Infrared (IR) Spectroscopy

from chapter(s) _____ in the recommended text

A. Introduction

B. Origin Of IR Absorbance

Quanta in IR transitions are *less* energetic than those associated with ultraviolet

NMR (nuclear magnetic resonance) involves *lower* frequency quanta

FT-IR is *accumulated after multiple scans* to increase signal-to-noise

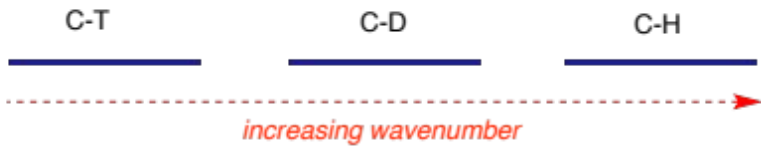
IR is most sensitive to *dipole* changes, so it provides a way of observing functional groups, particularly *unsymmetrical* ones like *C=O*, *N-H*, *N=O*.

Energies in IR are *greater* than in NMR

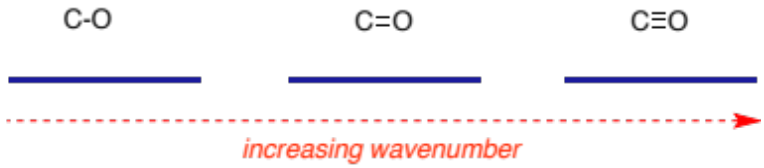
Strong bonds between the same atoms vibrate *faster* than weaker ones, *ie* at *higher* wavenumbers, for which the units are cm^{-1}.

bonds between carbon and heavy atoms tends to be *slower* than those between carbon and lighter ones, *ie* at a *lower* wavenumber.

write C-H, C-D, and C-T
above the appropriate lines



write
C≡O C−O C=O
above the appropriate lines



Symmetrical stretches of carbonyl groups in organic molecules involve *large* changes of dipole moment, hence they are *strong* and tend to be a *useful* indicator of molecular structure.

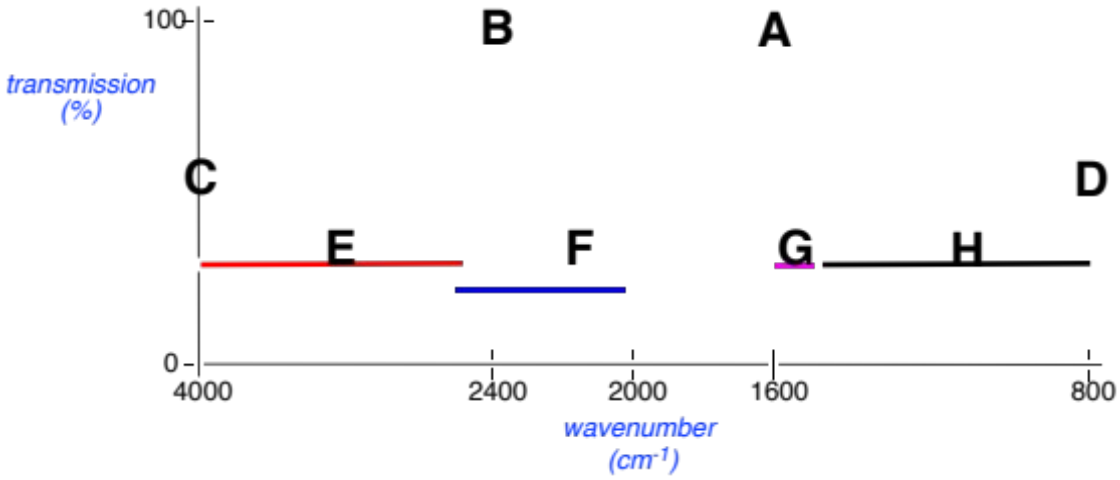
Wavenumbers for symmetrical *C=O* stretches tend to *increase* along the series ester, ketone, amide, carboxylate

Esters and carboxylates also have *C-O* symmetrical stretches.

Wavenumbers in IR spectra *are* proportional to frequencies.
Transmission in IR is *inversely* correlated to absorbance.
Vibrations of the same energy generally have *the same* absorbance wavelength maxima in IR spectra.

The wavenumber axis in IR spectra is *expanded below 2000 relative to the 4000 – 2000 cm^{-1}*.

so each bond *can* be associated with more than one IR peak.



C-H stretches occur at about *3000* cm^{-1}.

N-H stretches tend to occur around *3300* cm^{-1}.

O-H that are not strongly H-bonded stretch at around *3500* cm^{-1}

Aromatic C=C bonds vibrate around *1600 - 1500* cm^{-1}

C=O bonds stretch between *1900 – 1500* cm^{-1}.

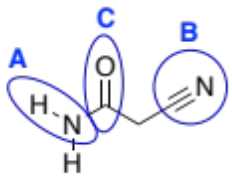
C=*C* bonds vibrate around *1640* cm^{-1} and absorb much *less* strongly than *C*=*O* because
Aromatic *C*-*C* bonds vibrate at *lower* frequencies because those

NO_2 groups give two intense bands at about *1550 & 1350* cm^{-1}.

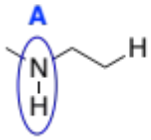
Sulfoxide S^+-O^- bonds absorb at *1030 – 1080* cm^{-1}.

This is called the *fingerprint* region because it is unique to

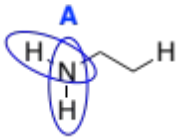
C. Functional Group Assignments



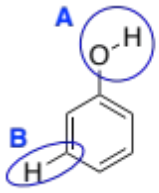
A 3300; **B** 2300; **C** 1690 cm^{-1}



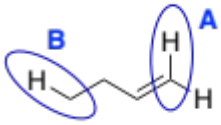
A 3300 cm^{-1}



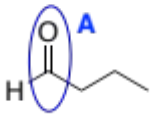
A 3300 and 3250 cm^{-1}



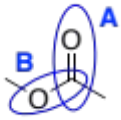
A 3400; **B** 3050 cm^{-1}



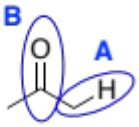
A 3050; **B** 2950 cm^{-1}



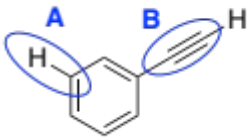
A 1730 cm^{-1}



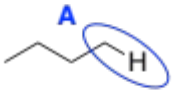
A 1735; **B** 1250 cm^{-1}



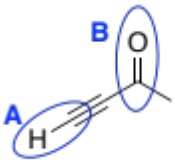
A 2950; **B** 1715 cm^{-1}



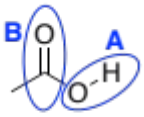
A 3050; **B** 2100 cm^{-1}



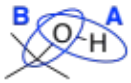
A 2950 cm^{-1}



A 2100; **B** 1680 cm^{-1}

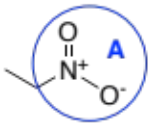


A 2900 (br); **B** 1690 cm^{-1}

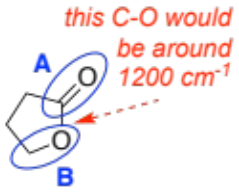


A 3400 (br); **B** 1100 cm^{-1}

A 1100 cm^{-1}



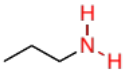
A 1560 and 1380 cm^{-1}



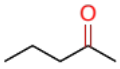
A 1770; **B** 1100 cm^{-1}

a "the "fingerprint region"

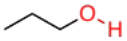
b



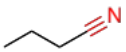
c



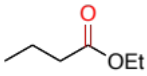
d



e

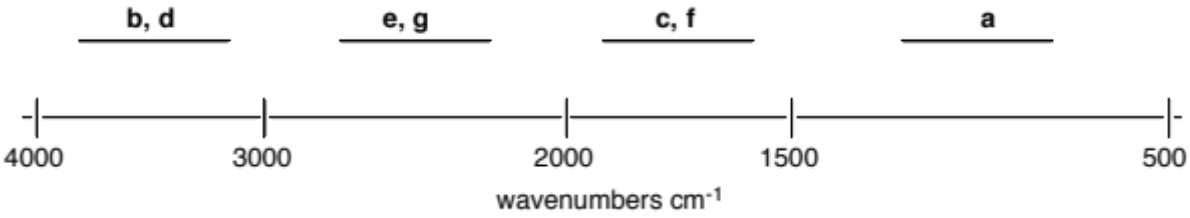


f



g

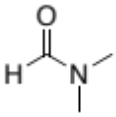
put letters on these lines to indicate the functional groups that absorb here



D. Assigning Structures From Spectra

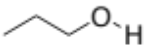
acetone

acetonitrile



DMF

DMSO



n-propyl alcohol

pyridine

is ____acetone_____ .

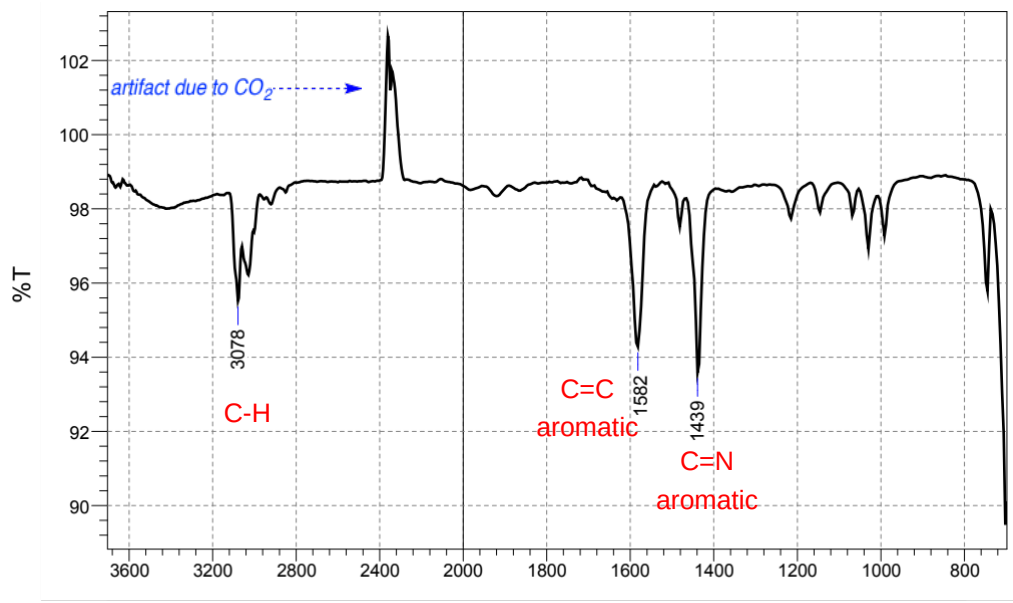
a ____C-H___ bond.

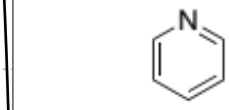
a ____C=O_____ bond.

is _____acetonitrile_____ .

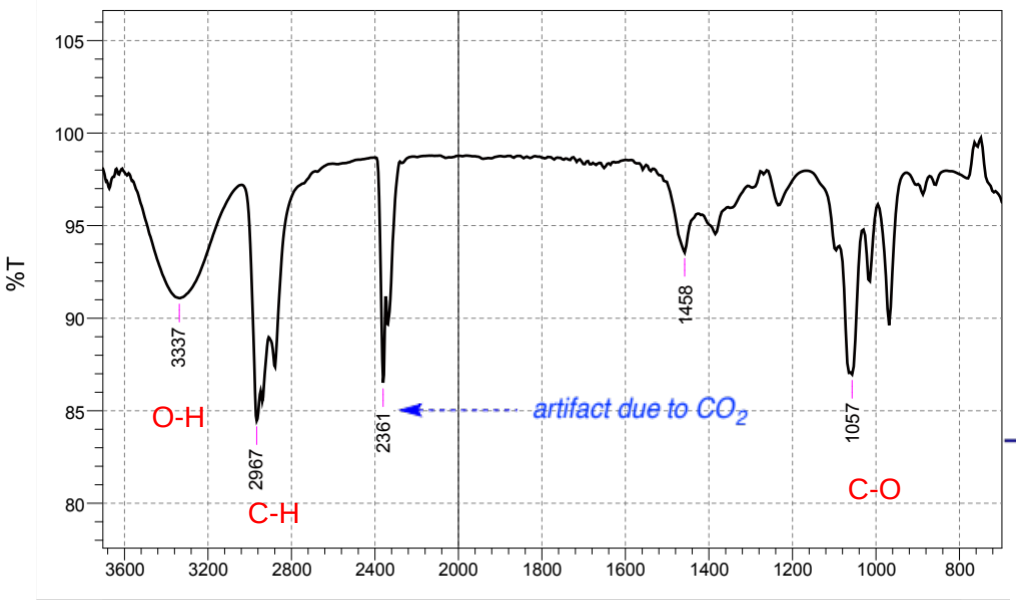
a _____C-H____ bond.

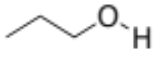
a ____C≡N_____ bond.



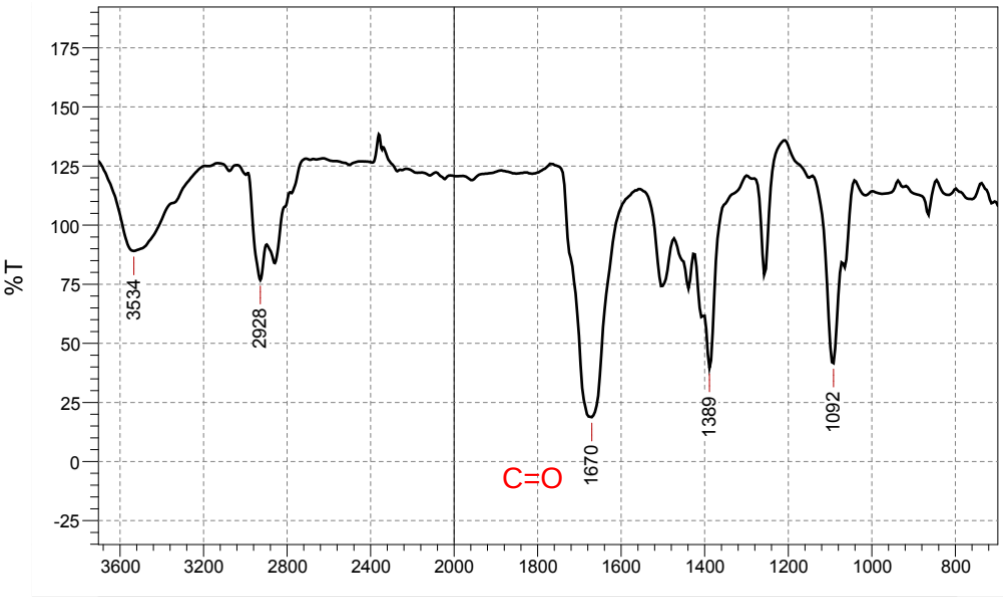


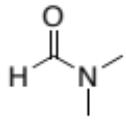
draw structure and attribute numbered IR stretches to particular bonds



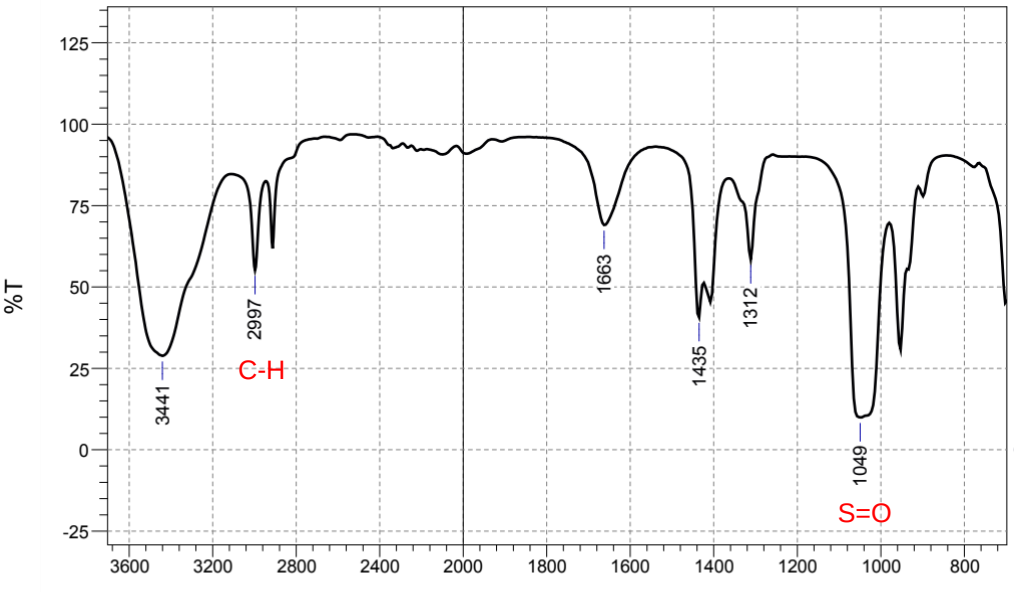


draw structure and attribute numbered IR stretches to particular bonds

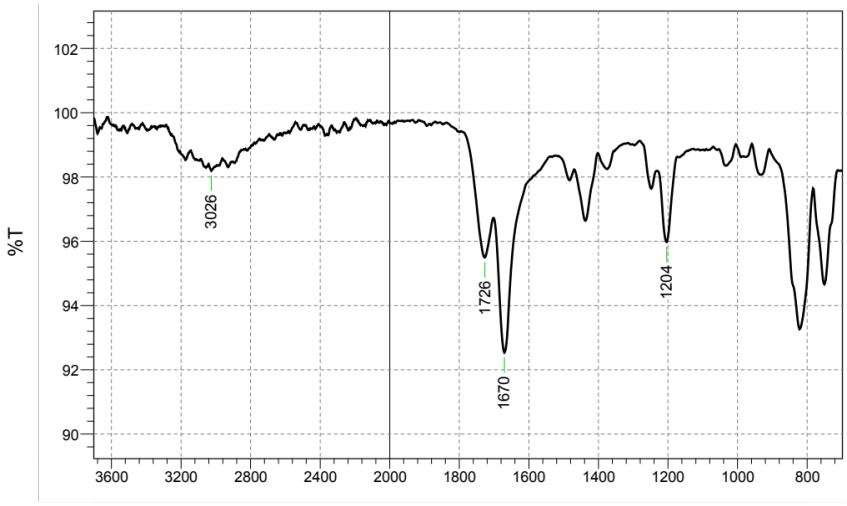




draw structure and attribute numbered IR stretches to particular bonds

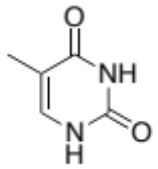


draw structure and attribute numbered IR stretches to particular bonds

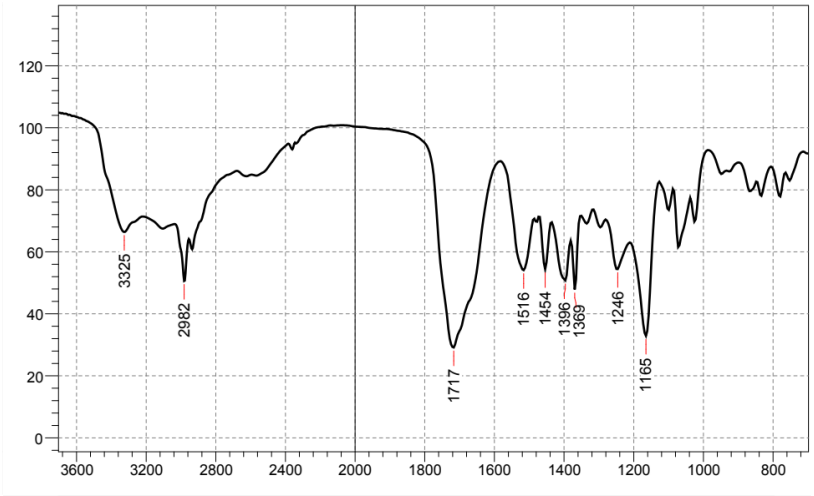


thymine

compound name

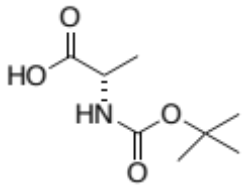


compound structure

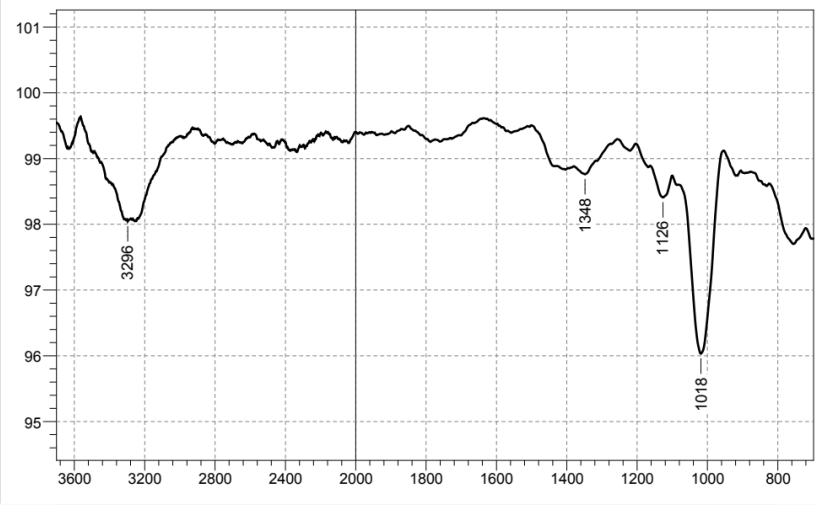


Boc-Ala

compound name

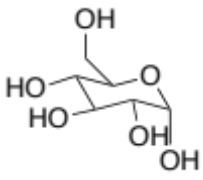


compound structure

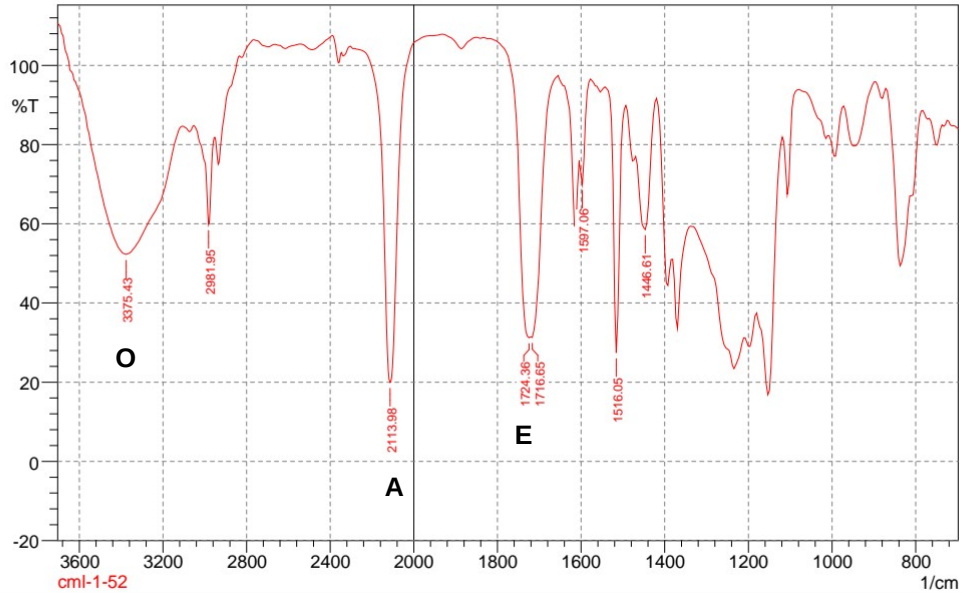


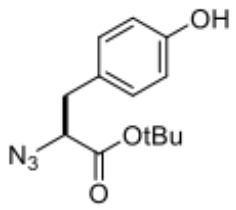
glucose

compound name

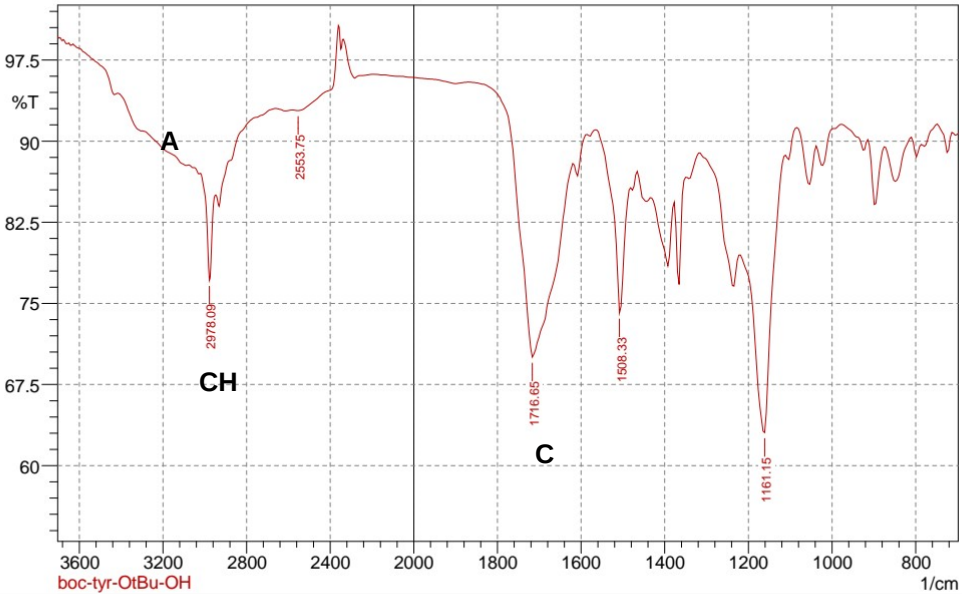


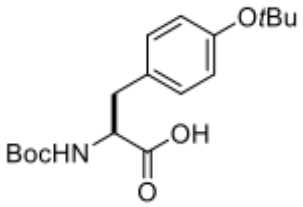
compound structure



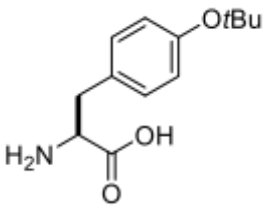


cml-1-52

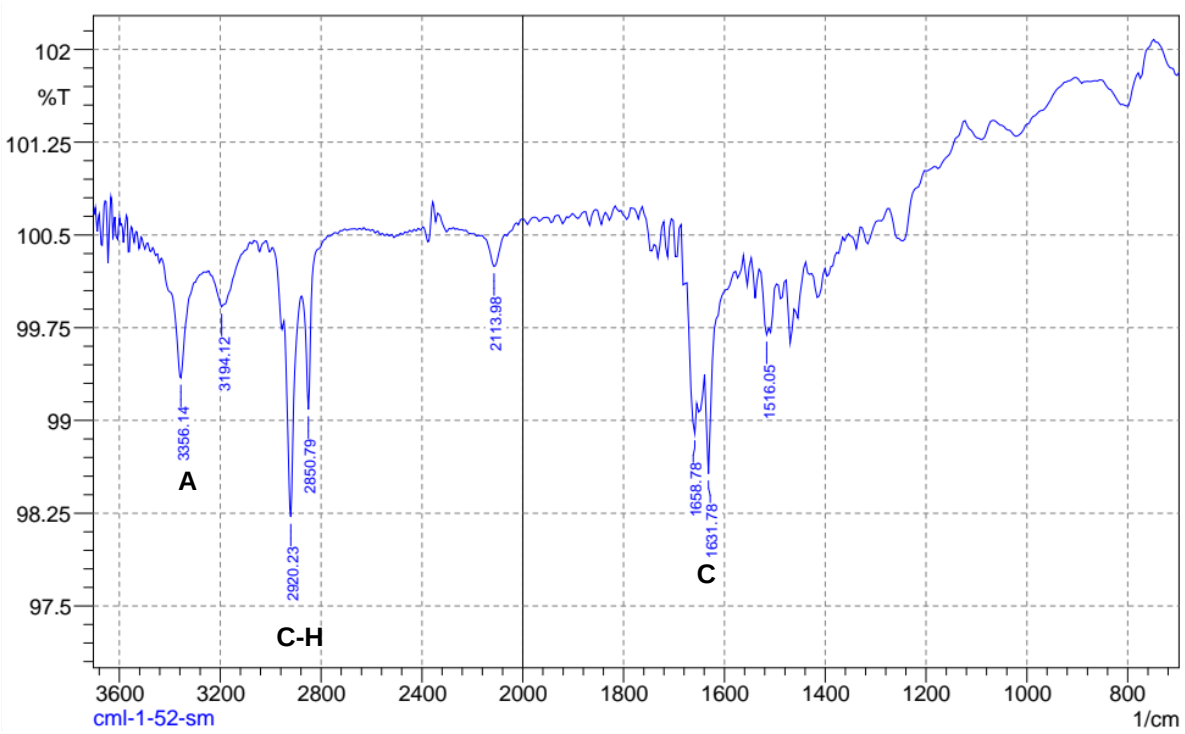




boc-tyr-OtBu-OH


OtBu
OH
H2N
O

cml-1-52-sm


102
%T
101.25
100.5
99.75
99
98.25
97.5
3356.14
3194.12
2920.23
2850.79
2113.98
1658.78
1631.78
1516.05
A
C-H
C
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
1/cm
cml-1-52-sm