Chapter 2

- Infrared (IR) Spectroscopy

❖ Dipole moment of some compounds

Compound	Dipole Moment	Compound	Dipole Moment
NaCl	9.0	H_2O	1.85
CH_3NO_2	3.45	CH_3OH	1.70
CH_3Cl	1.87	CH_3COOH	1.52
CH_3Br	1.79	NH_3	1.47
CH_3I	1.64	CH_4	0
$CHCl_3$	1.02	CCl_4	0

12. Summary of Important Families of Organic Compounds

TABLE 2.3 Important Families of Organic Compounds

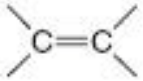
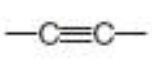
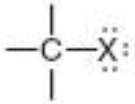
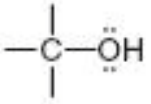
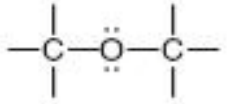
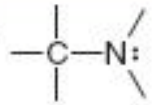
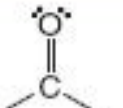
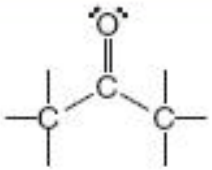
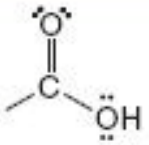
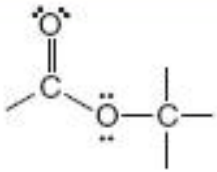
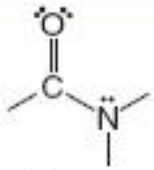
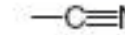
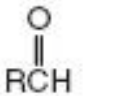
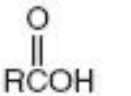
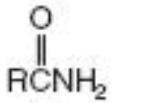
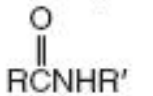
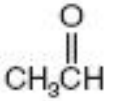
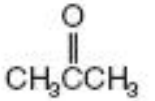
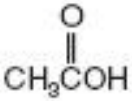
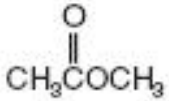
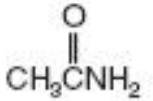
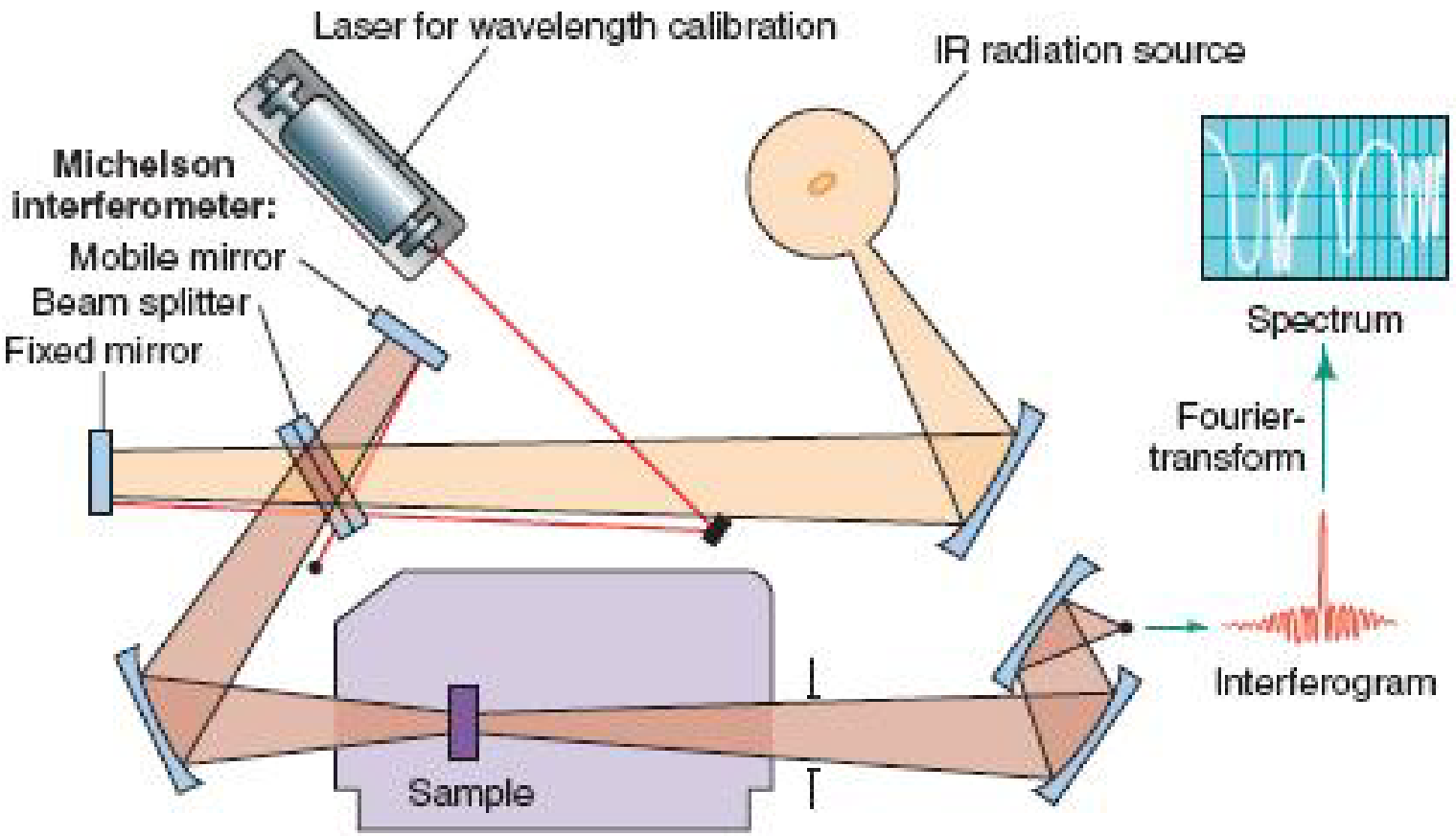
	Family						
	Alkane	**Alkene**	**Alkyne**	**Aromatic**	**Haloalkane**	**Alcohol**	**Ether**
Functional group	C—H and C—C bonds			Aromatic ring			
General formula	RH	$RCH{=}CH_2$ $RCH{=}CHR$ $R_2C{=}CHR$ $R_2C{=}CR_2$	$RC{\equiv}CH$ $RC{\equiv}CR$	ArH	RX	ROH	ROR
Specific example	CH_3CH_3	$CH_2{=}CH_2$	$HC{\equiv}CH$		CH_3CH_2Cl	CH_3CH_2OH	CH_3OCH_3
IUPAC name	Ethane	Ethene	Ethyne	Benzene	Chloroethane	Ethanol	Methoxymethane
Common name[a]	Ethane	Ethylene	Acetylene	Benzene	Ethyl chloride	Ethyl alcohol	Dimethyl ether

TABLE 2.3 Important Families of Organic Compounds (*cont.*)

	Family						
	Amine	**Aldehyde**	**Ketone**	**Carboxylic Acid**	**Ester**	**Amide**	**Nitrile**
Functional group							
General formula	RNH_2 R_2NH R_3N					  	RCN
Specific example	CH_3NH_2						$CH_3C{\equiv}N$
IUPAC name	Methanamine	Ethanal	Propanone	Ethanoic acid	Methyl ethanoate	Ethanamide	Ethanenitrile
Common name	Methylamine	Acetaldehyde	Acetone	Acetic acid	Methyl acetate	Acetamide	Acetonitrile

15. Infrared Spectroscopy



- The position of an absorption band (peak) in an IR spectrum is specified in units of wavenumbers ($\bar{\nu}$)

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

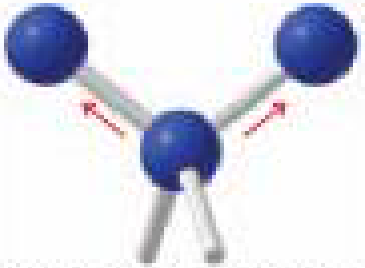
$$\because \Delta E = h\nu$$
$$\therefore E \propto \nu$$

(λ = wavelength in cm)
(E = energy)
(ν = frequency of radiation)

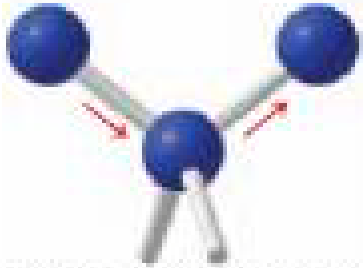
$$\because \nu = \frac{c}{\lambda}$$

$$\therefore \Delta E = \frac{hc}{\lambda}$$

A stretching vibration

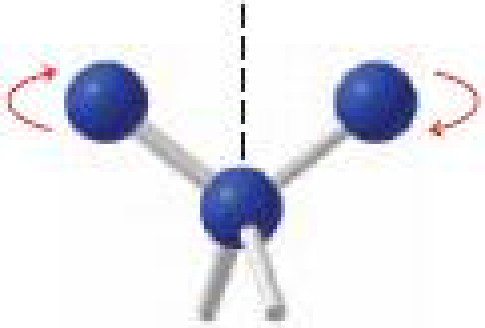


Symmetric stretching



Asymmetric stretching

An in-plane
bending vibration
(scissoring)



An out-of-plane
bending vibration
(twisting)

❖ Characteristic IR absorptions

Intensity: s = strong, m = medium, w = weak, v = variable

Group	Freq. Range (cm^{-1})	Intensity
Alkyl		
C–H (stretching)	2853–2962	(m–s)
Alkenyl		
C–H (stretching)	3010–3095	(m)
C=H (stretching)	1620–1680	(v)
cis-RCH=CHR	675–730	(s)
trans-RCH=CHR	960–975	(s)
Alkynyl		
≡C–H (stretching)	~3300	(s)
C≡C (stretching)	2100–2260	(v)

❖ Characteristic IR absorptions

Intensity: s = strong, m = medium, w = weak, v = variable

Group	Freq. Range (cm^{-1})	Intensity
Aromatic		
Ar–H (stretching)	~3300	(v)
- monosubstituted	690–710	(very s)
	730–770	(very s)
- o-disubstituted	735–770	(s)
- m-disubstituted	680–725	(s)
	750–810	(very s)
- p-disubstituted	800–860	(very s)

❖ Characteristic IR absorptions

Intensity: s = strong, m = medium, w = weak, v = variable

Group	Freq. Range (cm^{-1})	Intensity
Alcohols, Phenols & Carboxylic Acids		
O–H (stretching)		
- alcohols & phenols (*dilute solutions*)	3590–3650	(sharp, v)
- alcohols & phenols (*hydrogen bonded*)	3200–3550	(broad, s)
- carboxylic acids (*hydrogen bonded*)	2500–3000	(broad, v)

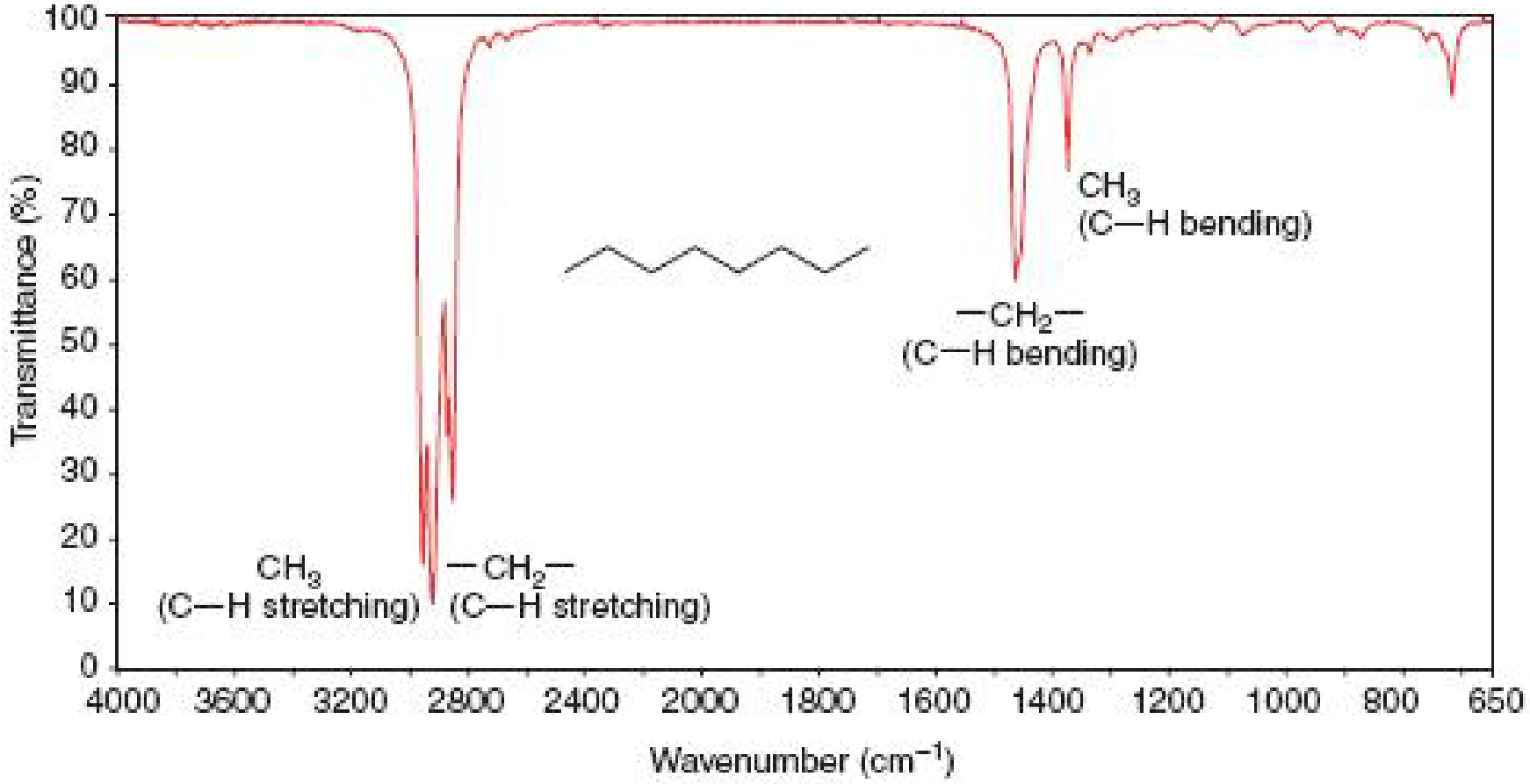
❖ Characteristic IR absorptions

Intensity: s = strong, m = medium, w = weak, v = variable

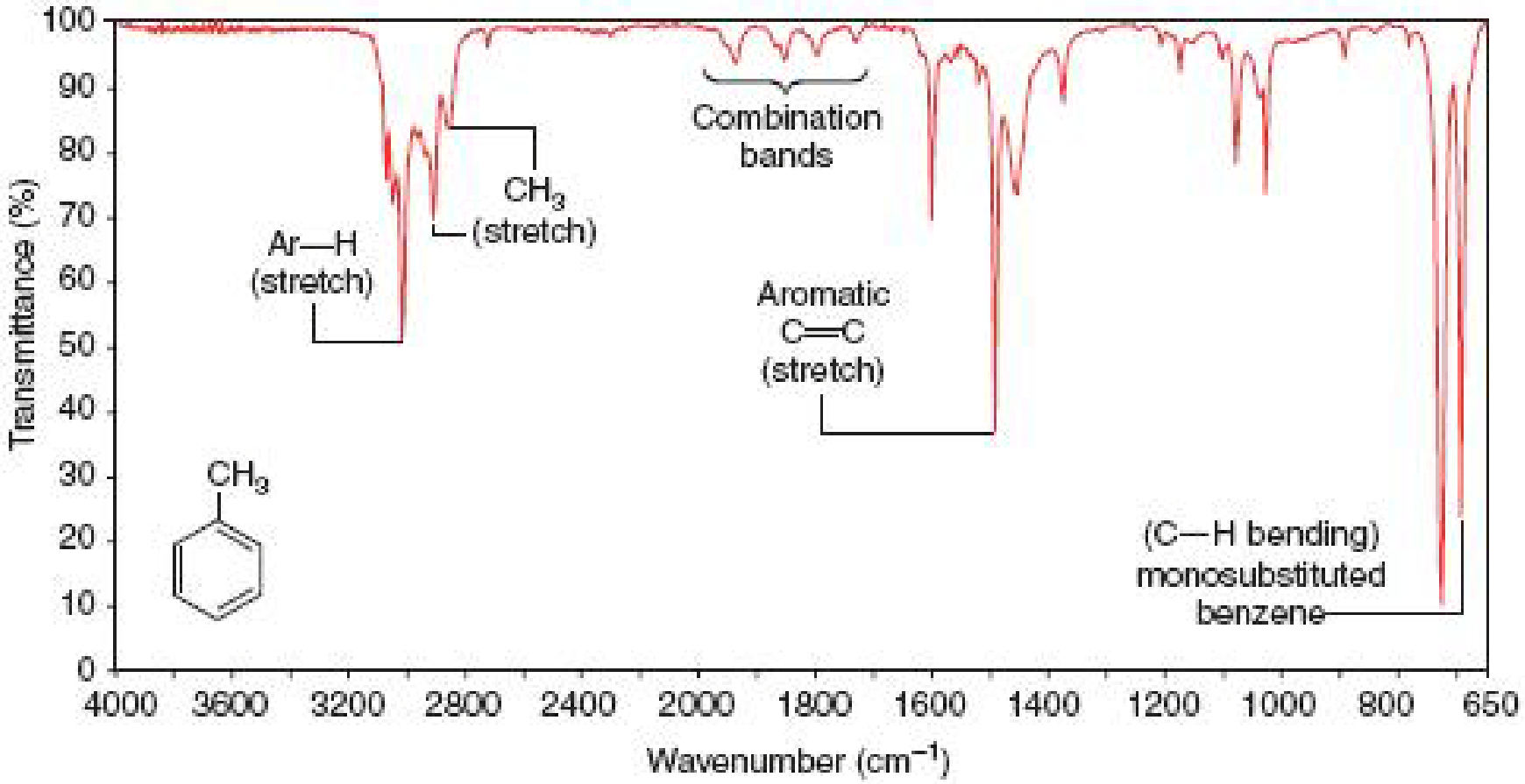
Group	Freq. Range (cm^{-1})	Intensity
Aldehydes, Ketones, Esters, Carboxylic Acids, Amides		
C=O (stretching)	1630–1780	(s)
Aldehydes	1690–1740	(s)
Ketones	1680–1750	(s)
Esters	1735–1750	(s)
Carboxylic Acids	1710–1780	(s)
Amides	1630–1690	(s)
Amines		
N–H	3300–3500	(m)
Nitriles		
C≡N	2220–2260	(m)

16. Interpreting IR Spectra

- IR spectrum of octane

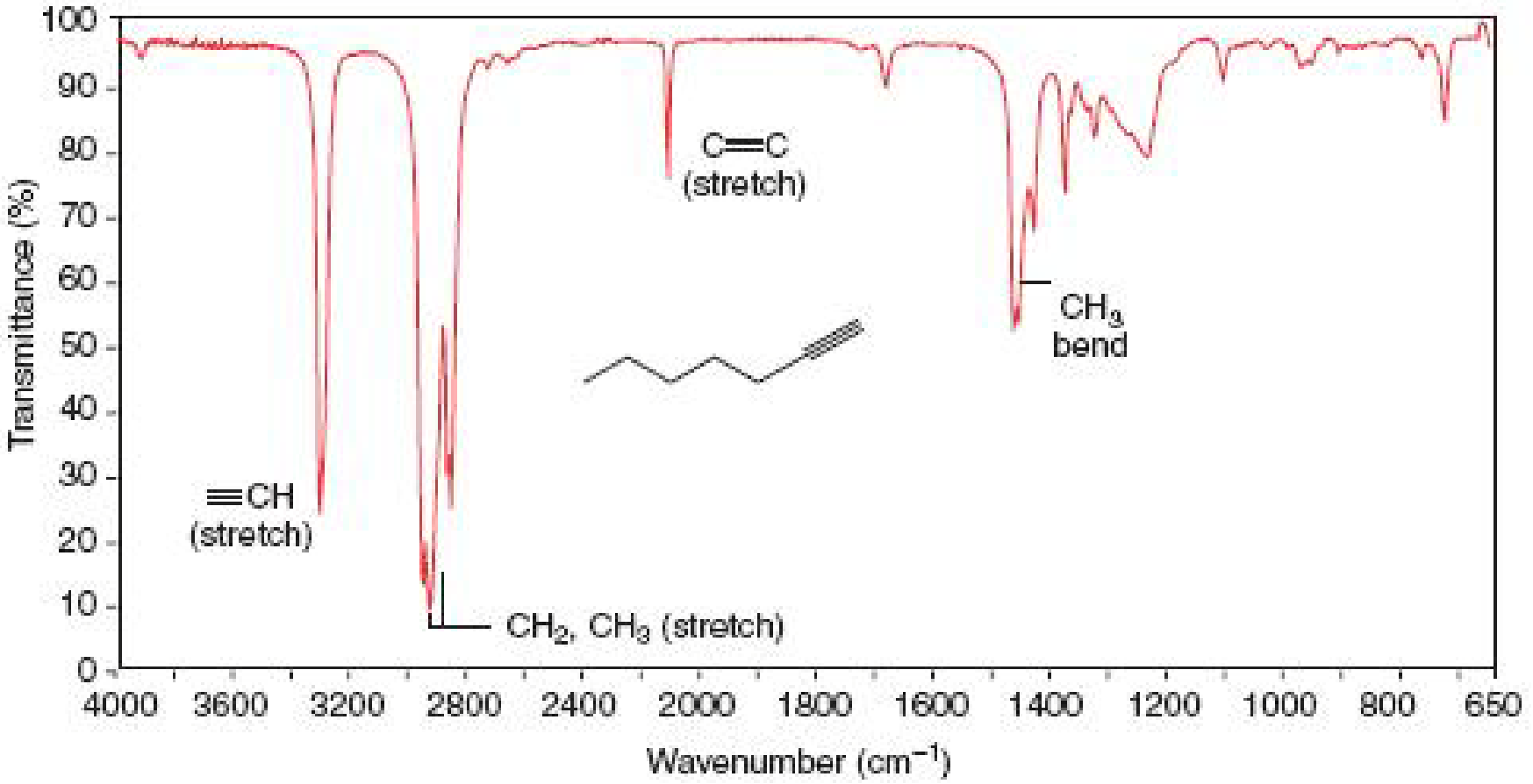


❖ IR spectrum of toluene

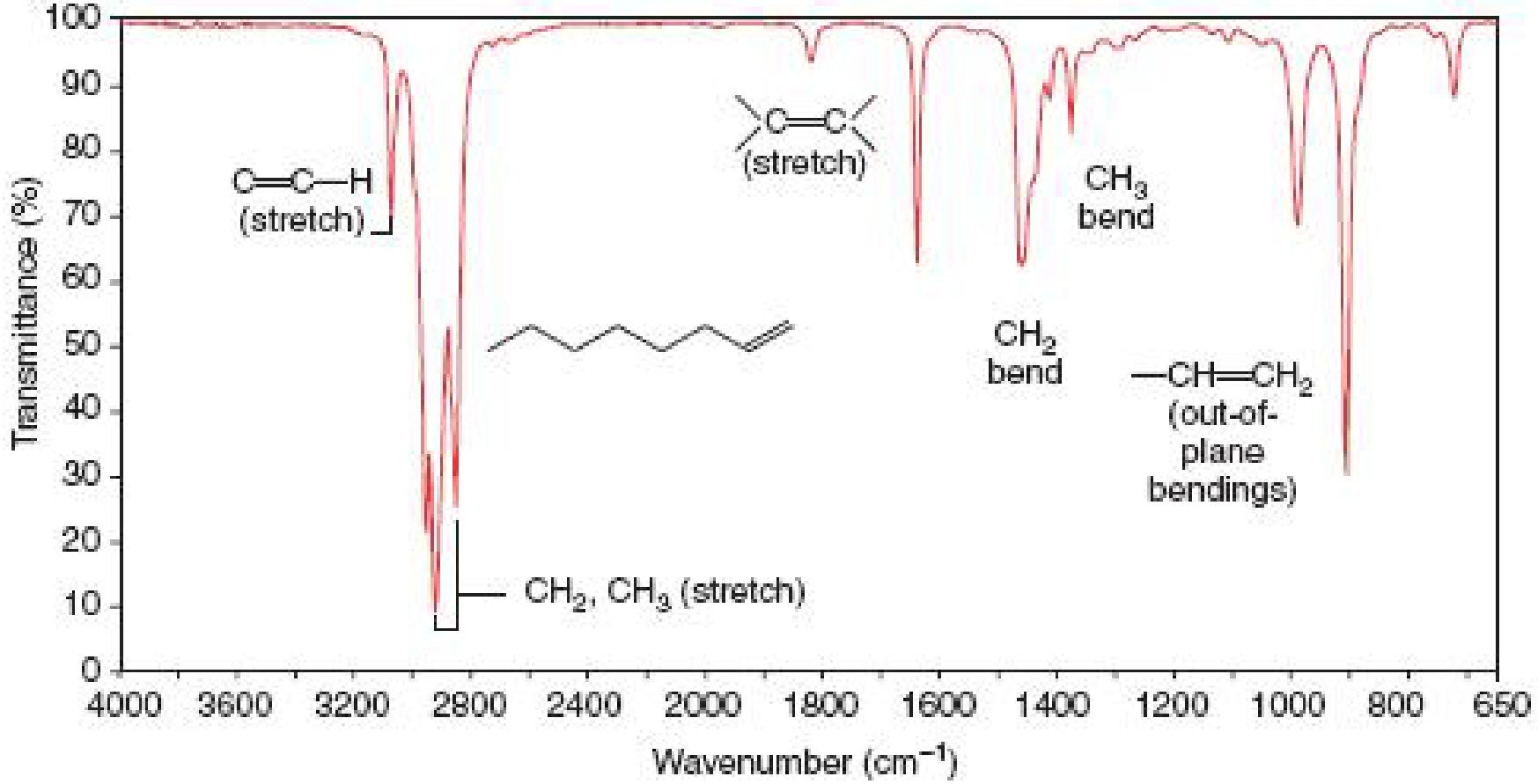


16B. IR Spectra of Hydrocarbons

- IR spectrum of 1-heptyne

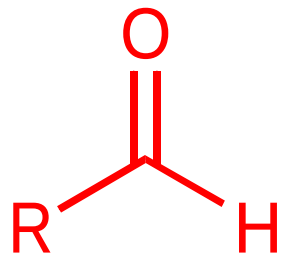


❖ IR spectrum of 1-octene



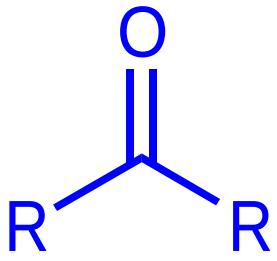
16B. IR Spectra of Some Functional Groups Containing

- Carbonyl Functional Groups



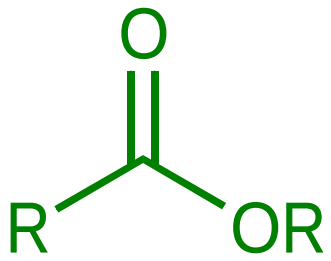
(aldehyde)

1690-1740 cm^{-1}



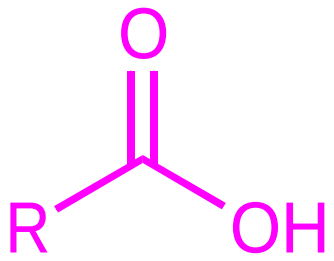
(ketone)

1680-1750 cm^{-1}



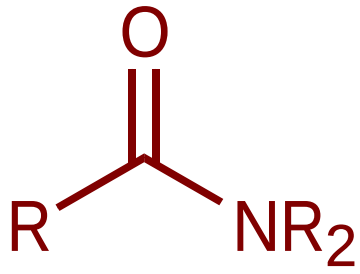
(ester)

1735-1750 cm^{-1}



(carboxylic acid)

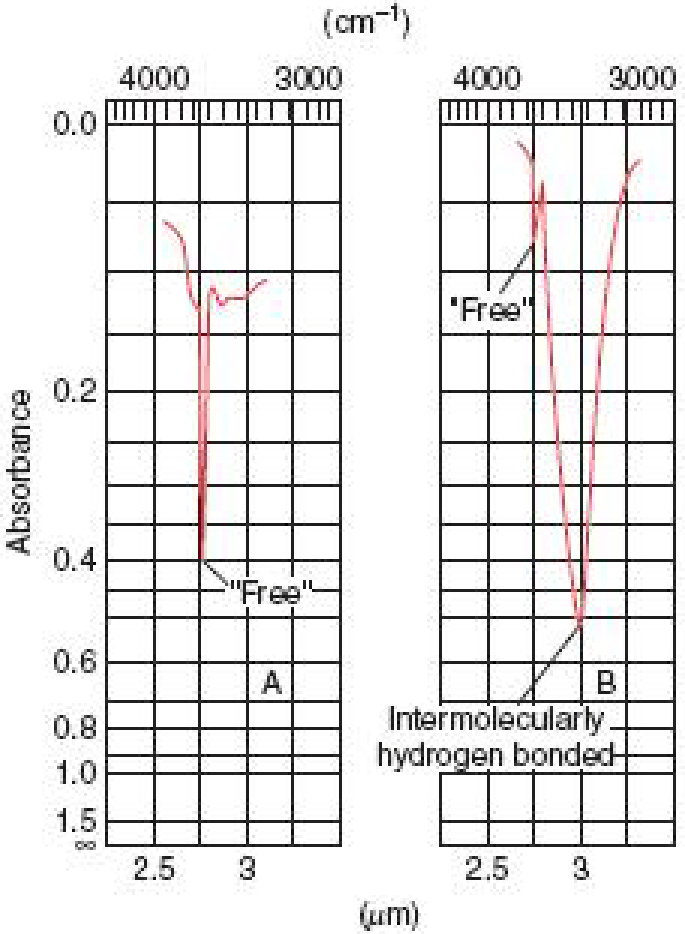
1710-1780 cm^{-1}



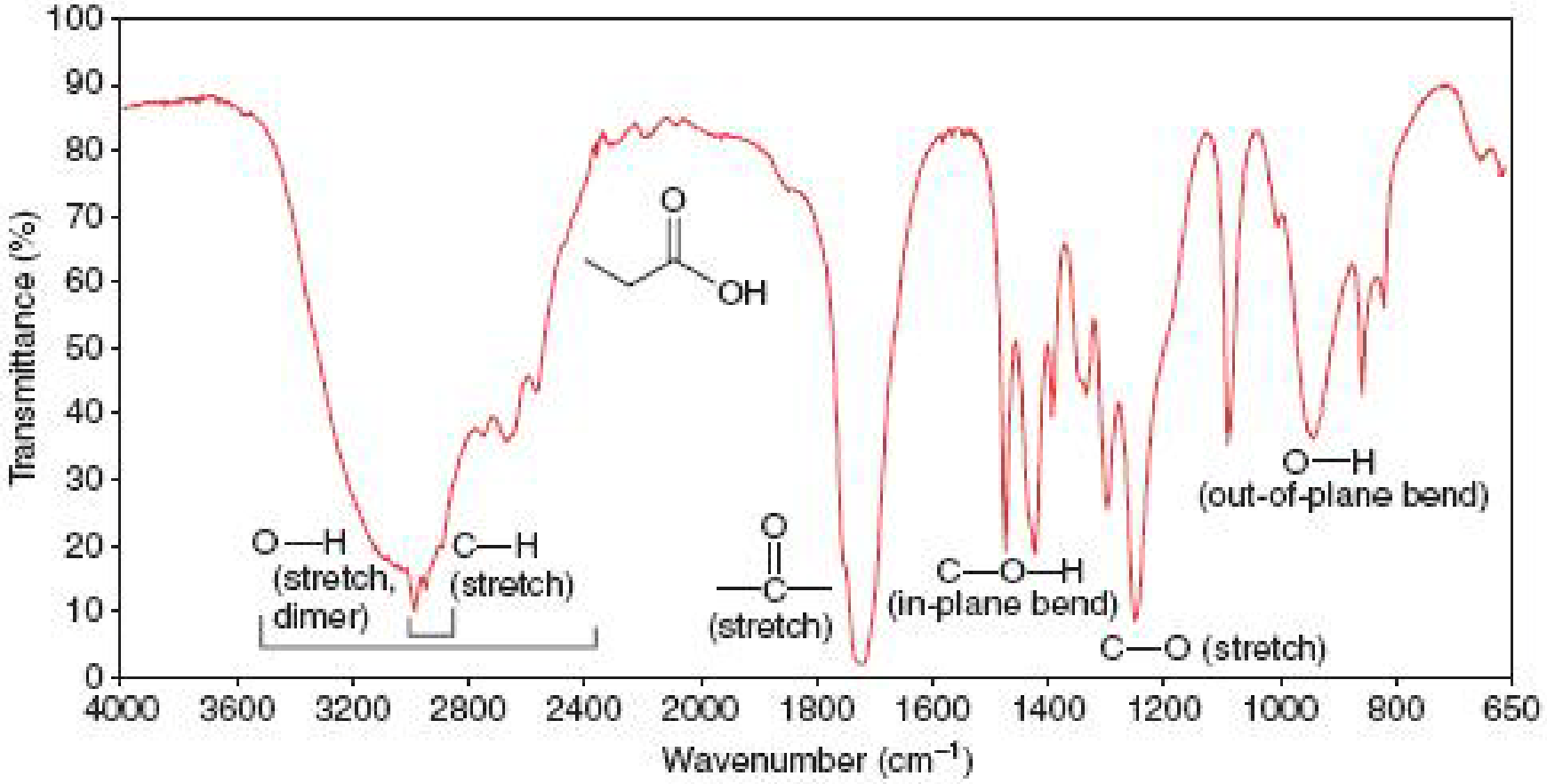
(amid)

1630-1690 cm^{-1}

- Alcohols and phenols
  - The IR absorption of an alcohol or phenol O–H group is in the 3200–3550 cm^{-1} range, and most often it is broad



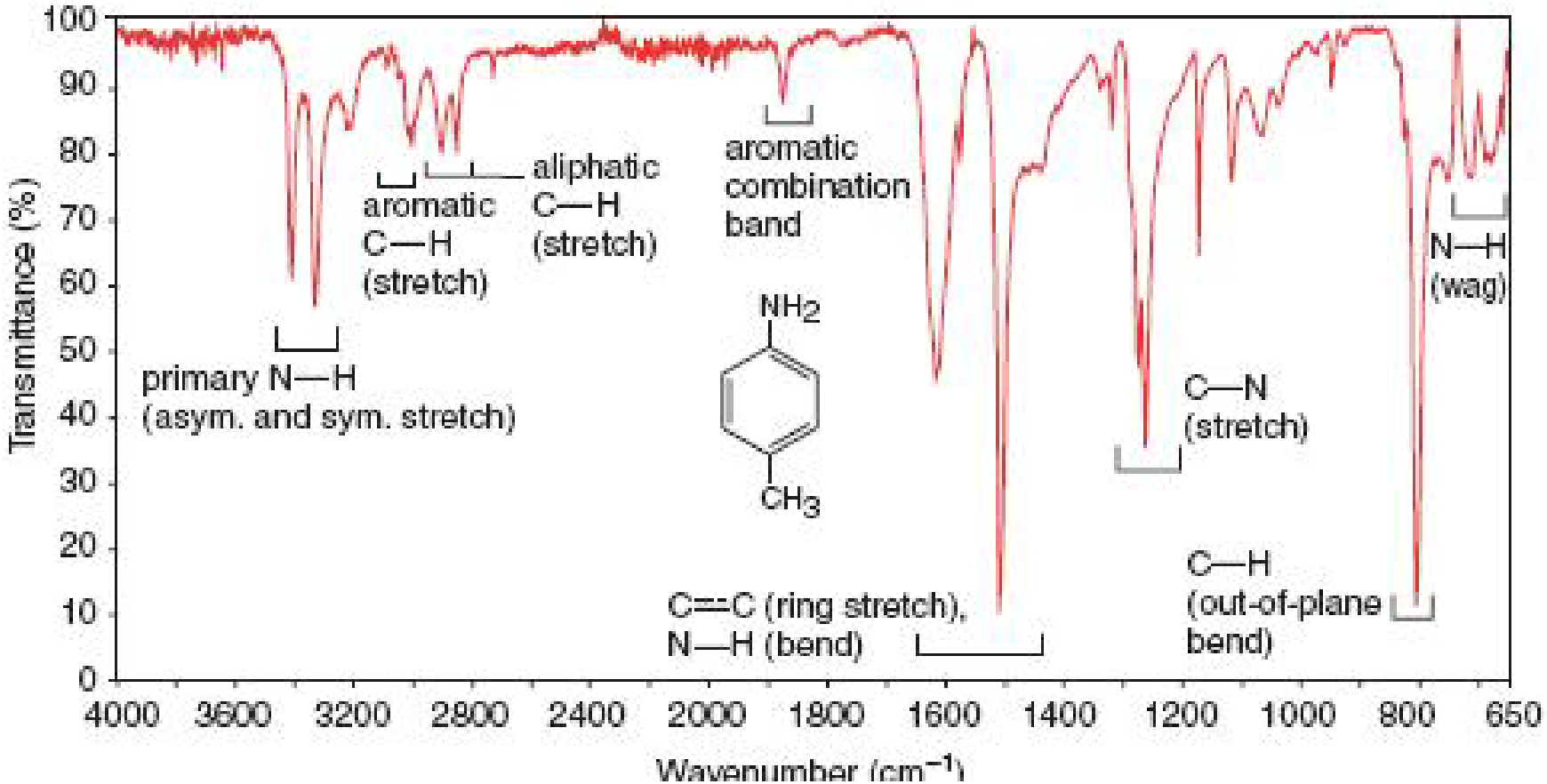
- Carboxylic Acids
  - IR spectrum of propanoic acid



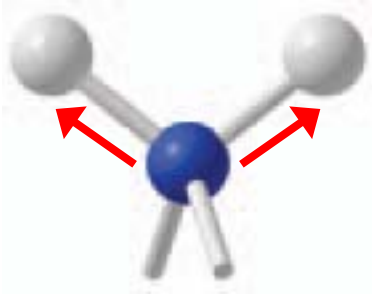
- Amines
  - 1^{o} and 2^{o} amines give absorptions of moderate strength in the 3300–3500 cm^{-1} region
  - 1^{o} amines exhibit two peaks in this region due to symmetric & asymmetric
  - stretching of the two N–H bonds
  - 2^{o} amines exhibit a single peak
  - 3^{o} amines show no N–H absorption because they have no such bond
  - A basic pH is evidence for any class of amines

❖ Amines

- IR spectrum of 4-methylaniline

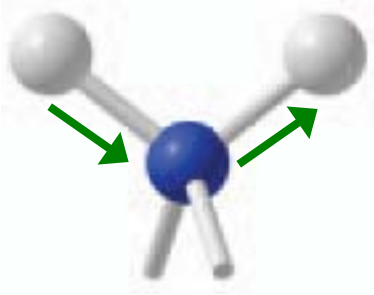


RNH_2 (1° Amine)
Two peaks in
3300–3500 cm^{-1}
region

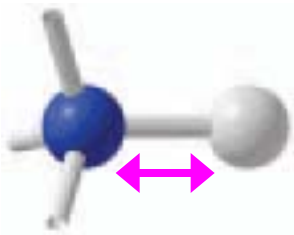


symmetric
stretching

R_2NH (2° Amine)
One peak in
3300–3500 cm^{-1}
region



asymmetric
stretching



END OF CHAPTER 2