

Spettroscopia infrarossa

tecnica principe per il riconoscimento di polimeri

Importante anche in fase di riciclo!

	<i>Energy</i> kcal/mol	<i>Molecular effects</i>
gamma rays	10^6	
X rays	10^4	ionization
vacuum UV	10^2	
near UV		electronic transitions
visible	10	
infrared (IR)	1	molecular vibrations
microwave	10^{-2} 10^{-4}	rotational motion
radio	10^{-6}	nuclear spin transitions

FT-IR spectroscopy ←

Classical vibrational model:

Hooke's law $\mathbf{F} = -\mathbf{k} \cdot \mathbf{y}$

Energy: force*distance: $dE = -Fdy$ $E = \frac{1}{2}ky^2$

Classical vibrational frequency:

$$\nu_{\text{classical}} = \frac{1}{2\pi} \sqrt{\frac{k}{m}}$$

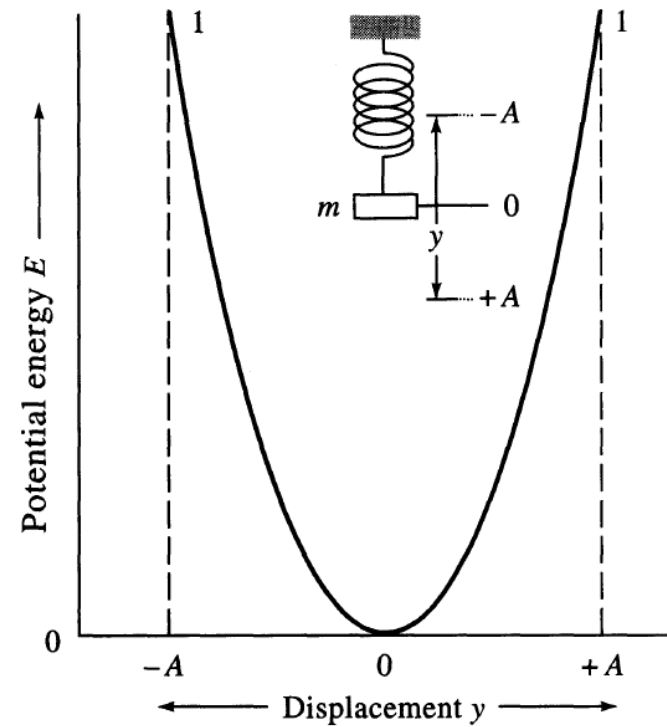
Quantum mechanics: energy is quantized

$$E = \left(\nu + \frac{1}{2} \right) \frac{h}{2\pi} \sqrt{\frac{k}{\mu}} = \left(\nu + \frac{1}{2} \right) h \cdot \nu_{\text{classical}}$$

In any case, $\Delta E = h\nu_{\text{classical}}$

- **Mass - ATOMS**
- **Force constant - BOND**
- **Geometry**

Harmonic oscillator



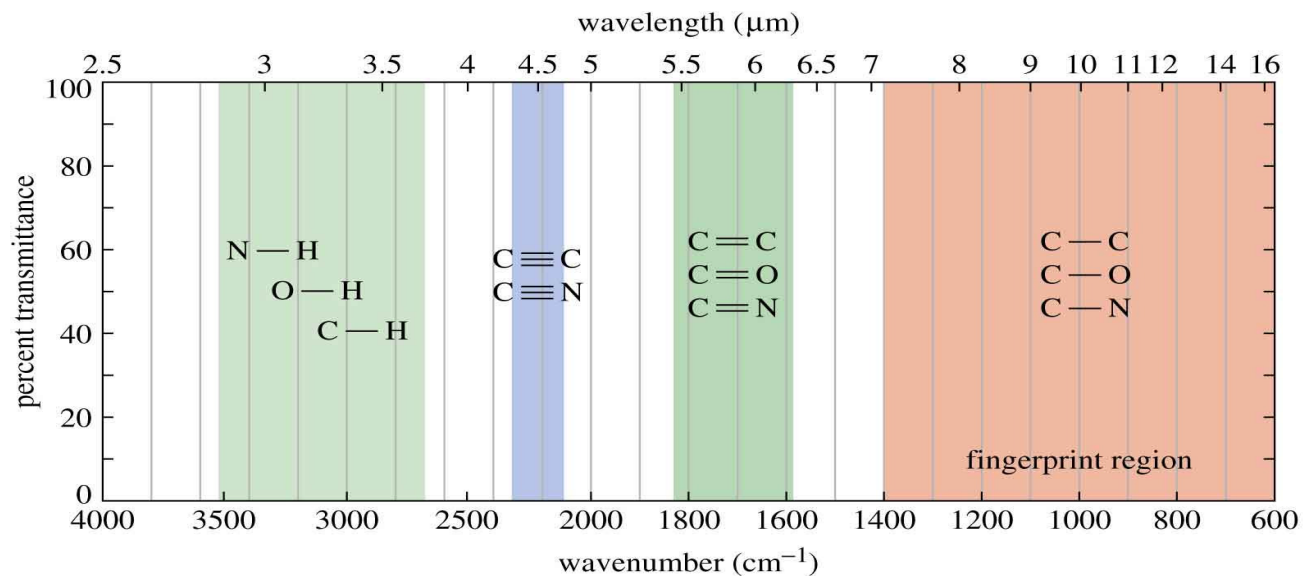
Bond	Bond Energy [kcal (kJ)]		Stretching Frequency (cm ⁻¹)
<i>Frequency dependence on atomic masses</i>			
C—H	100	(420)	3000
C—D	100	(420)	2100
C—C	83	(350)	1200
	↓ heavier atoms		↓ $\bar{\nu}$ decreases
<i>Frequency dependence on bond energies</i>			
C—C	83	(350)	1200
C=C	146	(611)	1660
C≡C	200	(840)	2200
	↓ stronger bond		↓ $\bar{\nu}$ increases

➤ **Mass**

➤ **Force constant**

$$v_{\text{classical}} = \frac{1}{2\pi} \sqrt{\frac{k}{m}}$$

$$\text{Reduced mass} = \frac{m_1 \cdot m_2}{m_1 + m_2}$$



Group frequency region

Identify functional groups

Fingerprint region

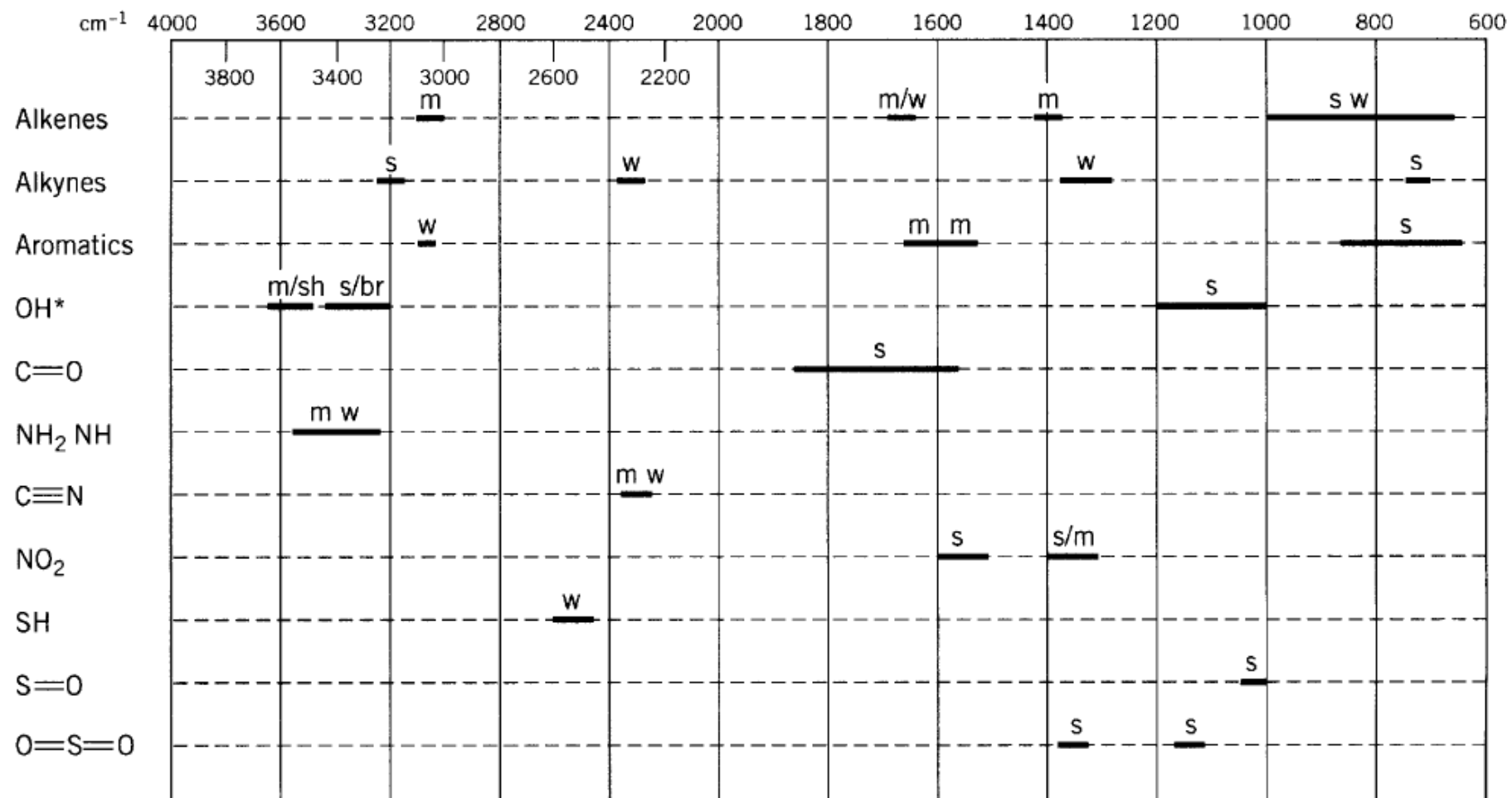
Compare with known spectra

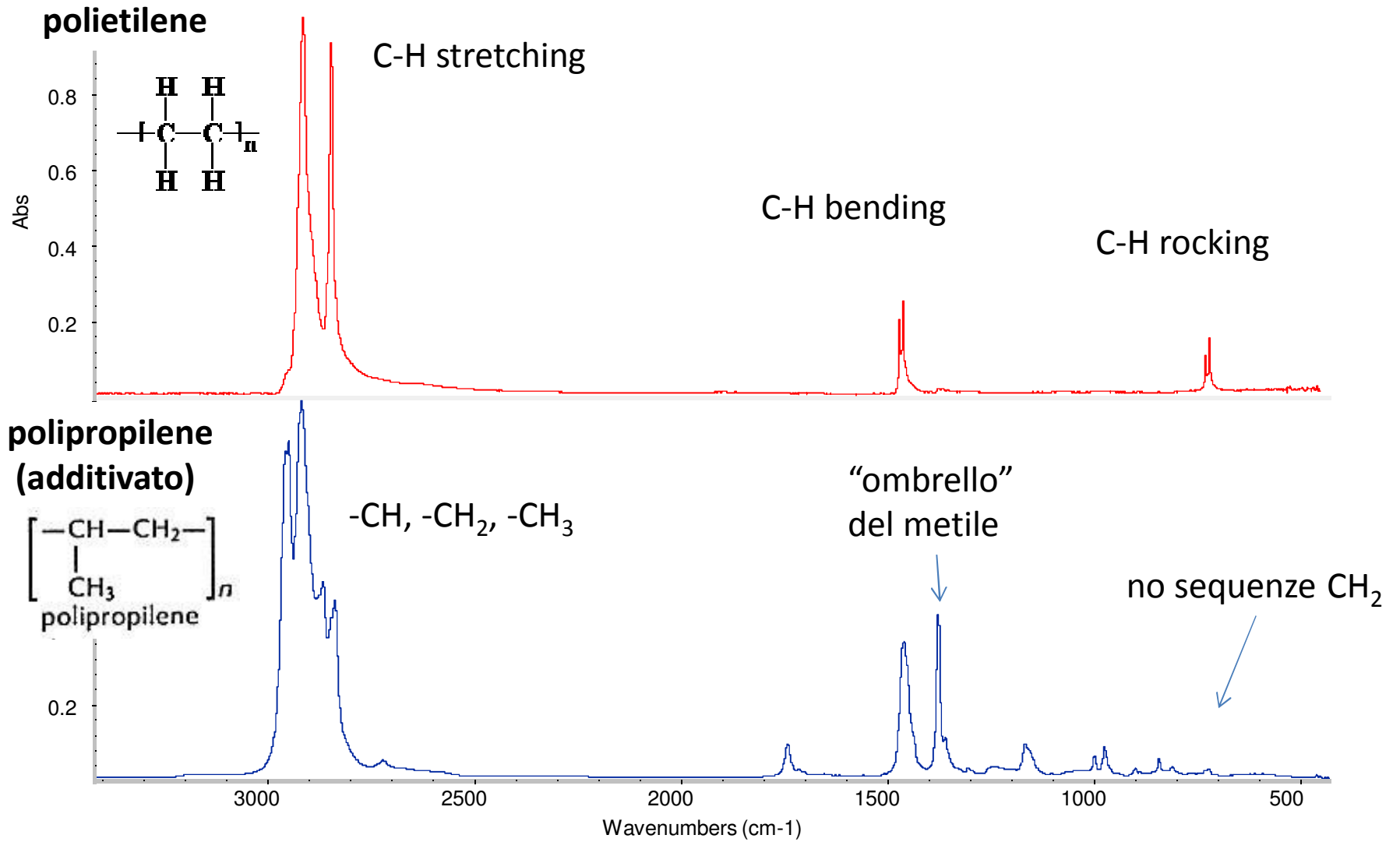


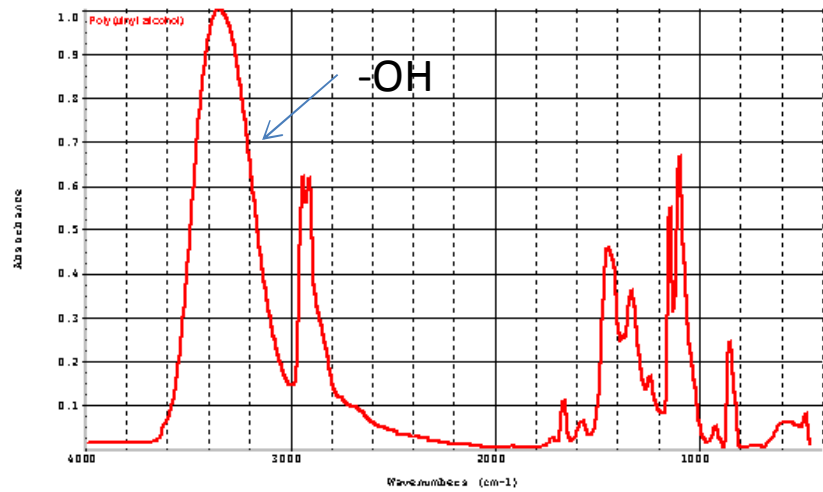
No two molecules will give exactly the same IR spectrum (except enantiomers)

Qualitative analysis

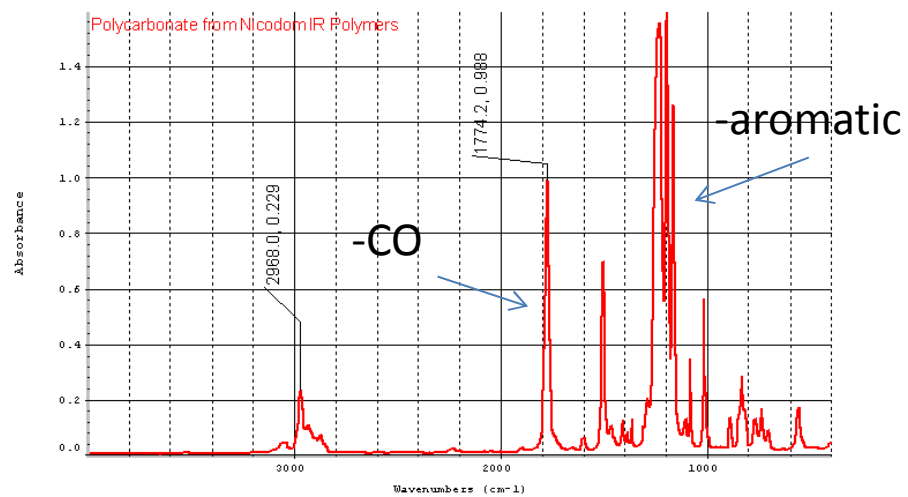
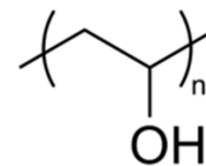
- spectra superimposition is evidence of identity
- recognition of specific chemical groups







PVA



PC

