IR-Spectroscopy: Functional Group Identification

HOW TO APPROACH FOR THE ANALYSIS OF AN IR SPECTRUM

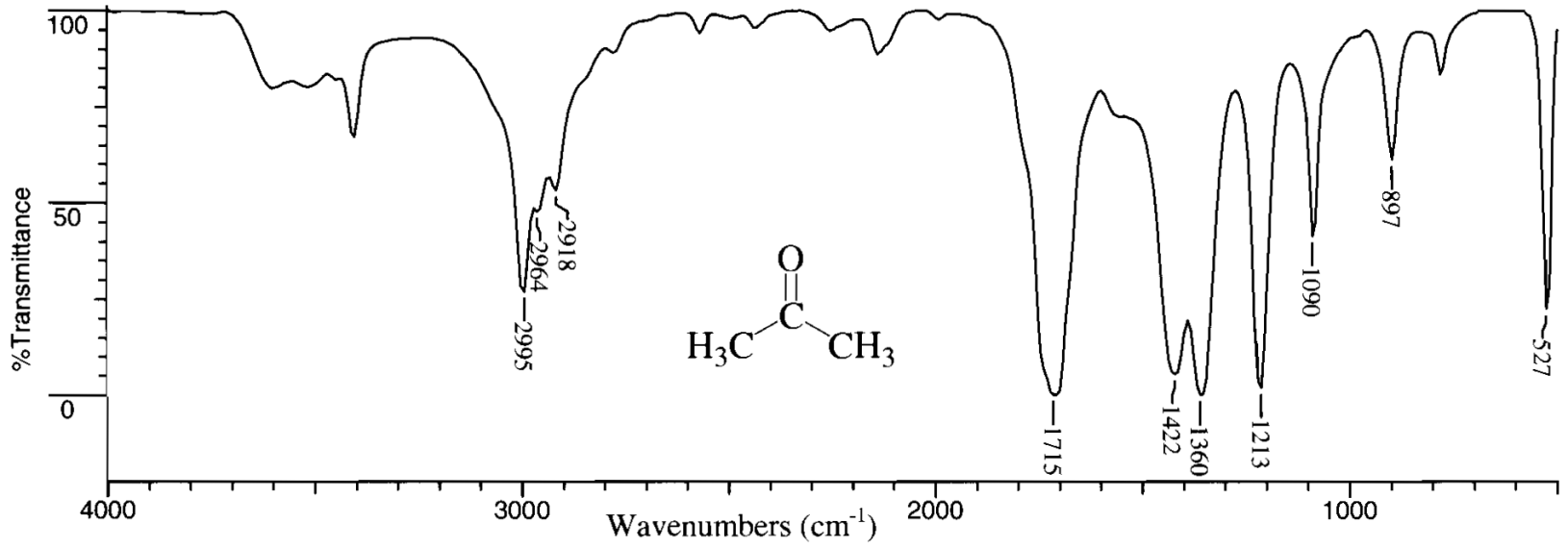
Look for the presence (or absence) of a few major functional groups:

C = O, O - H, N - H, C - O, C = C, C ≡ C and C ≡ N

Do not try to make a detailed analysis of the C - H absorptions near 3000 cm^{-1} almost all organic compounds have these absorptions

1. Is a carbonyl group present?

The C = O group gives rise to a strong absorption in the region 1820 –1660 cm^{-1}
The peak is often the strongest in the spectrum . One can't miss it.

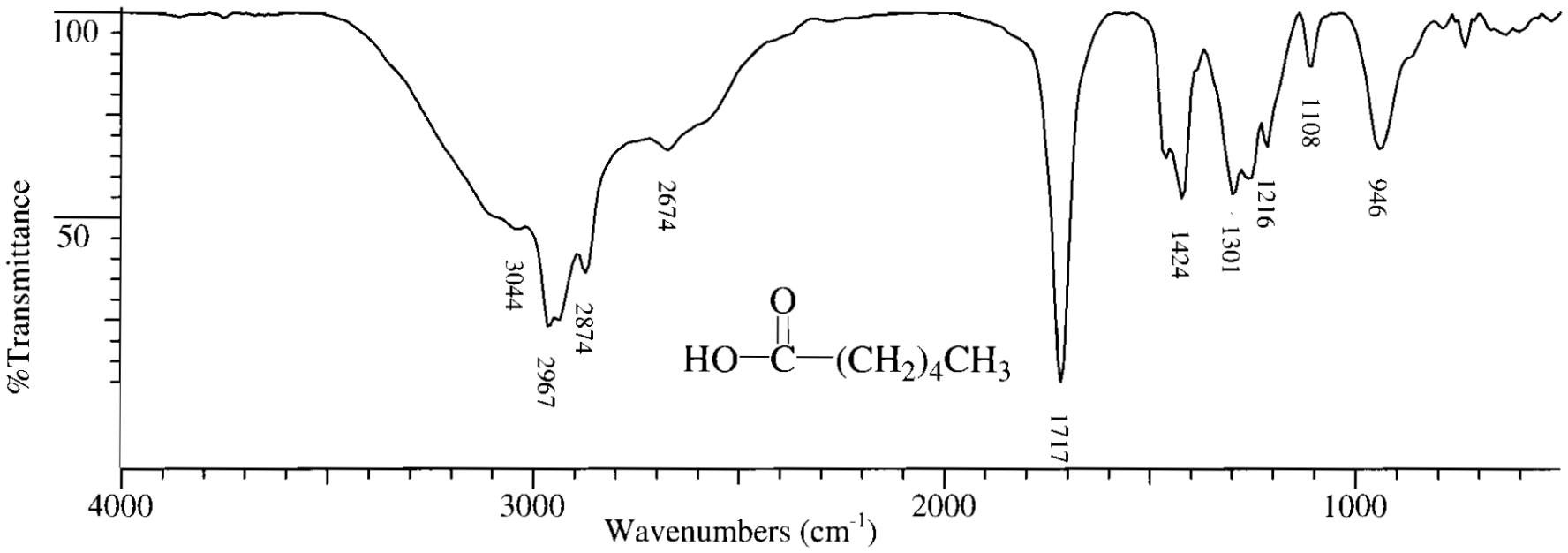


ANALYSIS OF AN IR SPECTRUM

2. If C=O is present, check the following types (if it is absent, go to step 3):

ACIDS — Is O—H also present?

- *Broad* absorption near 3400–2400 cm^{-1} (usually overlaps C—H).

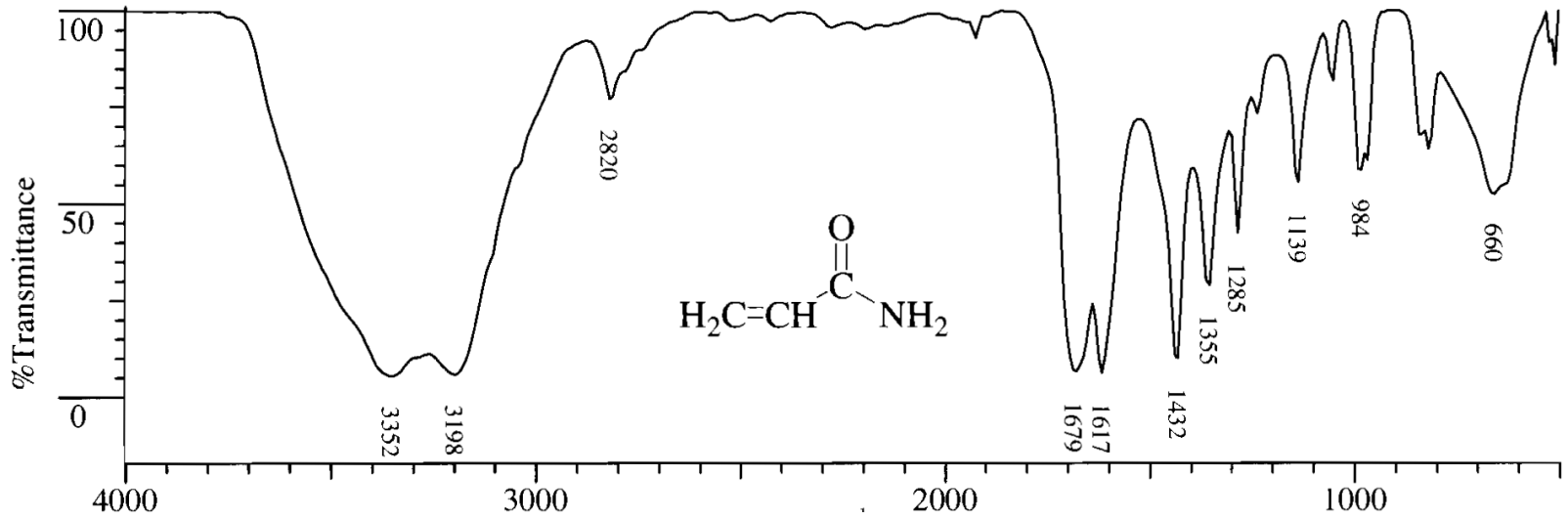


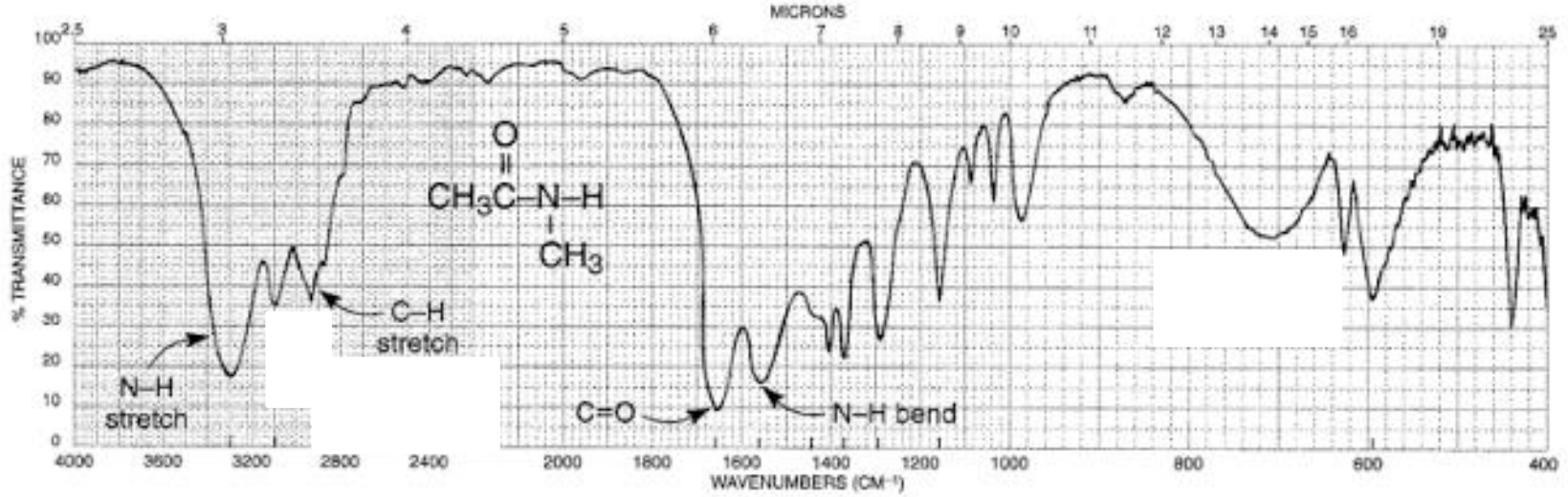
ANALYSIS OF AN IR SPECTRUM

AMIDES

Is N−H also present?

- Medium absorption near 3400 cm^{-1}; sometimes a double peak with equivalent halves.



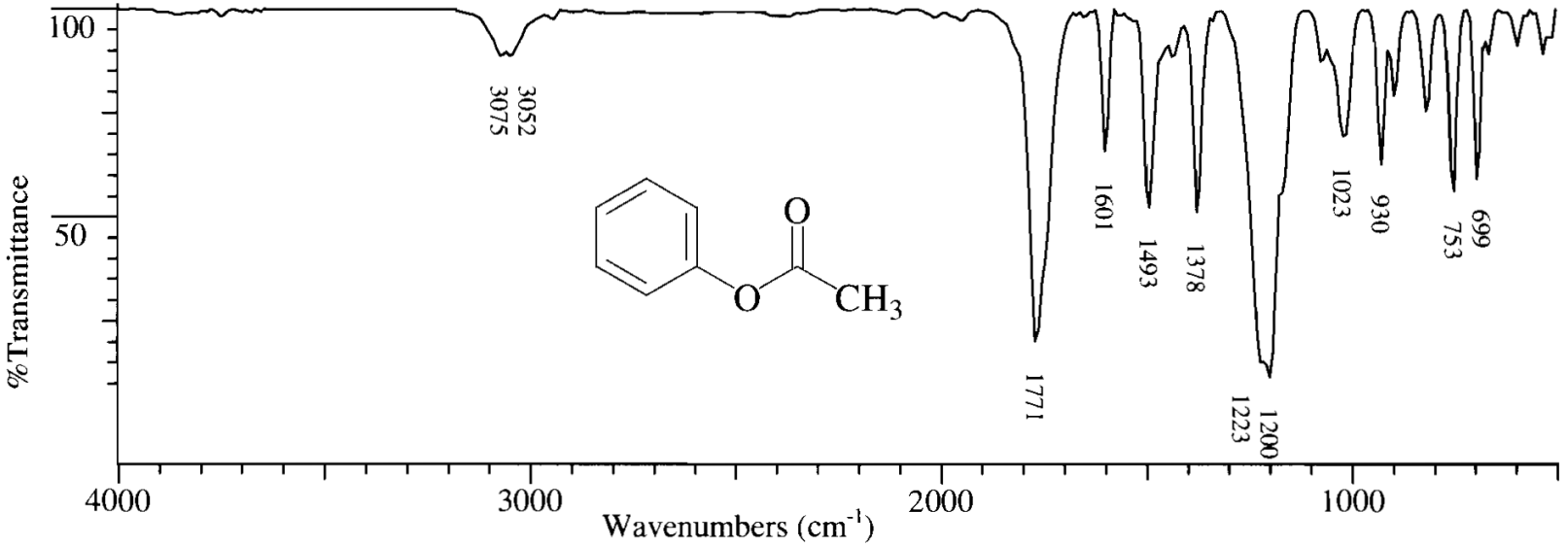


ANALYSIS OF AN IR SPECTRUM

ESTERS

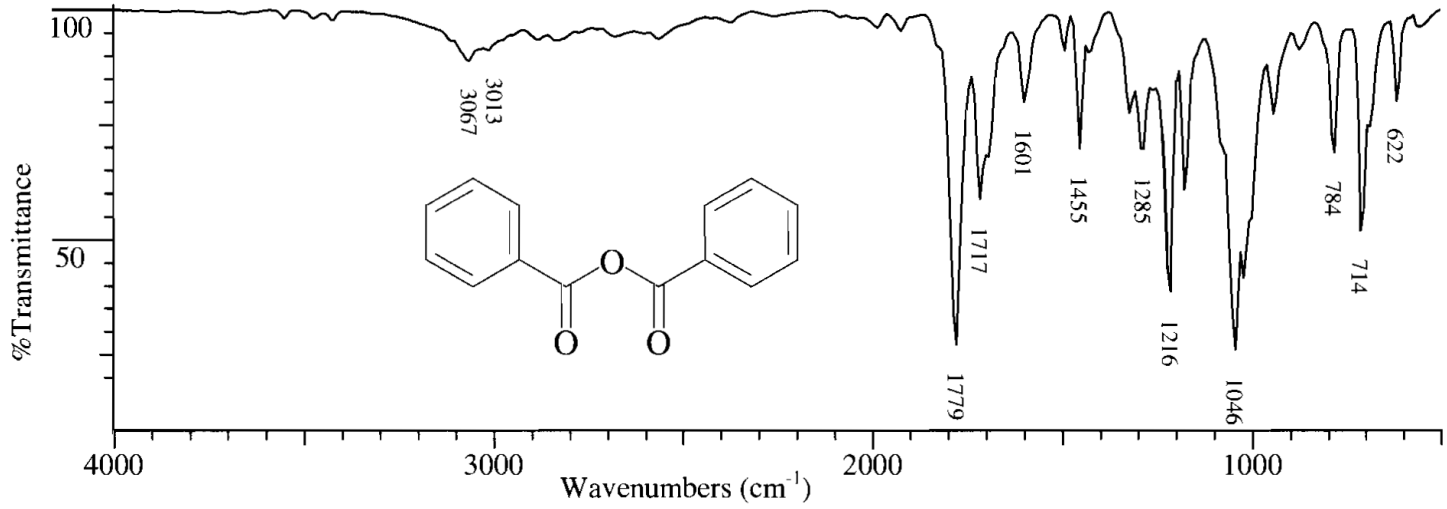
Is C—O also present?

- Strong-intensity absorptions near 1300–1000 cm^{-1}.



ANHYDRIDES

Two C=O absorptions near 1810 and 1760 cm^{-1}.

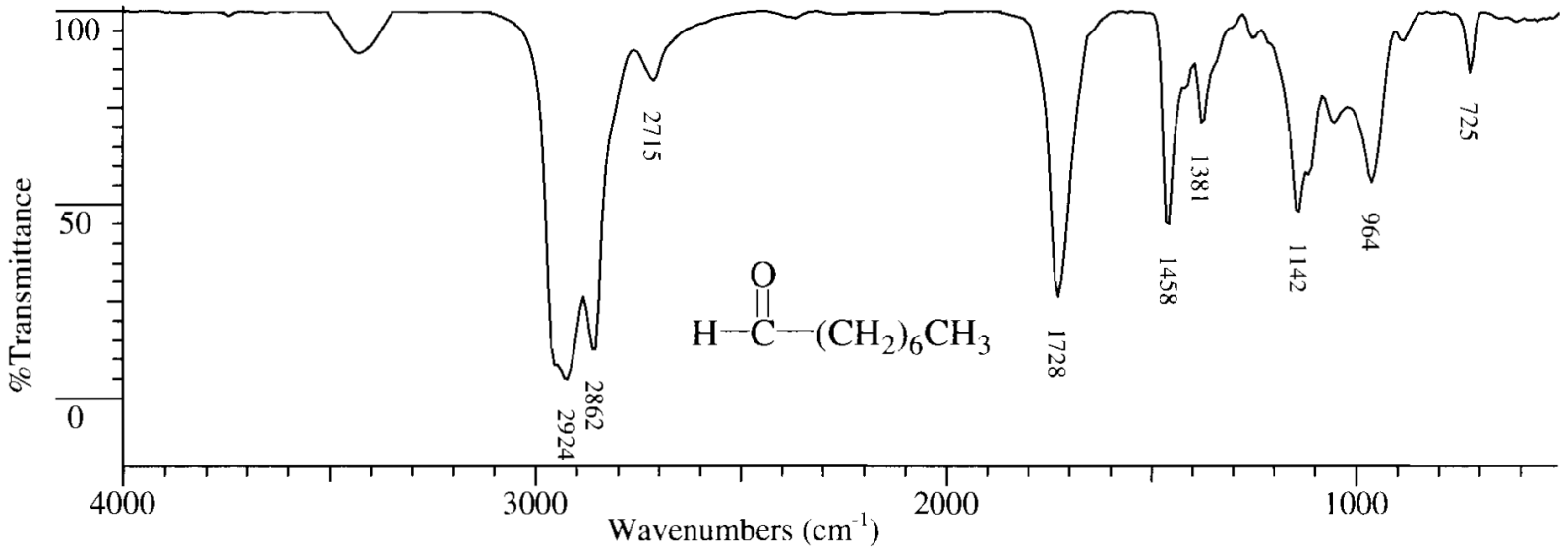


ANALYSIS OF AN IR SPECTRUM

ALDEHYDES

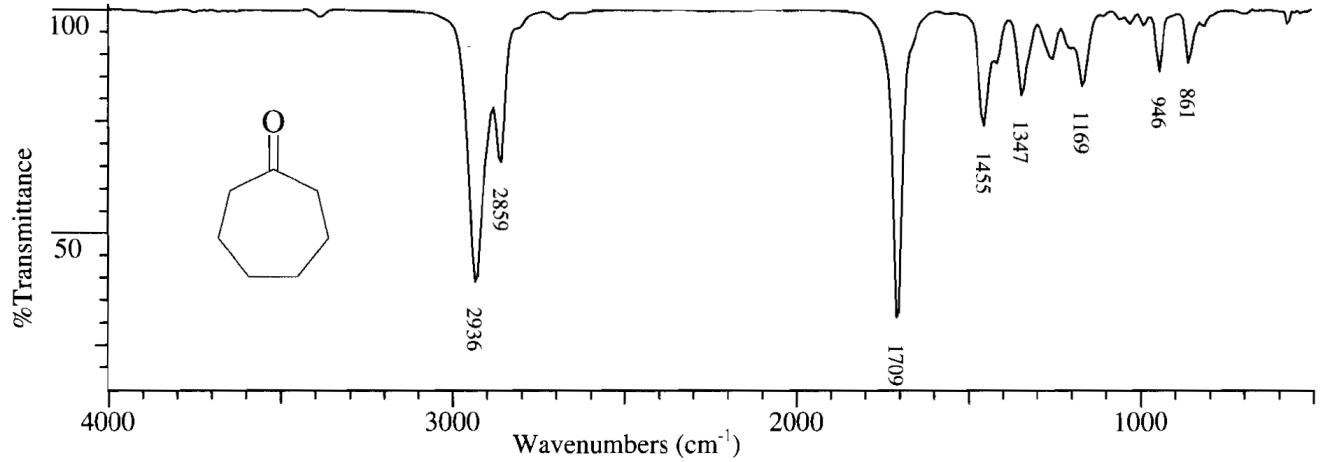
Is aldehyde C—H present?

- Two weak absorptions near 2850 and 2750 cm^{-1} on right side of the aliphatic C—H absorptions.



KETONES

The preceding five choices have been eliminated.

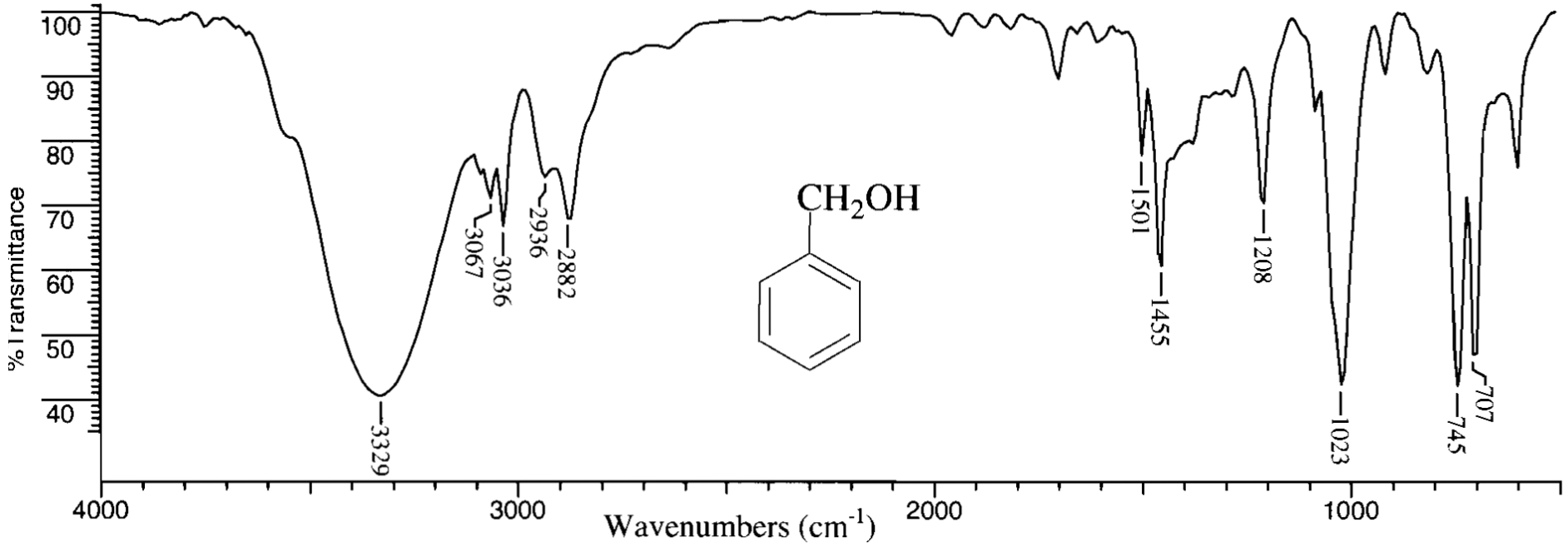


ANALYSIS OF AN IR SPECTRUM

3. If C=O is absent:

ALCOHOLS, PHENOLS — Check for O—H.

- *Broad* absorption near 3400–3300 cm^{-1}.
- Confirm this by finding C—O near 1300–1000 cm^{-1}.

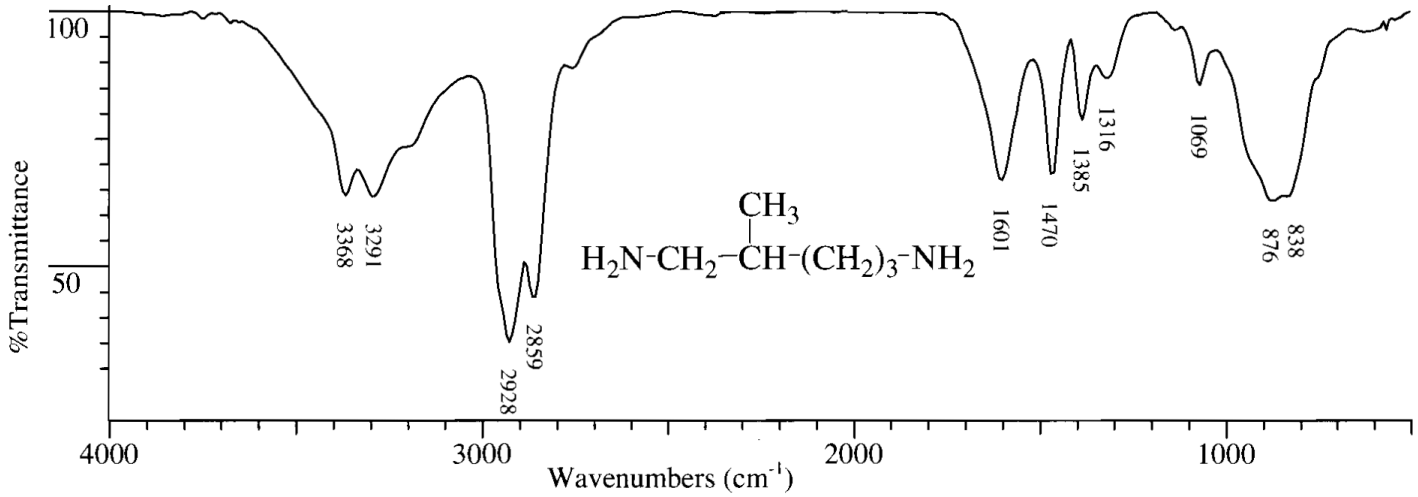


ANALYSIS OF AN IR SPECTRUM

AMINES

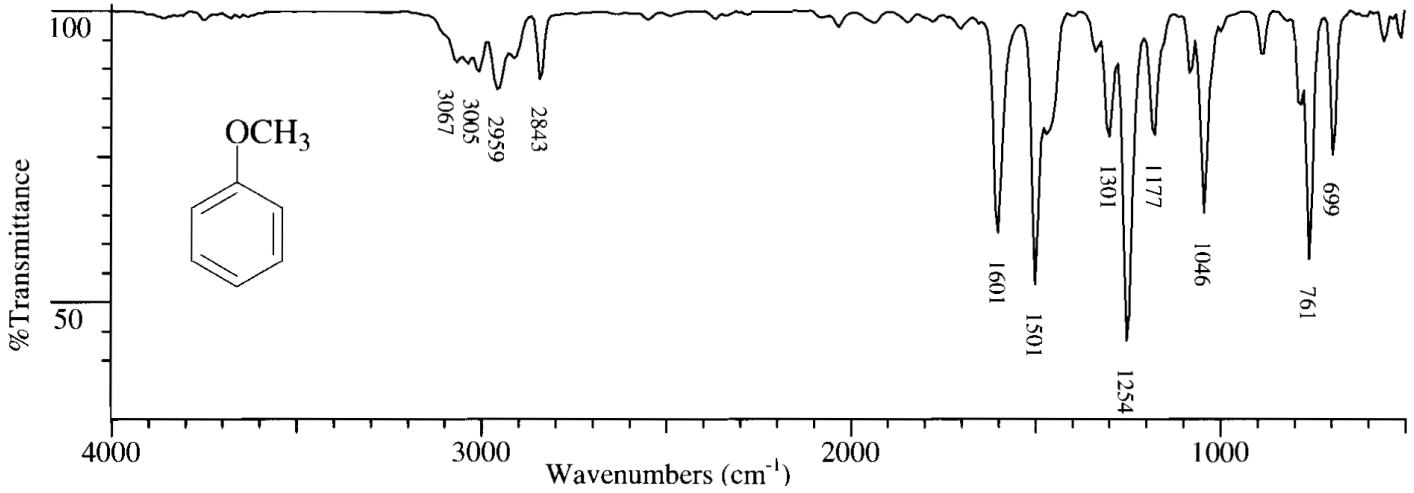
Check for N—H.

- Medium absorption(s) near 3400 cm^{-1}.



ETHERS

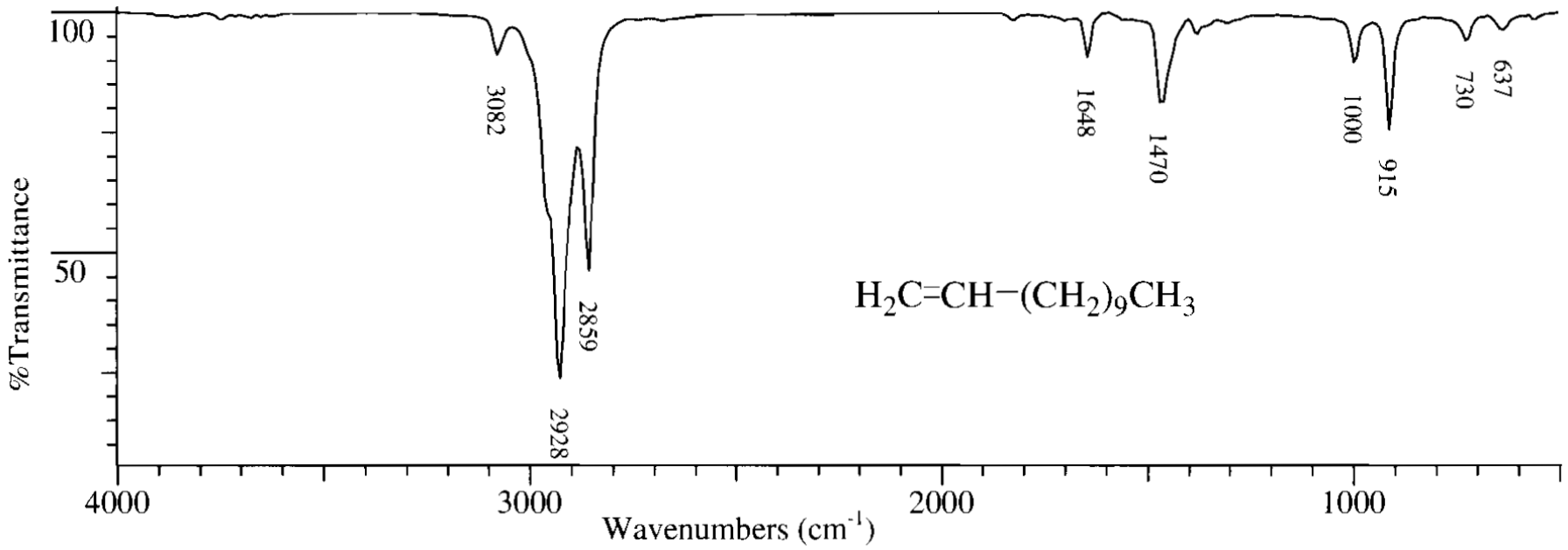
Check for C—O near 1300–1000 cm^{-1} (and absence of O—H near 3400 cm^{-1}).



ANALYSIS OF AN IR SPECTRUM

4. Double bonds and/or aromatic rings

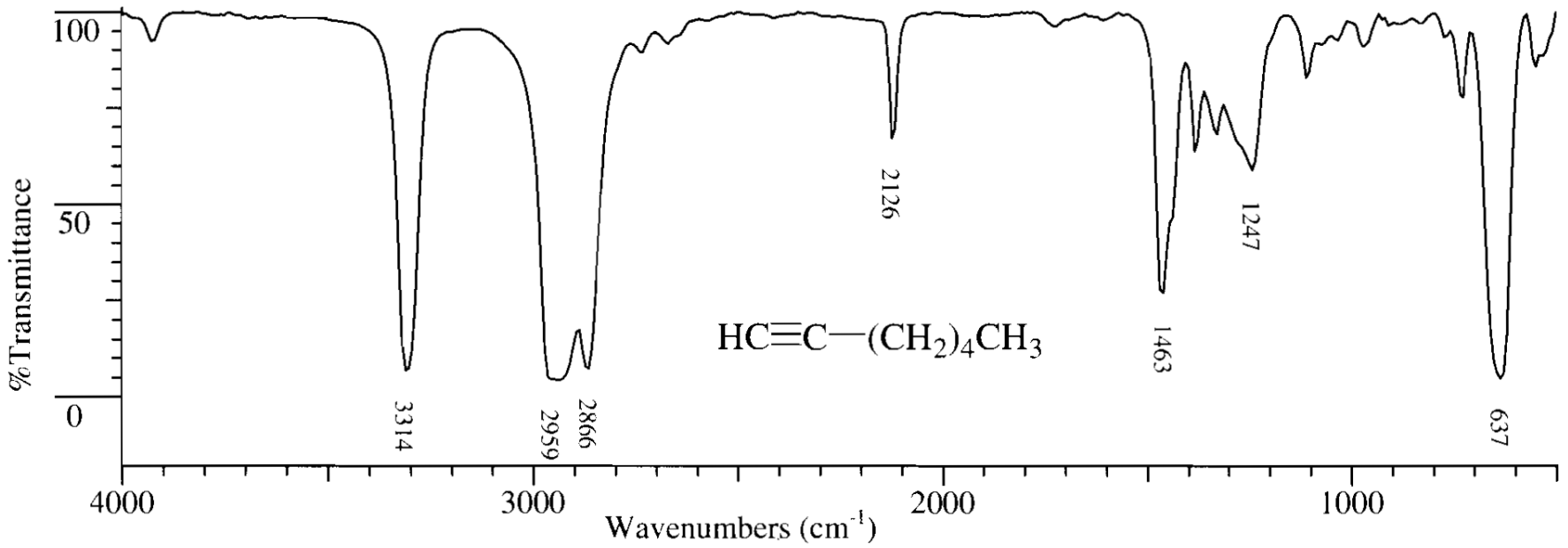
- C=C is a weak absorption near 1650 cm.



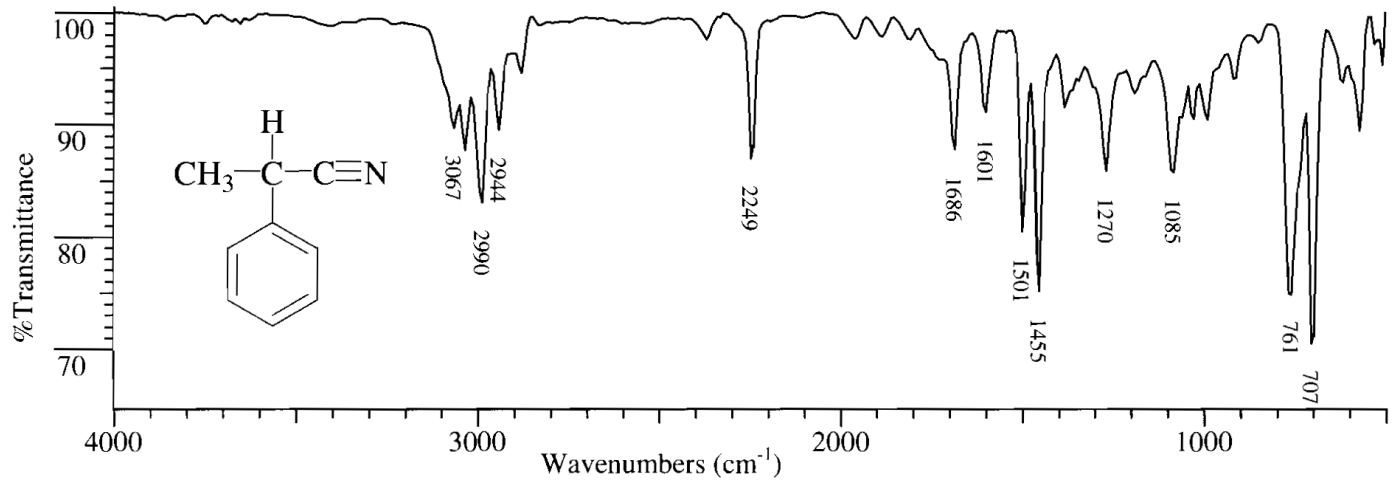
ANALYSIS OF AN IR SPECTRUM

5. Triple bonds

- C≡C is a weak, sharp absorption near 2150 cm^{-1}.
- Check also for acetylenic C—H near 3300 cm^{-1}.

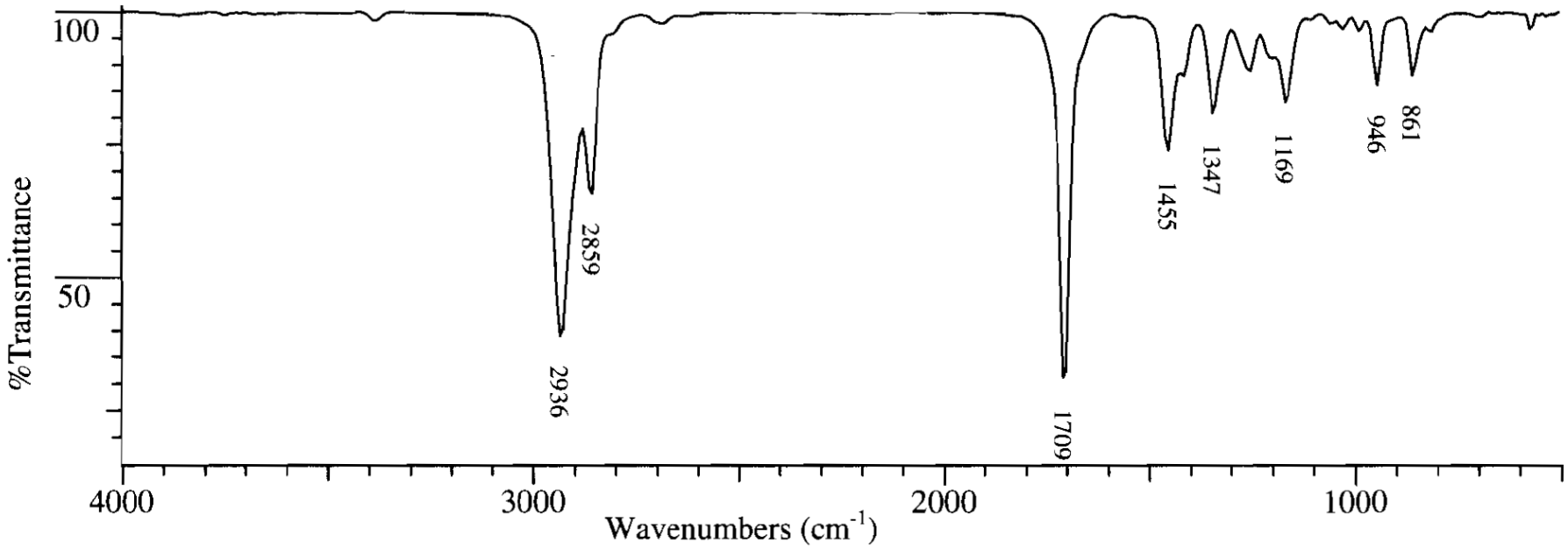


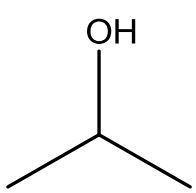
- C≡N is a medium, sharp absorption near 2250 cm^{-1}.



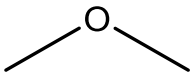
Infrared Spectroscopy: Problem

IR of an oxygen-containing compound is given below. What class of compound is it?

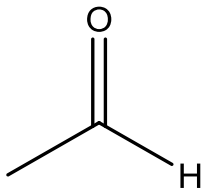




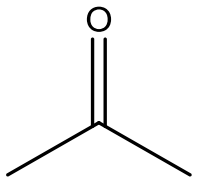
Alcohol



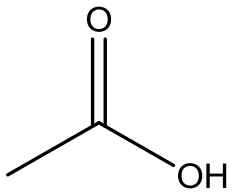
ether



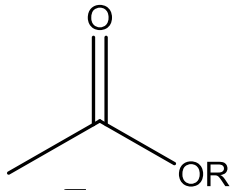
Aldehyde



Ketone



Acid



Ester

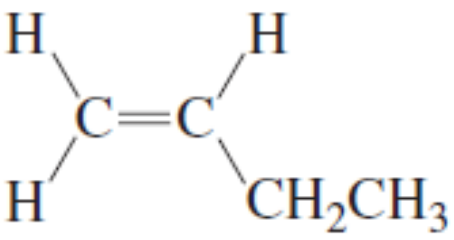
Peaks Absent: **~3400 cm^{-1}** **~1050 cm^{-1}** **~2720 cm^{-1}** **~1050 cm^{-1}** **~1250 & ~1050 cm^{-1}**

The class of the compound is ketone

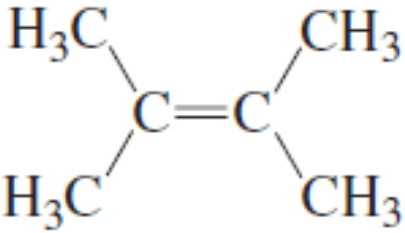
Infrared Spectroscopy: Infrared Inactive Vibrations

Not all vibrations give rise to absorption bands

In order for a vibration to absorb IR radiation, the dipole moment of the molecule must change when the vibration occurs



1-butene



2,3-dimethyl-2-butene

Other IR-inactive molecules are

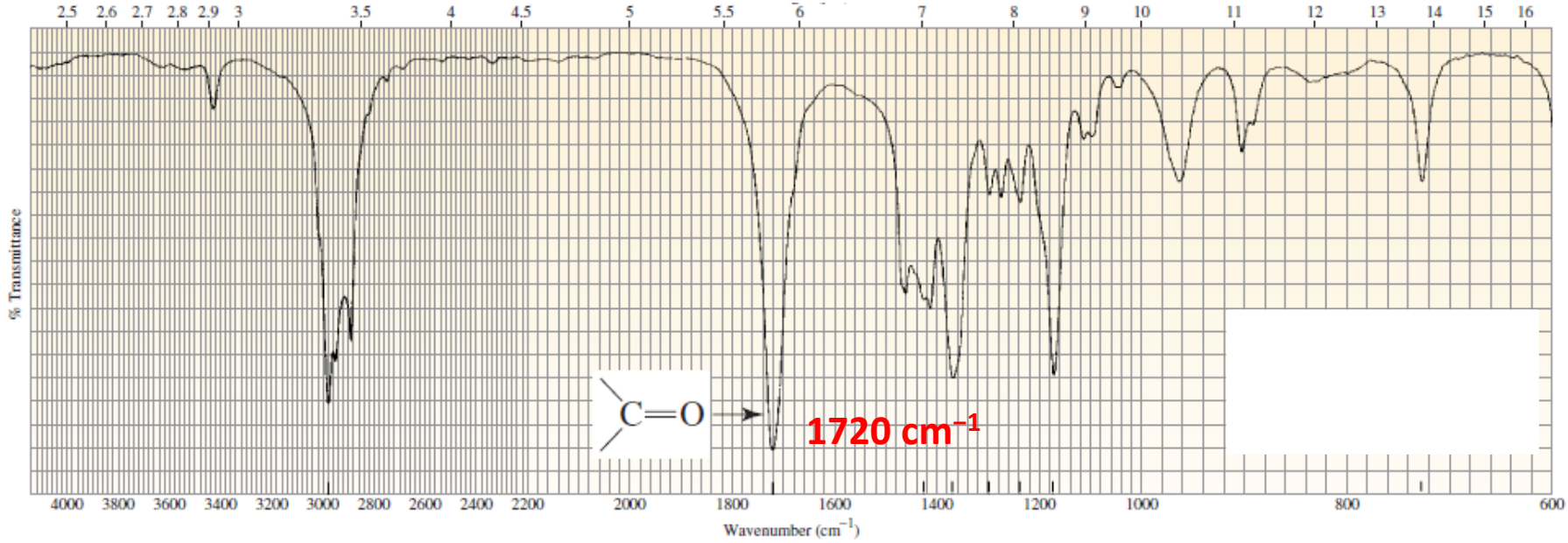
For example, the C = C bond in 1-butene has a dipole moment because the molecule is not symmetrical about this bond.

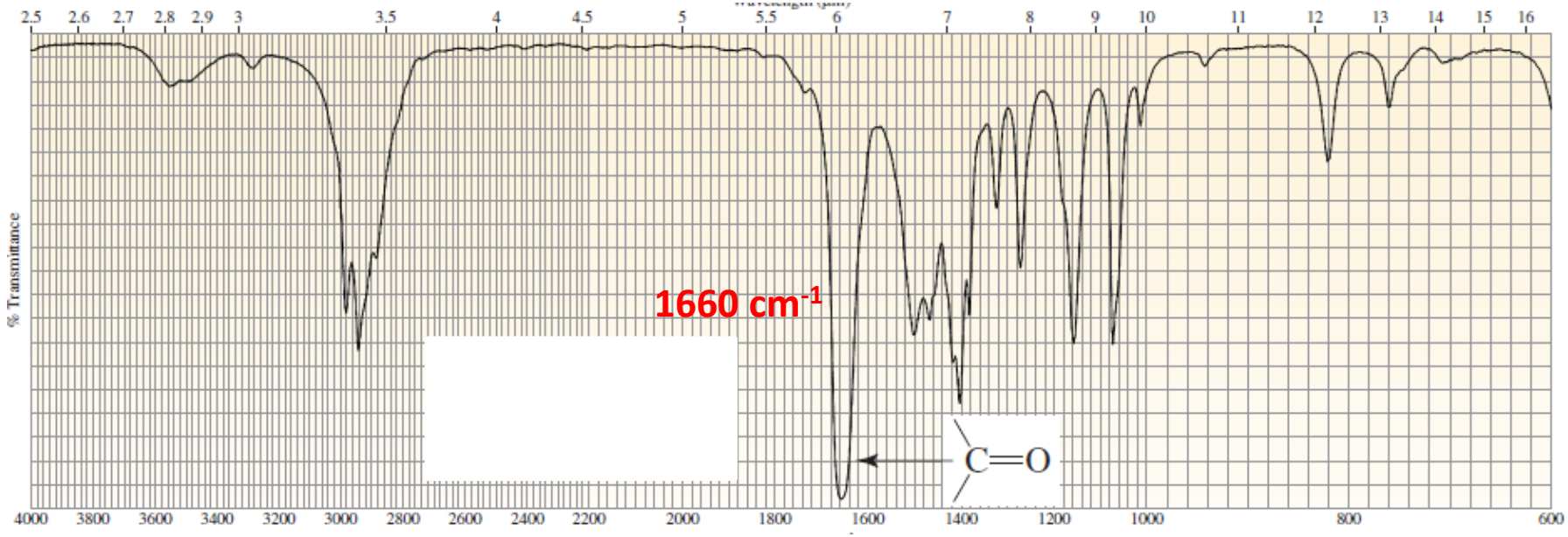
2,3-Dimethyl-2-butene, in contrast, is a symmetrical molecule, so its bond has no dipole moment

When the C = C bond stretches, it still has no dipole moment. Since stretching is not accompanied by a change in dipole moment, no absorption band is observed. The vibration is *infrared inactive*

Infrared Spectroscopy: Problem

Identify the functional groups corresponding to the following IR-spectra





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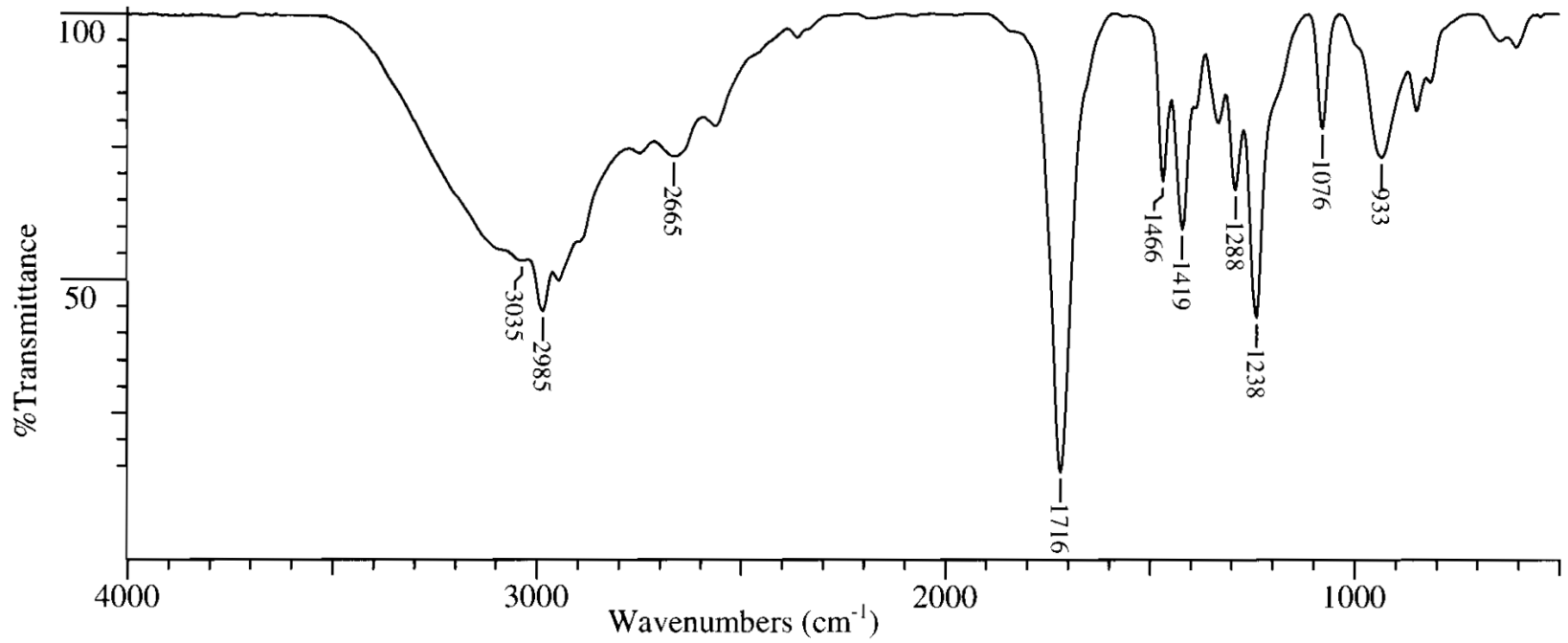
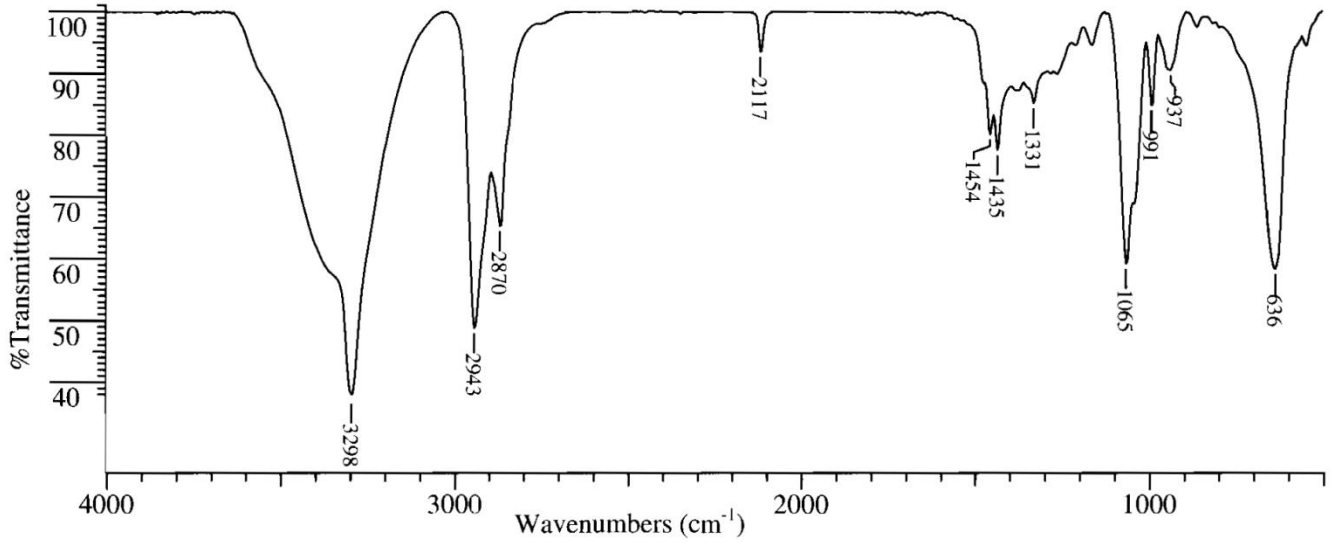
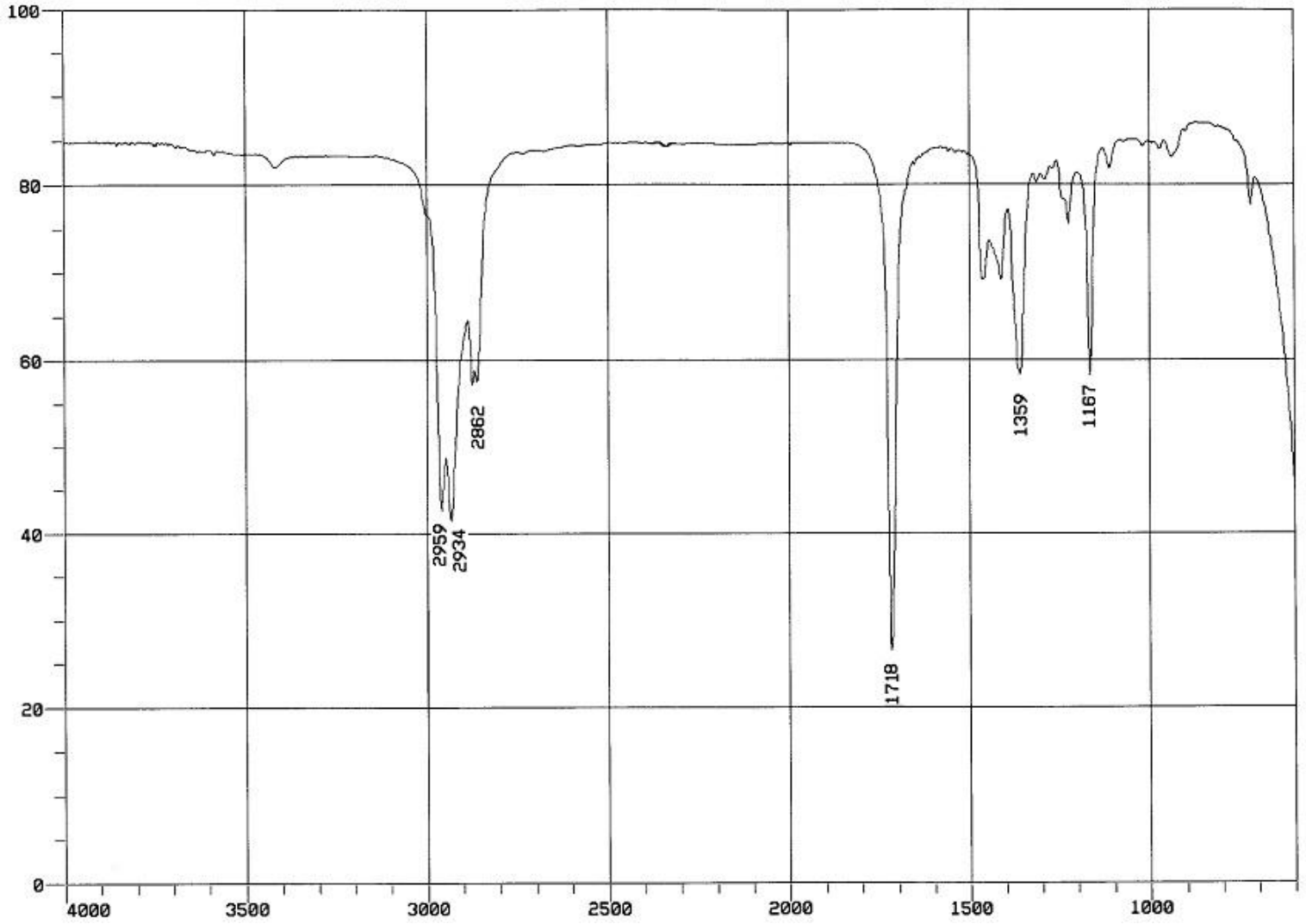




Infrared Spectroscopy: Problem

Molecular formula: $C_7H_{14}O$



Looking forward

NMR -spectroscopy