Infra-Red (IR)
&
Fourier Transform Infra-Red (FT-IR) Spectroscopy

Molecular Motions & Degree of Freedom (D.F)

- Translational motion
- Rotational motion
- Vibrational motion

- Total internal D.F: includes vibrational motion; excludes translational & rotational motions

✓ for linear molecules: 3n – 5

✓ for cyclic molecules: 3n – 6

* n = number of atoms

IR Spectrum Report

- Relation of transmittance percent (%T) to wavenumber (υ)
- The pattern of IR spectrum is reverse type of absorption spectrum

IR Absorption Wavenumber (Values) for Bond between Carbon & Hydrogen: Stretching & Bending

C–H stretching	C–H bending
~3000 cm^{-1}	~1340 cm^{-1}

sp	sp^2	sp^3
≡C–H	=C–H	–C–H
3300 cm^{-1}	3100 cm^{-1}	2900 cm^{-1}

IR Absorption Wavenumbers (Values) for Various Types of "C-H": Stretching

sp	sp^2	sp^3
≡C−H	=C−H	−C−H
3300 cm^{-1}	3100 cm^{-1}	2900 cm^{-1}

TABLE 2.5
PHYSICAL CONSTANTS FOR *sp*-, sp^2-, AND sp^3-HYBRIDIZED CARBON AND THE RESULTING C−H ABSORPTION VALUES

Bond	≡C−H	=C−H	−C−H
Type	*sp*-1*s*	sp^2-1*s*	sp^3-1*s*
Length	1.08 Å	1.10 Å	1.12 Å
Strength	506 kJ	444 kJ	422 kJ
IR frequency	3300 cm^{-1}	~3100 cm^{-1}	~2900 cm^{-1}

IR Absorption Wavenumber (Values) for Bond Between Carbon & Hydrogen: Stretching

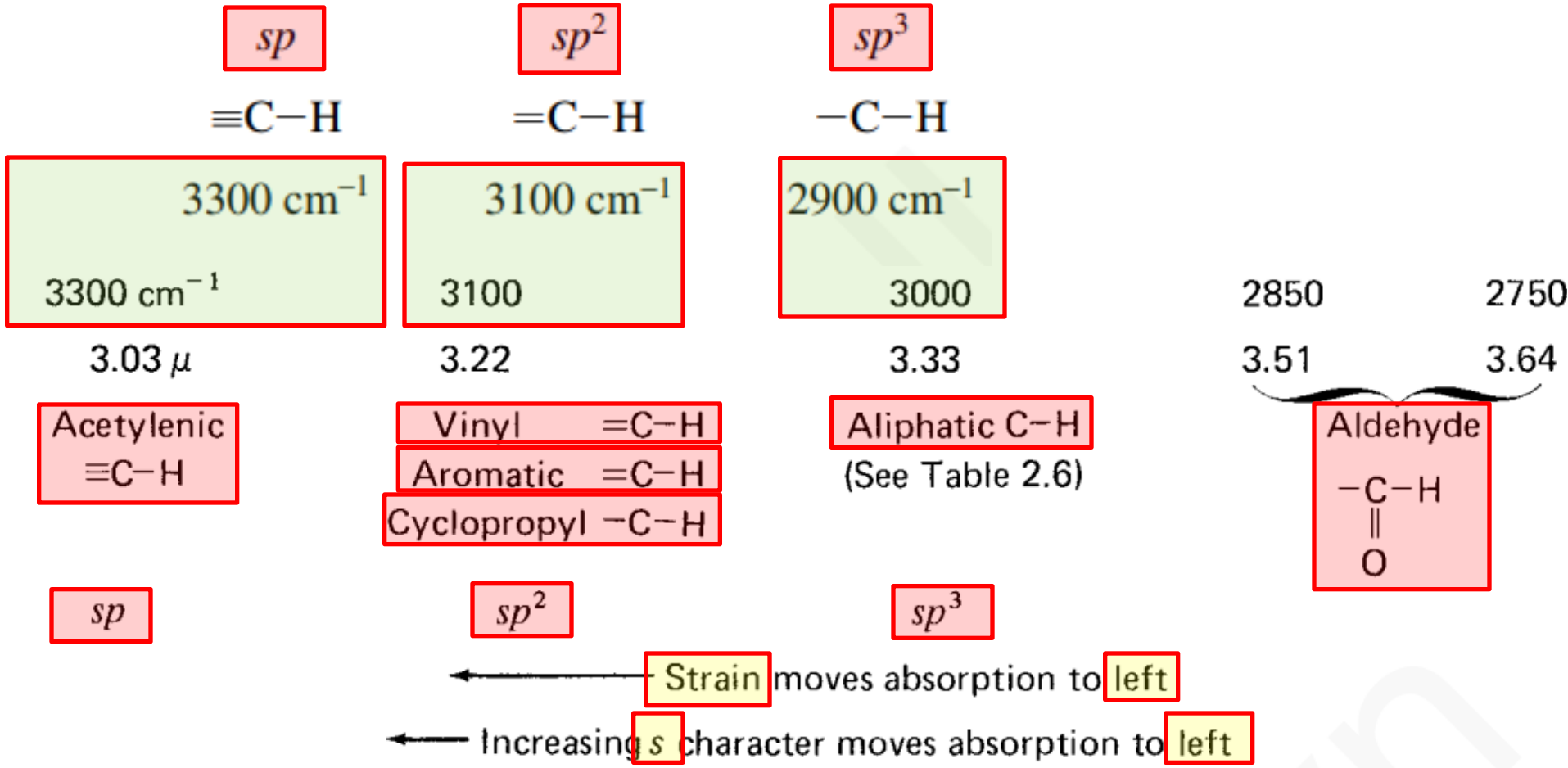


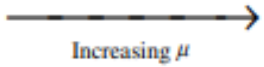
FIGURE 2.16 The C–H stretch region.

IR Absorption Wavenumber (Values) for Bond Between Carbon & Various Atoms: Stretching

- Follow Hook law for magnitude of wavenumber of IR for each type of bonds.

$$\bar{\nu}(\text{cm}^{-1}) = 4.12\sqrt{\frac{K}{\mu}}$$

C–H	C–C	C–O	C–Cl	C–Br	C–I
3000 cm^{-1}	1200 cm^{-1}	1100 cm^{-1}	750 cm^{-1}	600 cm^{-1}	500 cm^{-1}



IR Absorption Wavenumber (Values) for C-H in Methyl & Methylene: Bending

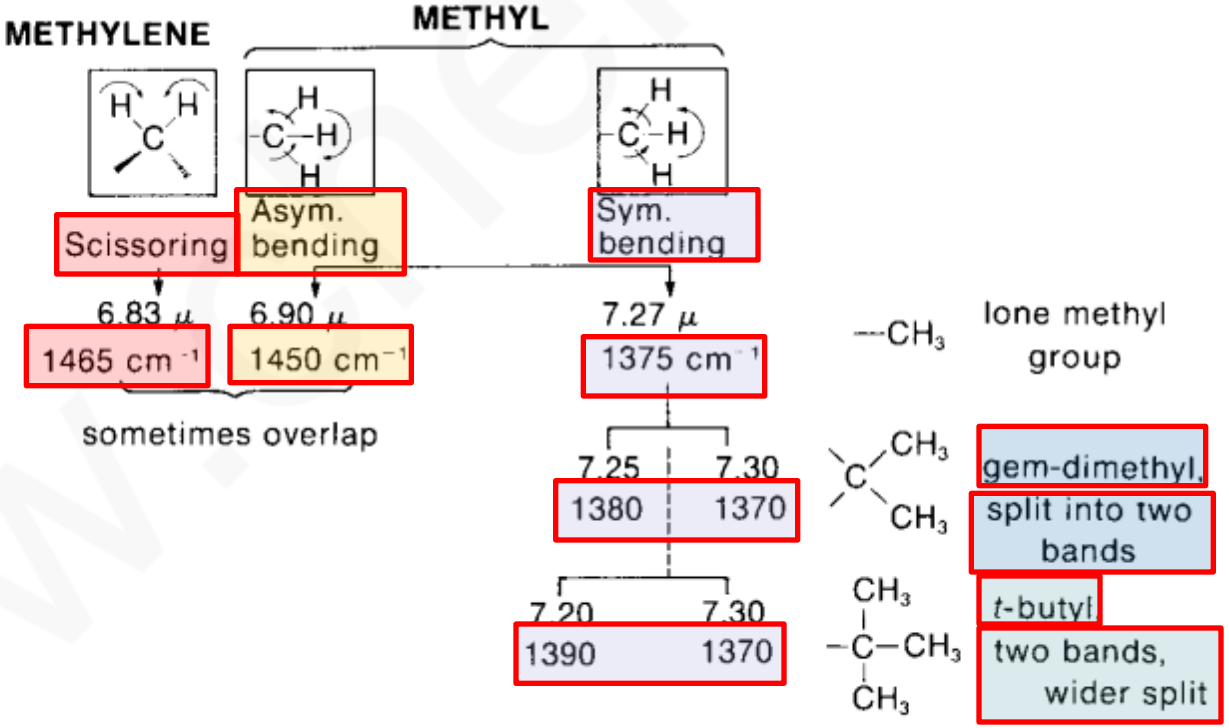
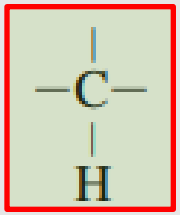


FIGURE 2.17 The C—H bending vibrations for methyl and methylene groups.

IR Absorption Wavenumber (Values) for sp^3-C-H Stretching

TABLE 2.6
STRETCHING VIBRATIONS FOR VARIOUS sp^3-HYBRIDIZED C—H BONDS

Group		Stretching Vibration (cm^{-1})	
		Asymmetric	*Symmetric*
Methyl	CH_3-	2962	2872
Methylene	$-CH_2-$	2926	2853
Methine		2890 Very weak	

IR Absorption Wavenumber (Values) for sp^3 C-H in Isopropyl & t-Butyl: Bending

- Isopropyl: two geminal methyls
- Compare intensity of split peaks

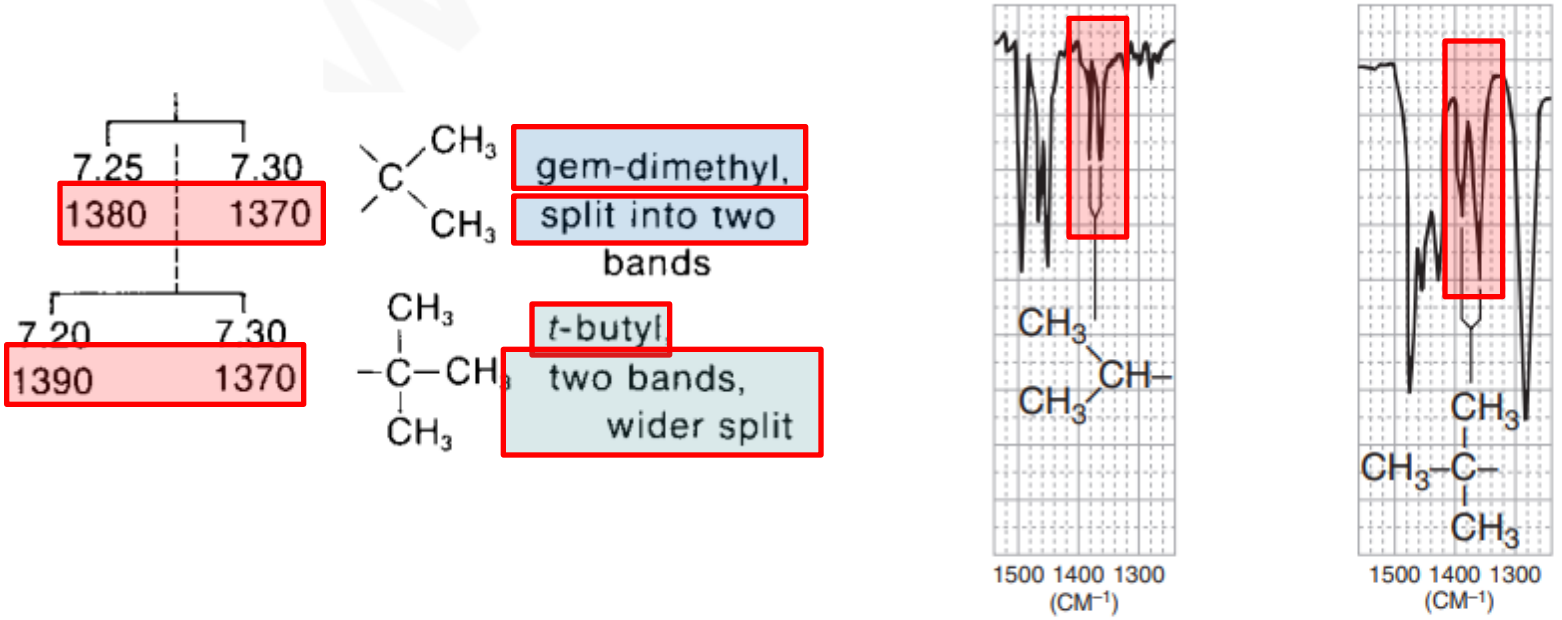


FIGURE 2.18 C—H bending patterns for the isopropyl and *tert*-butyl groups.

Example of IR Spectrum: Infrared Spectroscopy for Decan ($C_{10}H_{22}$)

IR(υ(cm^{-1}), KBr): ~2900 (s, C-H stretching), ~1450 (s, C-H bending), ~1360 (s, C-H bending), ~720 (s, $(CH_2)_4$ bending)

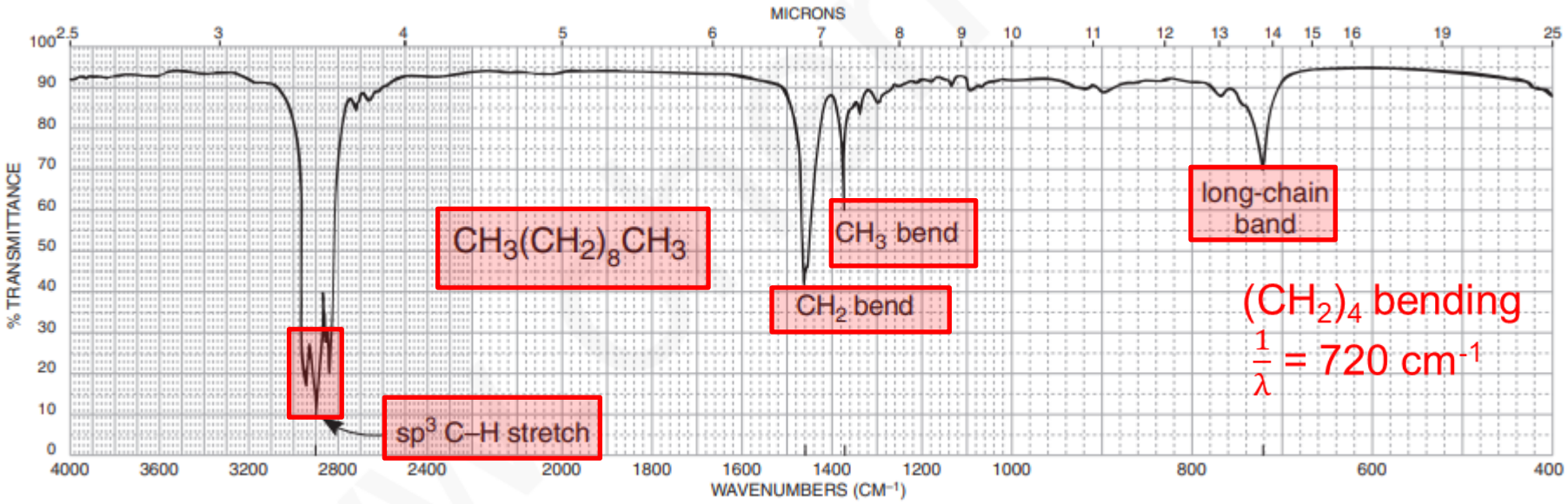


FIGURE 2.7 The infrared spectrum of decane (neat liquid, KBr plates).

C−H stretching	C−H bending	sp^3 −C−H
~3000 cm^{-1}	~1340 cm^{-1}	2900 cm^{-1}

Recyclable Polymers

1 PETE — Poly(ethylene terephthalate) (PET)

2 HDPE — High Density Poly(ethylene)

3 V — Poly(vinyl chloride)

4 LDPE — Low Density Poly(ethylene)

5 PP — Poly(propylene)

6 PS — Poly(styrene)

7 OTHER — Composites:

eg. PET with Poly(ethylene vinyl alcohol)

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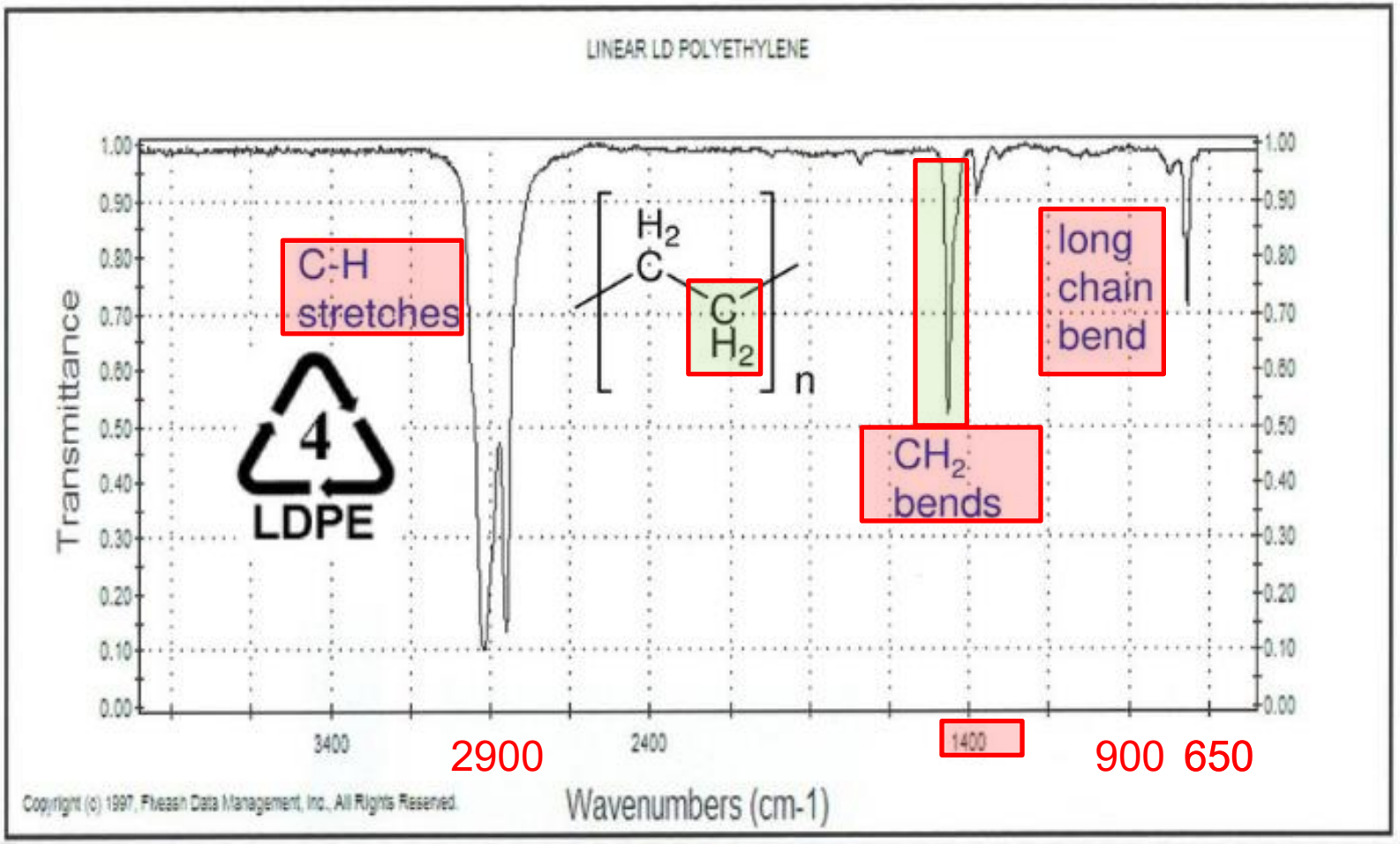
Infrared Spectrum of Low Density Polyethylene



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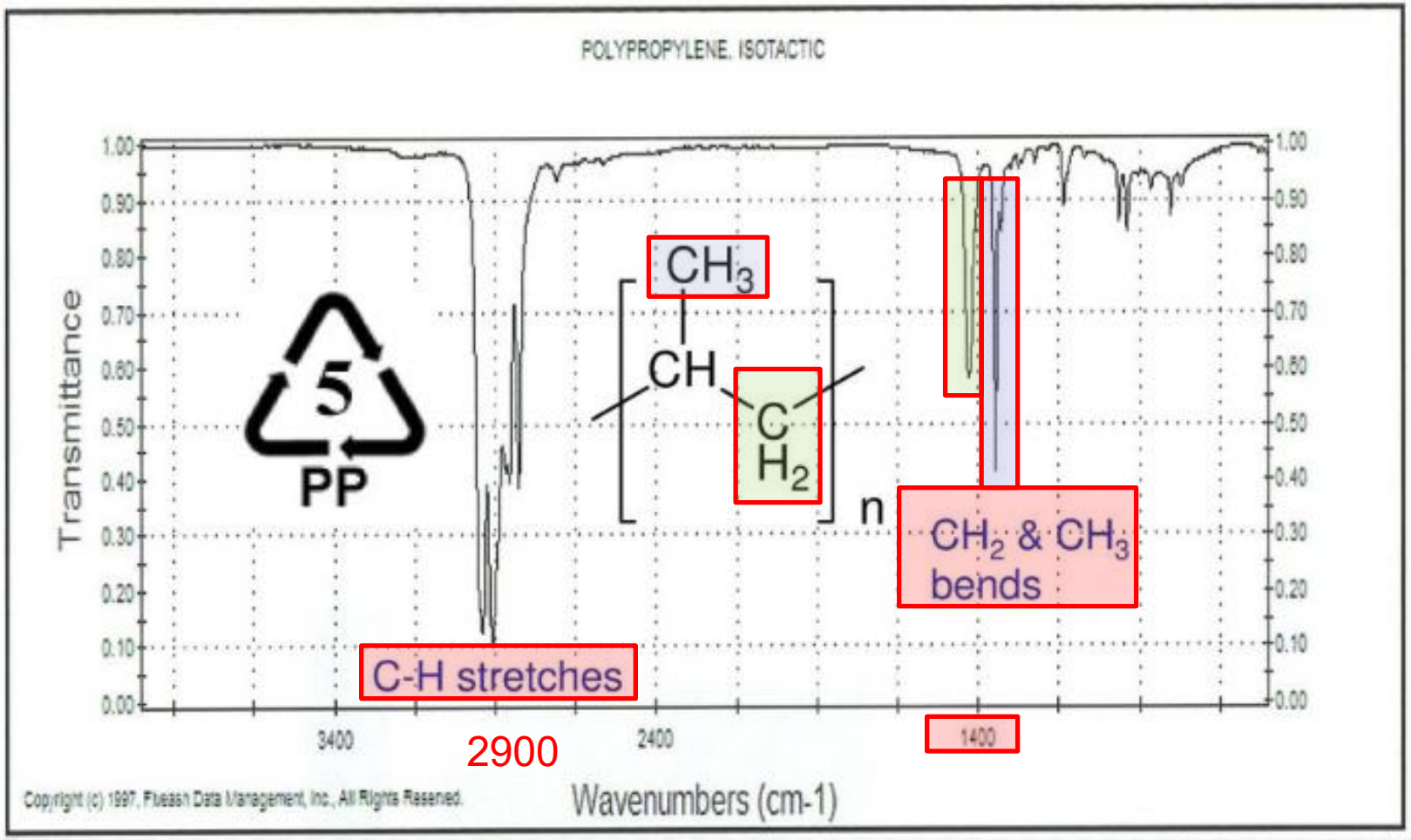
Infrared Spectrum of Polypropylene



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Example of IR Spectrum: Infrared Spectroscopy for Cyclohexane (C_6H_{12})

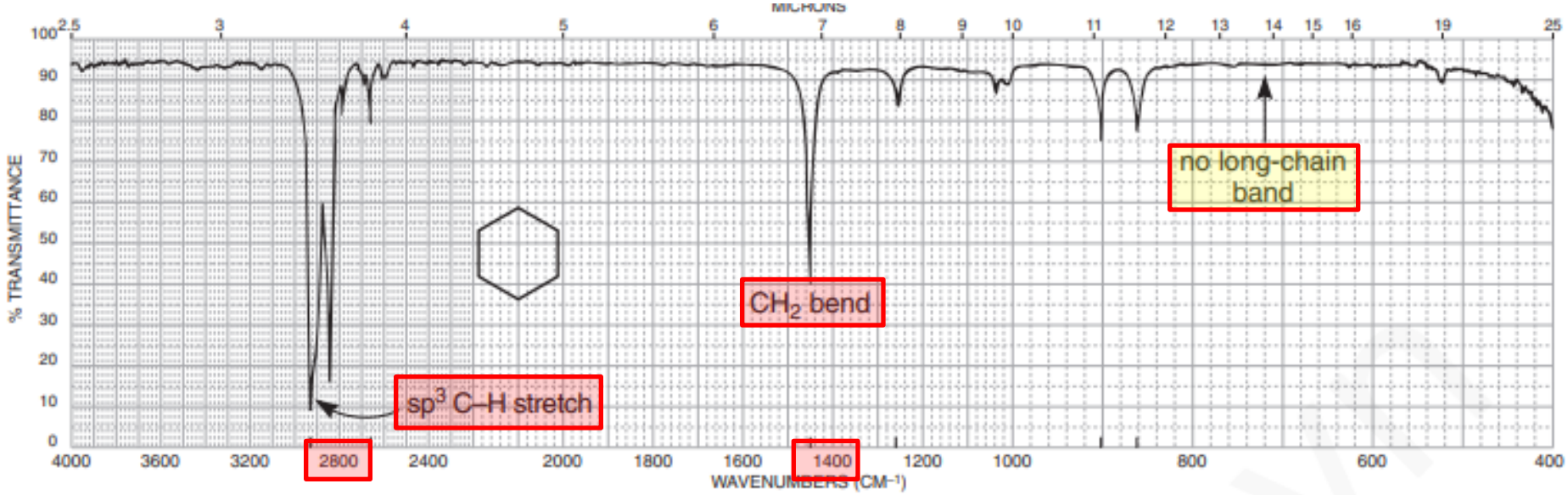
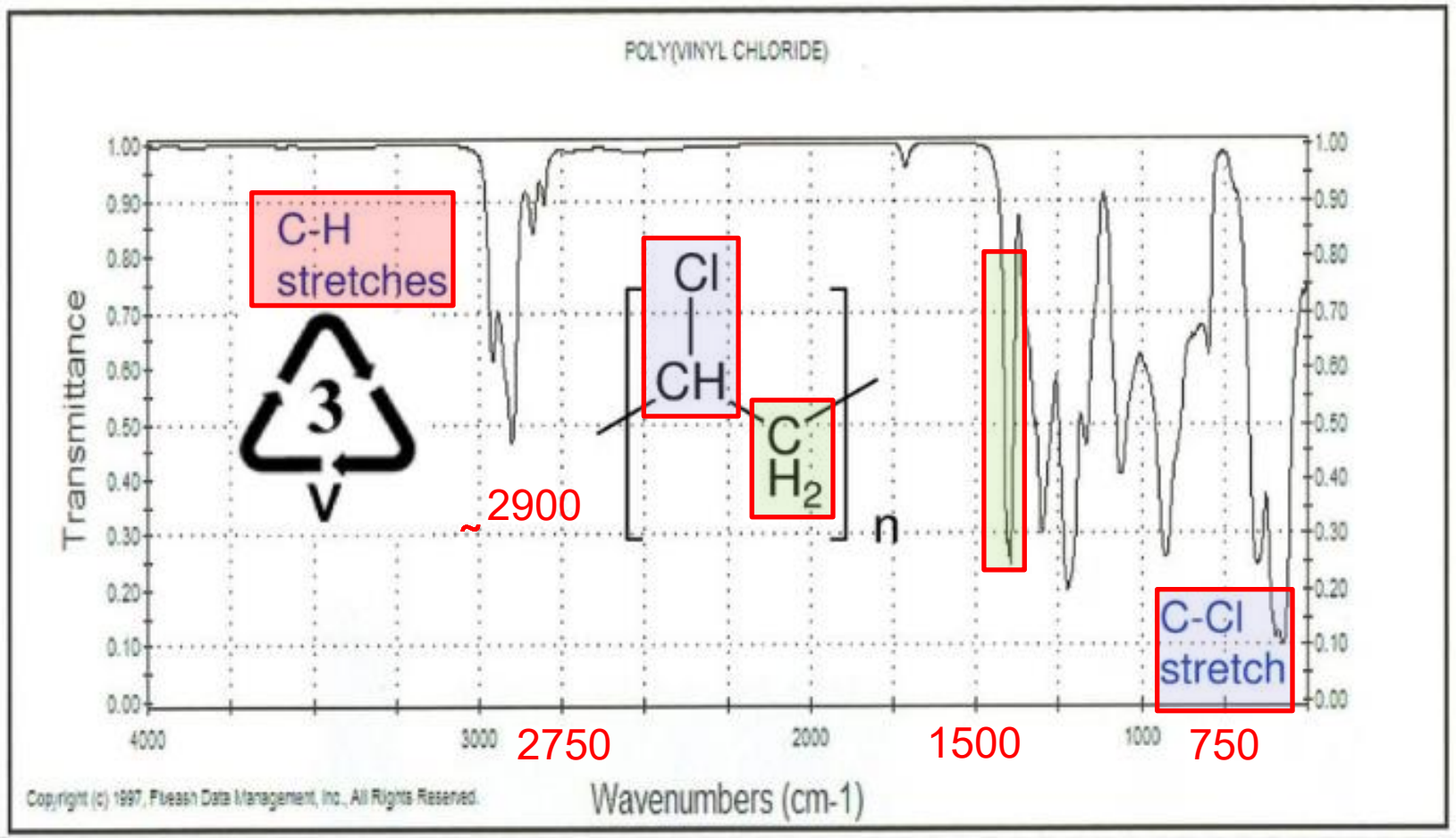


FIGURE 2.9 The infrared spectrum of cyclohexane (neat liquid, KBr plates).

Infrared Spectrum of Poly(vinyl chloride)



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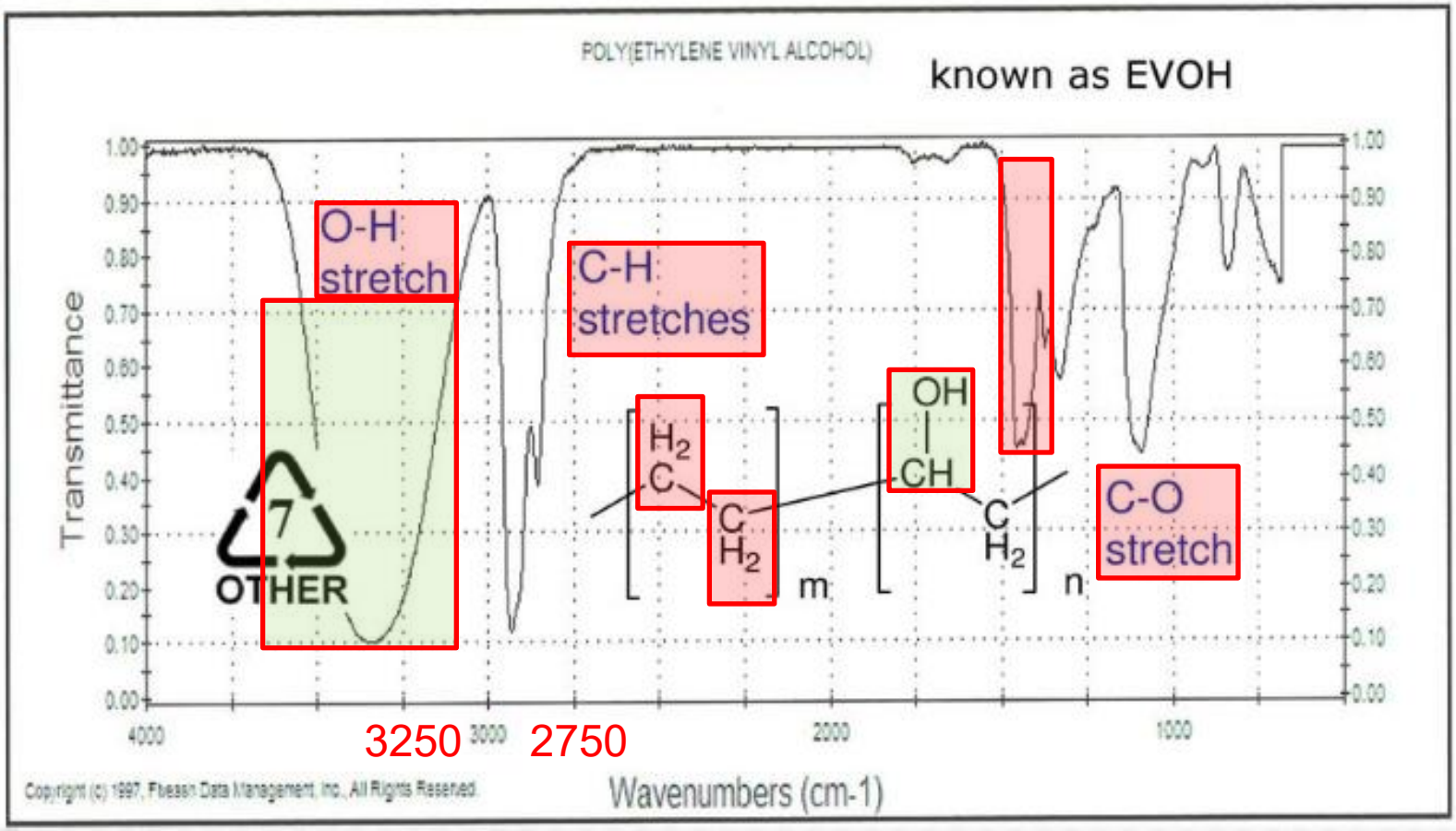
Infrared Spectrum of Poly(ethylene vinyl alcohol)



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