

Today

Infrared Spectroscopy

Next Class

Spectroscopy Practice?

Chapter 21

Second Class from Today

Chapter 21

Third Class from Today

Chapter 21

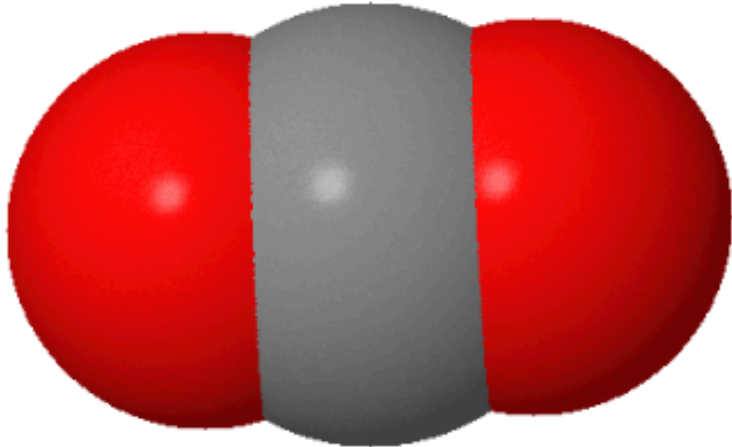
Monday office hours rescheduled to 1:10 to 2:10 from now on.

Please rework, on a separate piece of paper, test 1 and hand in on Wednesday, March 19.

Rework means for each question that your did not receive full credit provide a more complete answer.

I do not need your test back, please just hand in the reworked answers.

Carbon Dioxide vibrations



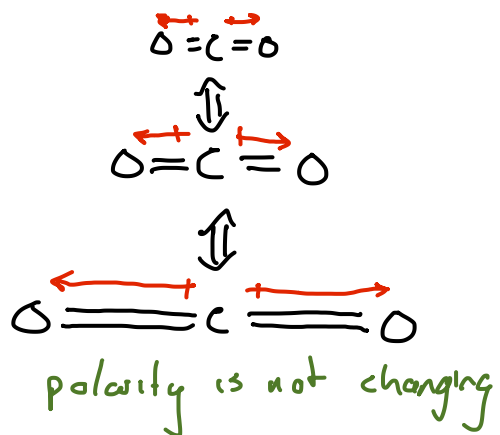
no vibration
bend
bend
symmetric stretch
antisymmetric stretch

vibration
 vectors
 color vectors yellow color vectors purple
 spacefill off spacefill 20% spacefill 100%
 wireframe on wireframe 0.1
 spin

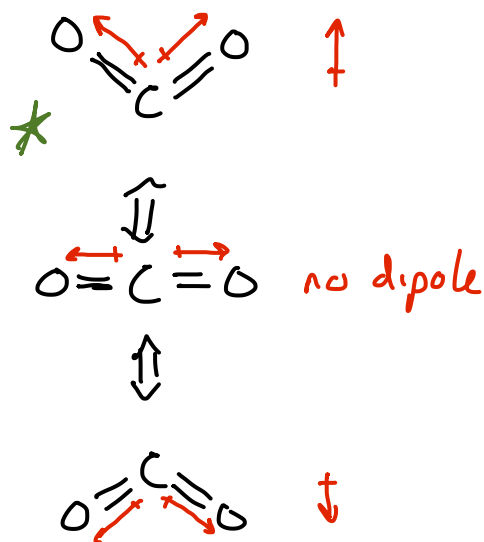
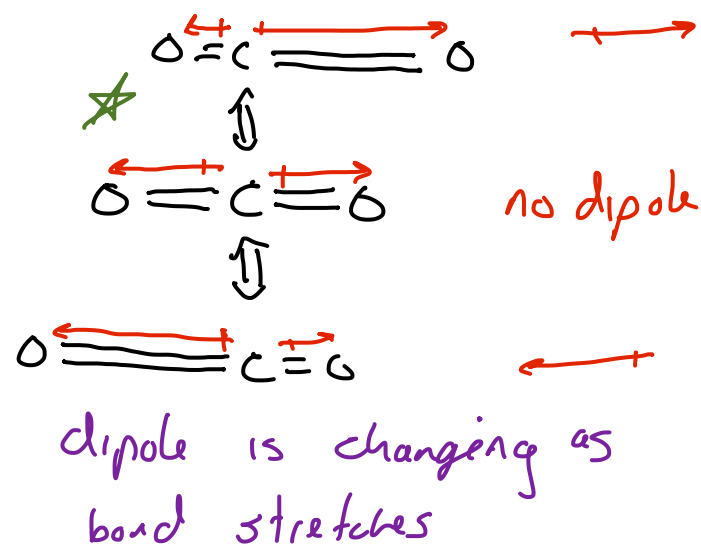
JSmol



A **vibration that changes the dipole of a molecule** creates an oscillating electric field that **can interact with Infra-red light**. Consider the vibrations of the greenhouse gas CO₂.

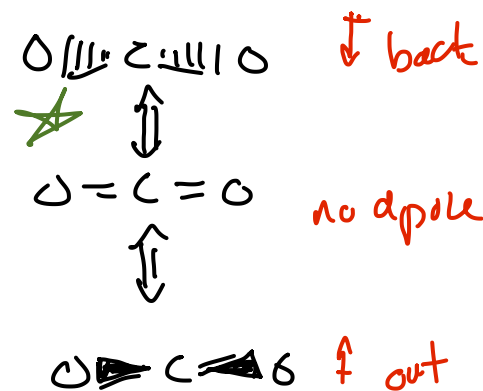


trying to show snapshots of the C=O stretching vibration



dipole is changing as bond bends

these oscillating electromagnetic fields can interact with electromagnetic radiation... IR



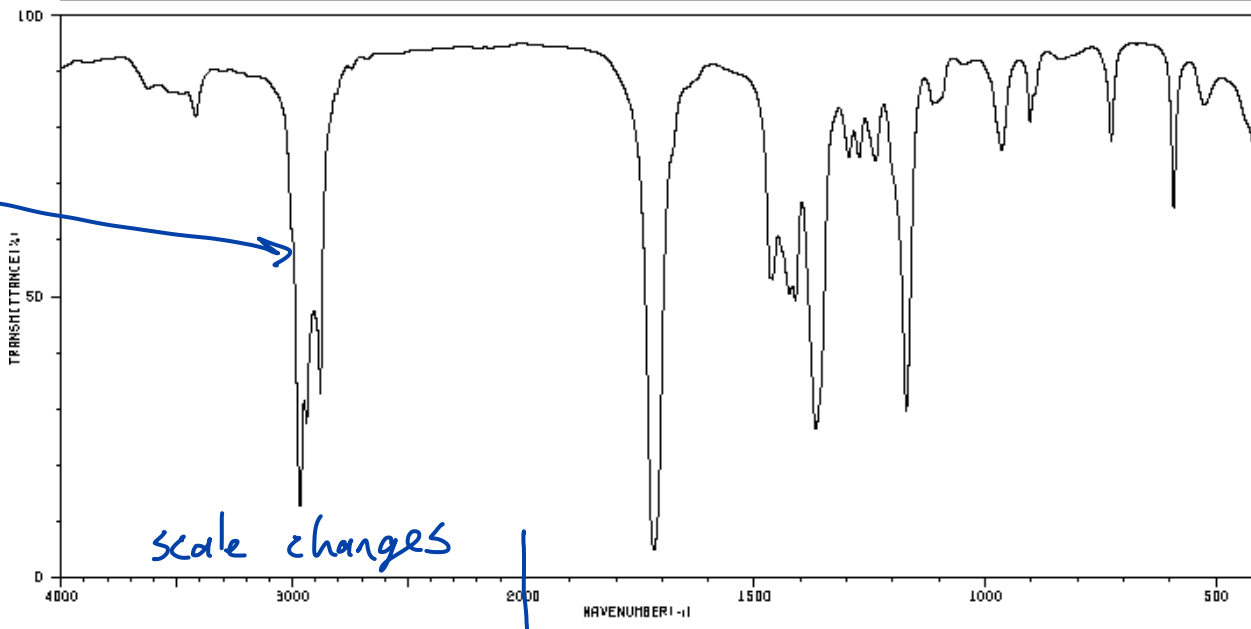
dipole is changing as bond bends

An Example Spectrum

Section

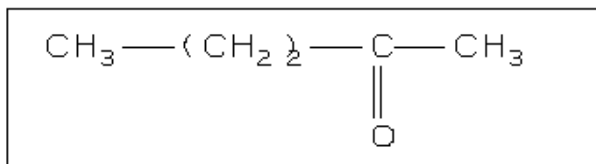
| | | | |
|----------------------------------|------------|--------------|-----------------------------|
| HIT-NO=1985 | SCORE= () | SDBS-NO=2673 | IR-NIDA-00433 : LIQUID FILM |
| 2-PENTANONE | | | |
| C ₅ H ₁₀ O | | | |

100% of IR light transmitted
 "Peaks" point down



wave numbers are "convenient"... α to energy
 αn 3500 cm⁻¹ is easier to write than the measurement in M, nm, of Hz

| | | | | | | | |
|------|----|------|----|------|----|-----|----|
| 3419 | 79 | 1426 | 49 | 1114 | 81 | 692 | 64 |
| 2966 | 12 | 1412 | 47 | 1105 | 81 | 526 | 81 |
| 2939 | 26 | 1367 | 25 | 1100 | 81 | | |
| 2879 | 31 | 1296 | 72 | 964 | 72 | | |
| 1717 | 4 | 1274 | 72 | 903 | 79 | | |
| 1467 | 50 | 1237 | 72 | 894 | 81 | | |
| 1461 | 60 | 1172 | 28 | 727 | 74 | | |



Hooke's Law

Force displacement

$$F = kx$$

Spring constant

Force constant

Harmonic Oscillator

$$\bar{\nu} = \frac{1}{2\pi} \sqrt{\frac{k}{m}}$$

Frequency

mass of the object

strong bond
high frequency vibrations
weak bond lower freq vibrations

Frequency of IR Absorbed

$$\bar{\nu} = \frac{1}{2\pi c} \left[\frac{f(m_1 + m_2)}{m_1 m_2} \right]$$

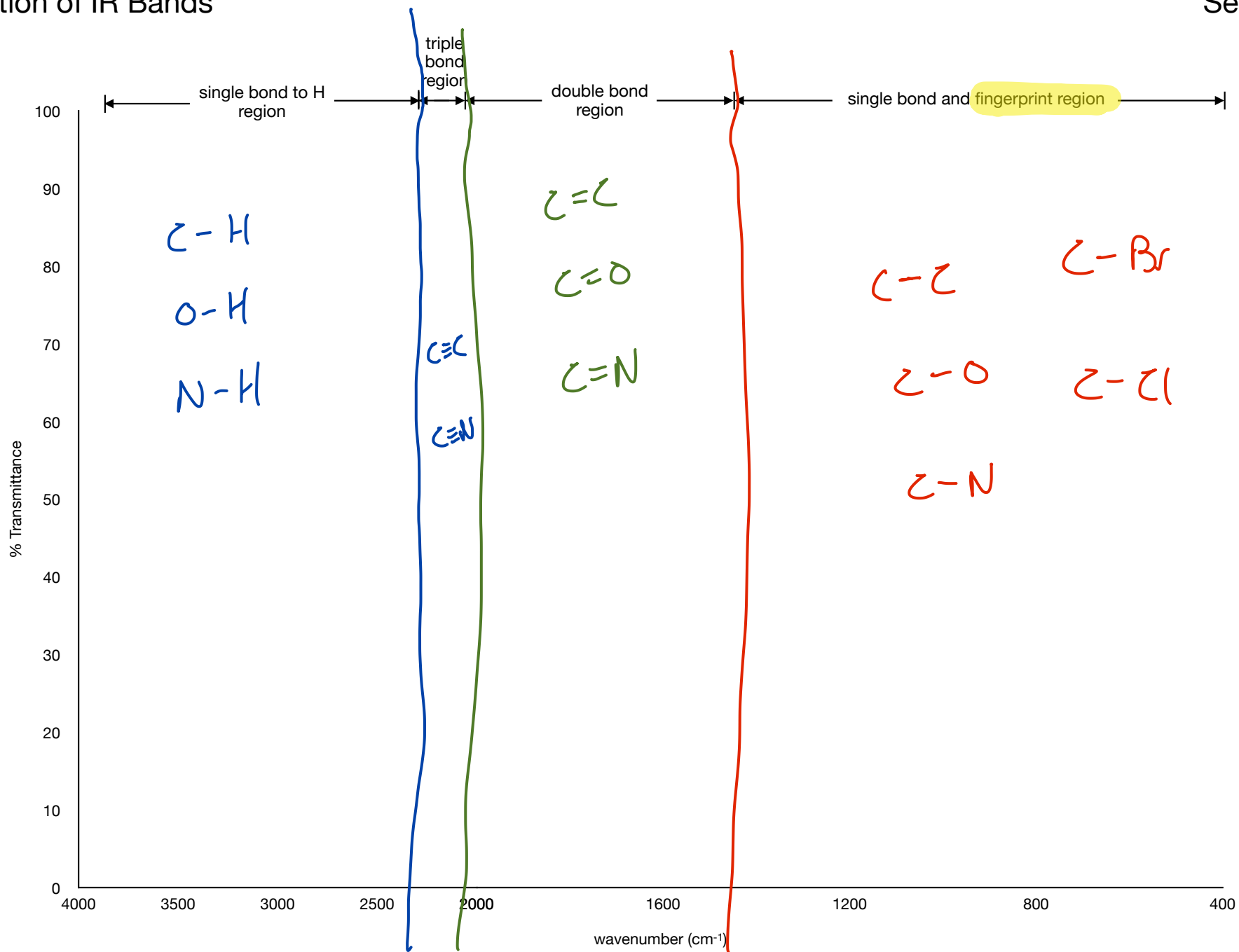
Force constant related to the strength of the bond

mass is the mass of the atoms

Small masses higher freq
larger masses lower freq

Position of IR Bands

Section



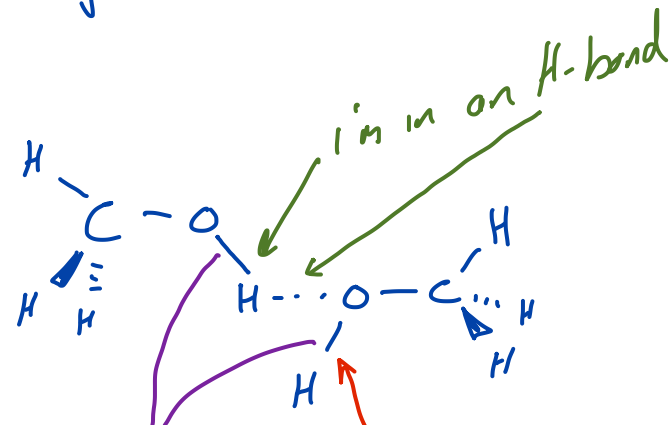
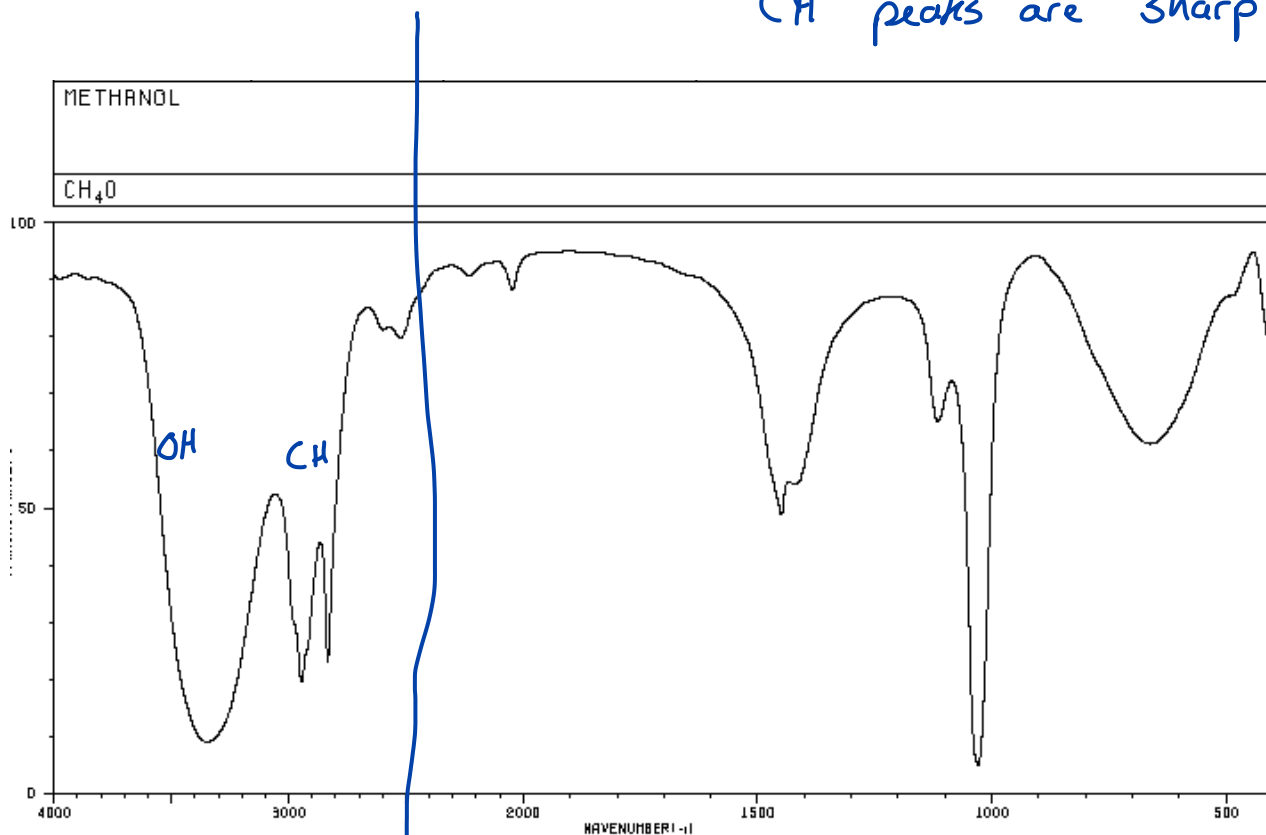
Intensity and Shape, OH vs CH

OH peaks tend to be broad.

CH peaks are sharp.

Why the difference?

Section

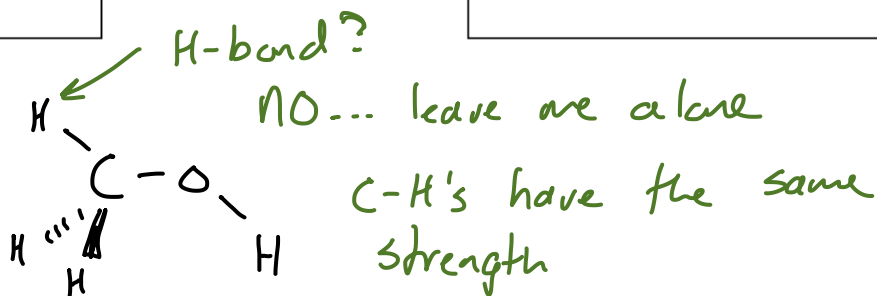


equally strong.

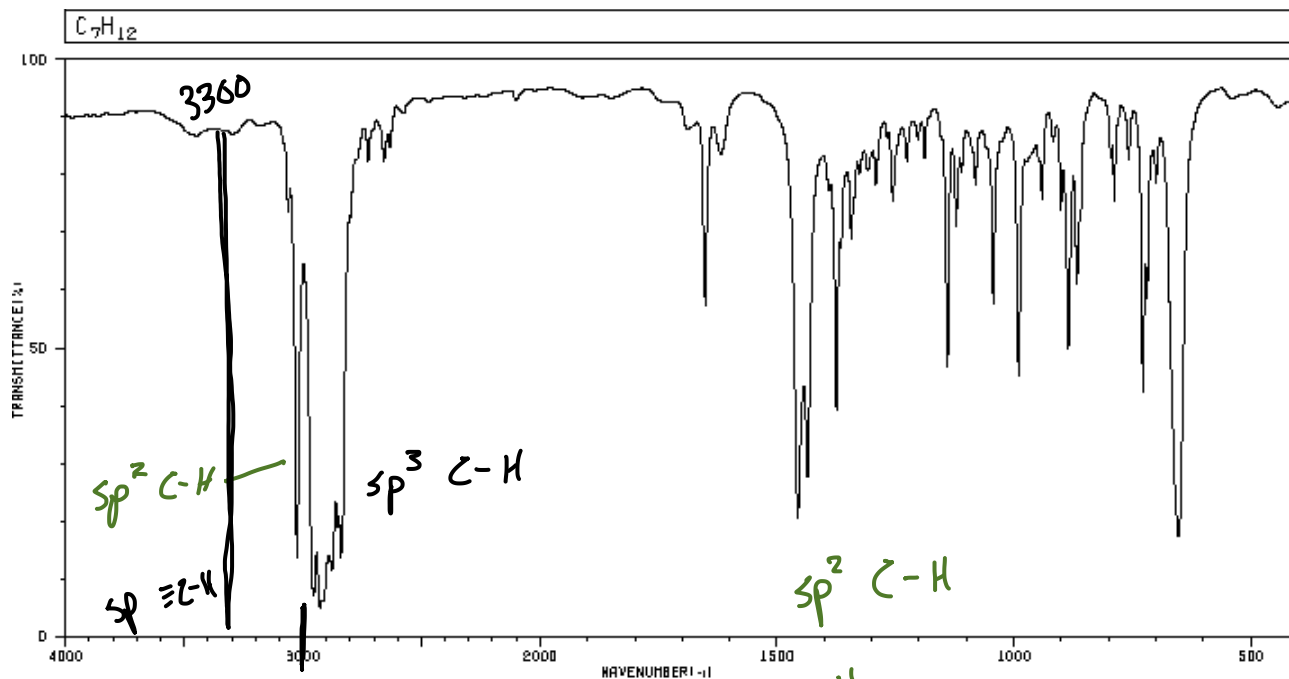
and I's not

Because the H's in OH are H-bonding to other O atoms the O-H bonds are the have a variety of strengths... sometimes stronger... sometimes weaker

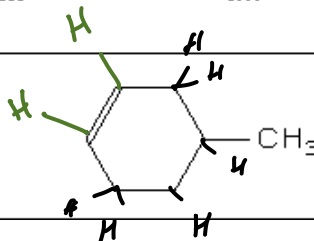
| | | | |
|------|----|------|----|
| 3347 | 6 | 1116 | 62 |
| 3336 | 8 | 1030 | 4 |
| 2945 | 16 | 662 | 56 |
| 2833 | 22 | | |
| 2522 | 77 | | |
| 2046 | 84 | | |
| 1450 | 47 | | |



Fine Tuning Position, CH's



| | | | | | | | | | |
|------|----|------|----|------|----|------|----|-----|----|
| 3063 | 70 | 2839 | 19 | 1344 | 66 | 1122 | 68 | 886 | 47 |
| 3025 | 13 | 1651 | 55 | 1326 | 77 | 1111 | 77 | 867 | 58 |
| 2954 | 6 | 1458 | 20 | 1309 | 77 | 1081 | 74 | 769 | 72 |
| 2928 | 4 | 1436 | 26 | 1292 | 74 | 1044 | 66 | 728 | 41 |
| 2915 | 6 | 1390 | 74 | 1256 | 72 | 990 | 43 | 719 | 57 |
| 2878 | 10 | 1375 | 37 | 1227 | 79 | 941 | 72 | 701 | 74 |
| 2852 | 18 | 1366 | 64 | 1141 | 44 | 901 | 70 | 653 | 16 |



sp^3 C-H