Lecture 12: Infrared Spectroscopy Part 2
Discussion Section Problems Solutions

1. **Compound A**
   
   **Zone 1:** Alcohol O–H: Present - peak at ~3350 cm⁻¹.  
   Amine N–H: Maybe - obscured by O–H.  
   Terminal alkyne ≡C–H: Absent - may be buried under O–H/N–H peak, but zone 3 is empty.

   **Zone 2:** Aryl or vinyl sp² C–H: Absent - nothing above 3000 cm⁻¹.  
   Alkyl sp³ C–H: Present - peaks below 3000 cm⁻¹.  
   Carboxylic acid O–H: Absent - no broad O-H; also no C=O in zone 4.  
   Aldehyde C–H: Absent - no peak at 2700 cm⁻¹; also no C=O in zone 4.

   **Zone 3:** C≡C or C≡N: Absent - no peaks.

   **Zone 4:** C=O: Absent - no peaks.

   **Zone 5:** Alkene and benzene: Both absent no peak ~1600 cm⁻¹.

   Actual structure (cannot be determined from IR alone):

   ![1-Octanol](https://via.placeholder.com/150)

   1-Octanol

**Compound B**

**Zone 1:** O–H (alcohol), N–H, ≡C–H: All absent.

**Zone 2:** Aryl or vinyl sp² C–H: Absent - no peaks above 3000 cm⁻¹.  
   Alkyl sp³ C–H: Present - peaks below 3000 cm⁻¹.  
   Carboxylic acid O–H: Absent - no broad O-H; also no C=O in zone 4.  
   Aldehyde C–H: Absent - no peak at 2700 cm⁻¹; also no C=O in zone 4.

**Zone 3:** C≡C or C≡N: Absent.

**Zone 4:** C=O: Absent.

**Zone 5:** Alkene and benzene: Both absent - no 1600 cm⁻¹ peak.

Actual structure (cannot be determined from IR alone):

![Octane](https://via.placeholder.com/150)

Octane
2. Phenylacetone (C₉H₁₀O)
   Zone 1: No alcohol O–H, N–H or =C–H so no peaks.
   Zone 2: Aryl C–H above 3000 cm⁻¹.
   Alkyl C–H below 3000 cm⁻¹.
   No aldehyde so no 2700 cm⁻¹.
   No COOH so no broadness.
   Zone 3: No C≡C or C≡N so no peaks.
   Zone 4: Ketone C=O at 1750–1705 cm⁻¹.
   Zone 5: Aromatic pattern: ~1600 cm⁻¹ and ~1500 cm⁻¹.
   No separate alkene peak.

Methamphetamine (C₁₀H₁₅N)
   Zone 1: N–H: 3500–3200 cm⁻¹.
   No alcohol O–H or =C–H so no peaks for these.
   Zone 2: Aryl C–H above 3000 cm⁻¹.
   Alkyl C–H below 3000 cm⁻¹.
   No aldehyde so no 2700 cm⁻¹.
   No COOH so no broadness.
   Zone 3: No C≡C or C≡N so no peaks.
   Zone 4: No C=O so no peaks.
   Zone 5: Aromatic pattern: peaks at ~1600 cm⁻¹ and ~1500 cm⁻¹.
   No separate alkene peak.

The main difference is the absence or presence of the C=O and N–H stretches.

3. Zone 1: 3550 and 3400 cm⁻¹: O–H (we can ignore N–H and =C–H for this problem).
   Zone 2: 3050 cm⁻¹: Aryl or vinyl C–H.
   Below 3000 cm⁻¹ is alkyl C–H.
   Not broad enough for COOH.
   No 2700 cm⁻¹ so no aldehyde.
   Zone 3: No peaks so no C≡C or C≡N (but we expected this!).
   Zone 4: 1675 cm⁻¹: Could be amide or aryl ketone, but these are not in the given structures. Looks good for a conjugated ketone.
   Zone 5: 1600 cm⁻¹: Alkene.
No 1500 cm\(^{-1}\) so no aromatic.

**Conclusion:** The presence of a carbonyl in Zone 4 rules out cholesterol. The carbonyl stretching peak at 1675 cm\(^{-1}\) is more consistent with a conjugated ketone (as in testosterone) than with a nonconjugated ketone (as in estrone).