Structural Elucidation: Infrared (IR) Spectroscopy

CHEM 8B Chapter 16 Homework

1. Consider the equations below with variables defined.



What is the relationship between wavenumber and frequency? Circle one.



Inversely proportional

2. Provide examples of a bond that would_absorb in each region below (ex. O-H, C=C). Draw one example



 \Rightarrow Which C=O bond has a lower stretching frequency (wavenumber)? Circle one.



3. Conjugation - Resonance

Used curved arrow notation and draw ONE resonance structure of the compound below. Be sure to include all charges on atoms where appropriate!



4. Predict Peaks: Use **Table 16-1** Characteristic Frequencies of IR absorption to list the **expected bond absorbance range (cm⁻¹)** in its IR spectrum.



a. How many N-H peaks are expected for the compound above? Circle one.

0



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5. Match spectrum to molecule: Which molecule best fits the IR spectrum?







7. Structure elucidation in a chemical reaction, using IR and Mass Spec data analysis of the product. Answer the prompts below to help confirm the structure of a reaction product.

- (a) The mass spectrum of the product in the reaction below displays a **M**⁺ **peak =** $\frac{1}{56}$. What is the molecular the **molecular formula** of the product?
- (b) The IR spectrum displays a **broad**, **strong signal at 3250cm**⁻¹.

What is the most likely **functional group** in the product?

(c) Draw the structure of the **product** in the box.



7. Structure elucidation in a chemical reaction, using IR and Mass Spec data analysis of the product. Answer the prompts below to guide you to the structure of the reaction product.

(a) The mass spectrum of the product in the reaction below displays a M^+ peak = 82.

What is the molecular the molecular formula of the product?

(b) The IR spectrum displays a medium-strength signal at 1627 cm⁻¹.

What is the most likely **functional group** in the product?

(d) **Circle the major product** of the reaction based on the spectroscopy data above.

