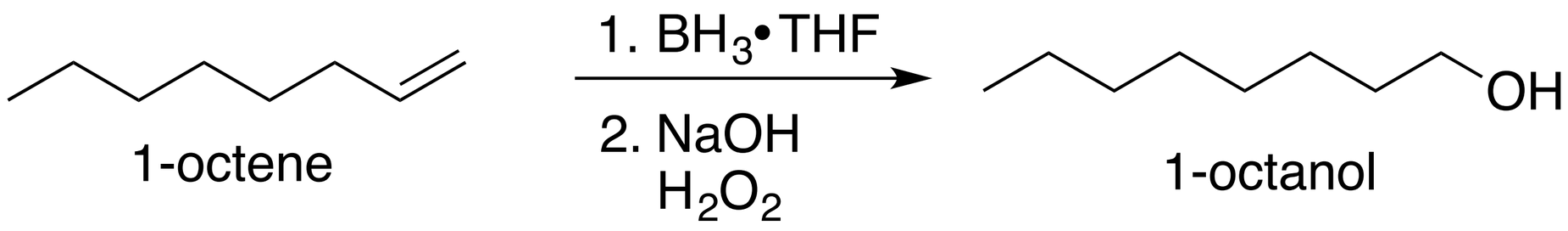
Infrared Spectroscopy

How do we know that the reaction has occurred as expected?

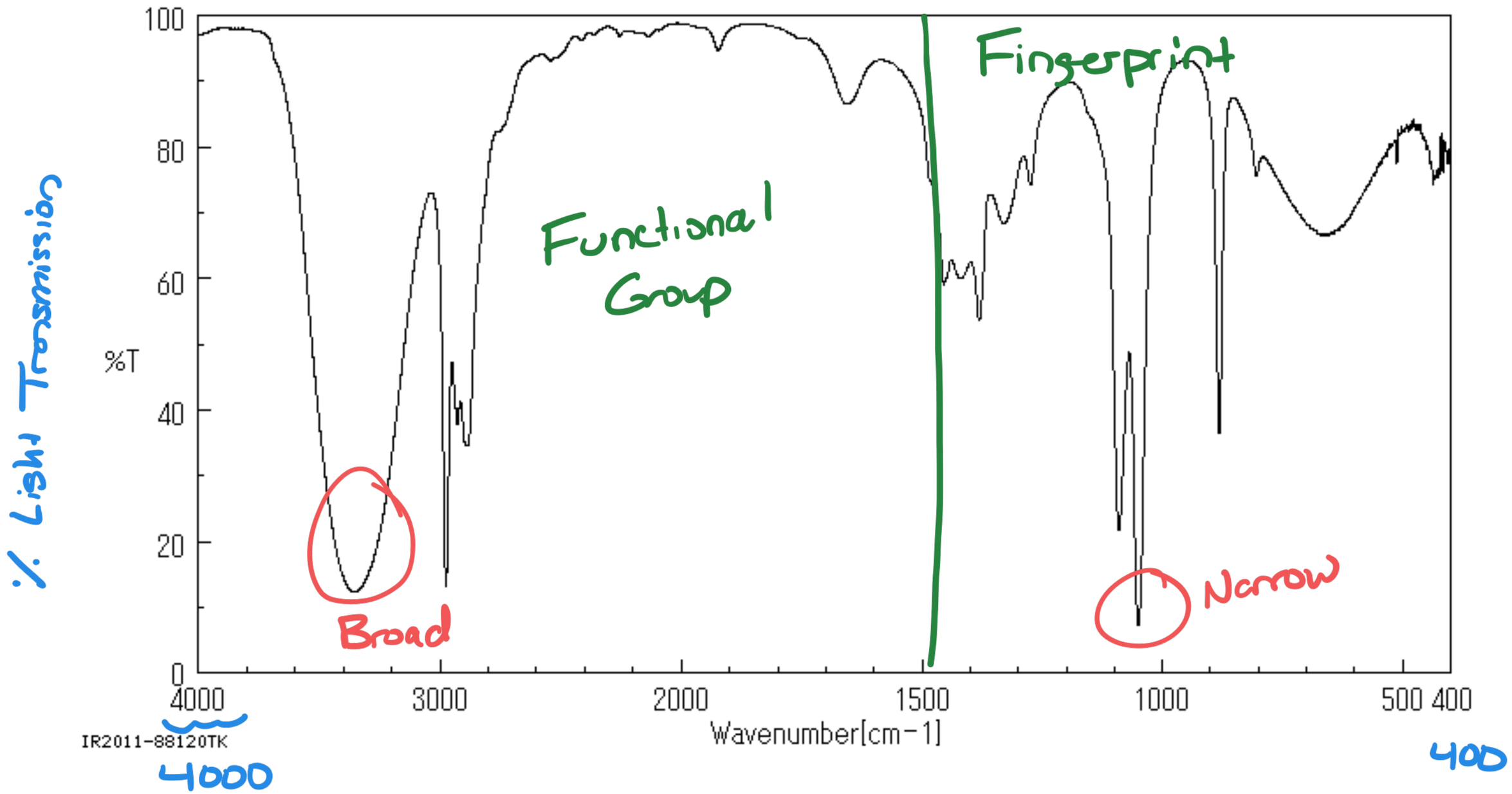


Purpose: Determination of functional groups in a molecule.

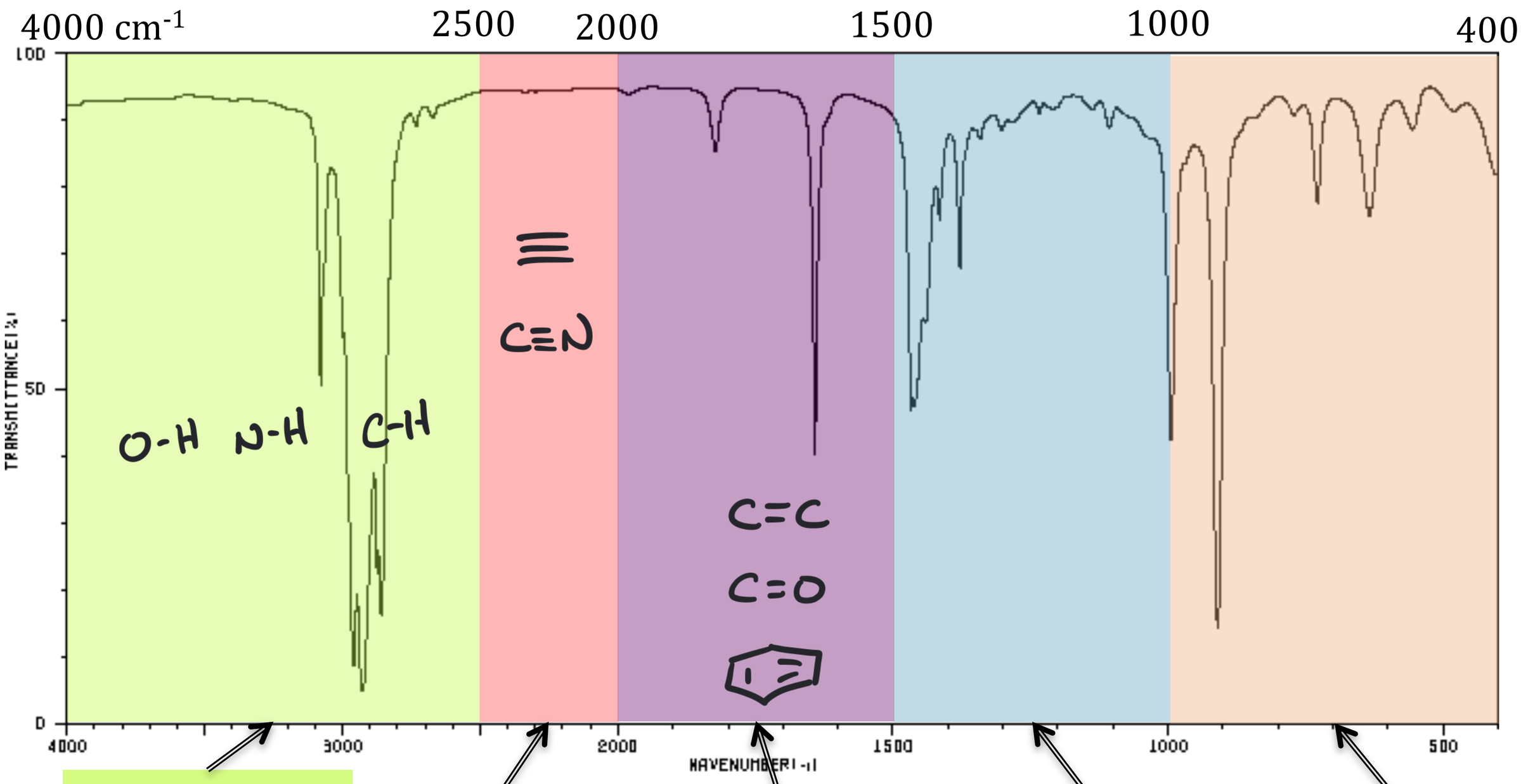
When IR light is passed through a molecule, the bonds will absorb IR light causing the bonds to stretch or bend.

This energy absorption is visualized on the IR spectrum.

A Sample IR Spectrum



General IR Regions



Z – H single bond stretches

Triple bond stretches

Double bond stretches

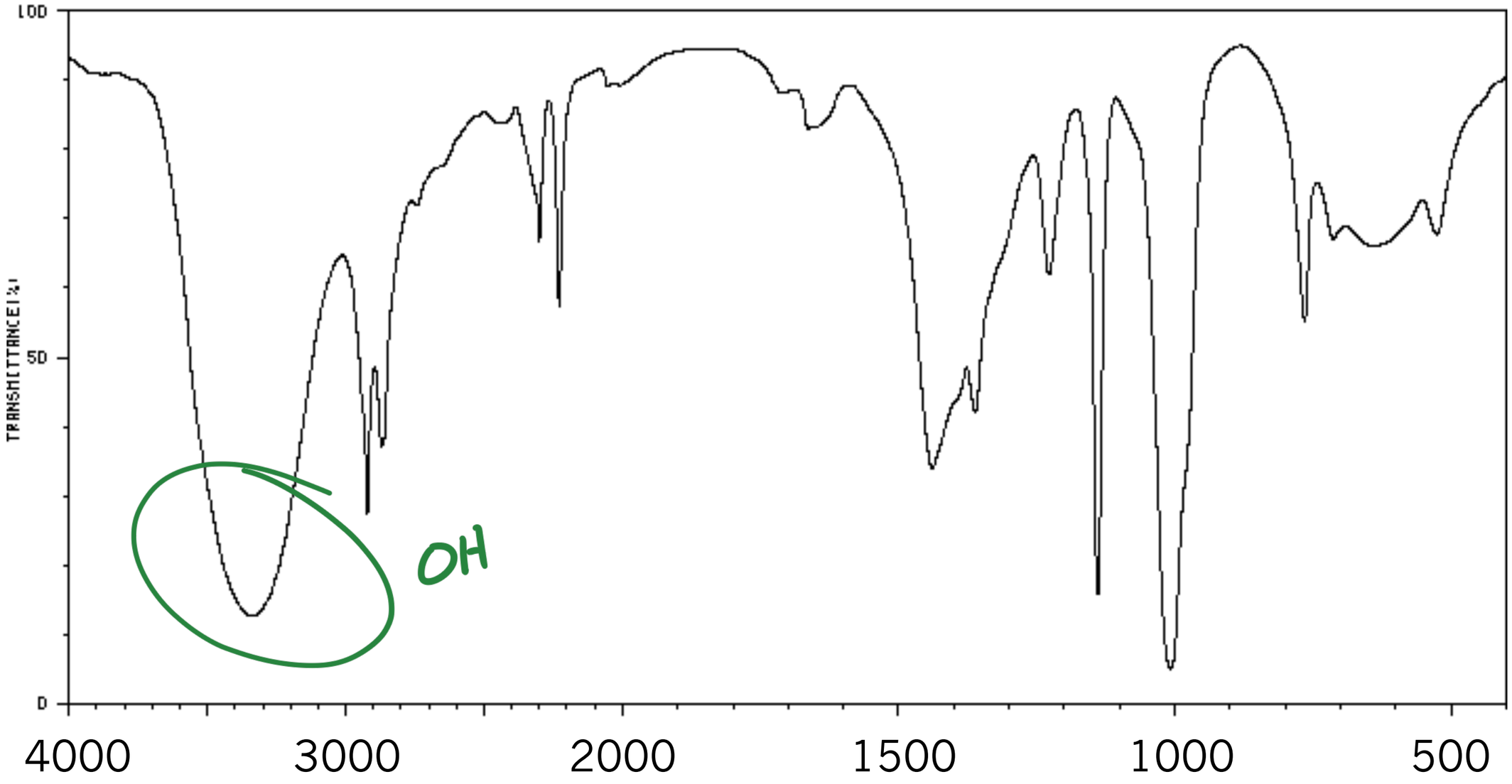
Single bond stretches

Bending vibrations

Key Functional Group Absorptions

1) Alcohol O-H Stretch

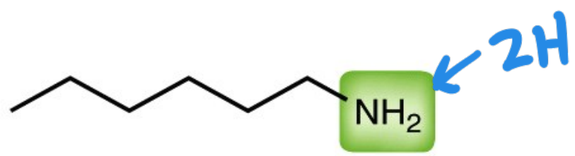
Broad Stretch, 3200-3600 cm^{-1}



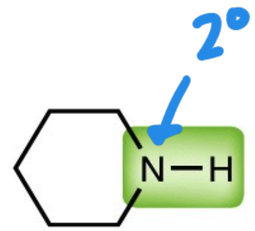
Key Functional Group Absorptions

2) Amine/Amide N-H Stretch

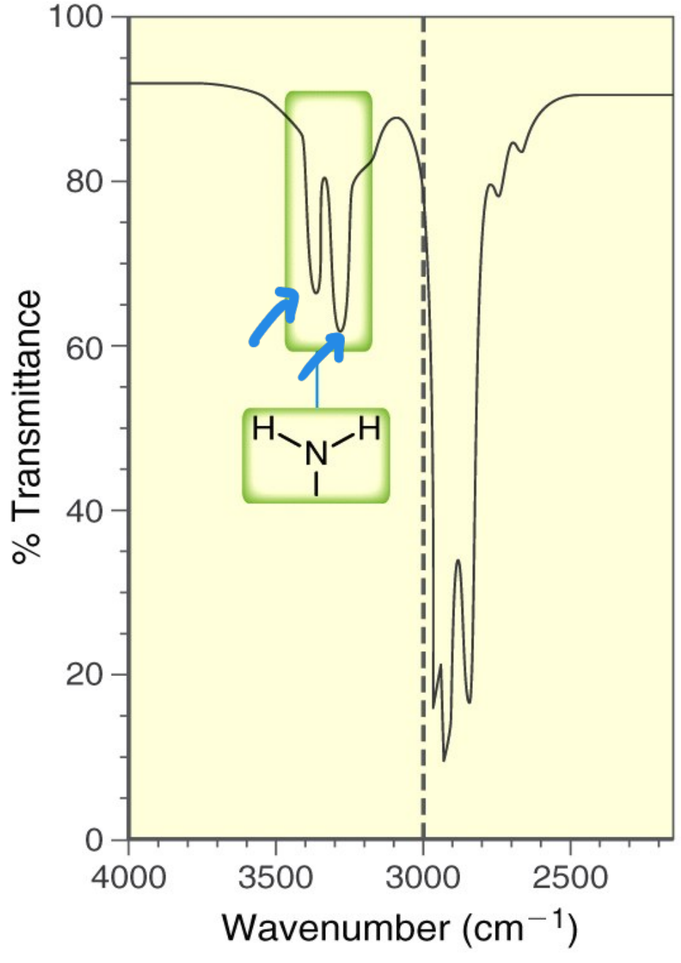
Medium Stretch, 3300-3500 cm^{-1}

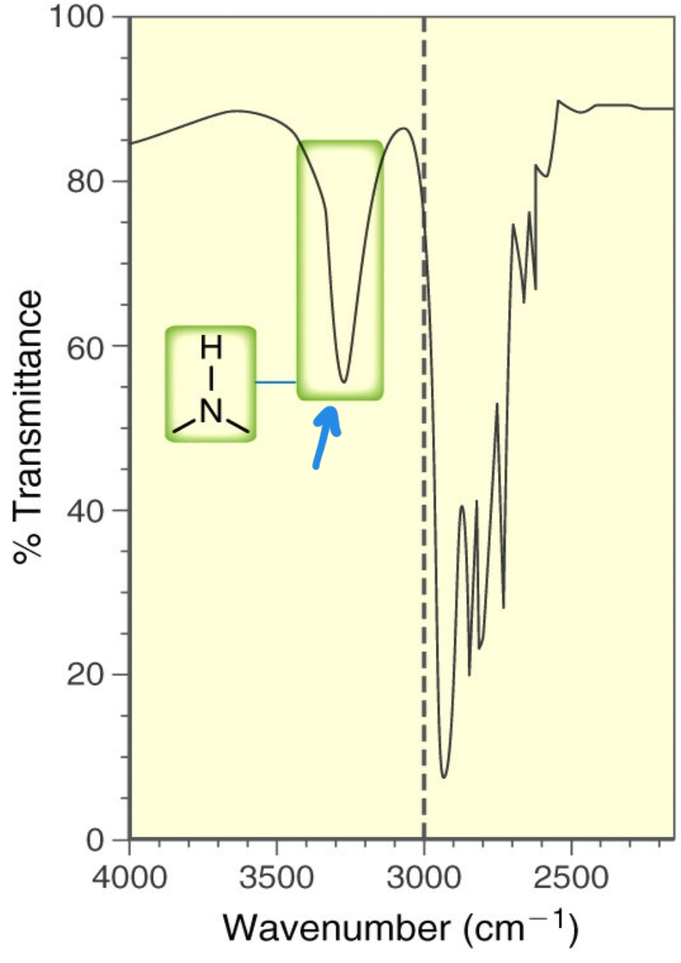


Hexylamine
(a primary amine)



Piperidine
(a secondary amine)

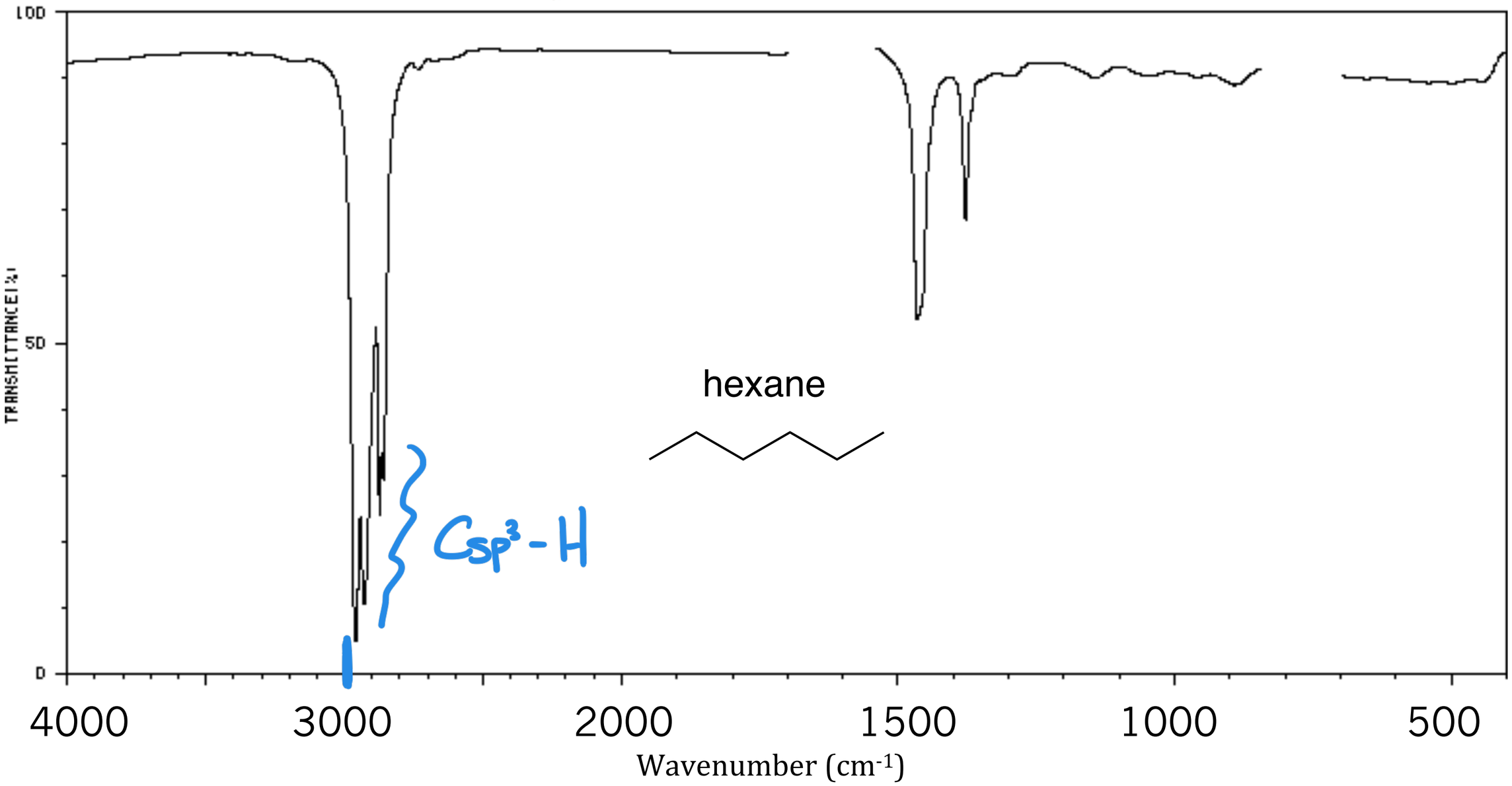




Key Functional Group Absorptions

3) Alkane – Csp^3-H Stretch

Stretches just below 3000 cm^{-1}

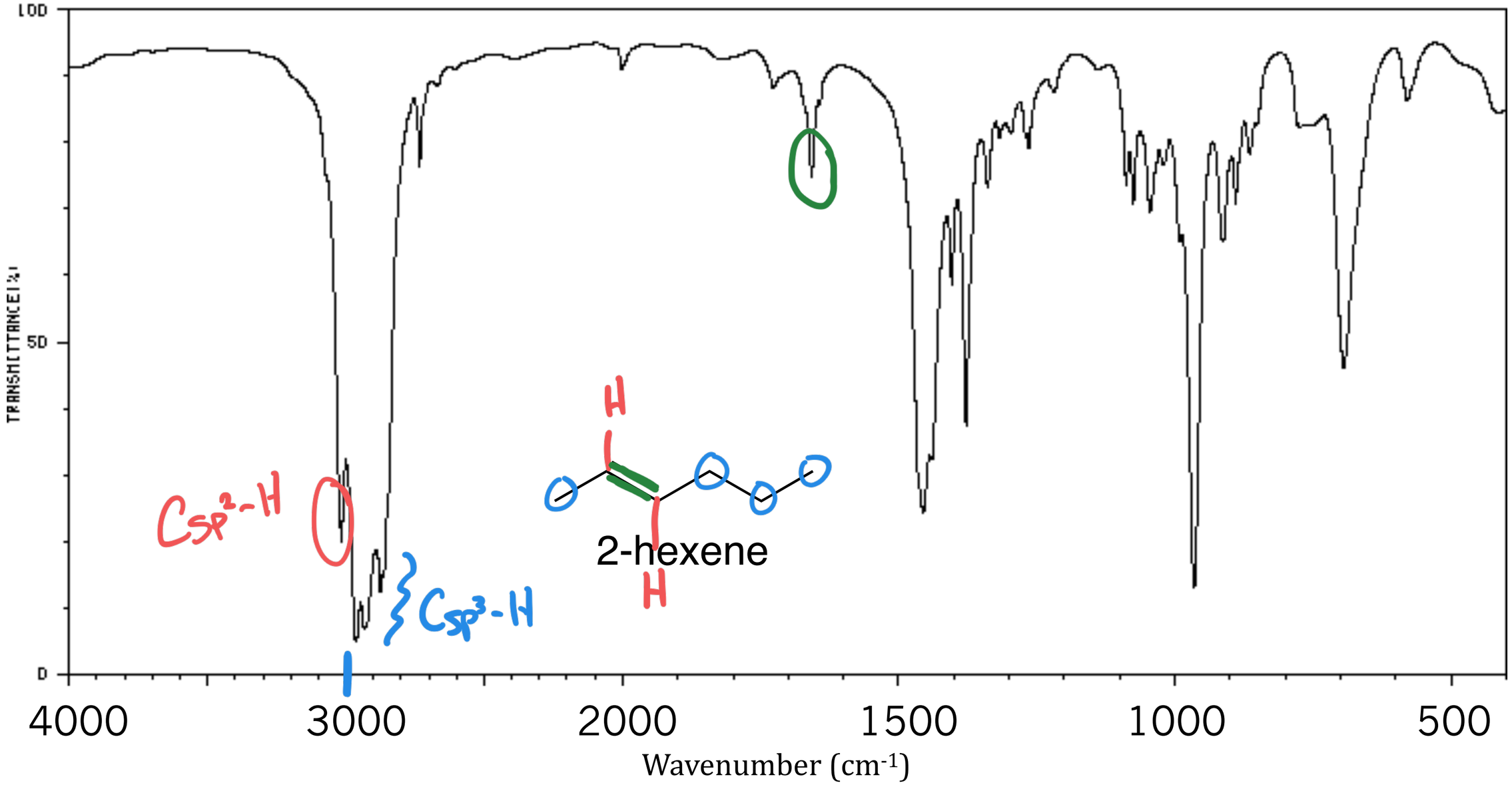


Key Functional Group Absorptions

4) Alkene

Csp^2-H just above 3000 cm^{-1}

C=C stretch 1600-1700 cm^{-1}

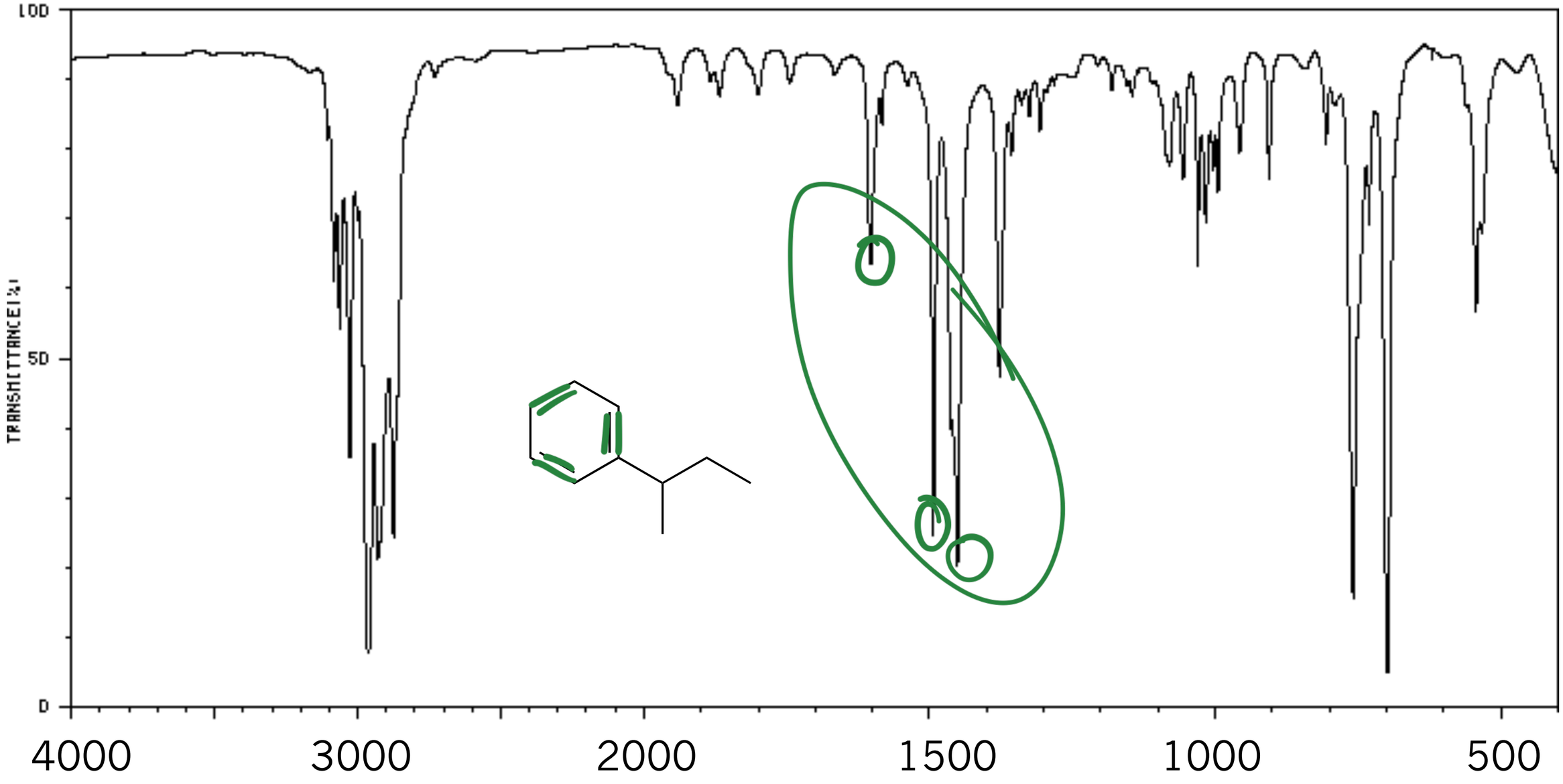


Key Functional Group Absorptions

5) Arene

Csp^2-H just above 3000 cm^{-1}

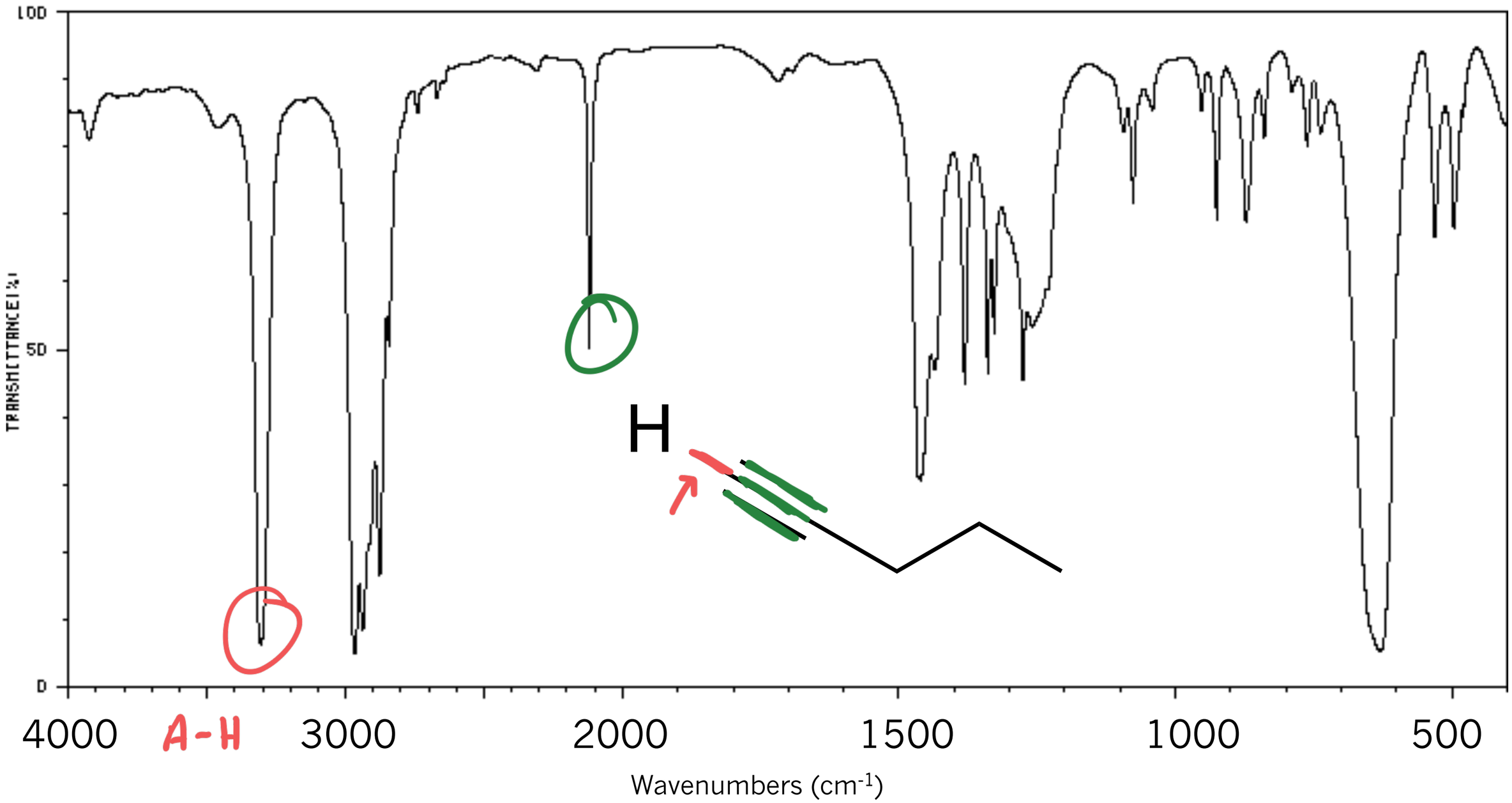
Arene stretches 1600, 1500, <1500 cm^{-1}



Key Functional Group Absorptions

6) Alkyne *Csp-H ~3300 cm^{-1} (terminal alkyne)*

C≡C stretch ~2150 cm^{-1}

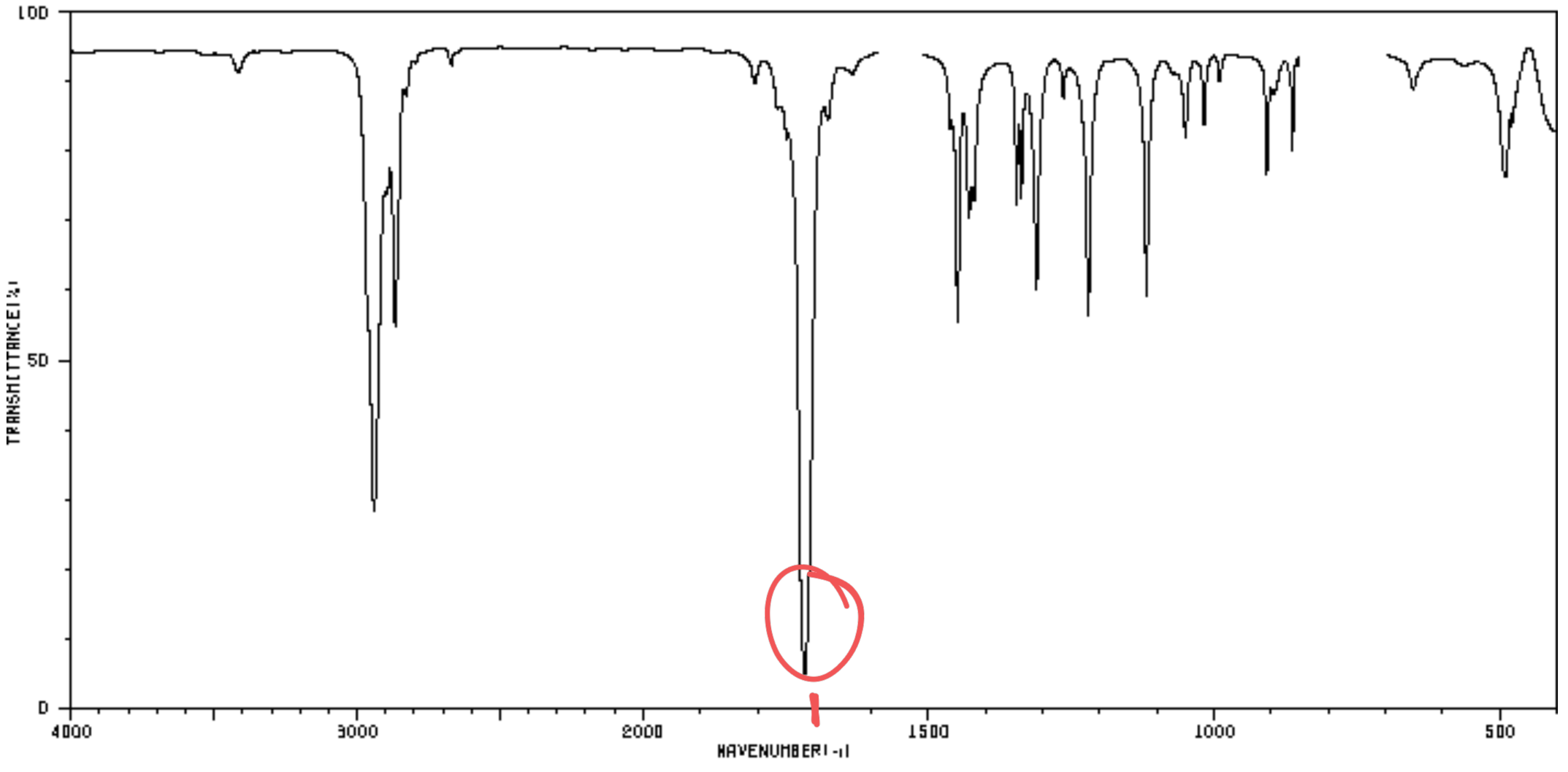


Key Functional Group Absorptions

7) Carbonyl Groups

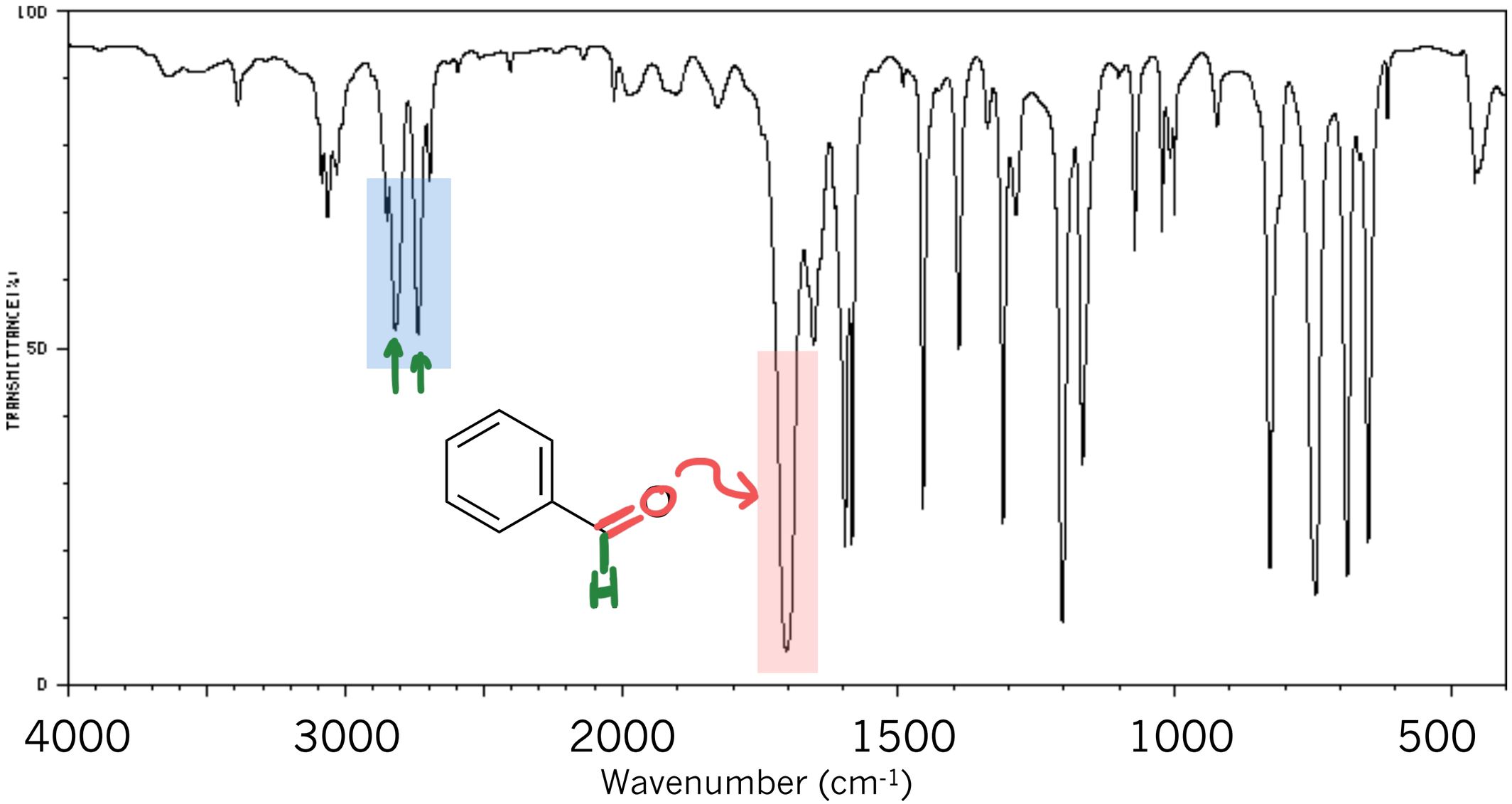
Look for the C=O group ~1700 cm^{-1}

C=C weak



Aldehydes

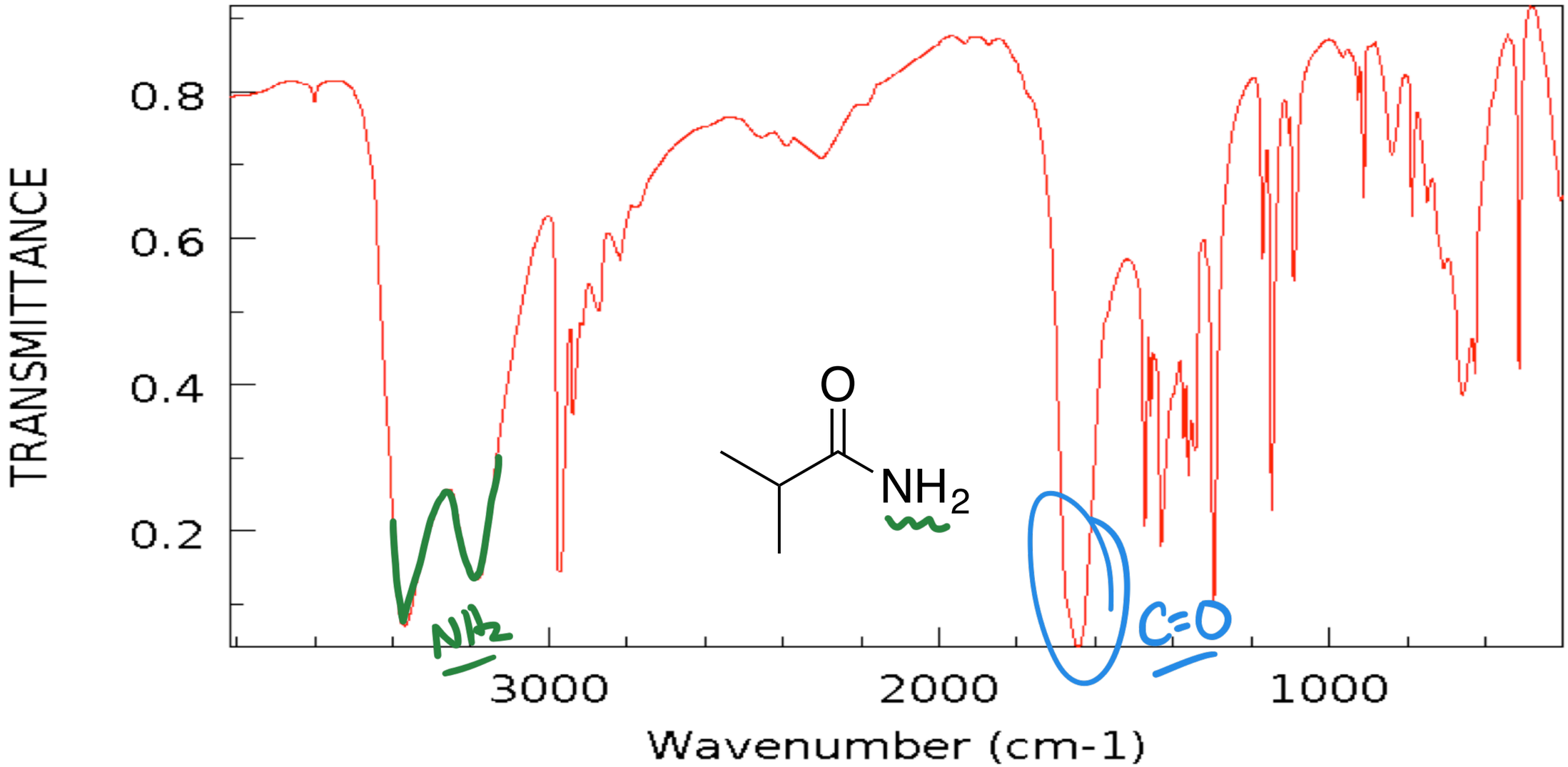
In aldehydes, look for specific aldehyde C-H stretches at ~2720 and ~2820 cm^{-1}.



Amides

Look for the C=O stretch ~1650 cm^{-1}

Also look for N-H stretches above 3000 cm^{-1}



Esters

Look for the C=O stretch ~1750 cm^{-1}

Csp^3-O stretch: 1000-1100 cm^{-1}

Csp^2-O stretch: 1200-1300 cm^{-1}