

ORGANIC CHEMISTRY 2 LECTURE GUIDE 2019

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Lesson VII.3. Interaction of Infrared Light with Molecules

Wavenumbers

Molecules absorb energy:

Ⓐ

Leading to:

Ⓑ

Expressing energy: $E = h\nu = \frac{hc}{\lambda}$

wavenumber ($\tilde{\nu}$):

Ⓒ

Larger wavenumbers =

Ⓓ

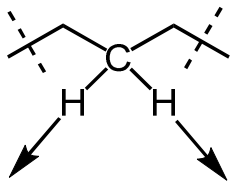
Notes

Lesson VII.3. Interaction of Infrared Light with Molecules

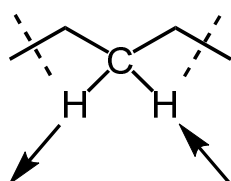
Vibrational modes; stretching modes and bending modes

Bonds can vibrate in different ways, and each of these **vibrational modes** requires a different energy:

Stretching modes

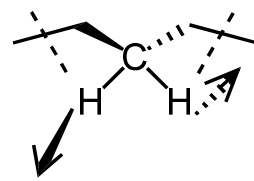
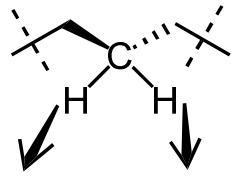


(A)

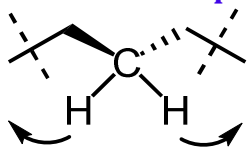


(B)

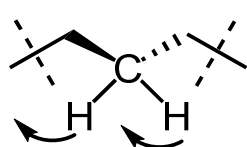
Out-of-plane bending modes



In-plane bending modes



(C)



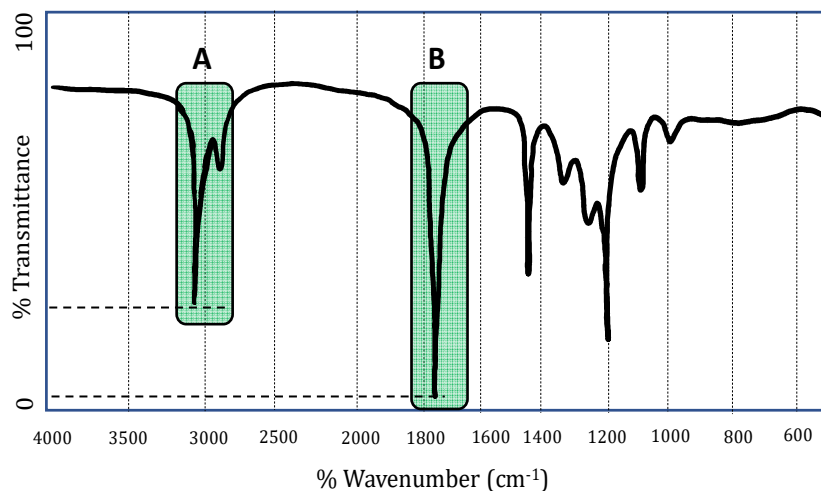
(D)

Notes

Lesson VII.4. Infrared Spectroscopy

Infrared spectrum and transmittance

A typical IR spectrum has this appearance:



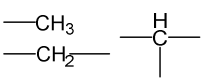
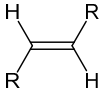
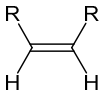
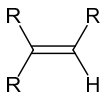
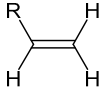
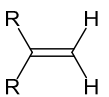


Band **A** corresponds to a set of bonds that absorbs ~75% of the IR light at 3000 cm^{-1} emitted by the source (i.e., 25% transmittance), whereas band **B** corresponds to a set of bonds that absorbs nearly 95% of the IR light at 1750 cm^{-1} (i.e., 5% transmittance).

Notes

Lesson VII.4. Infrared Spectroscopy*Infrared Table*

Each type of bond has a characteristic energy of absorption for IR radiation:

<u>Bond</u>	<u>Energy (cm⁻¹)</u>	<u>Intensity</u>	<u>C-H Bond (Stretch)</u>	<u>Energy (cm⁻¹)</u>
N≡C	2255-2220	m-s	C≡C-H	3300-ish
C≡C	2260-2100	w-m	C=C-H	3100-3000
C=C	1675-1660	m	C-C-H	2950-2850
N=C	1650-1550	m		2820-ish and 2720-ish
 {	1600 AND	w-s	C-H Bond (Bending)	
	1500-1425			1450-1400
C=O	1775-1650	s		980-960 trans
C-O	1250-1000	s		730-670 cis
C-N	1230-1000	m		840-800 trisubstituted
O-H	3650-3200	s (br)		990 and 910 monosubstituted
O-H	3300-2500	s (br)		890 disubstituted terminal
N-H	3500-3300	m (br)		
C-H	3300-2725	m		

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Lesson VII.4. Infrared Spectroscopy

Resonance effects on IR modes

There are several points worth noting:

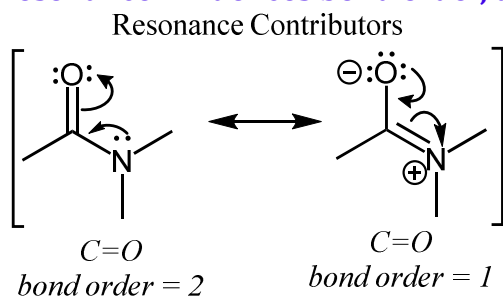
Stronger bonds:

(A)

More polar bonds:

(B)

Resonance influences bond order, and therefore bonds strength:



Resonance Hybrid

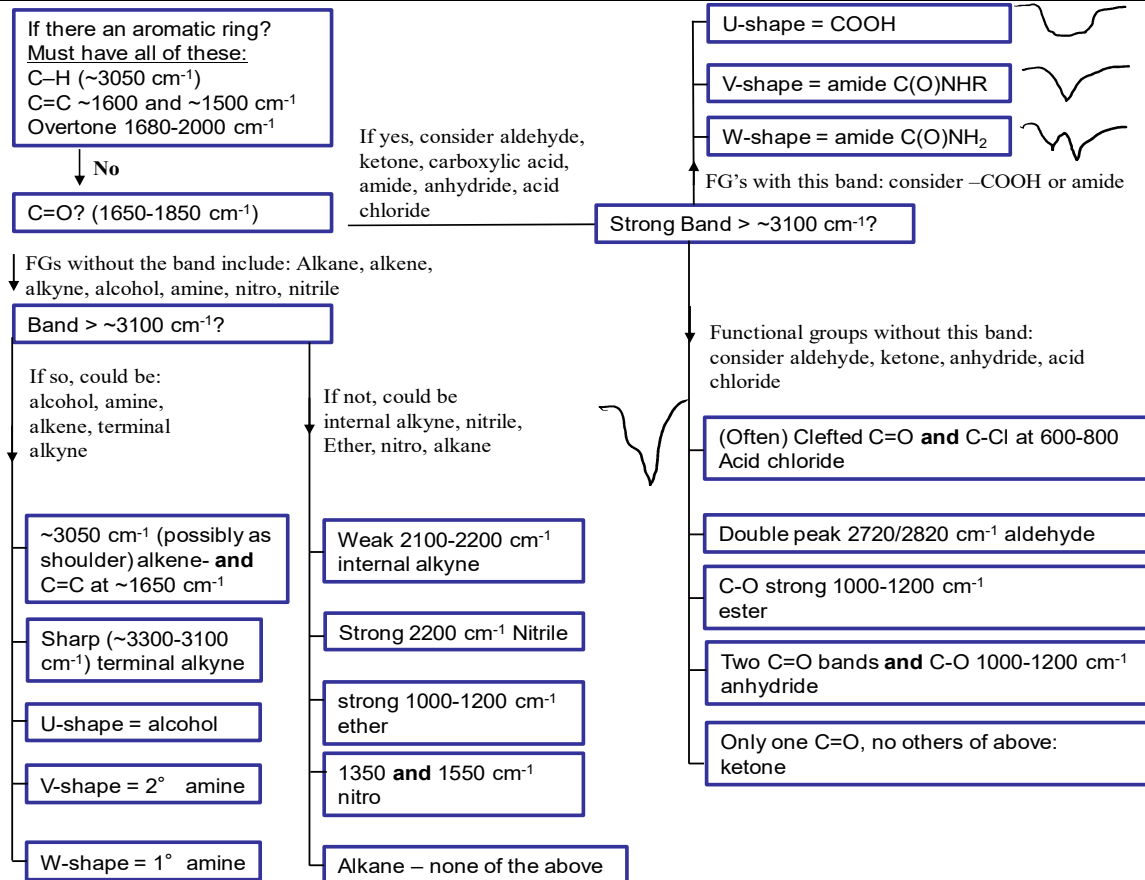
(C)

Amides have lower-energy C=O stretches than ketones

Notes

Lesson VII.4. Infrared Spectroscopy

IR decision tree

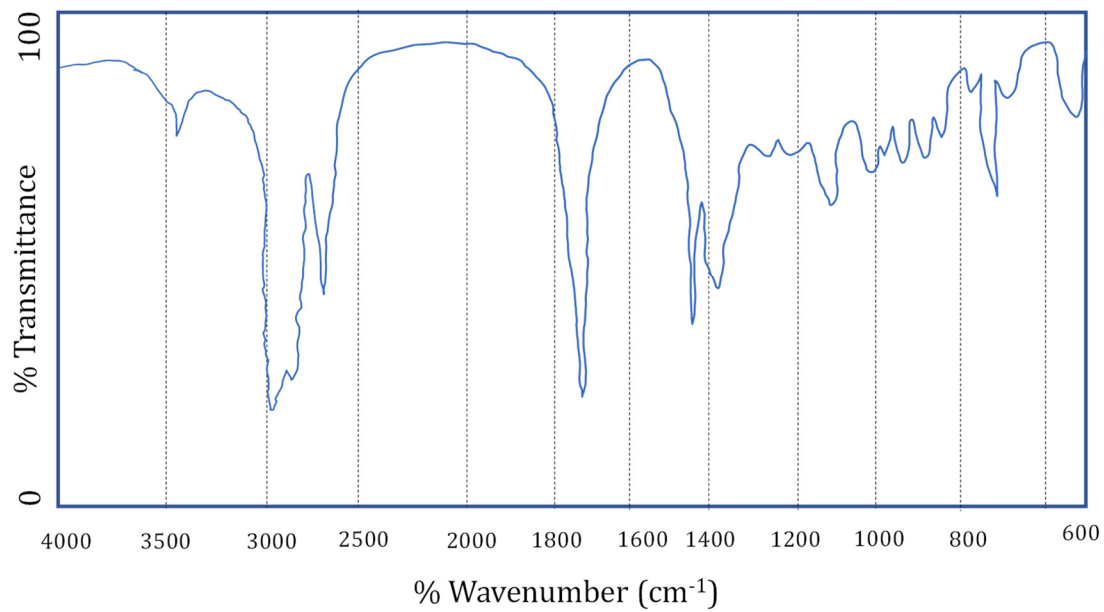


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Lesson VII.4. Infrared Spectroscopy

IR Practice

IR Spectrum for Hexanal

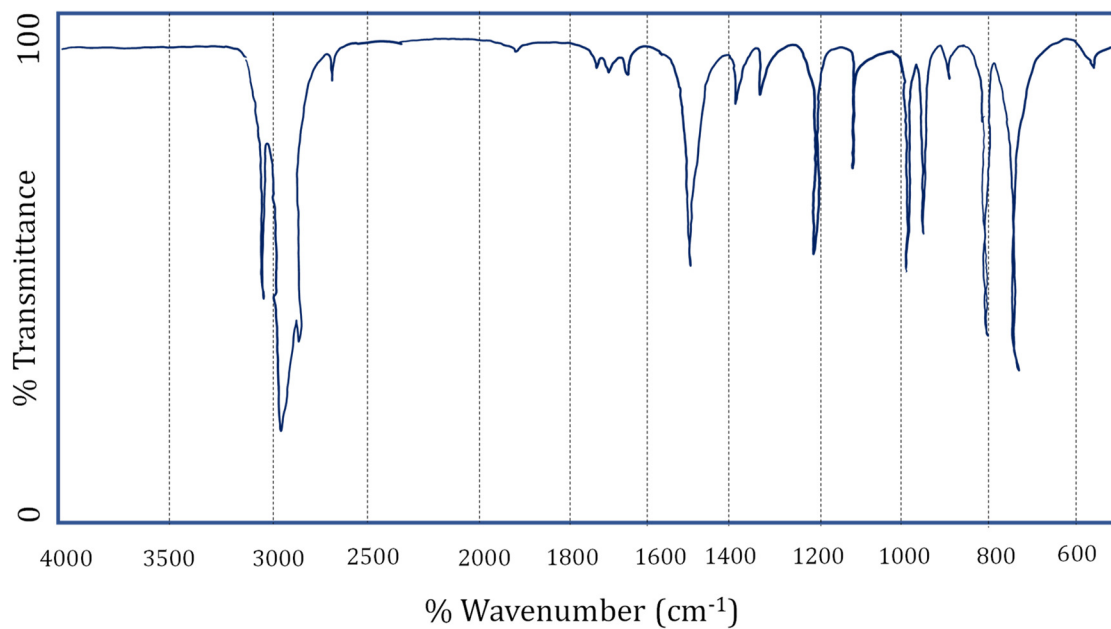


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Lesson VII.4. Infrared Spectroscopy

IR Practice

IR Spectrum for cyclohexene

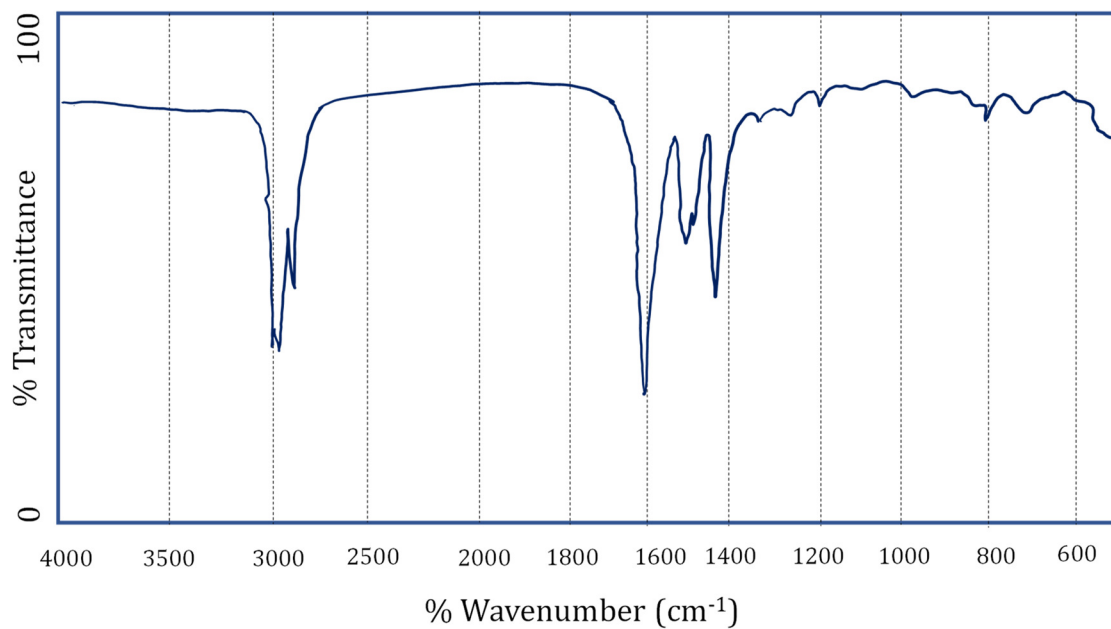


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Lesson VII.4. Infrared Spectroscopy

IR Practice

IR Spectrum for nitrohexane

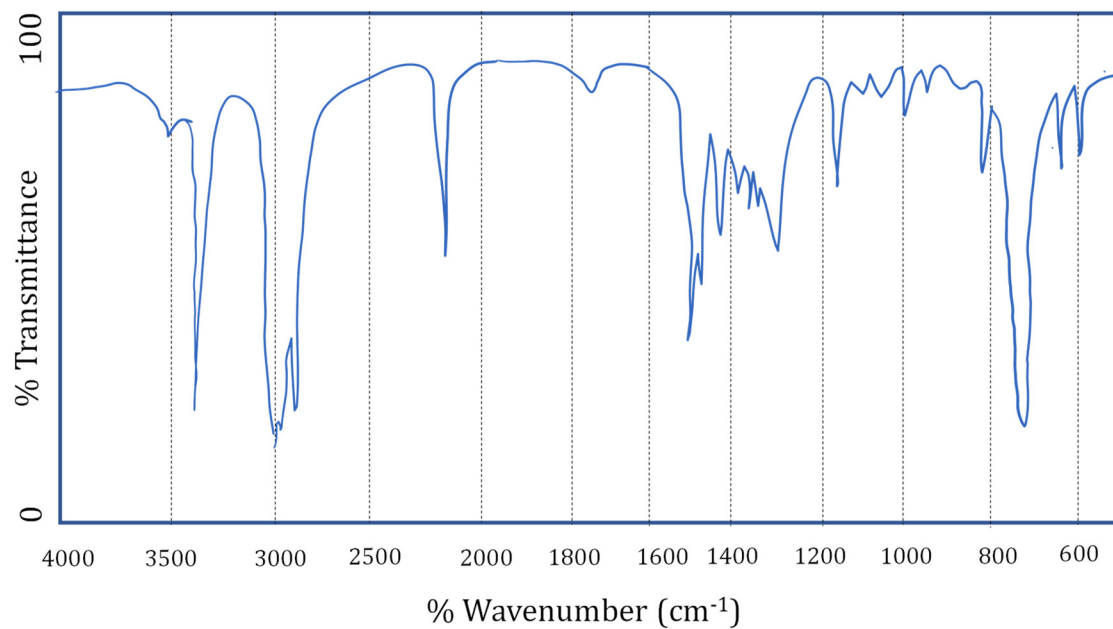


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Lesson VII.4. Infrared Spectroscopy

IR Practice

IR Spectrum for 1-hexyne

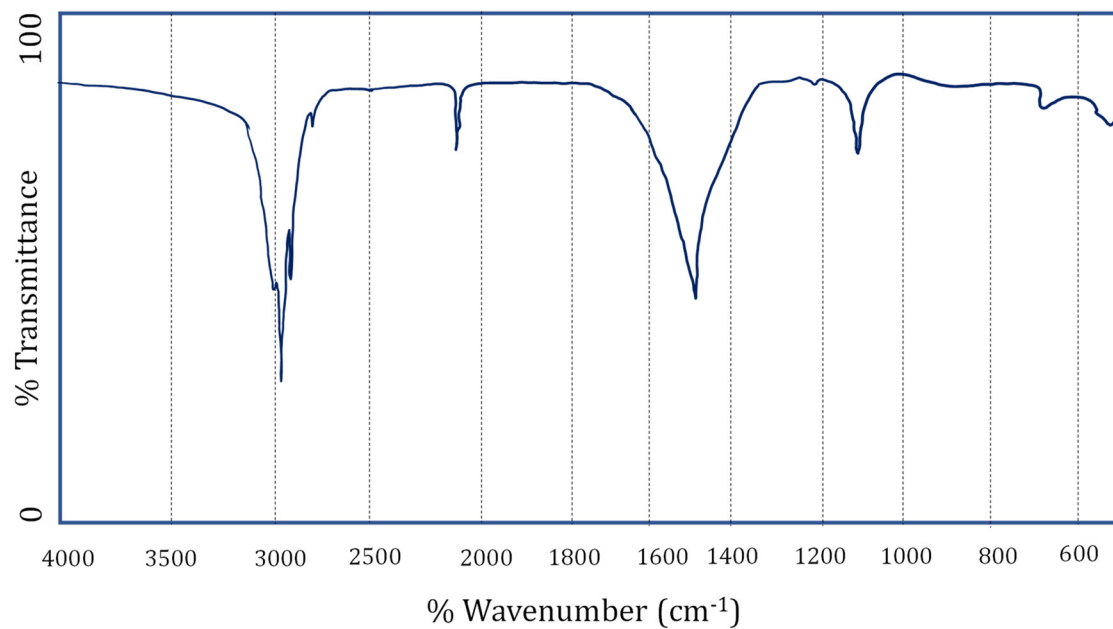


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Lesson VII.4. Infrared Spectroscopy

IR Practice

IR Spectrum for 2-butyne

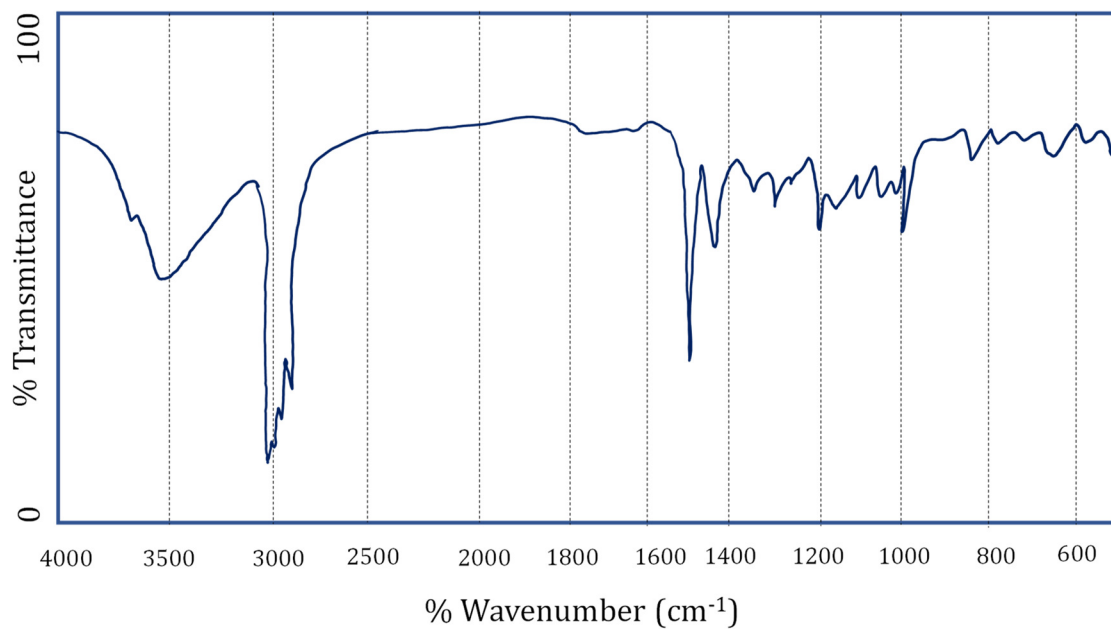


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Lesson VII.4. Infrared Spectroscopy

IR Practice

IR Spectrum for 3-octanol

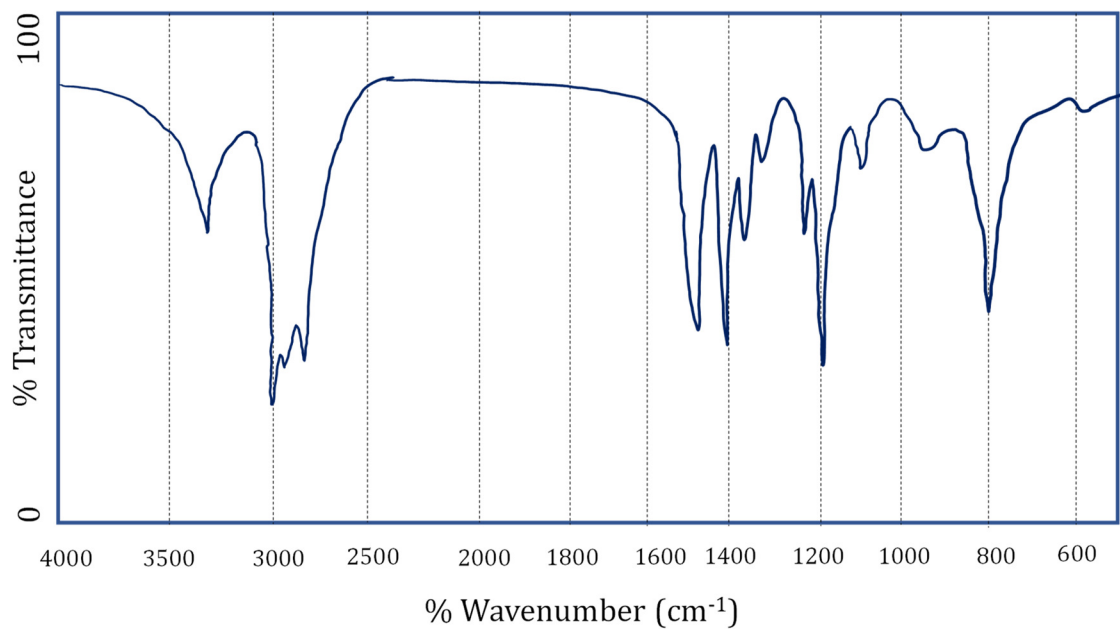


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Lesson VII.4. Infrared Spectroscopy

IR Practice

IR Spectrum for diethylamine

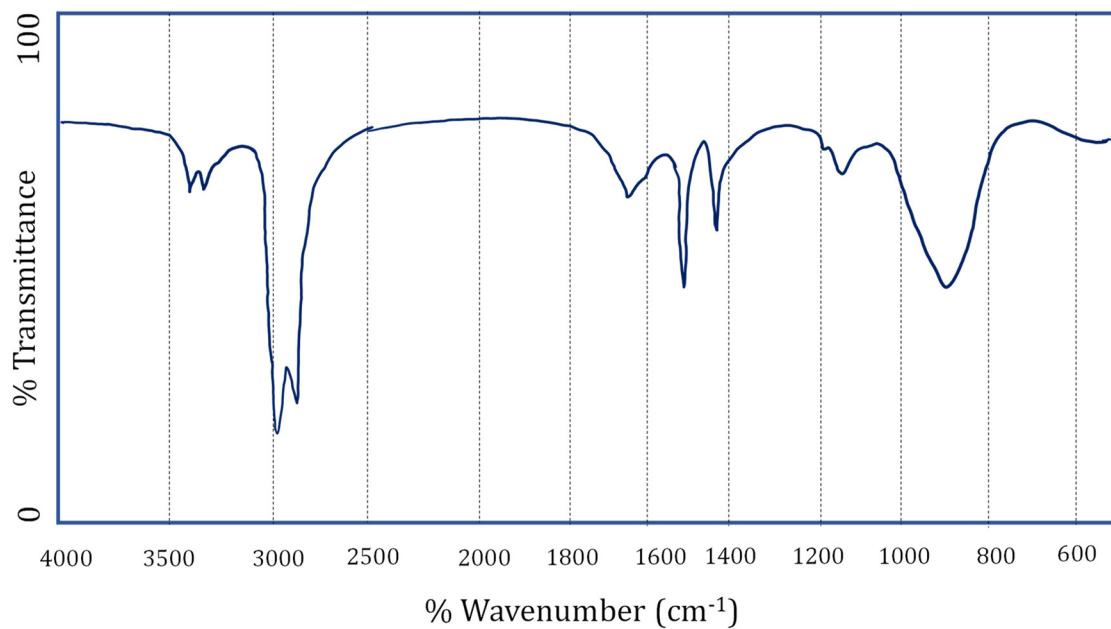


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Lesson VII.4. Infrared Spectroscopy

IR Practice

IR Spectrum for hexylamine

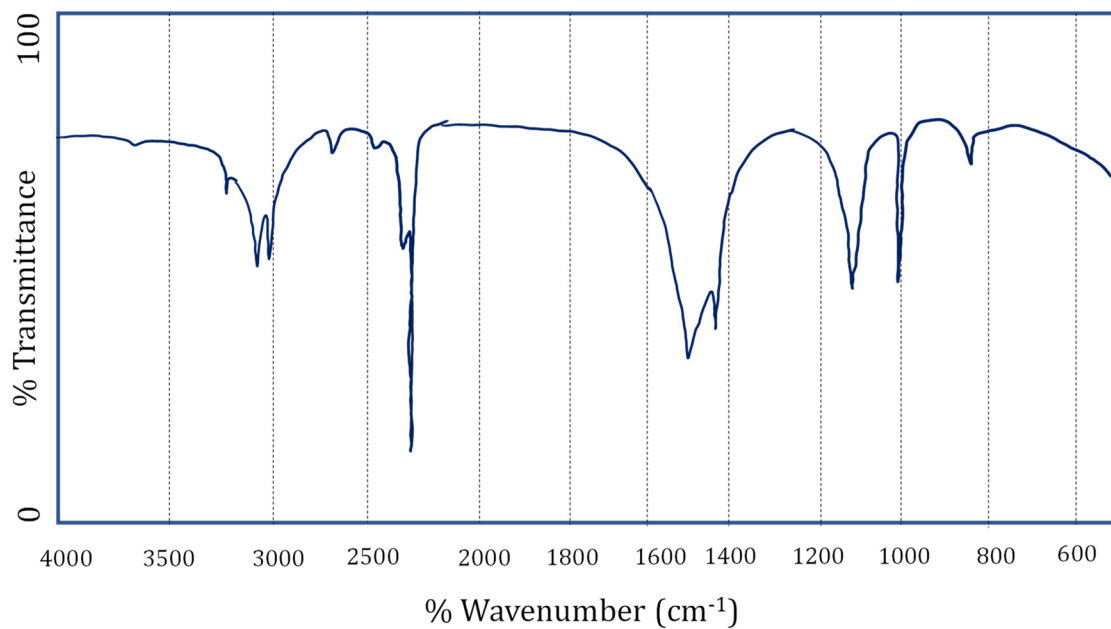


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Lesson VII.4. Infrared Spectroscopy

IR Practice

IR Spectrum for acetonitrile (CH_3CN)

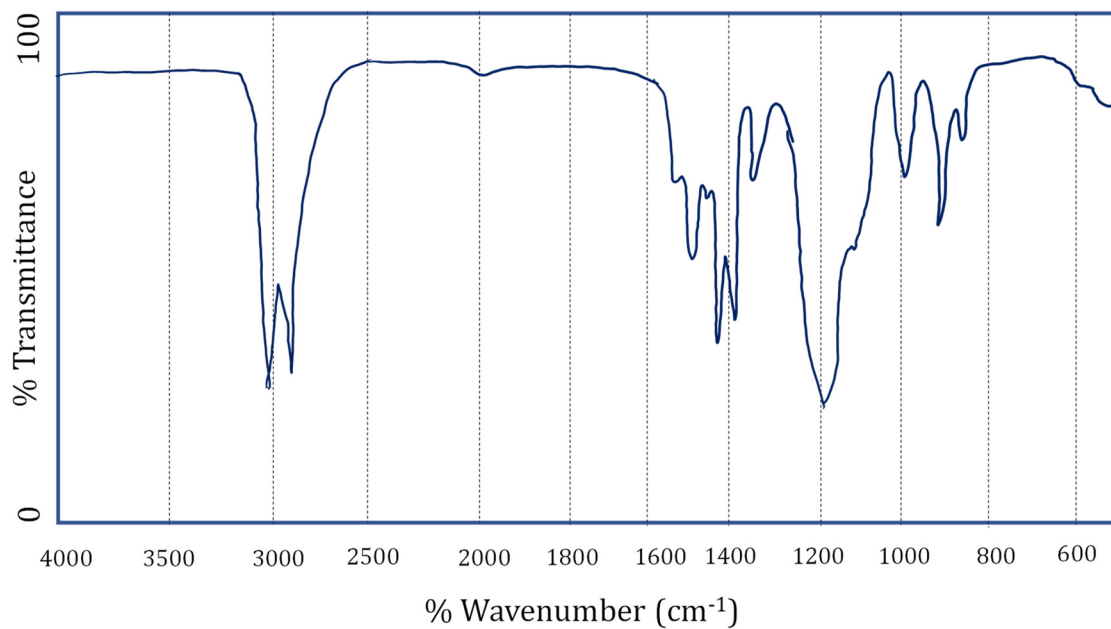


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Lesson VII.4. Infrared Spectroscopy

IR Practice

IR Spectrum for diethylether

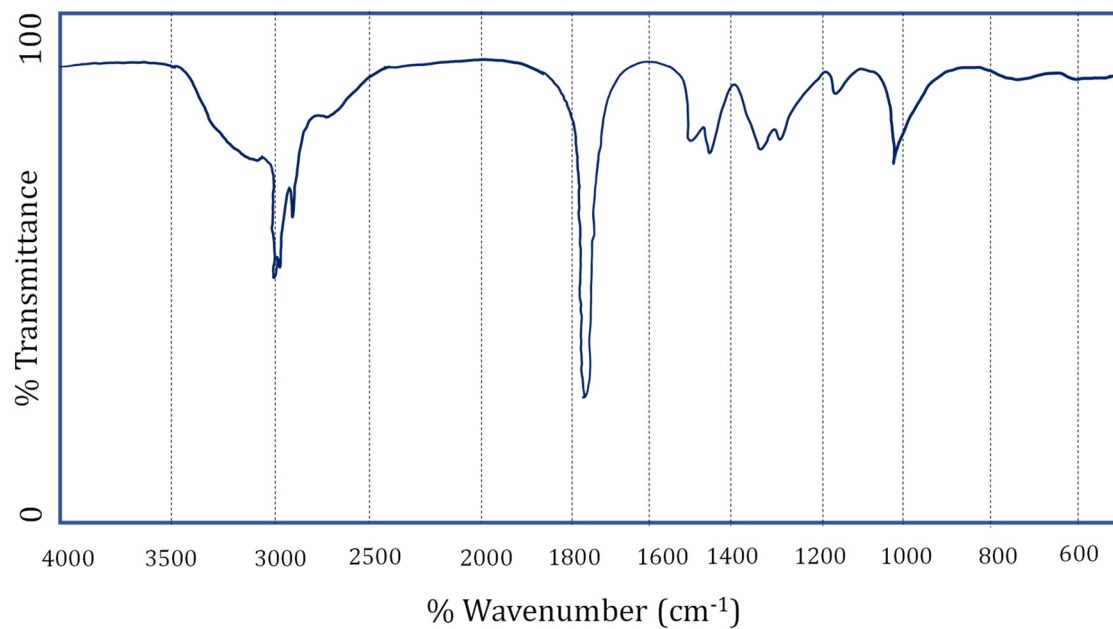


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Lesson VII.4. Infrared Spectroscopy

IR Practice

IR Spectrum for hexanoic acid

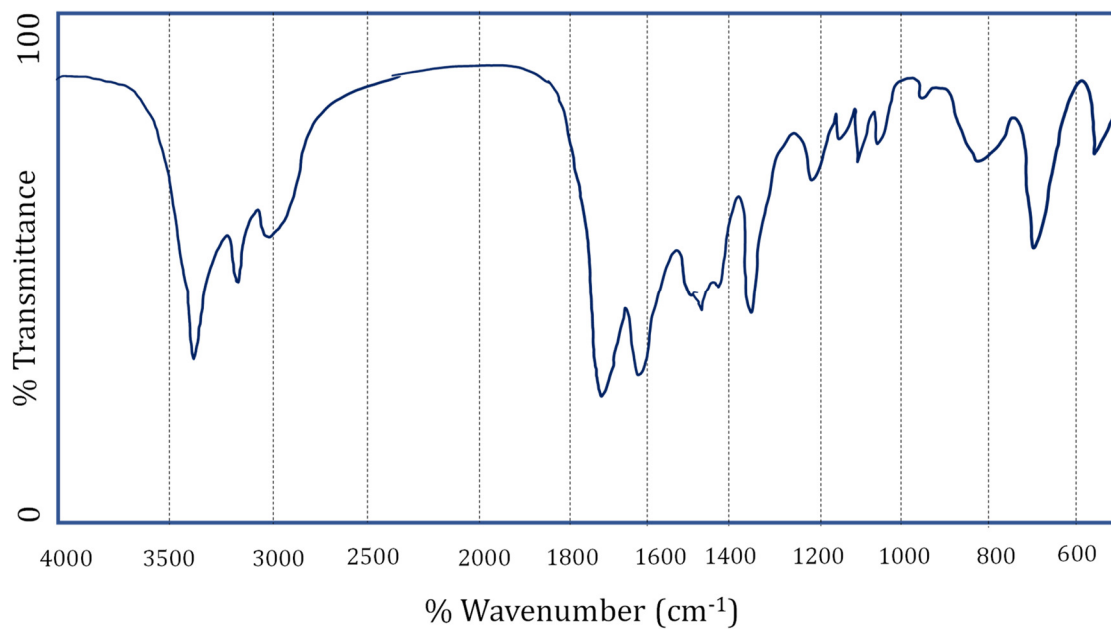


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Lesson VII.4. Infrared Spectroscopy

IR Practice

IR Spectrum for *N*-methylacetamide ($\text{CH}_3\text{C}(\text{O})\text{N}(\text{H})\text{CH}_3$)

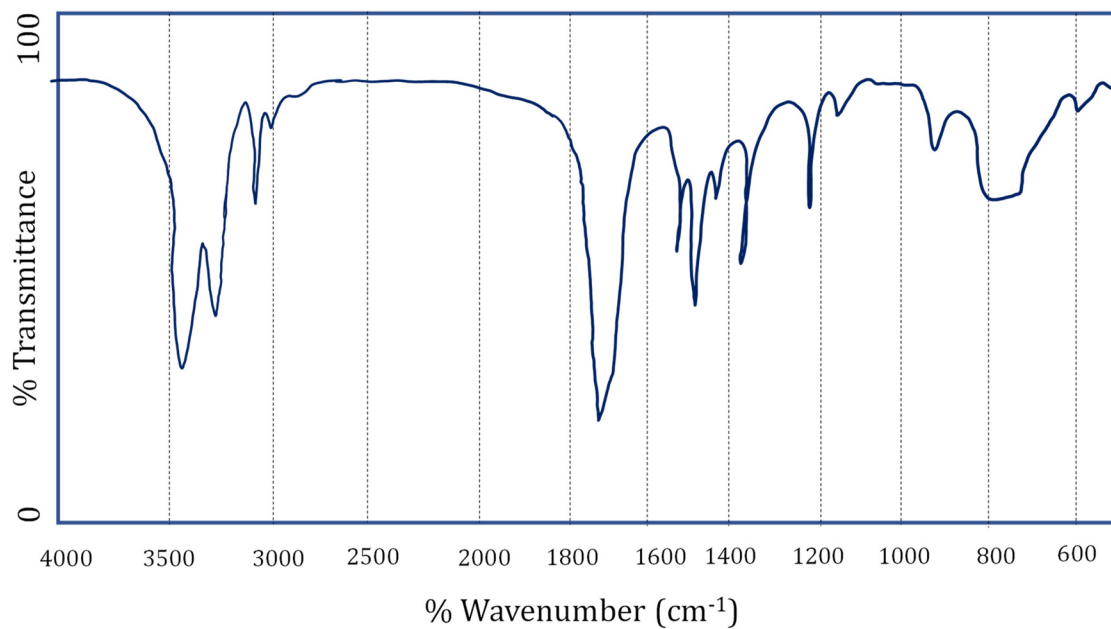


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Lesson VII.4. Infrared Spectroscopy

IR Practice

IR Spectrum for propamide ($\text{CH}_3\text{CH}_2\text{C}(\text{O})\text{NH}_2$)

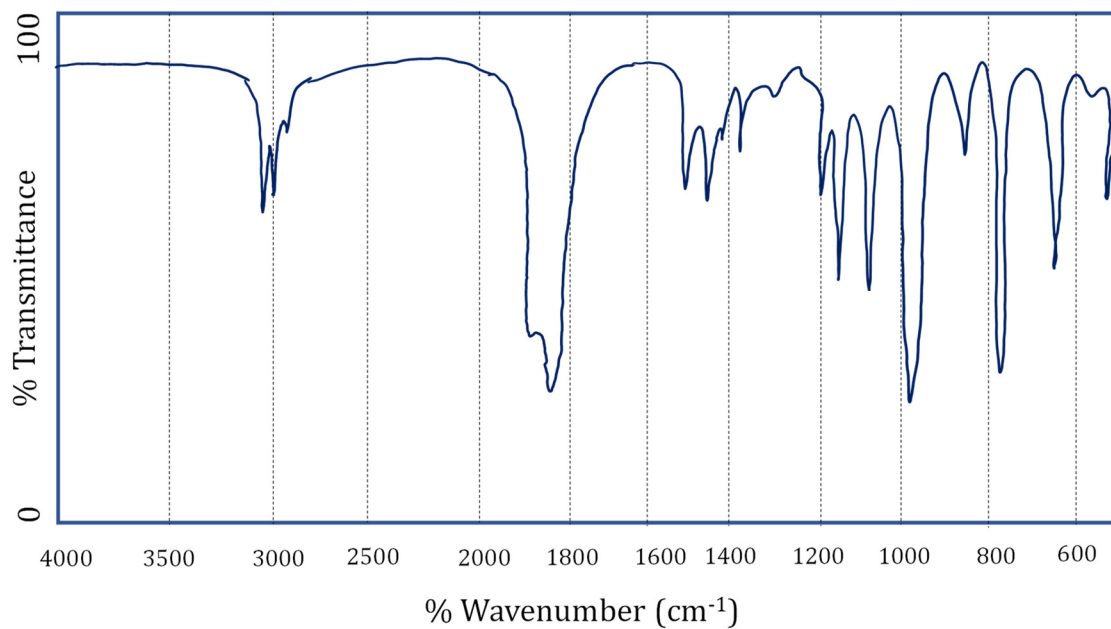


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Lesson VII.4. Infrared Spectroscopy

IR Practice

IR Spectrum for propanoyl chloride

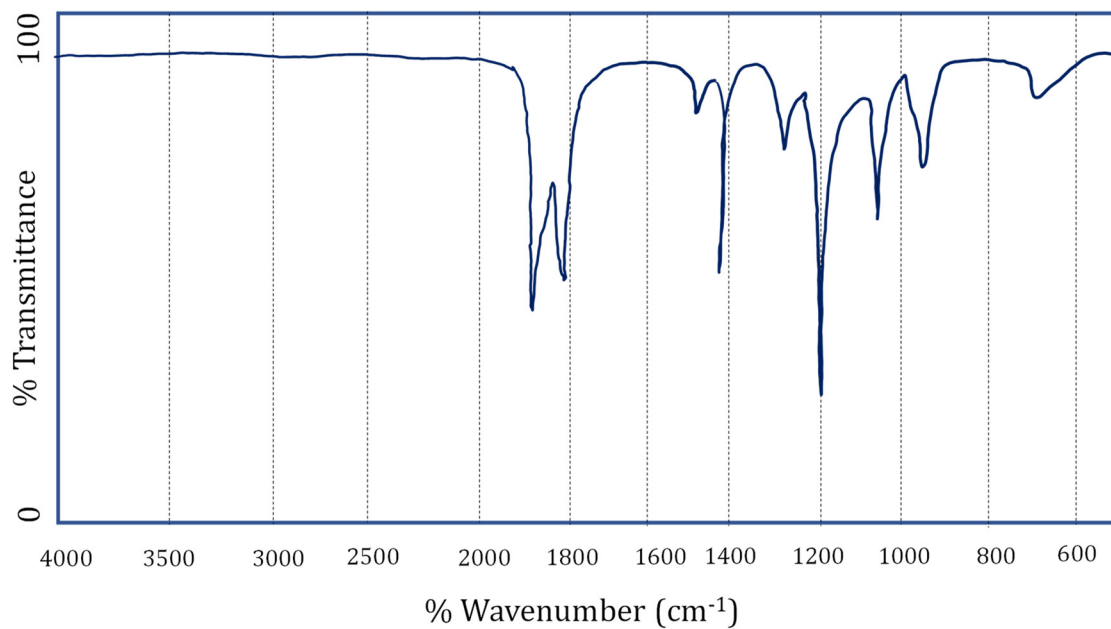


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Lesson VII.4. Infrared Spectroscopy

IR Practice

IR Spectrum for acetic anhydride

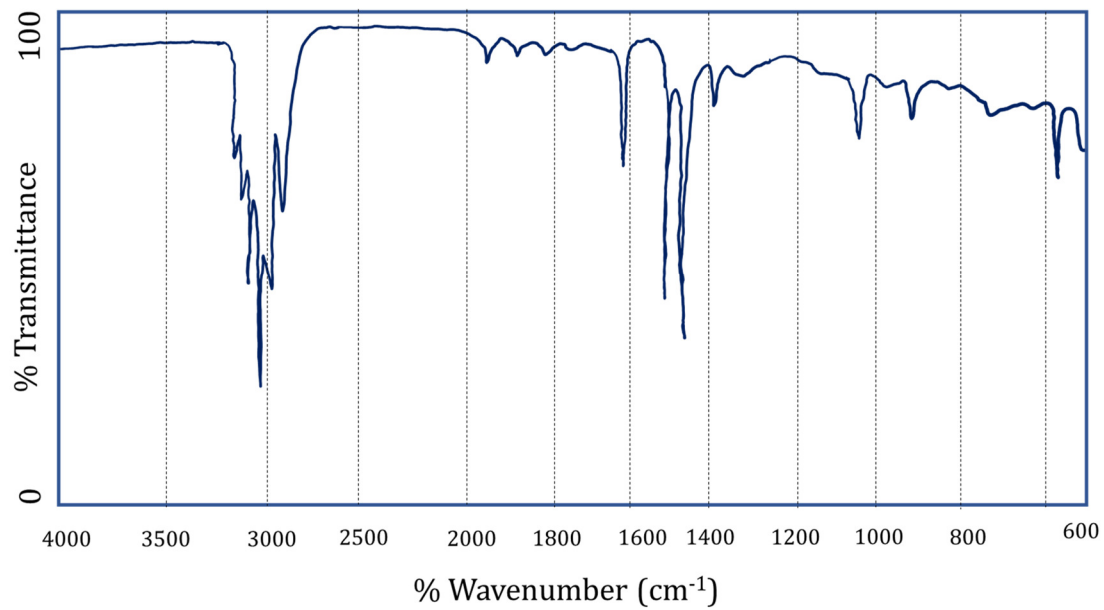


Notes

Lesson VII.4. Infrared Spectroscopy

IR Practice

IR Spectrum for ethylbenzene



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