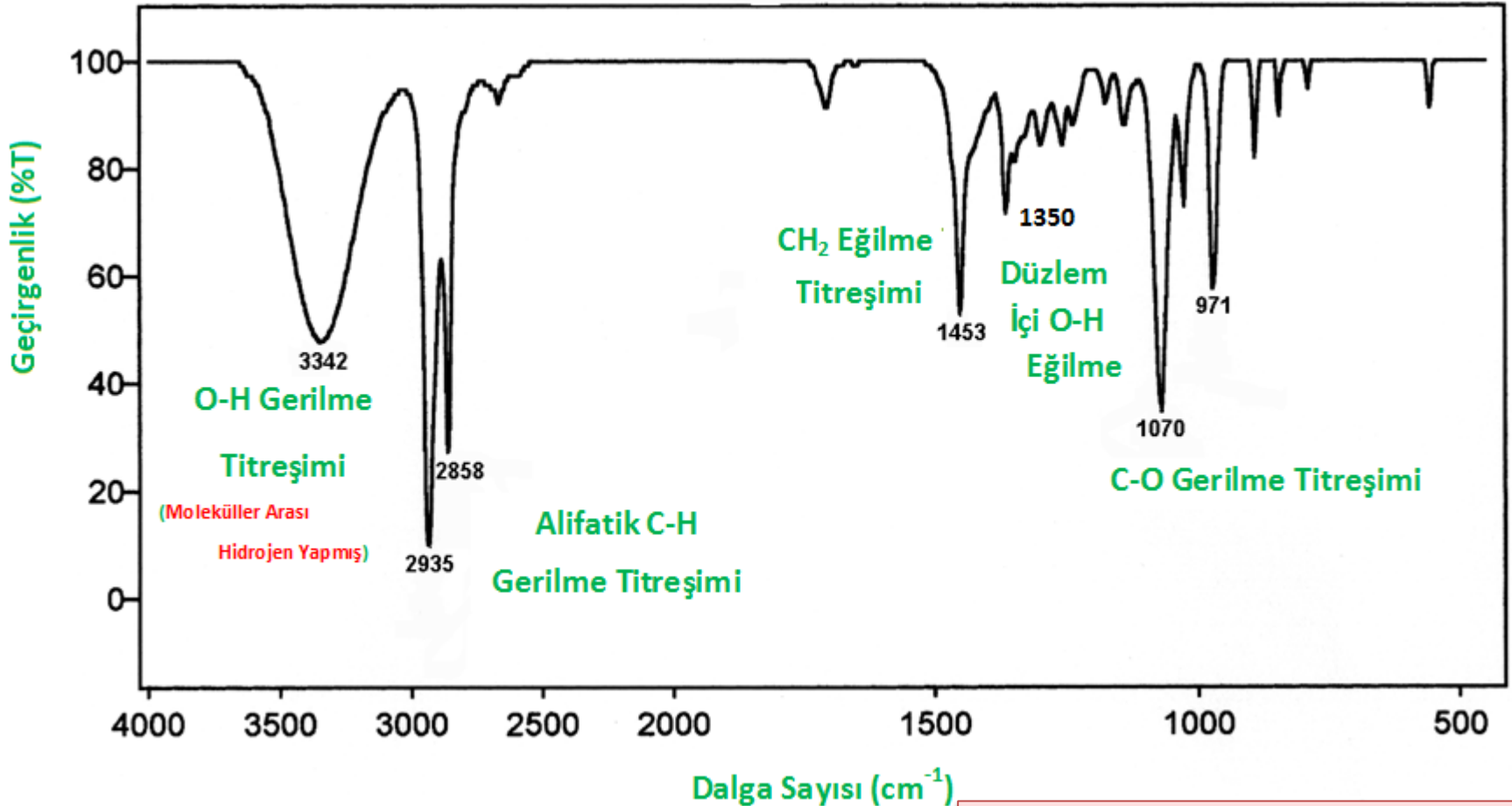
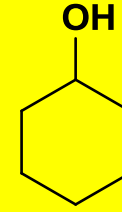
3



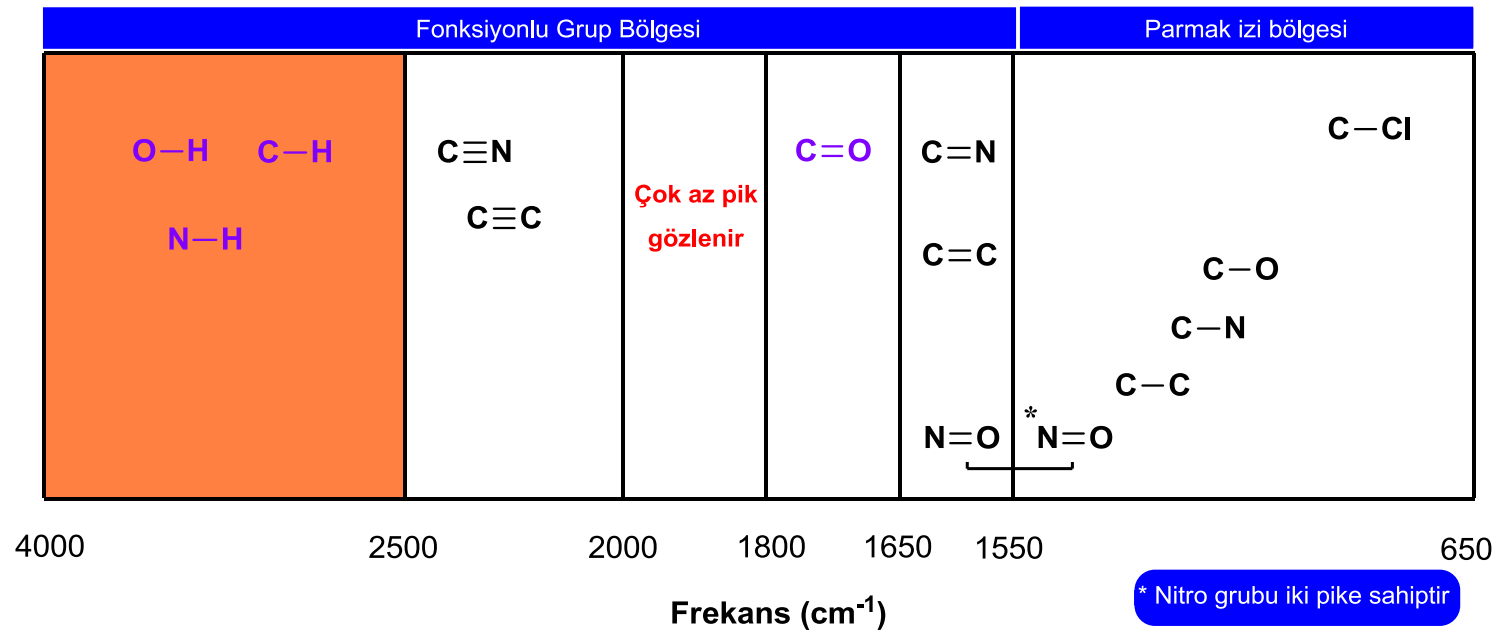
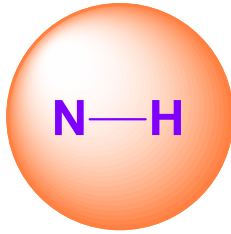
4

ALKOLLER

Sikloheksanol

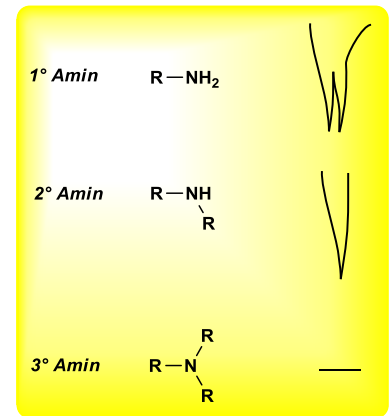


KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

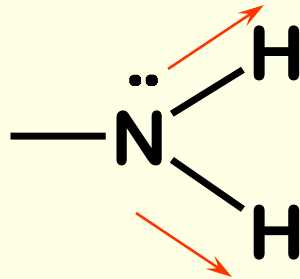


N-H gerilme bölgesi

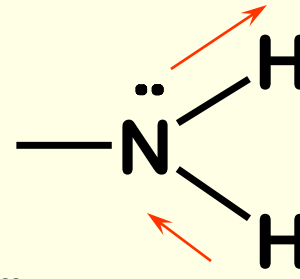
N-H 3300 - 3400 cm^{-1}



- Primer aminler iki pik verir.



simetrik

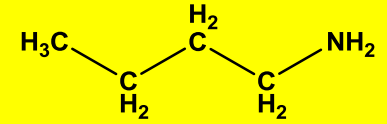


asimetrik

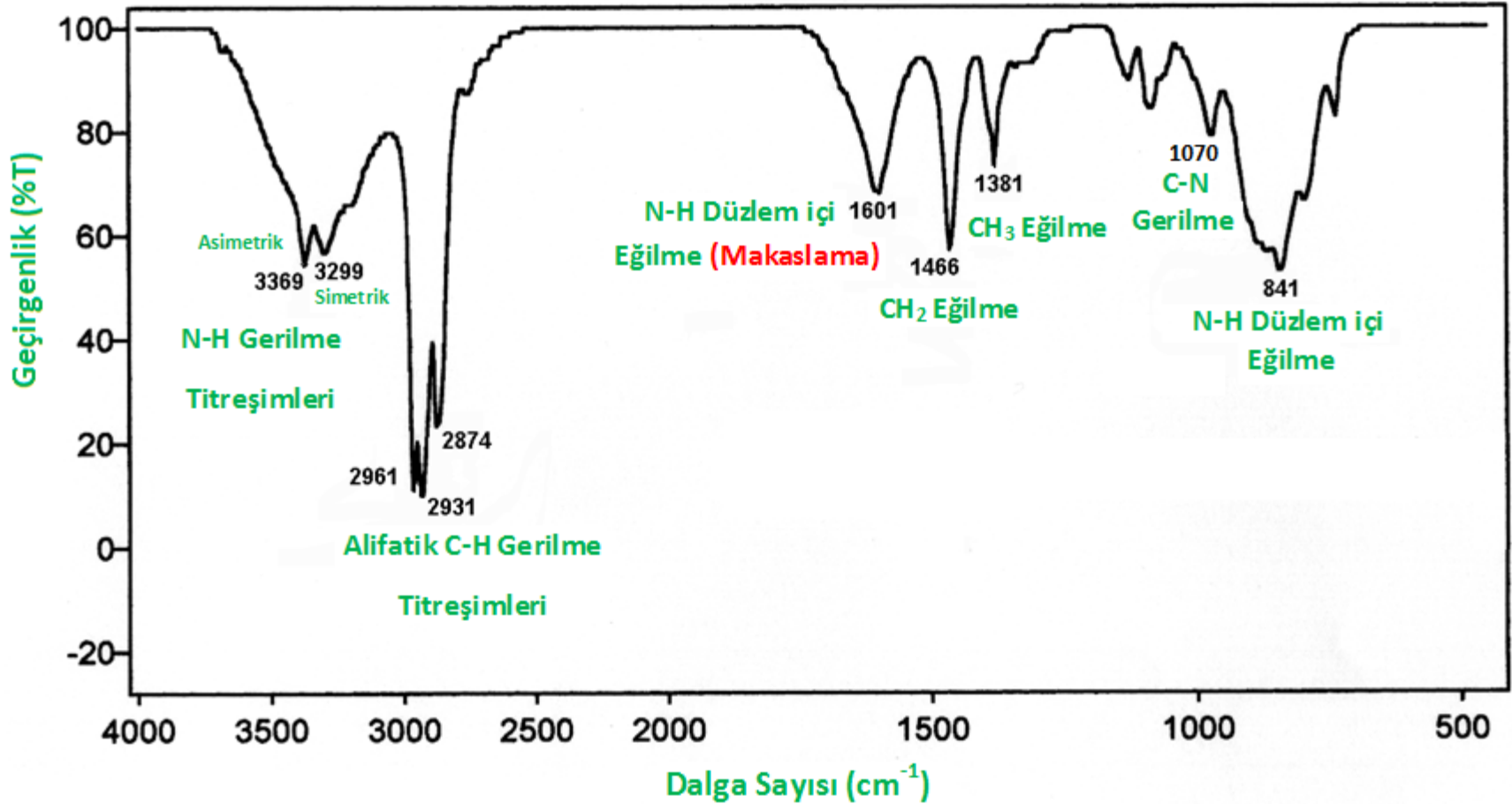
- Sekonder aminler tek pik verir.
- Tersiyer aminler pik vermez.

AMİNLER (Primer Aminler)

1-Bütanamin



1-Bütanamin



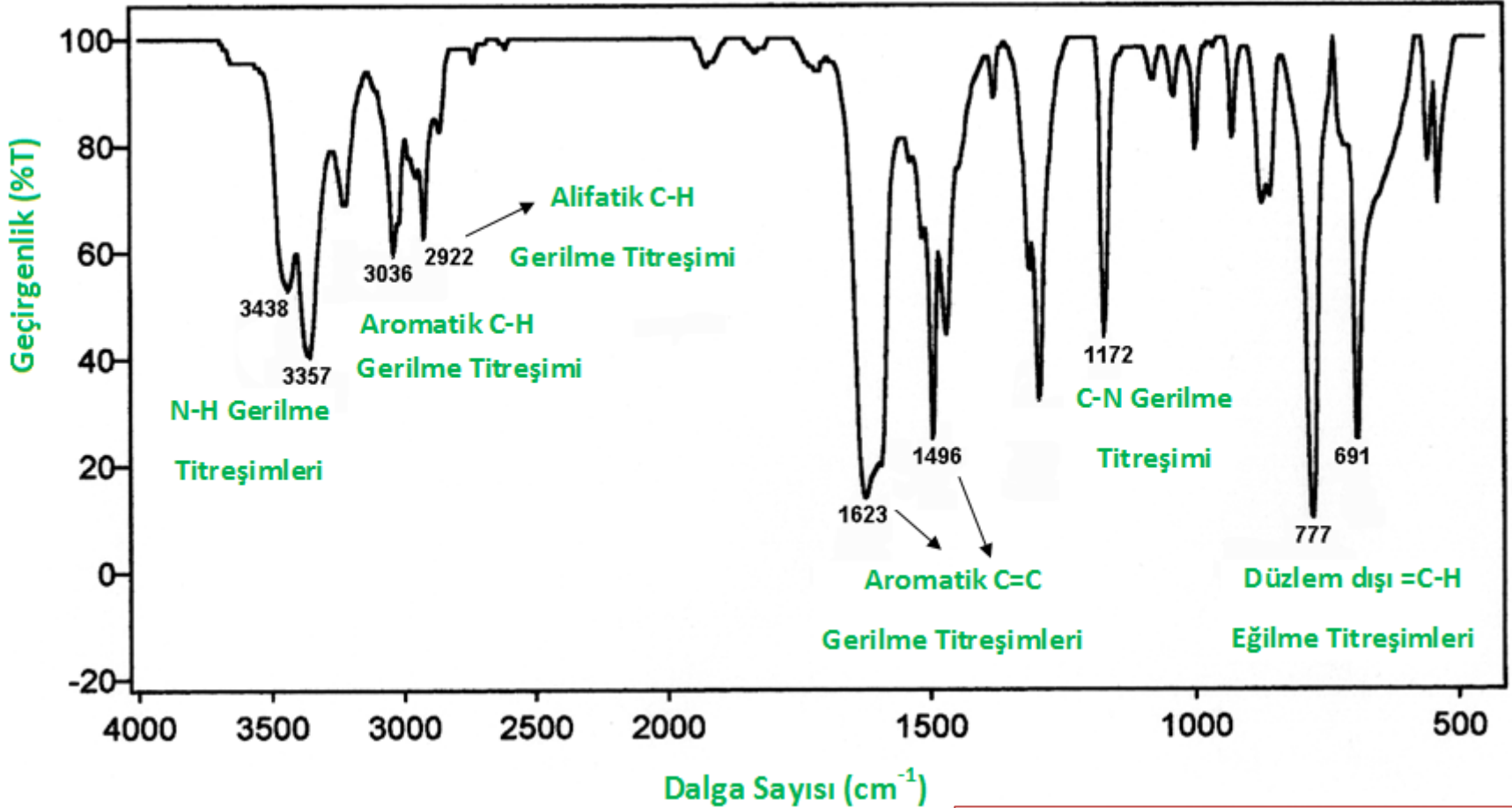
KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

PRİMER AROMATİK AMİN (Primer Aminler)

3-Metilanilin



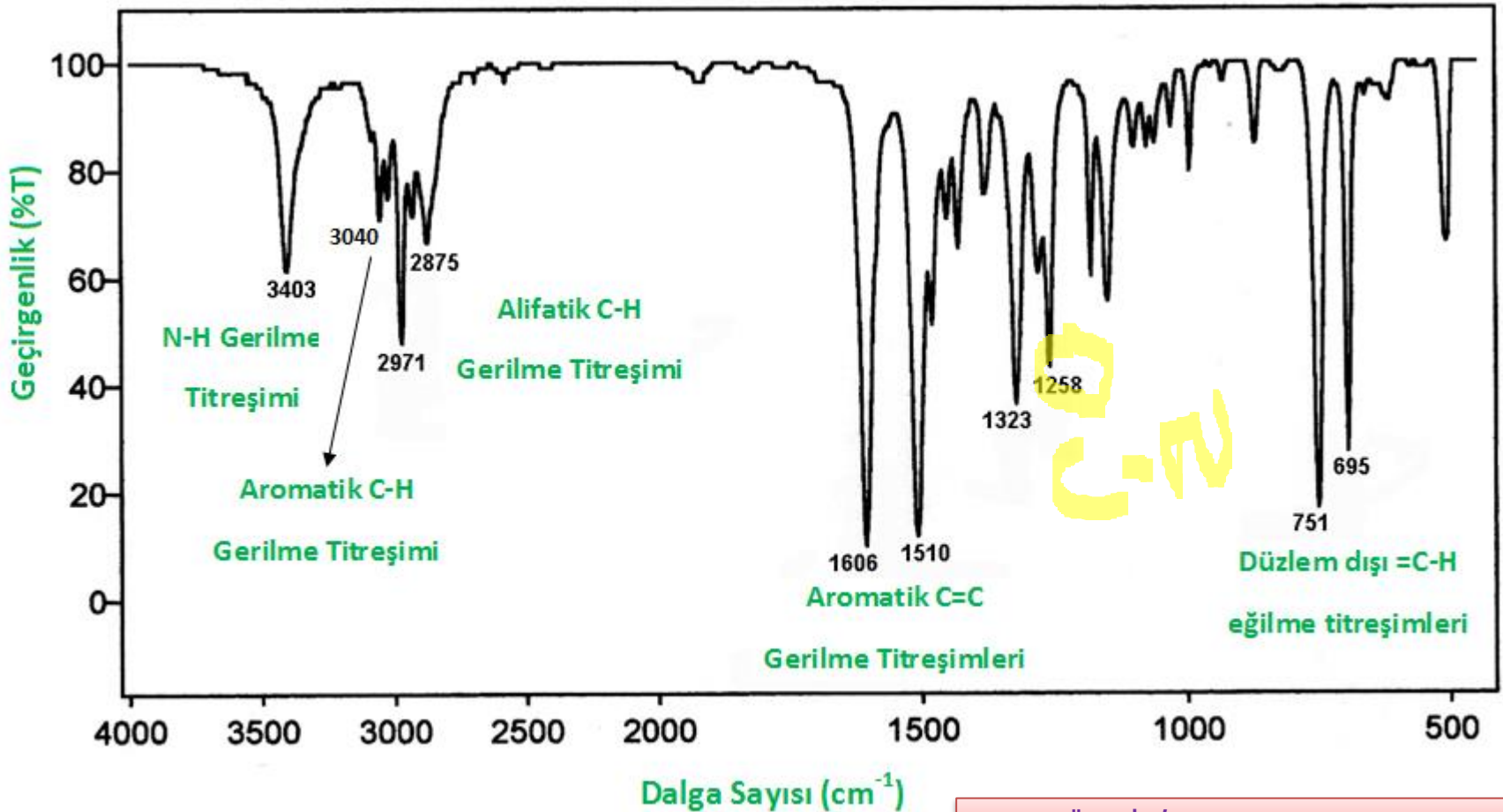
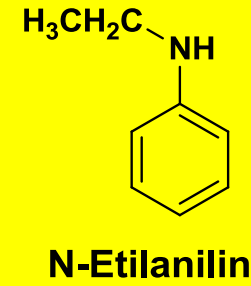
3-Metilanilin



KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

AMİNLER (Sekonder Aminler)

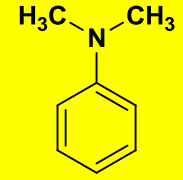
N-Etilanilin



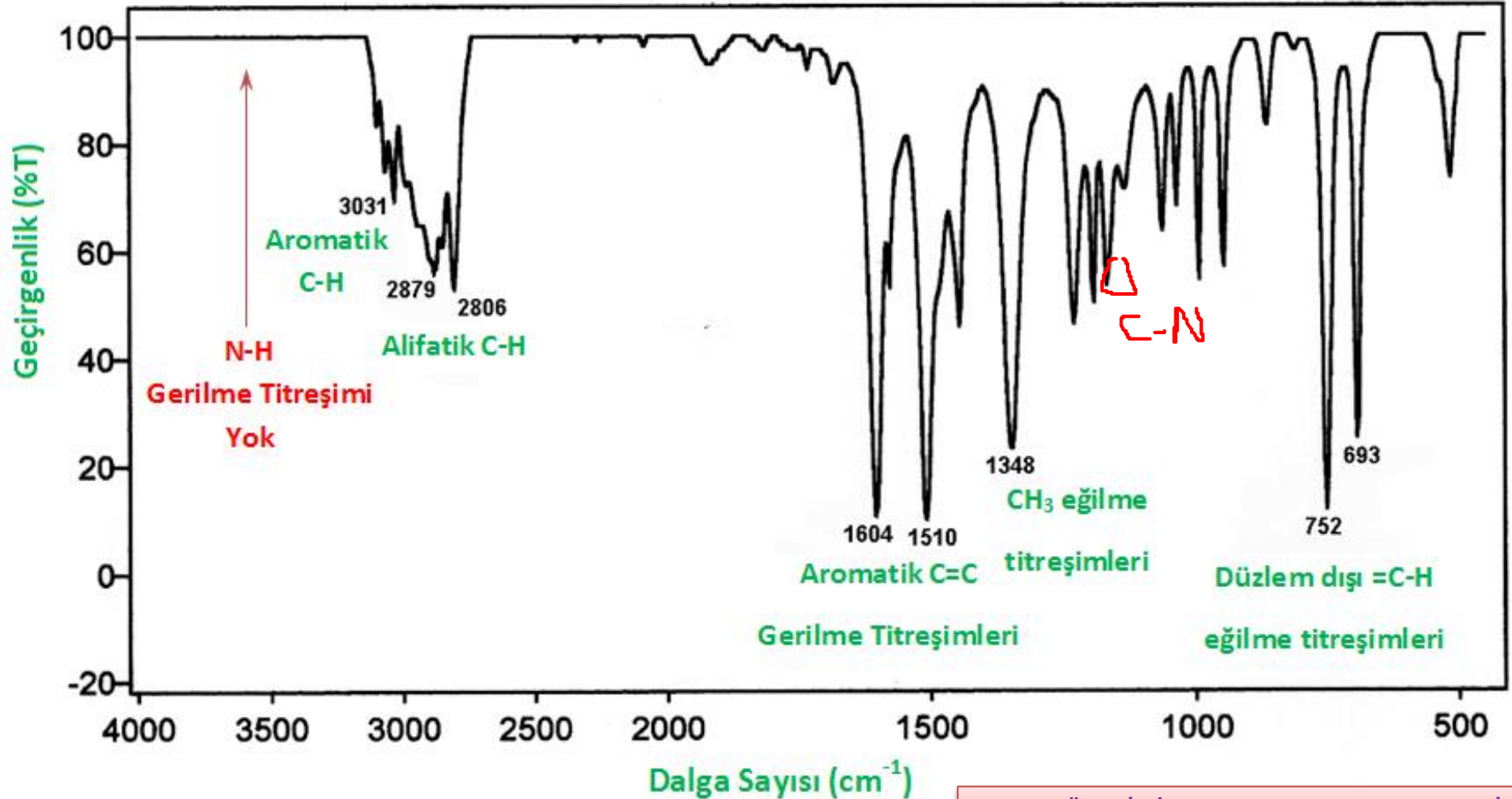
KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

AMİNLER (Tersiyer Aminler)

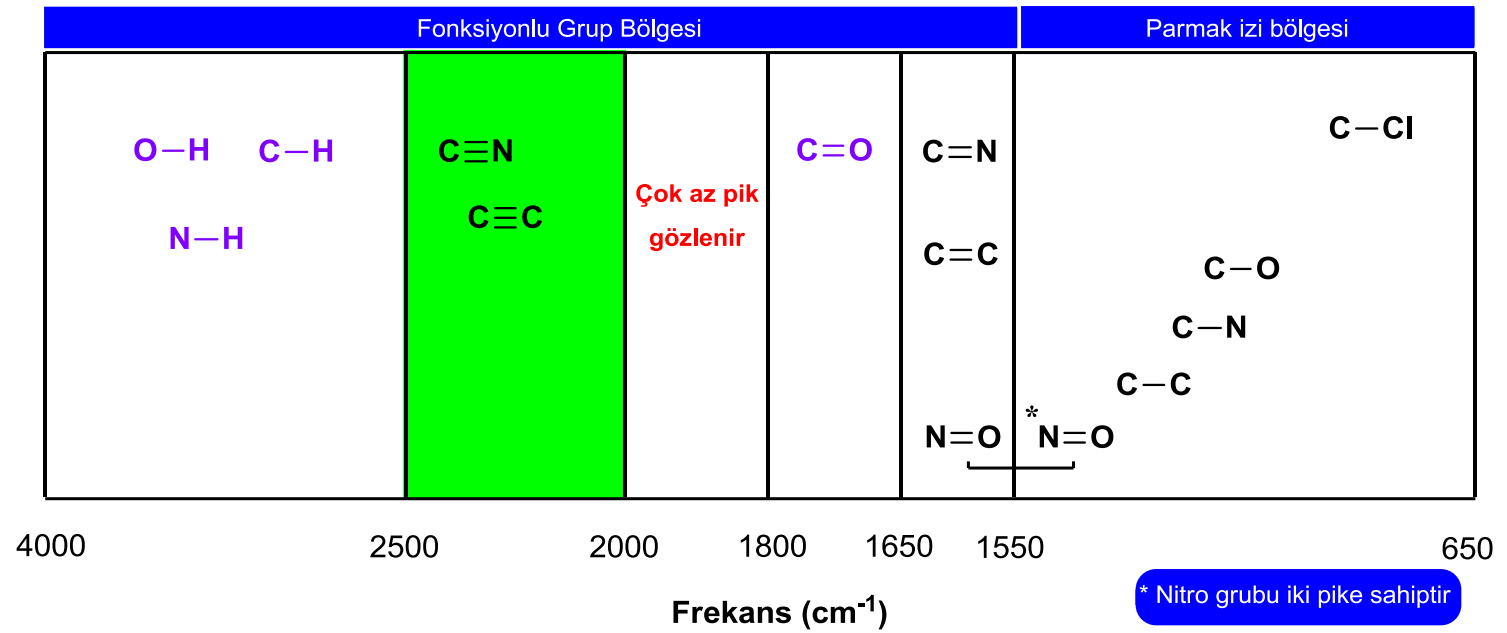
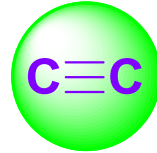
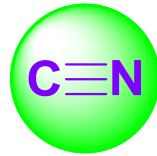
N,N -Dimetilanilin



N-Dimetilanilin



KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

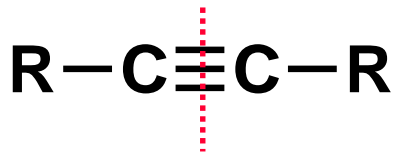


Üçlü Bağ Gerilme bölgesi

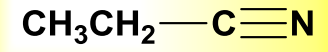
- $\text{C}\equiv\text{N}$ 2250 cm^{-1}
- $\text{C}\equiv\text{C}$ 2150 cm^{-1}

Siyano grubu büyük bir dipol momente sahip olduğundan keskin bir pik verir.

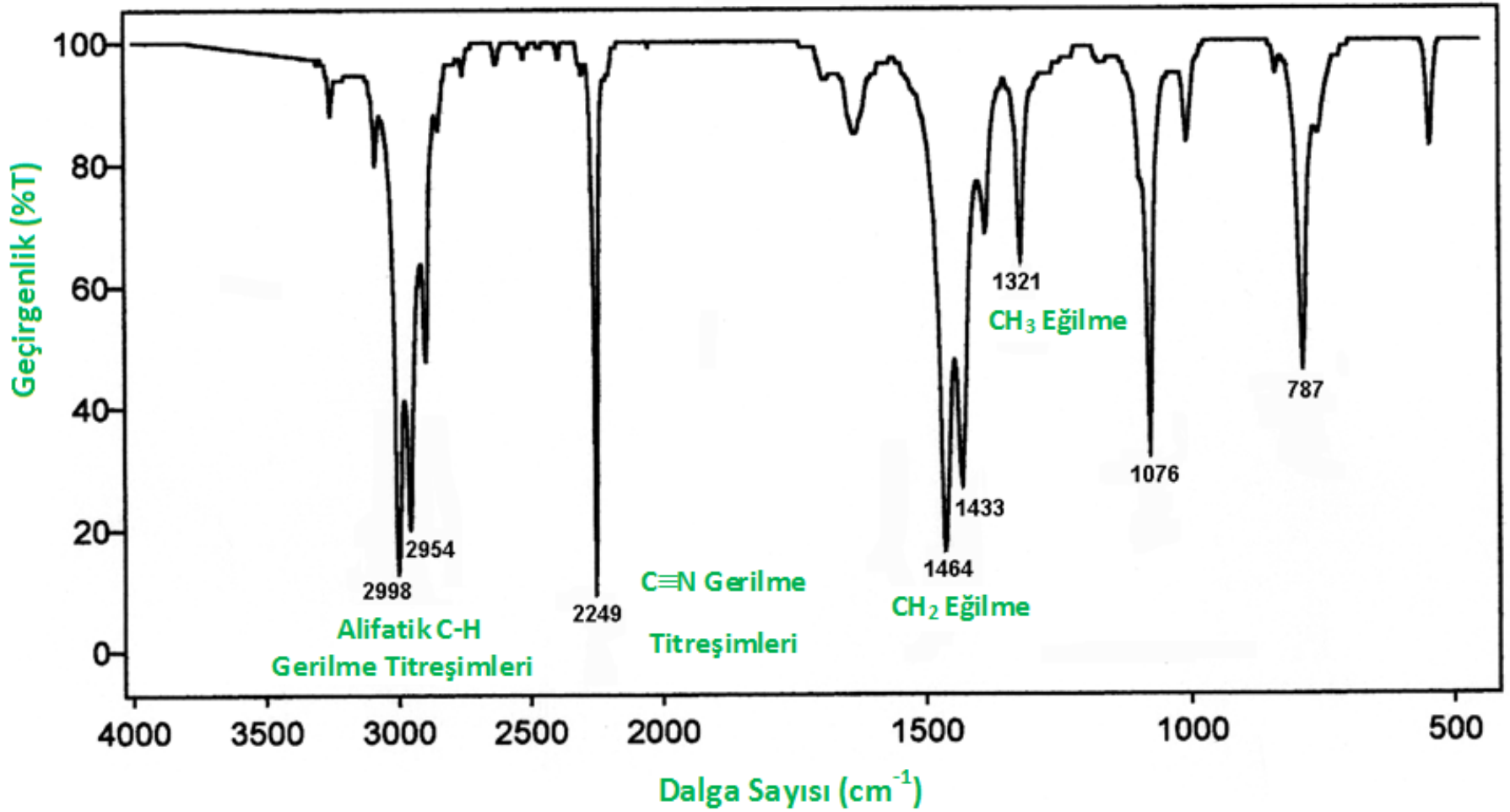
Karbon-Karbon Üçlü Bağı Keskin bir Pik verir, fakat molekül simetrik ise bu pik zayıftır.

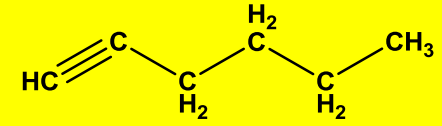


NİTRİLLER

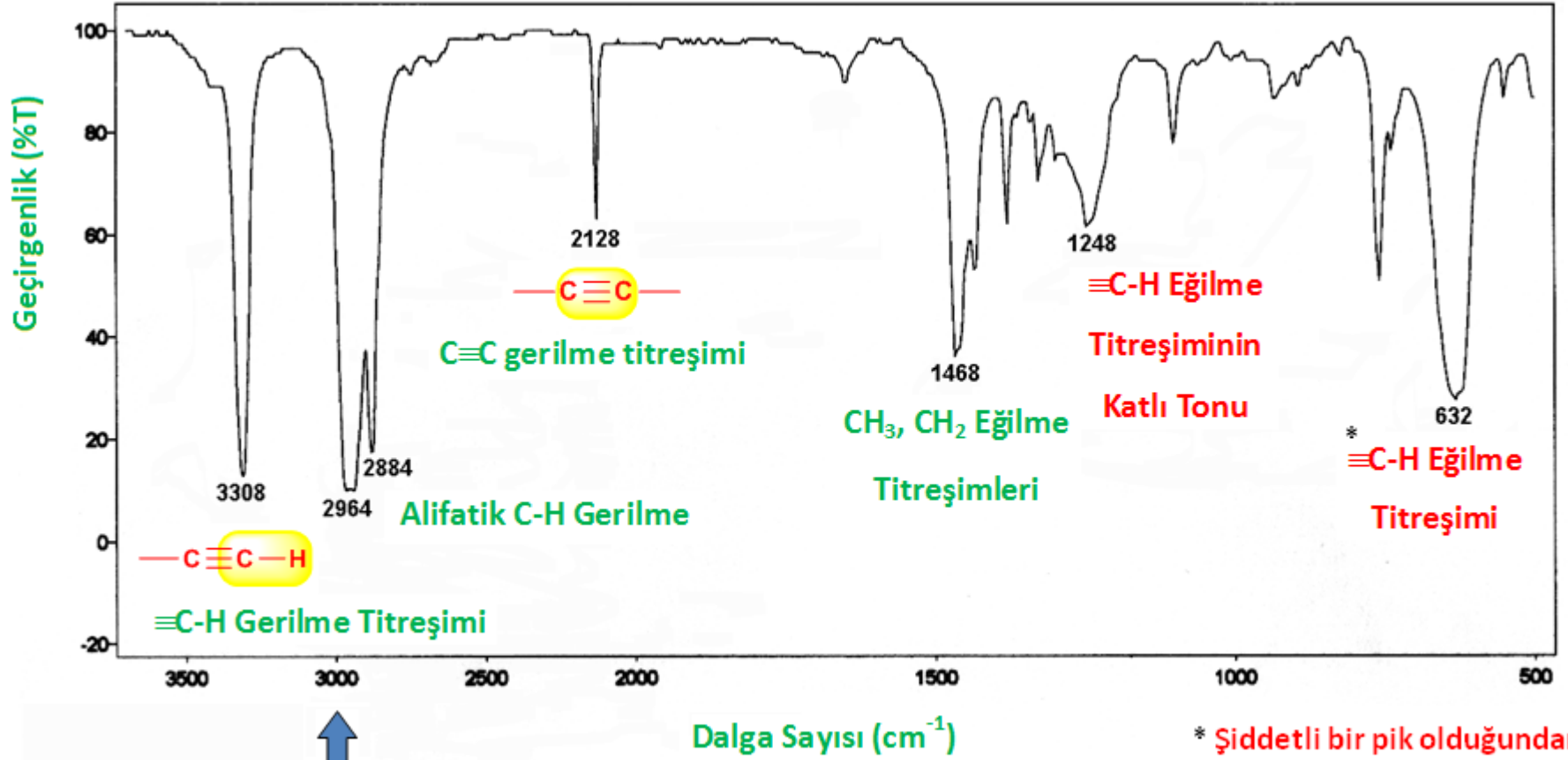


Propannitril

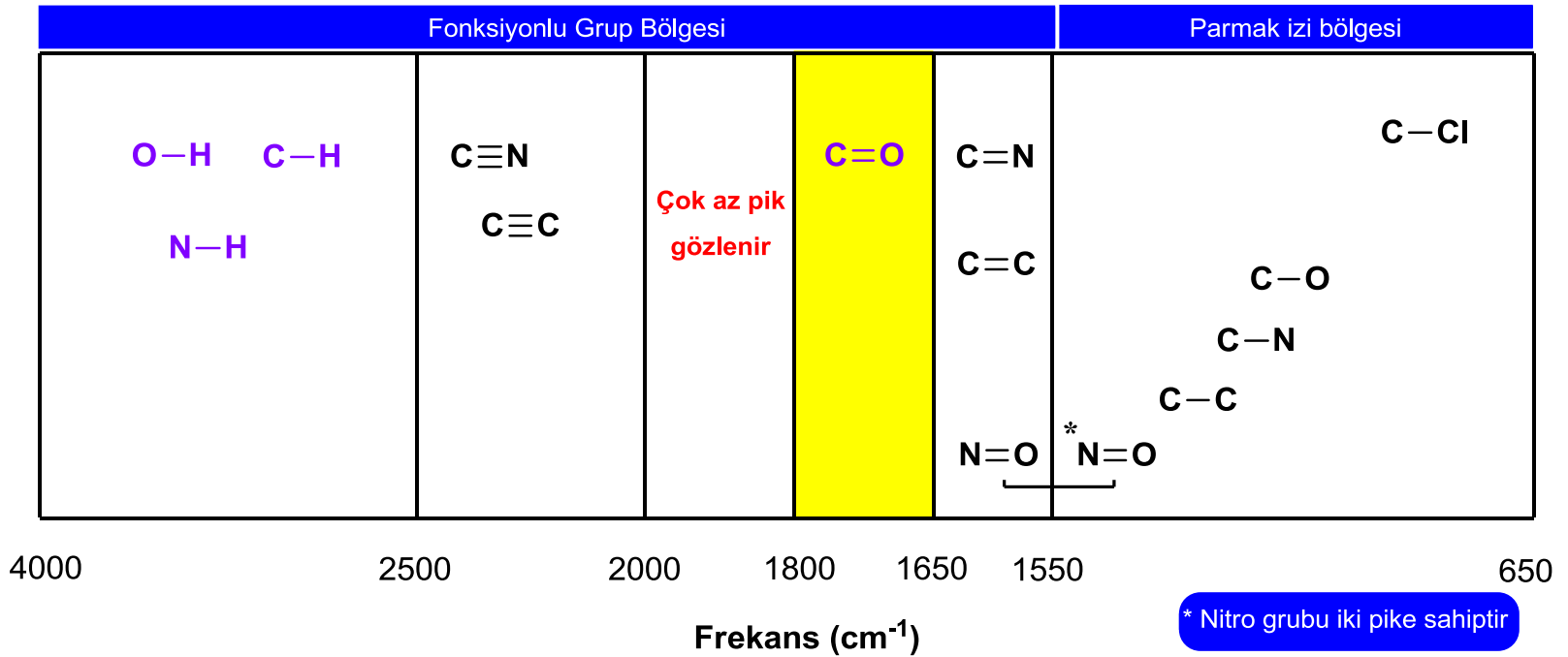
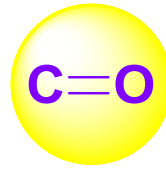




1-Hekzin



* Şiddetli bir pik olduğundan Overtonu (katlıtonu) gözlenir



KARBONİL GERİLME BÖLGESİ

- Bu bölge gerilmeleri $1650 - 1800 \text{ cm}^{-1}$
Spektrumun ortasının sağında bulunur

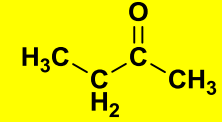
- Temel değer 1715 cm^{-1} (keton)

- Pikler çok güçlüdür!!! C=O büyük bir dipol momente sahip olduğundan.

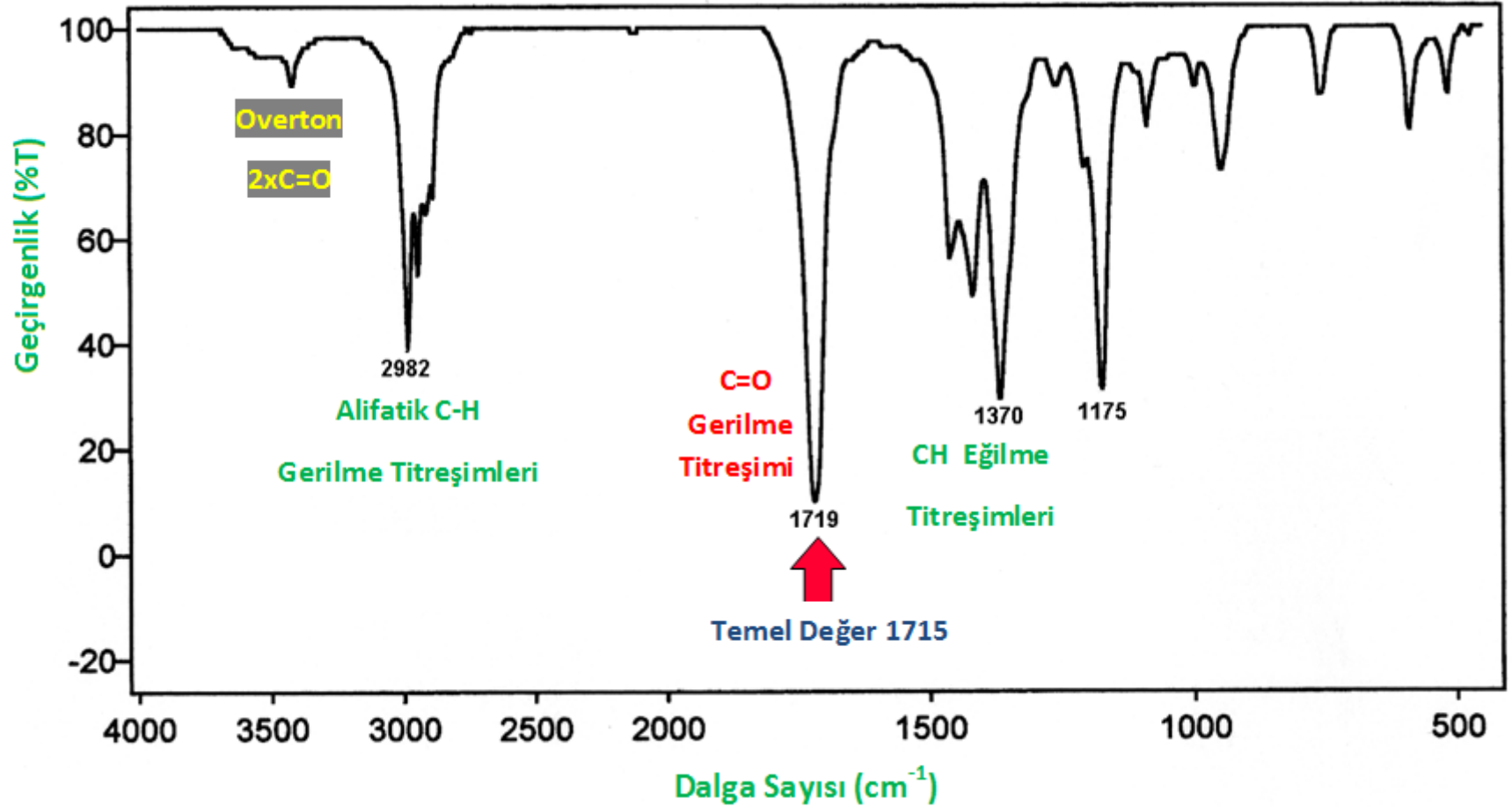
- C=O IR spektrumundaki en güçlü ve keskin pikdir.

KETONLAR

2-Bütanon



2-Bütanon

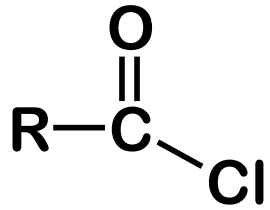


Temel Değer = 1715

KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

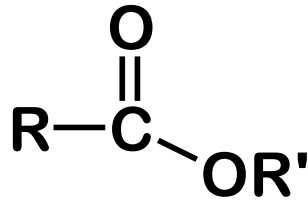
C=O ÇEVRESİNE GÖRE ÇOK HASSASTIR

Açıl klorür



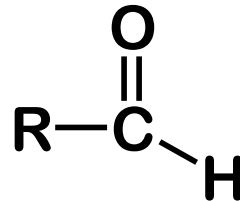
1800

Ester



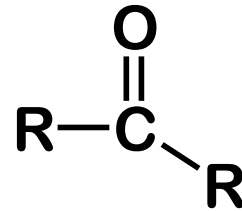
1735

Aldehit



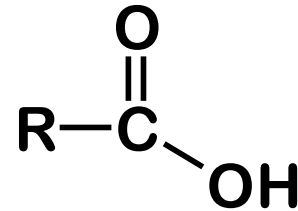
1725

Keton



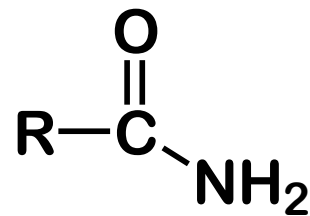
1715

Karboksilli
asit



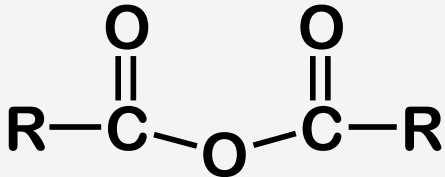
1710

Amit



1690

Anhidrit



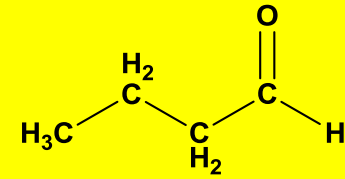
1810 and 1760
(iki pik)



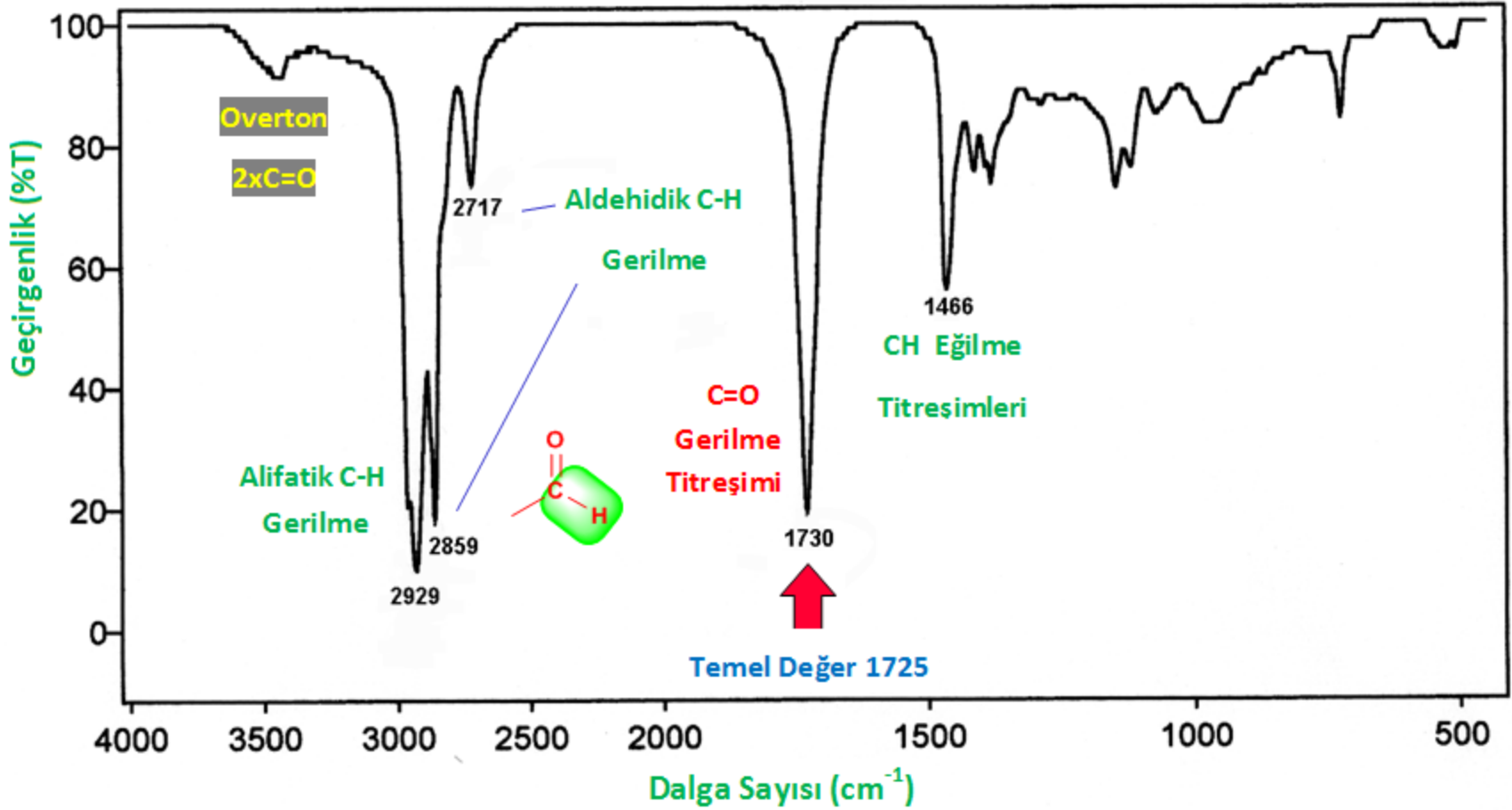
Temel
Değer

ALDEHİTLER

Bütanal

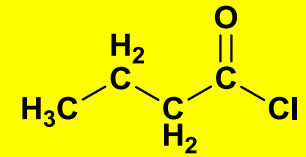


Bütanal

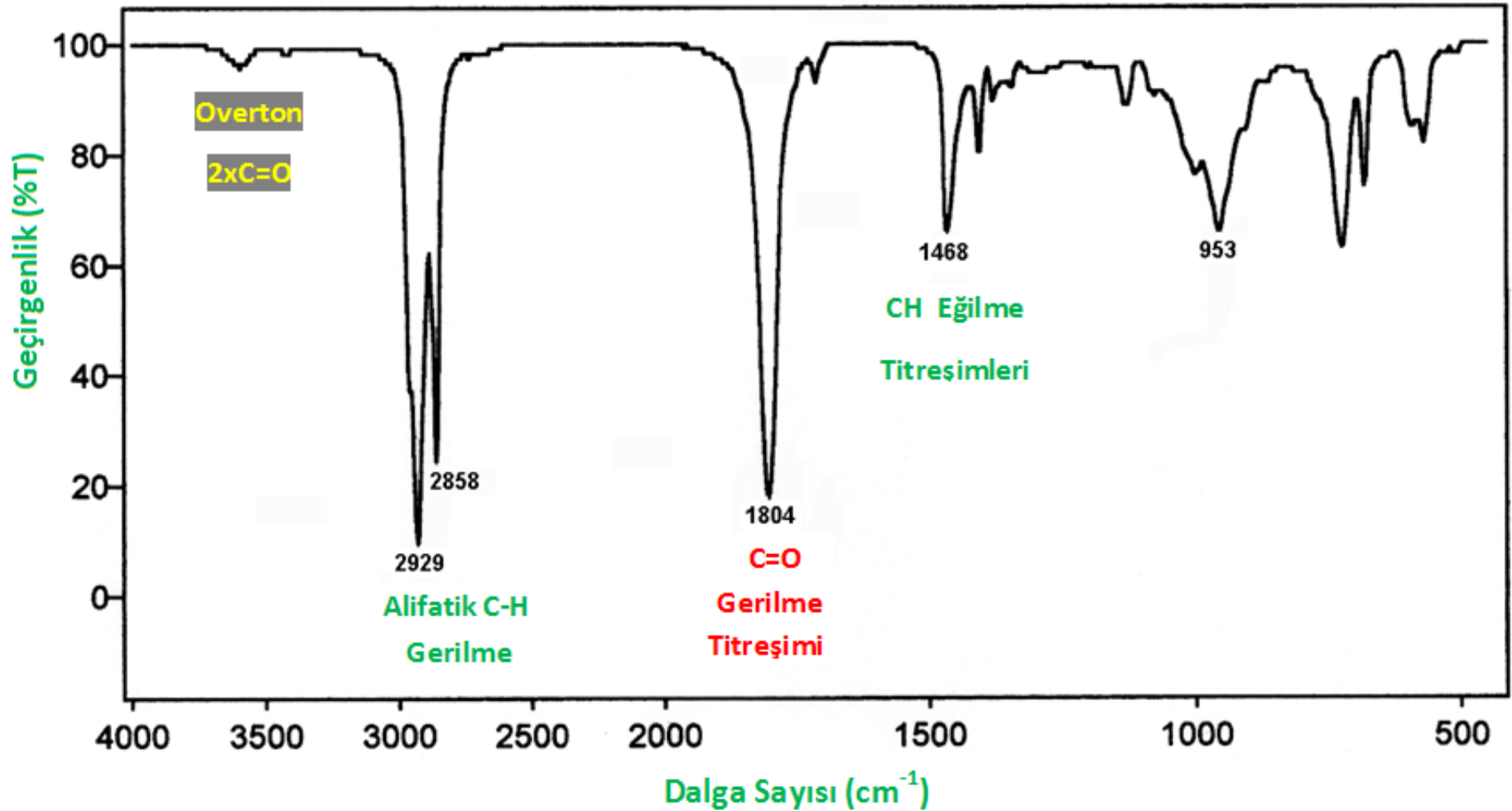


AÇIL KLORÜRLER

Bütanoil klorür



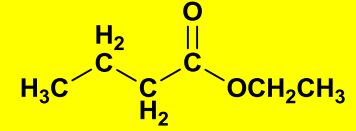
Bütanoil klorür



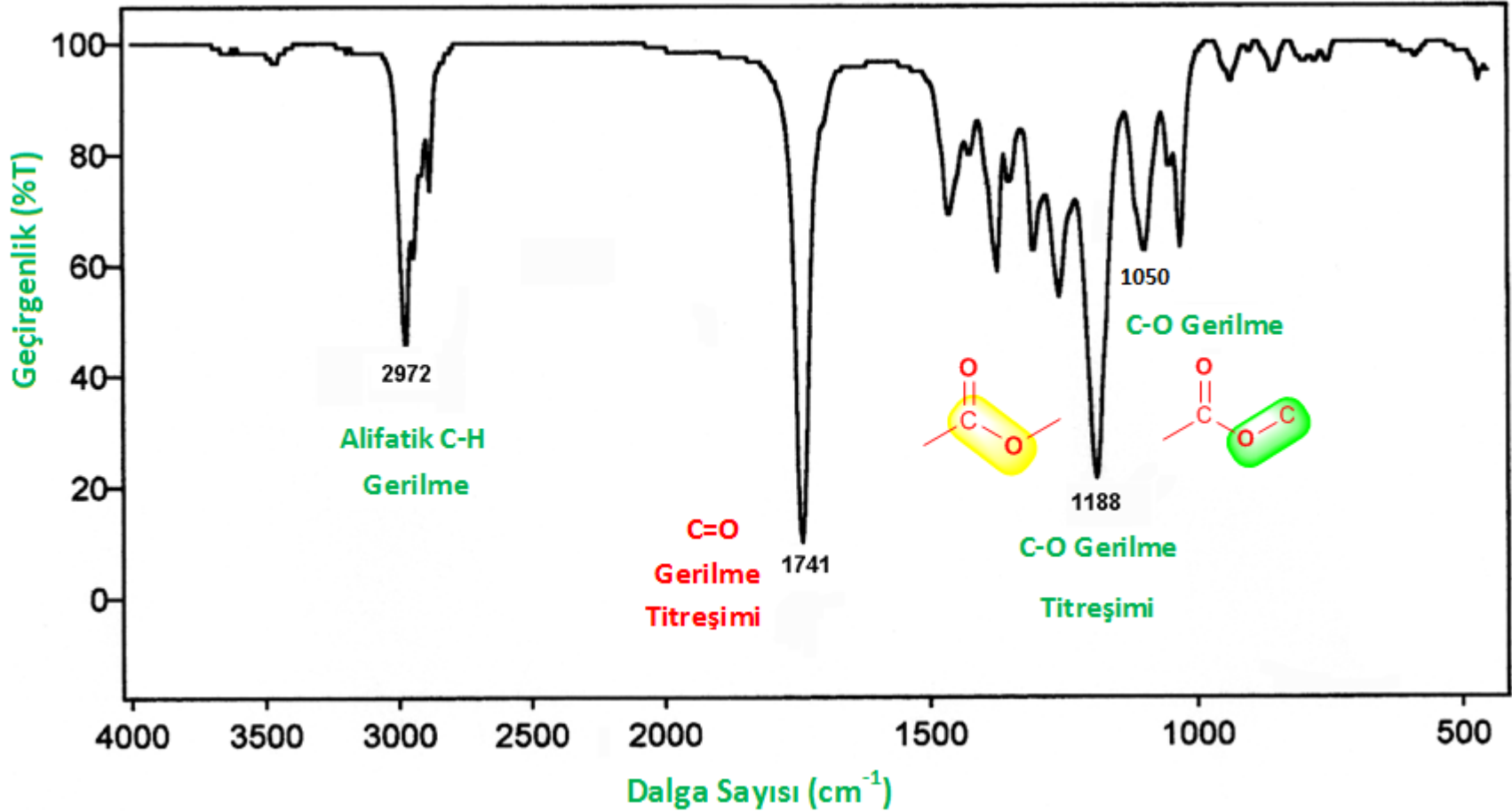
KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

ESTERLER

Etilbütanoat

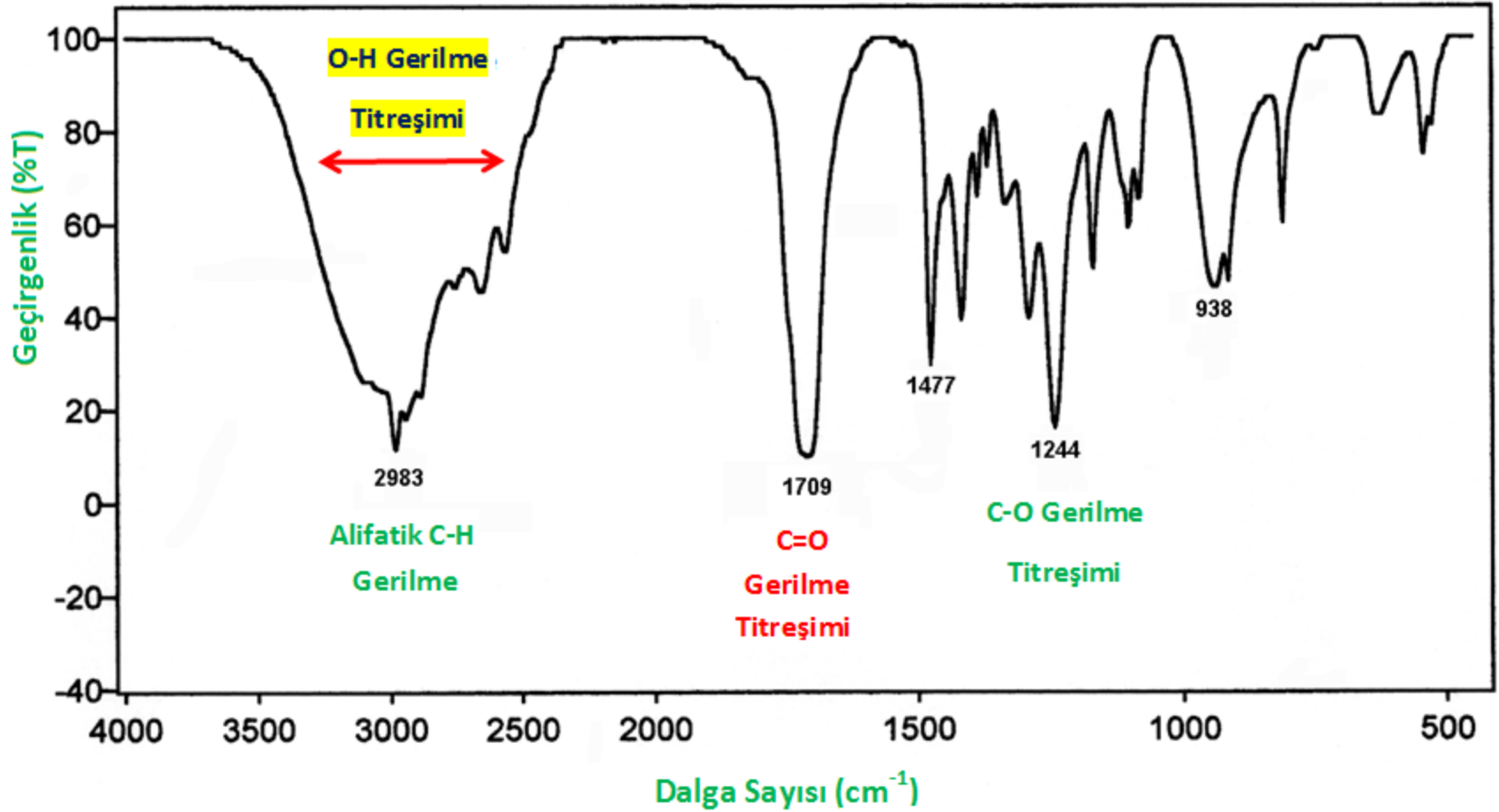
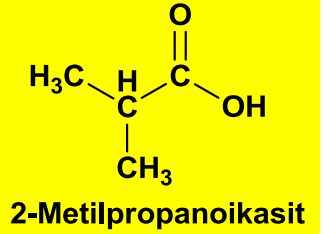


Etilbütanoat

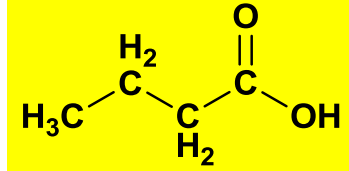


KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

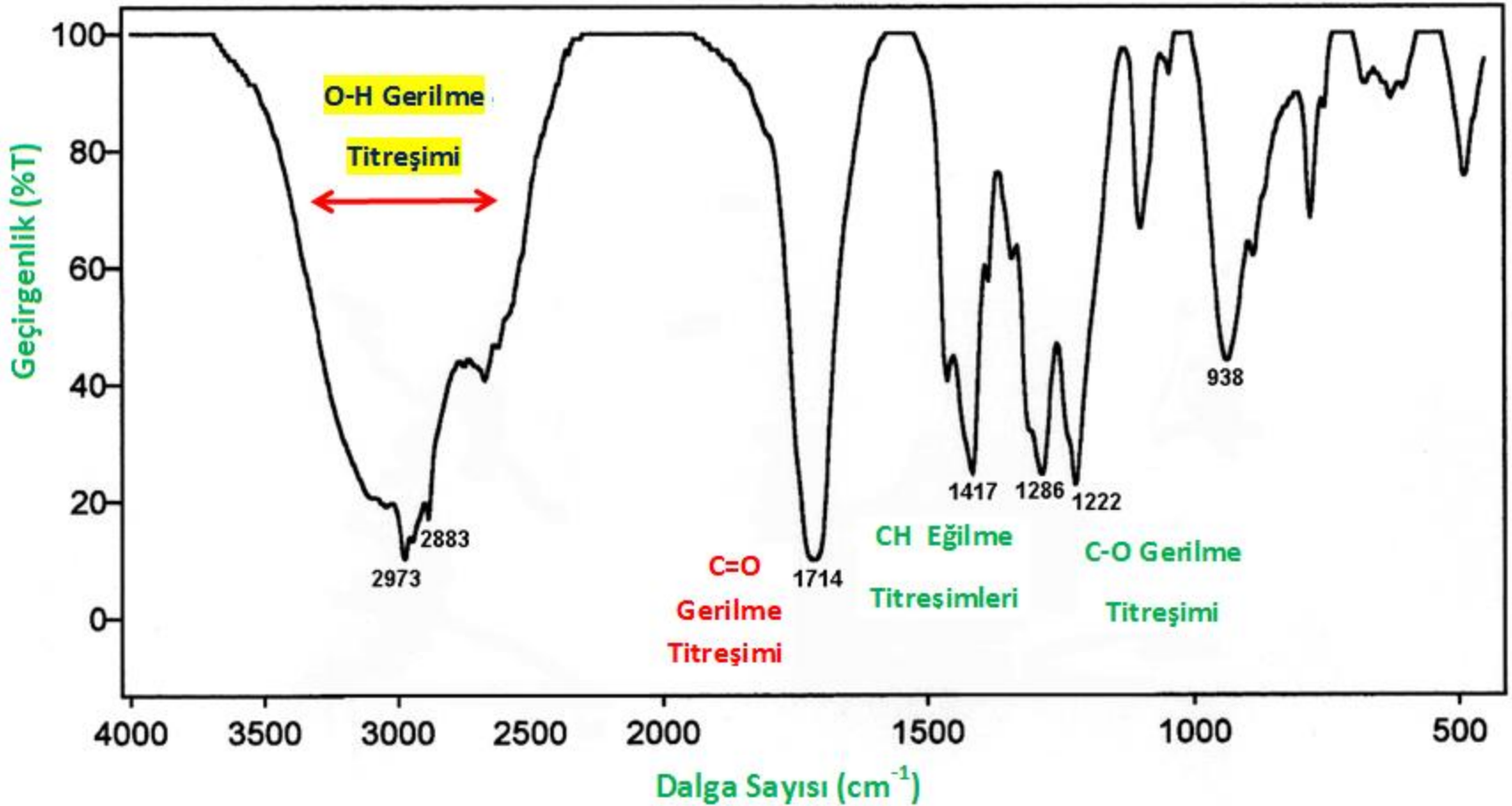
2-Metilpropanoik asit



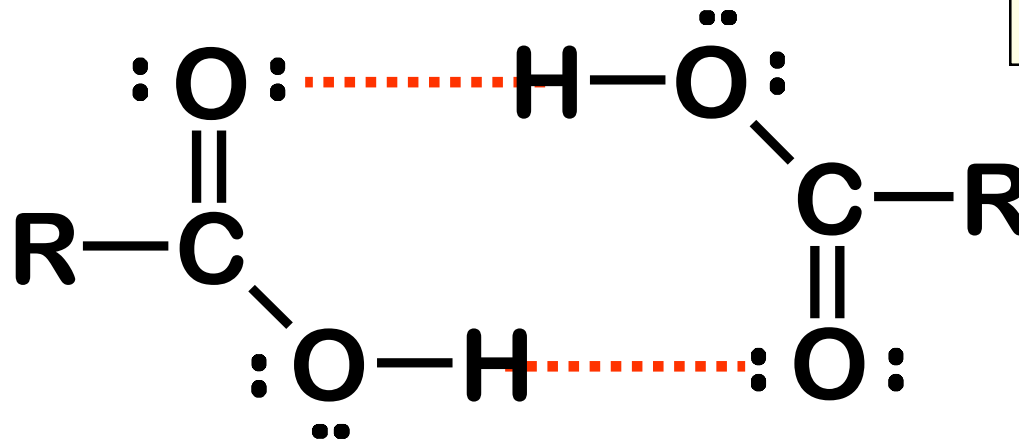
Bütanoik asit



Bütanoik asit



KARBOKSİLLİ ASİT DİMERLERİ



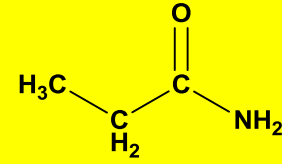
C=O titreşimi
düşük
frekansa
kayar

Aynı zamanda
O-H titreşimide

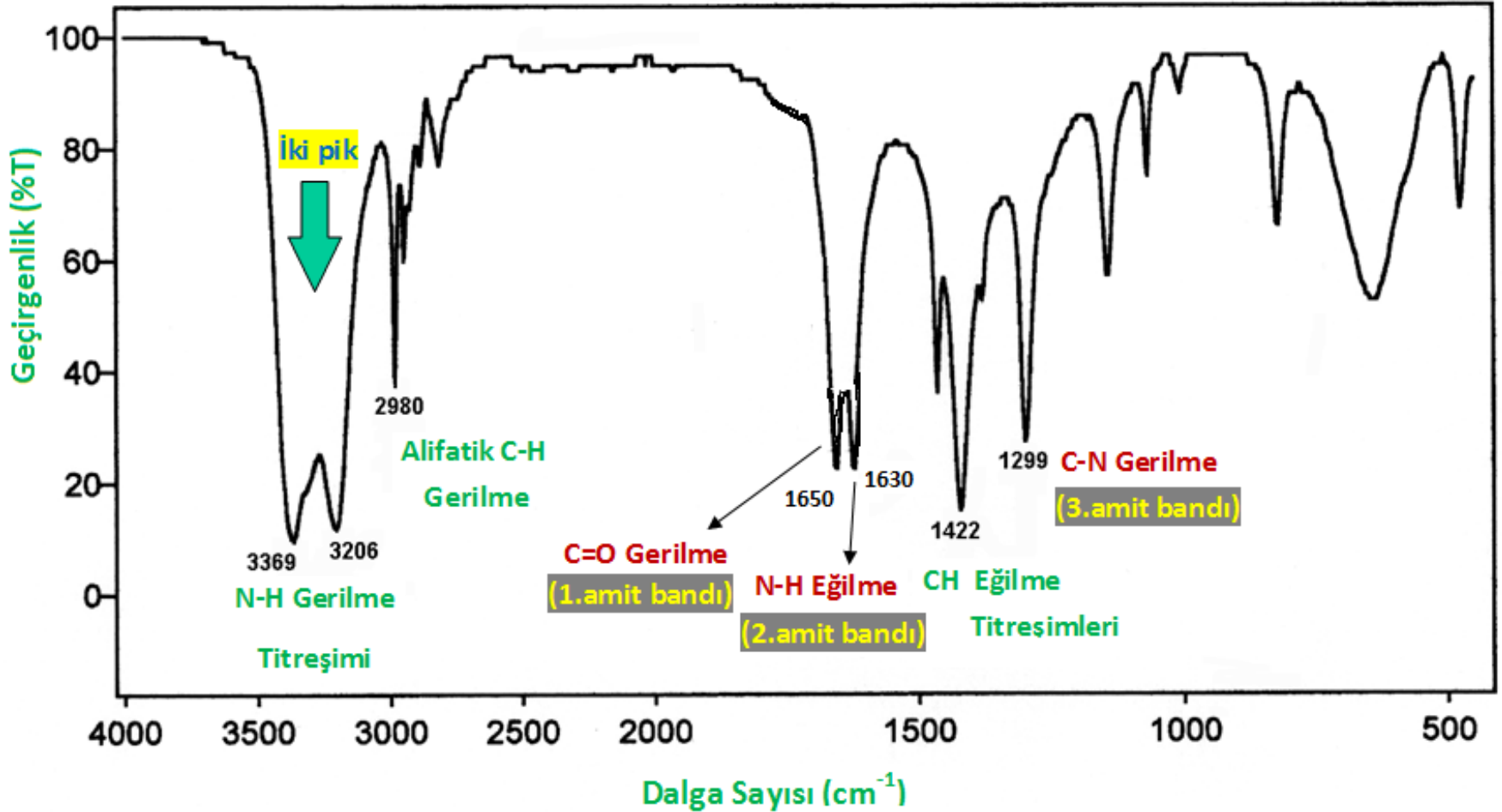
Dimerdeki güçlü H-bağları O-H ve C=O bağlarını zayıflatır
Bu sebeple bu titreşimler düşük frekansta gözlenir.

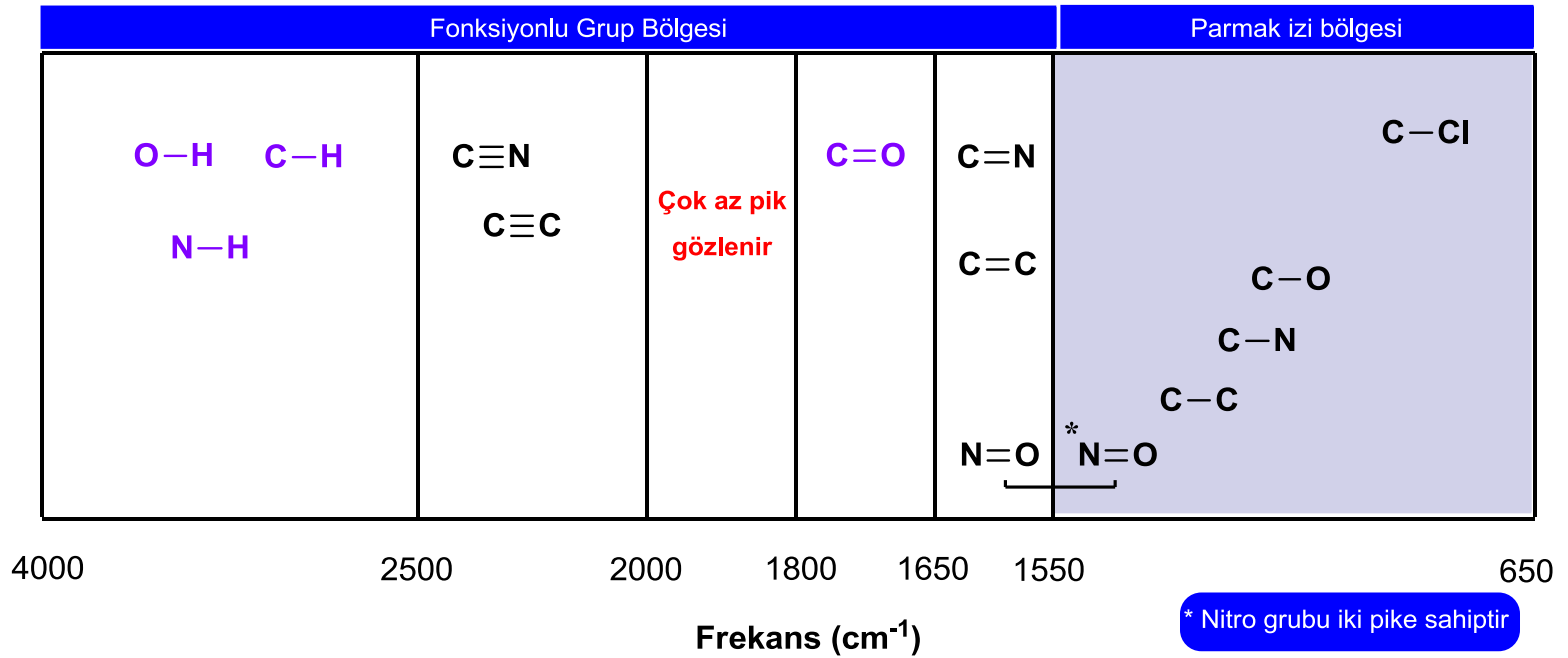
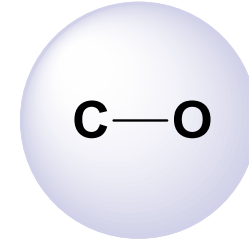
AMİTLER

Propanamit



Propanamit





C-O gerilme bölgesi

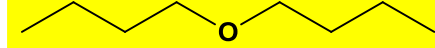
- C-O piki 1000-1300 cm^{-1} aralığında görülür

- Bu aralıkta tek veya daha fazla güçlü pikler görülür

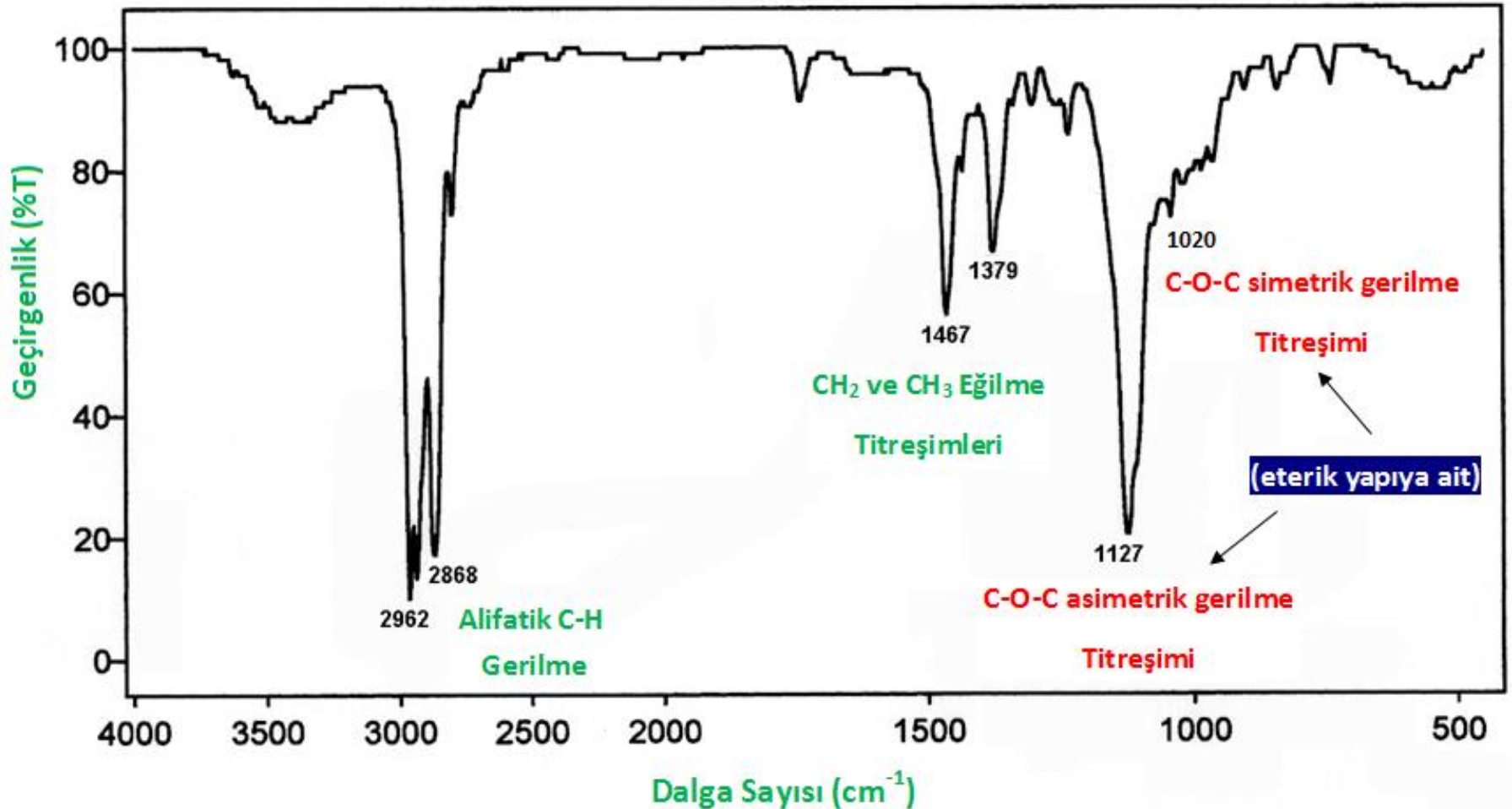
- Eterler, alkoller, esterler ve karboksilik asitler C-O piki ne sahiptirler.

ETERLER

Dibütleter



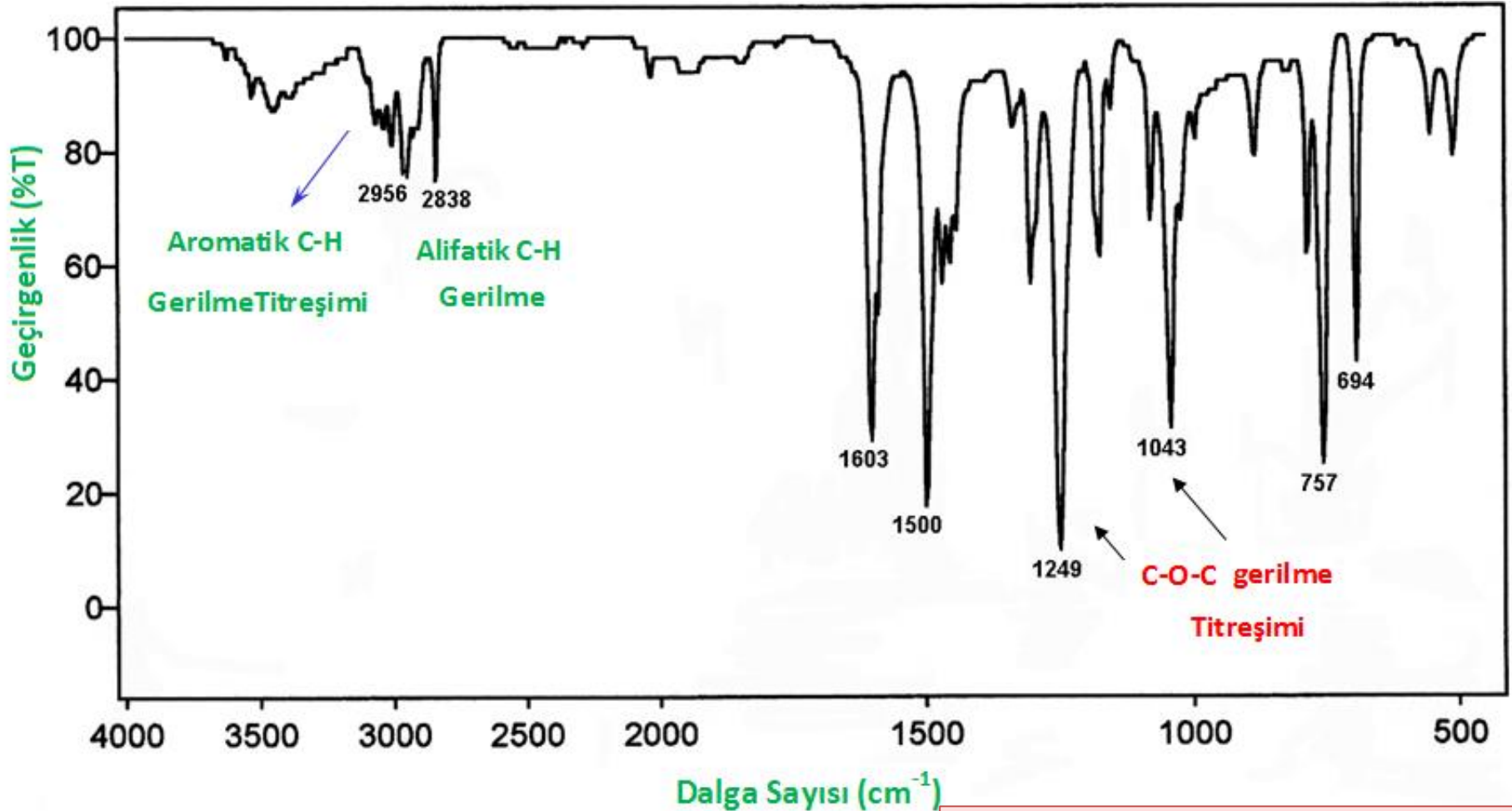
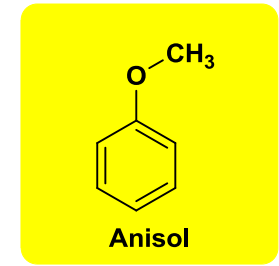
Dibütleter



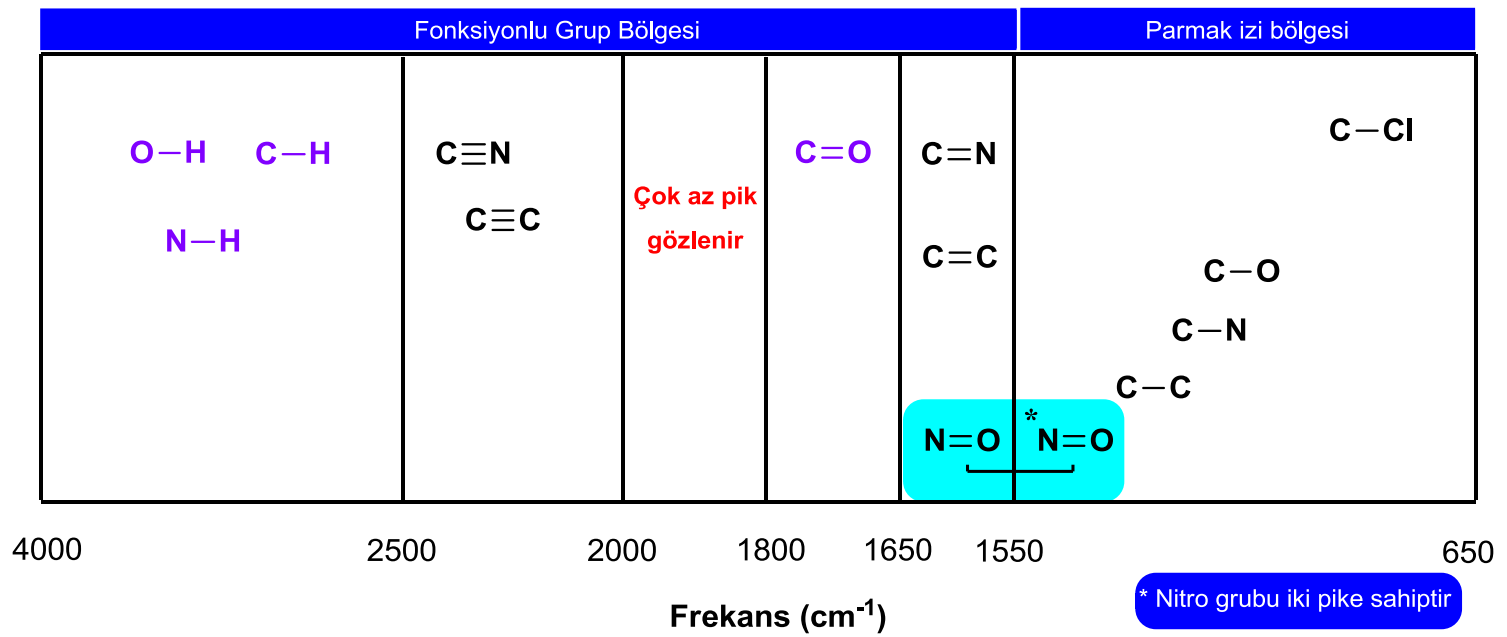
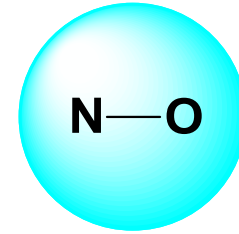
KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

ETERLER-2

Anisol (Metoksibenzen)



KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

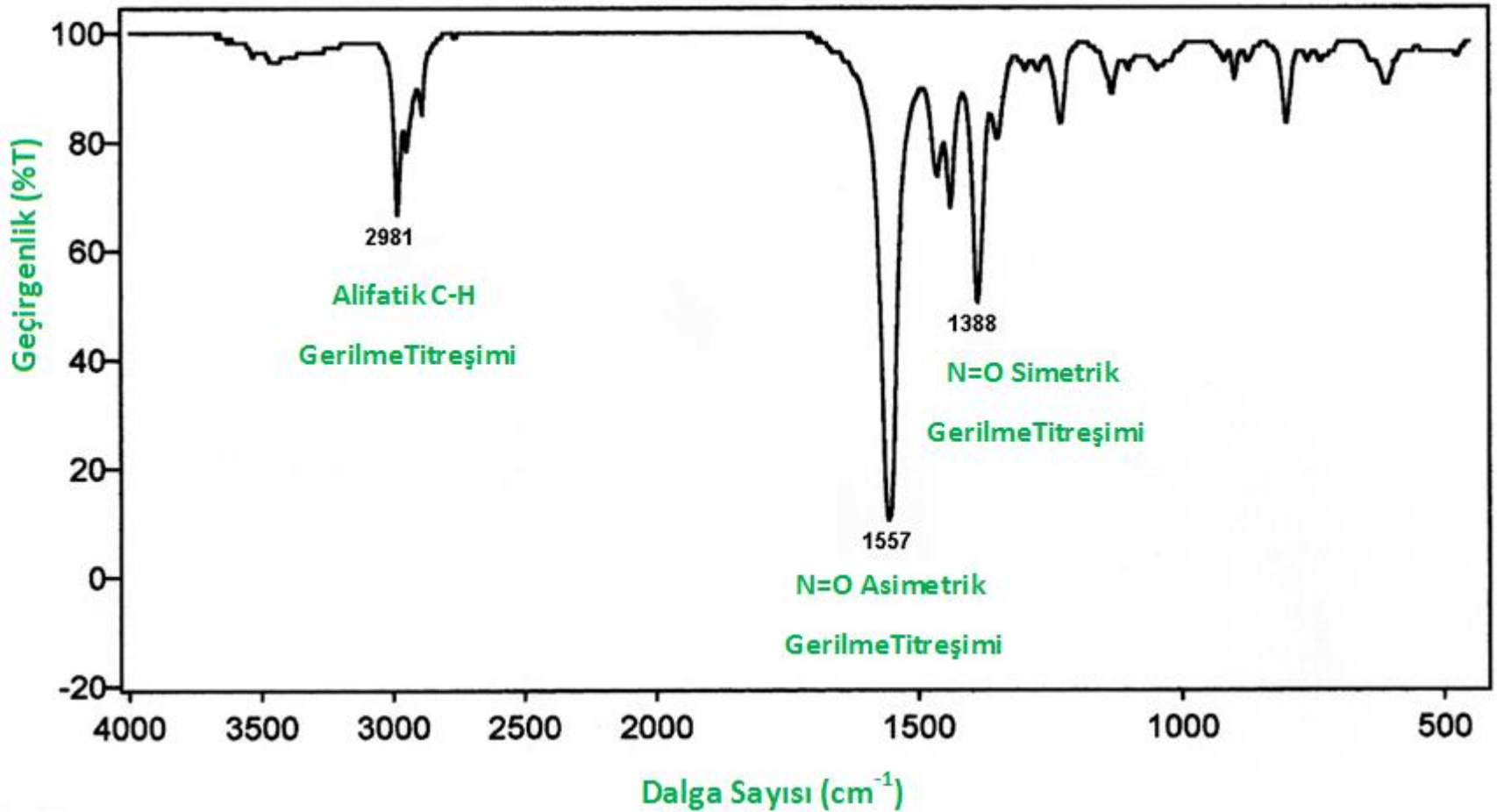
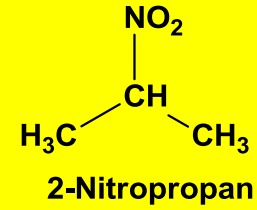


N=O gerilme bölgesi

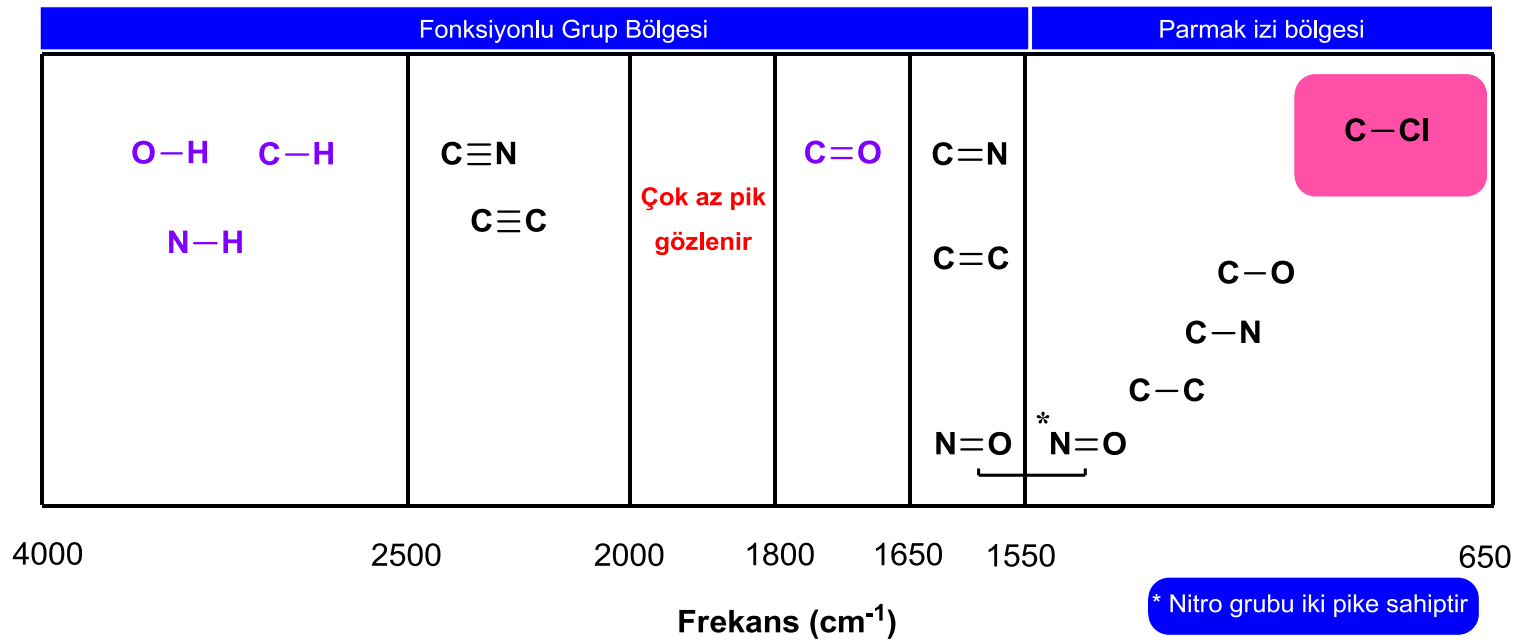
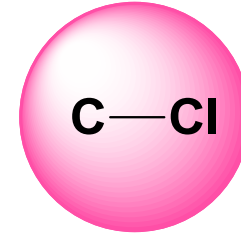
- N=O gerilmesi 1550 ve 1350 cm^{-1} asimetrik ve simetrik gerilmeler
- 1550 cm^{-1} asimetrik pik daha güçlüdür

NİTROALKANLAR

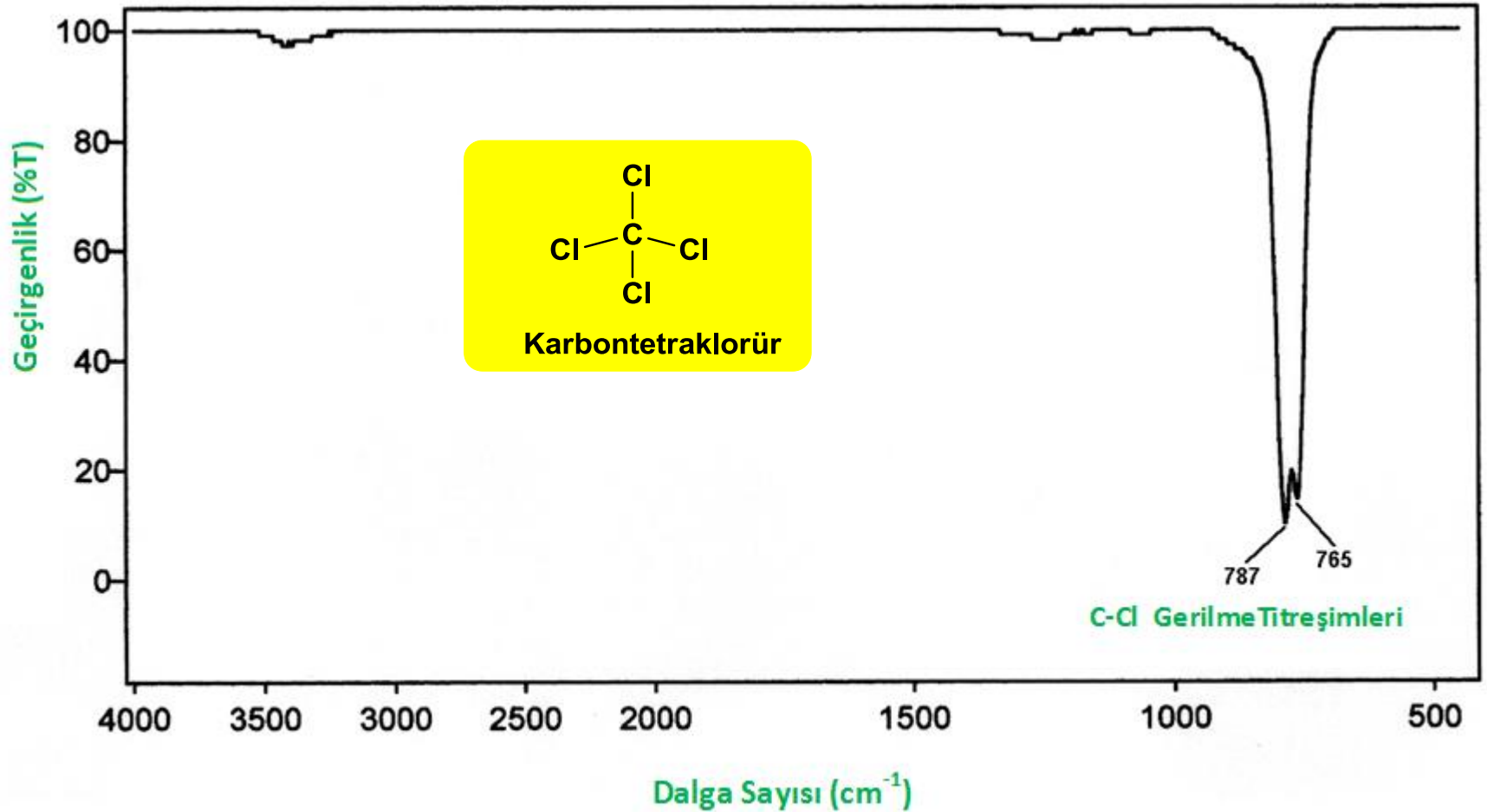
2-Nitropropane



KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

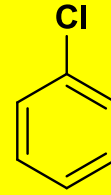


HALOJENÜR BİLEŞİKLERİ

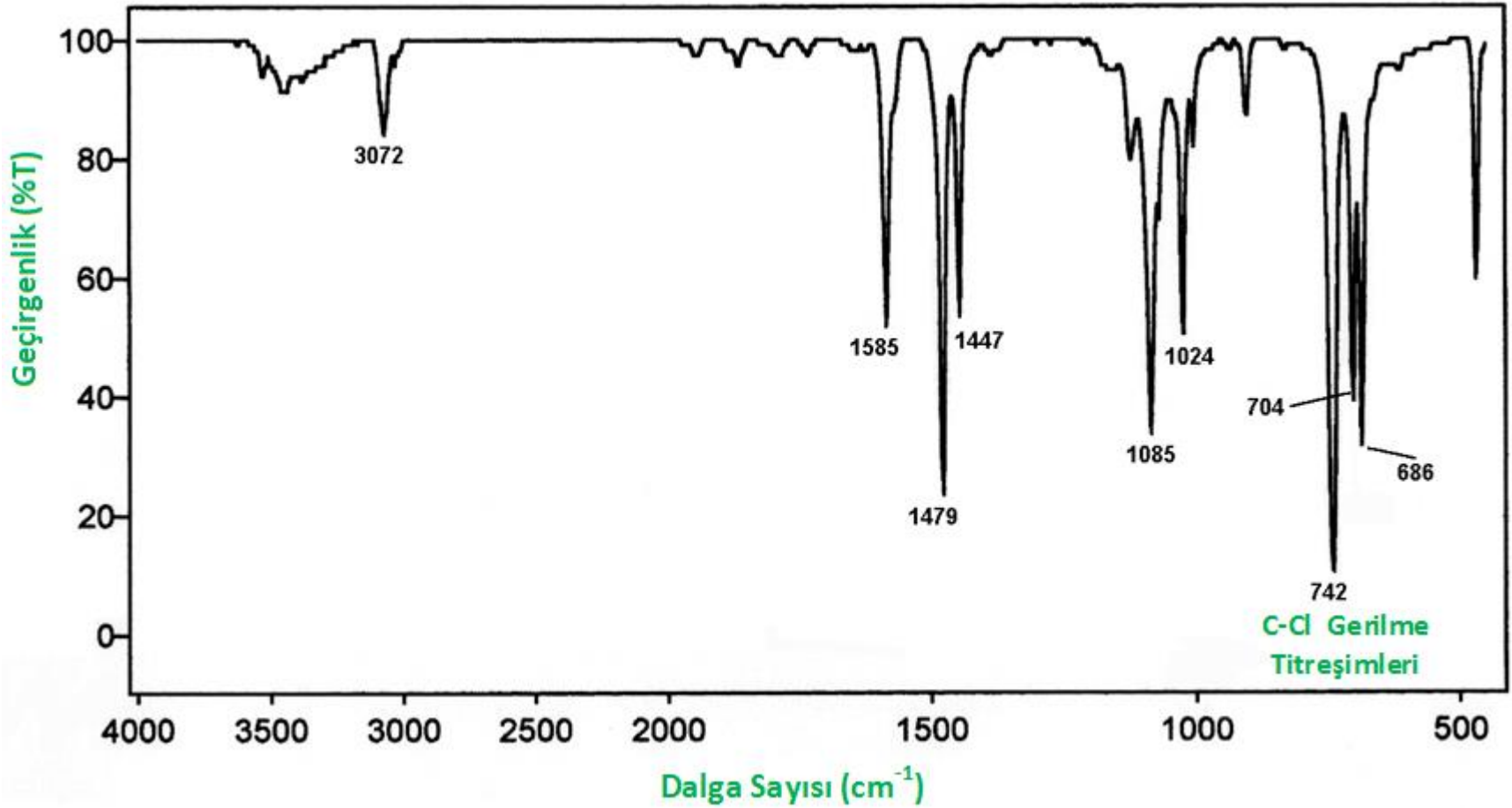


ARILHALOJENÜRLER

Klorbenzen



Klorbenzen



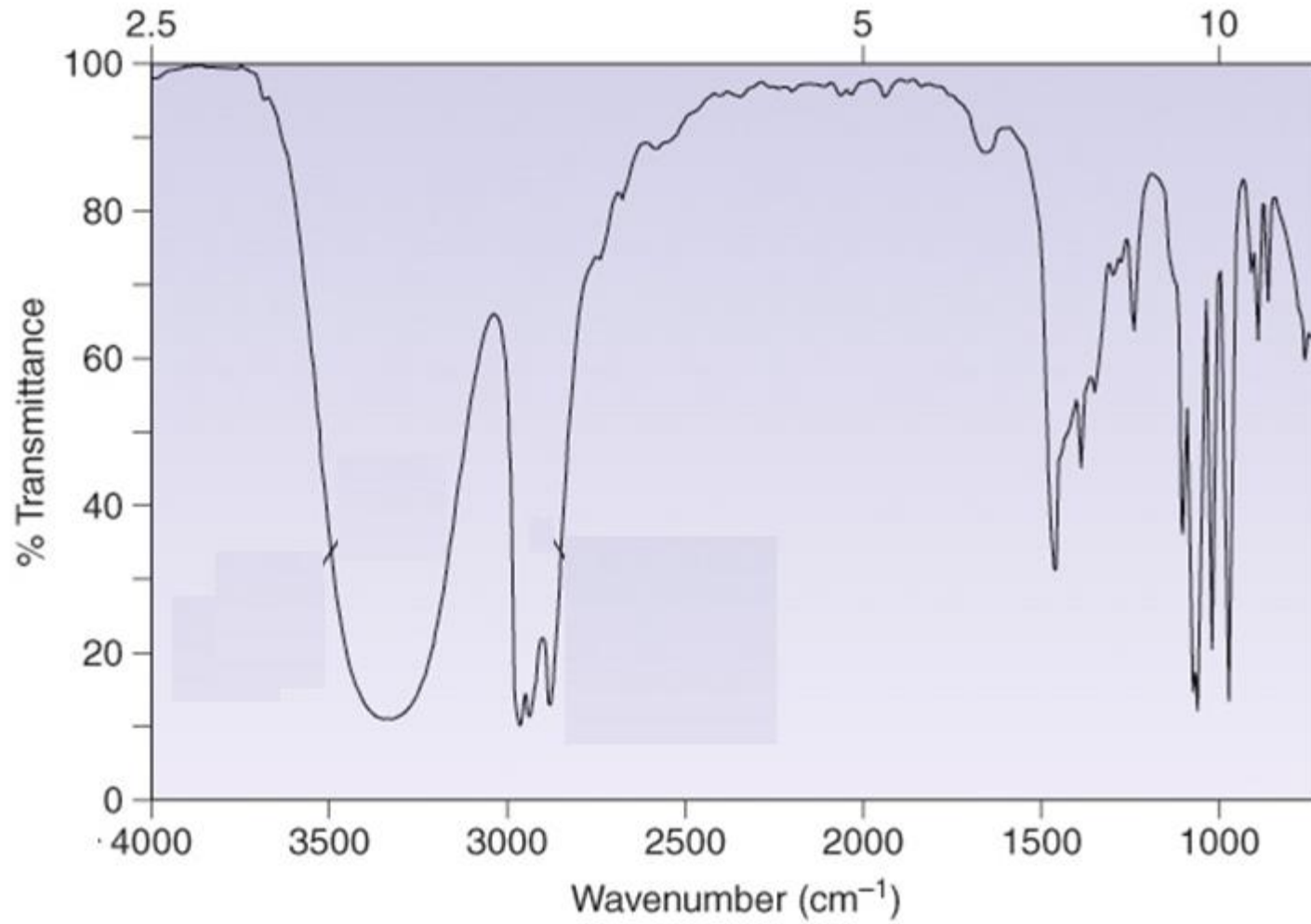
KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

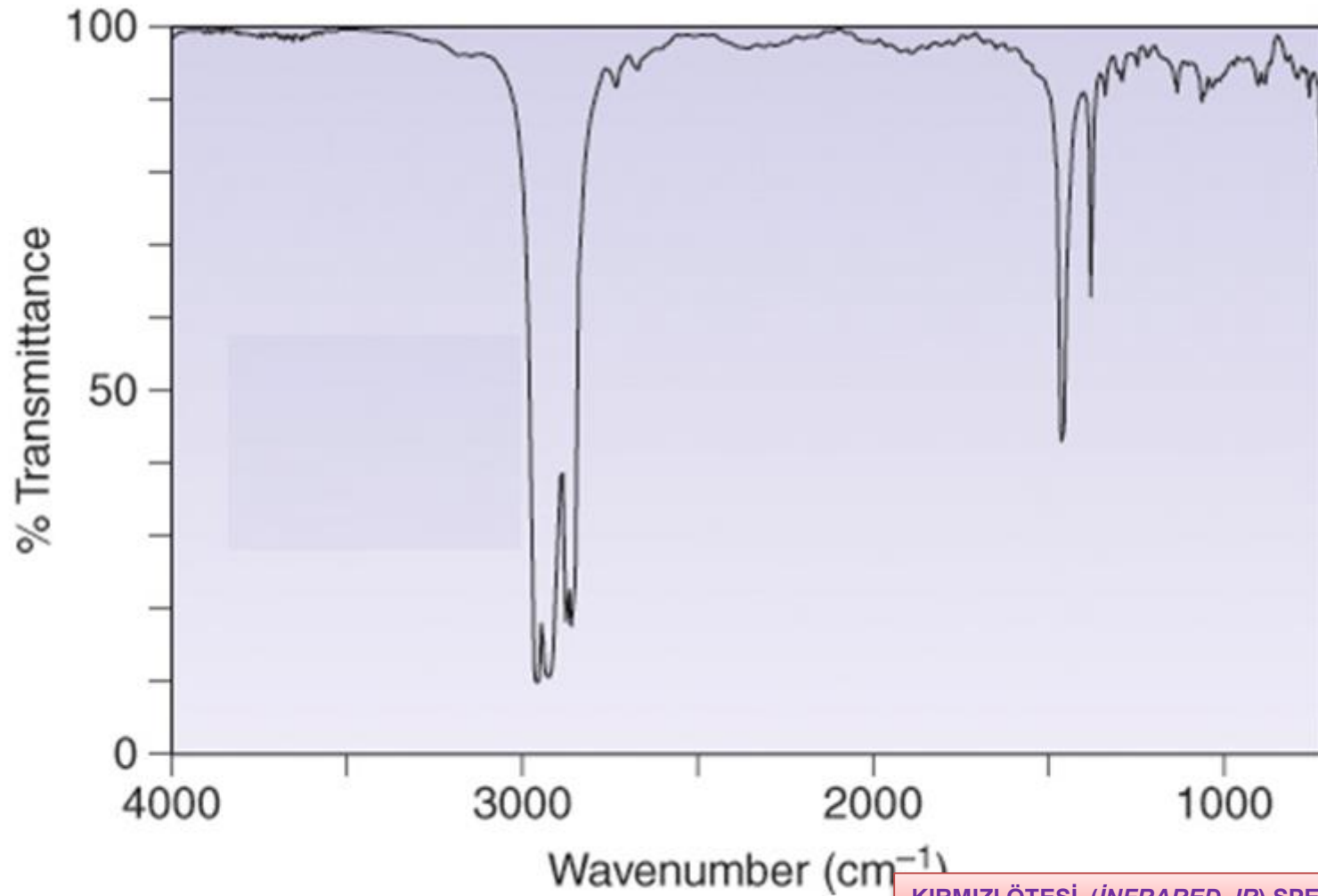
10.5. Kırmızı Ötesi (IR) Spektrumundan Yapı Analizi

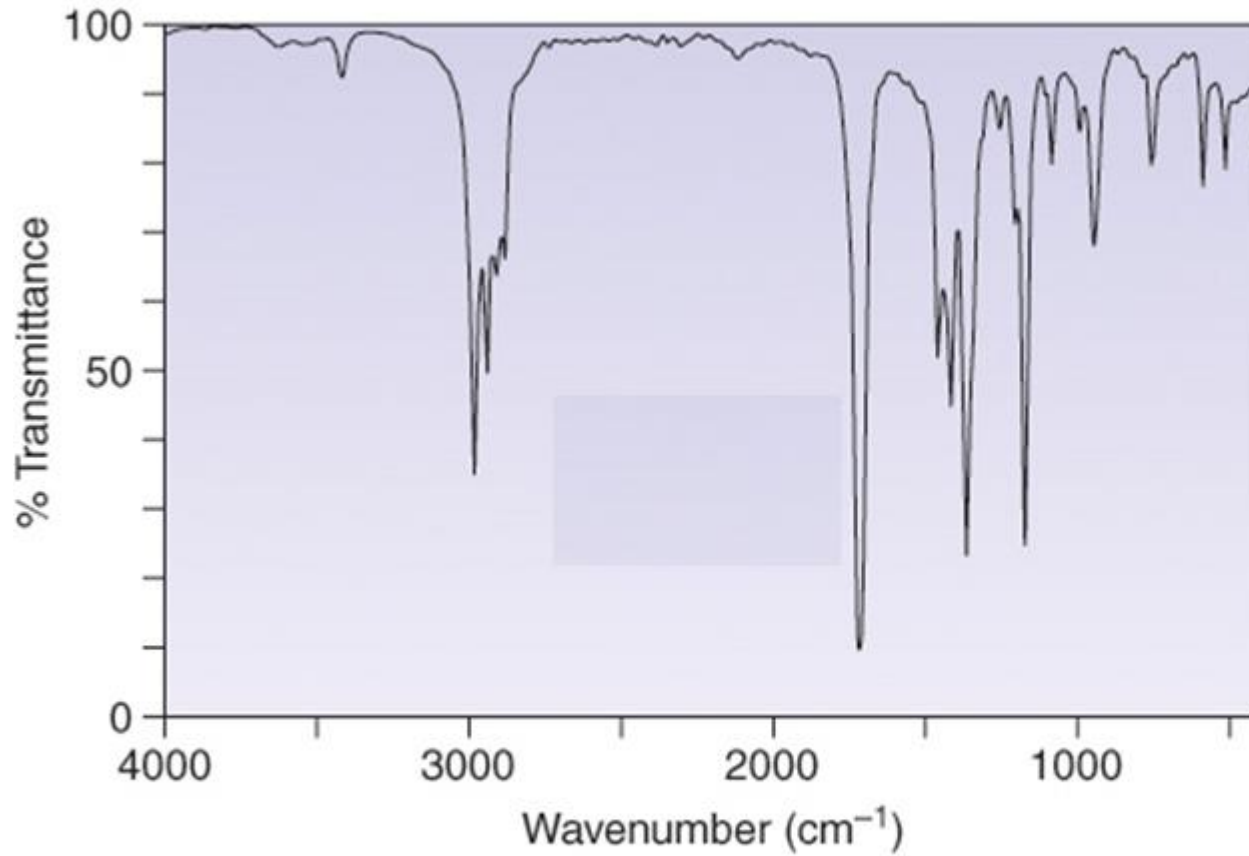
DBE (Double Bond Equivalent); Çift bağ eşdeğeri veya Doymamışlık Derecesi

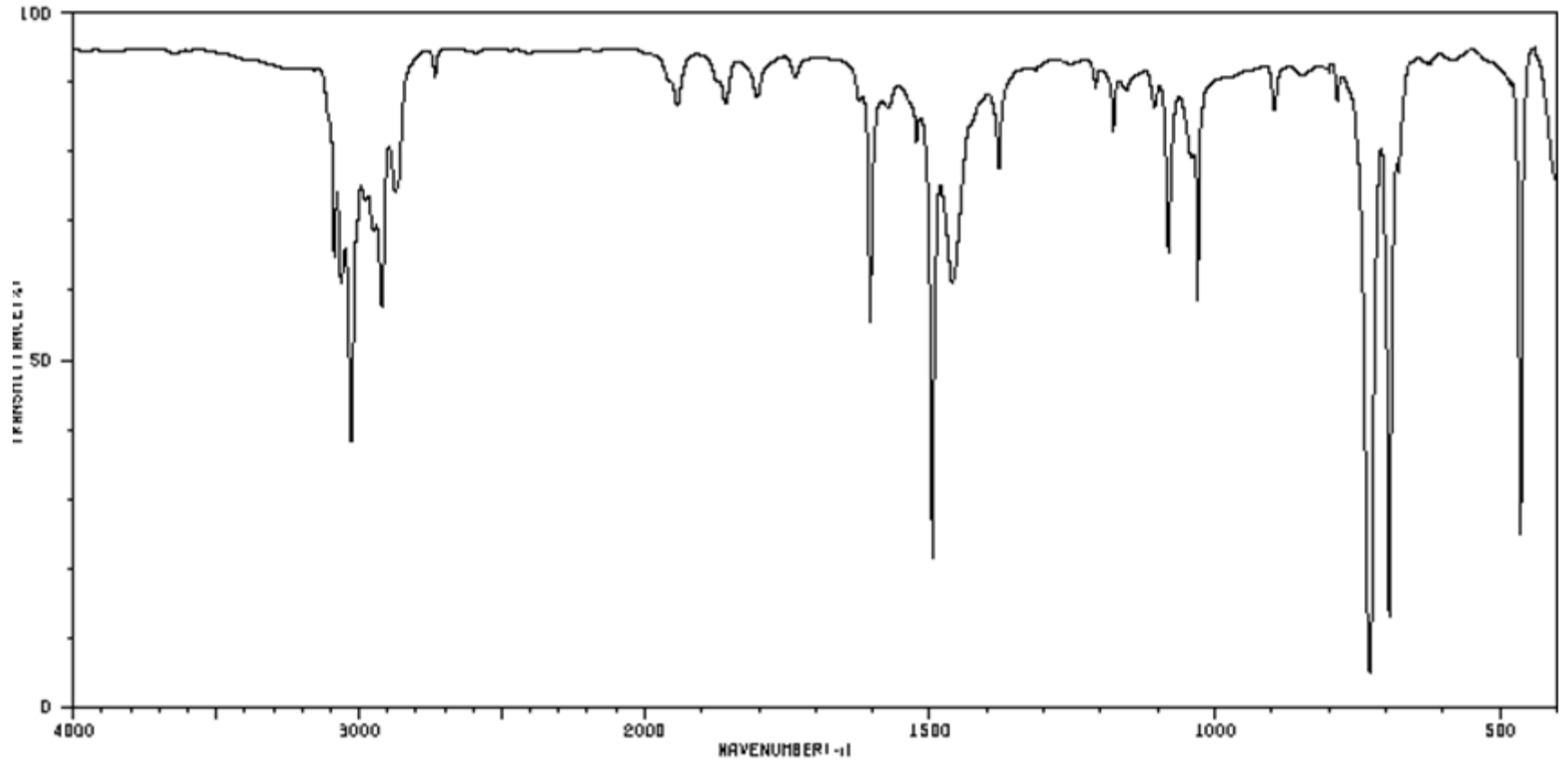
$$\text{DBE} = 1 + \frac{2N_{\text{C}} - N_{\text{H}} - N_{\text{x}} + N_{\text{N}}}{2}$$

N : Atom Sayısı

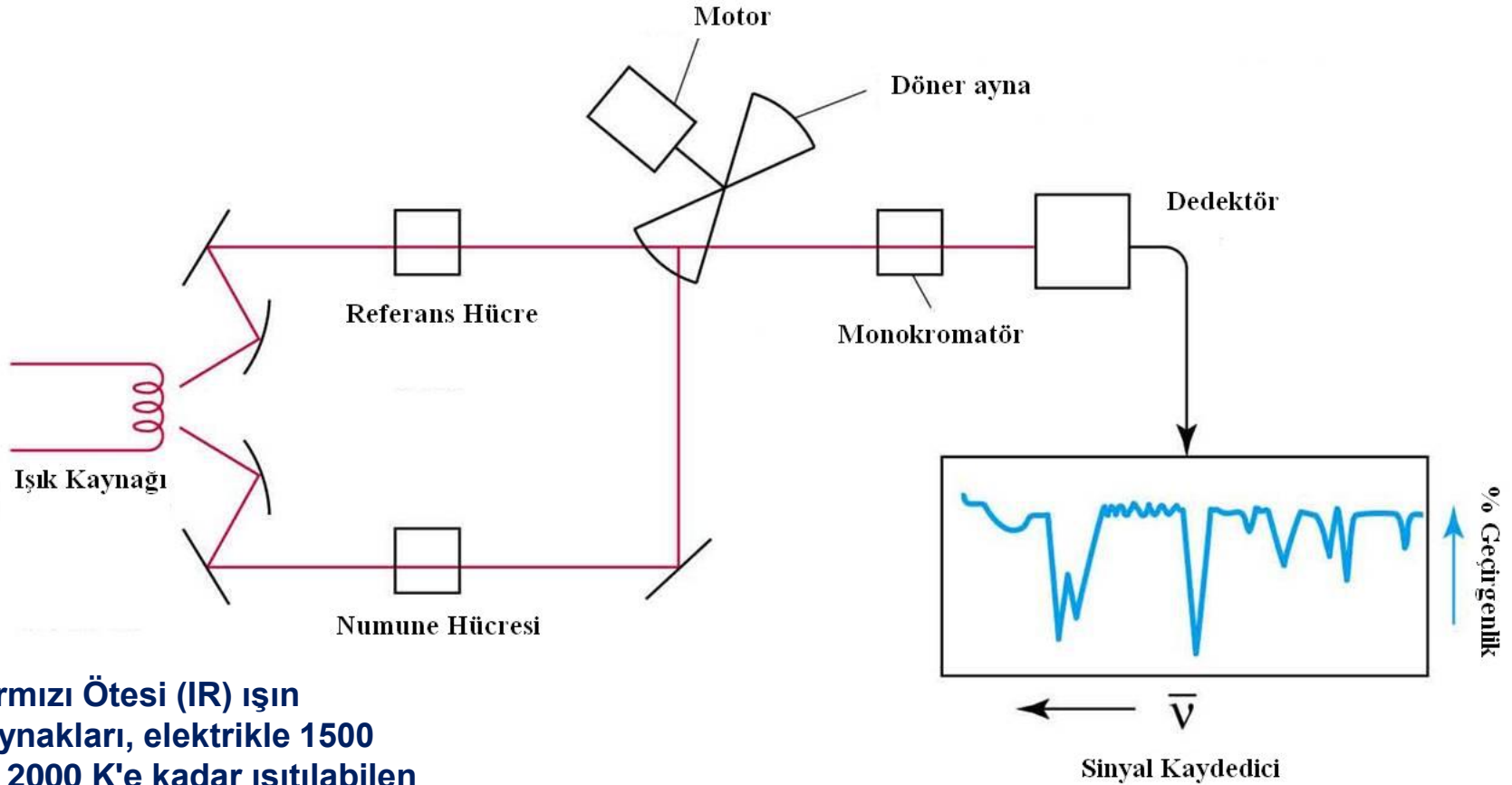
1) $\text{C}_3\text{H}_8\text{O}$ 

2) C_6H_{14} 

3) $\text{C}_4\text{H}_8\text{O}$ 

4) C_7H_8O 

11. Kırmızı Ötesi (IR) Cihazı ve Çalışma Prensipleri



Kırmızı Ötesi (IR) ışın kaynakları, elektrikle 1500 ile 2000 K'e kadar ısıtılabilen inert katılardır.

- Nernst çubuğu
- Gobar çubuğu
- Civa arkı
- Tungsten telli lamba

KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

12. Numune Hazırlama

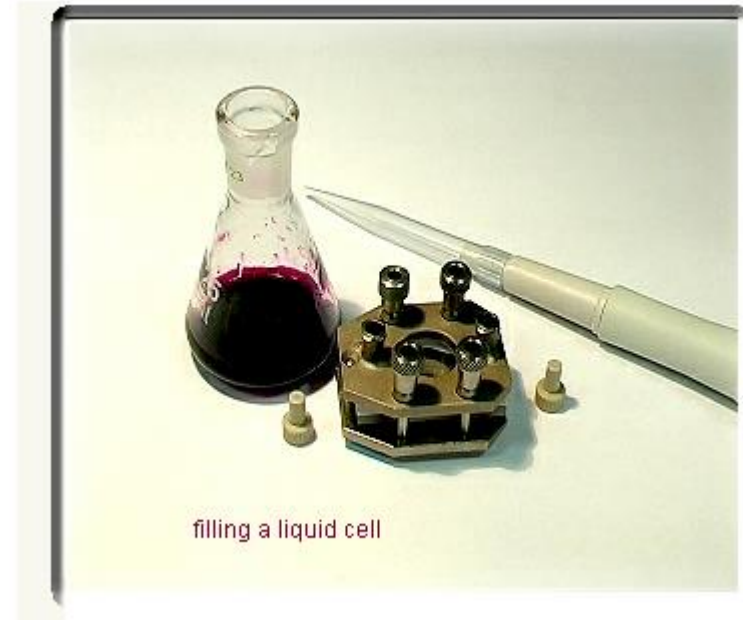


KIRMIZI ÖTESİ (INFRARED, IR) SPEKTROSKOPİSİ

SIVI



ÇÖZELTİ



KATI



GAZ



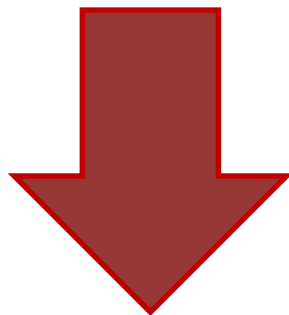
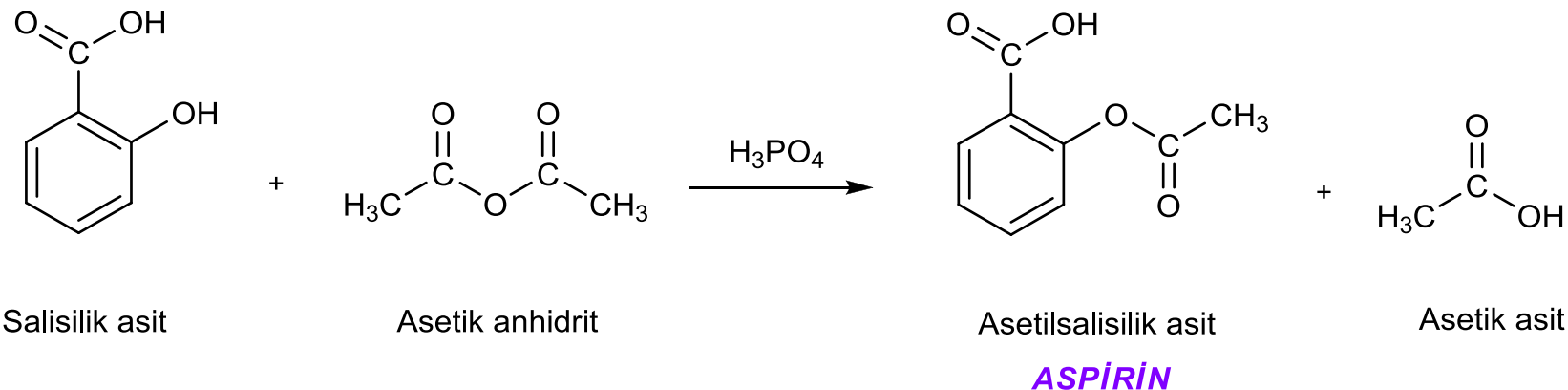
12. Kırmızı Ötesi (IR) Spektroskopisi Çalışma Soruları

Kırmızı Ötesi Spektroskopisi (IR) RAPOR

Fourier Transformlu Kırmızı Ötesi Spektroskopisi (FTIR)

IR ve UV arasındaki farklar

IR	UV-Vis
IR dalga sayısı olarak ifade edilir	UV dalgaboyu olarak ifade edilir
IR molekülde titreşim ve dönme hareketi yaptırır	UV elektronik uyarma yapar
IR de pikler daha keskindir	UV pikler geniştir
IR de maddeyi tanıma hakkında daha fazla bilgi elde edebiliriz	
IR de pik max. ları aşağı doğrudur	UV de pik max. ları yukarı doğrudur
Bir molekülün IR de absorpsiyon yapması için dipol momentinin olması gerekir. Molekülün polarlığından çok bağların polar olması gerekir. Molekül apolar olabilir.	



NMR (NÜKLEER MAGNETİK REZONANS SPEKTROSKOPİSİ)