

Objective

Determine the relative strength of the carbon-oxygen double bond in various carbonyl compounds. The compounds will be listed in order of double-bond strength, from strongest to weakest.

Procedure

1. Estimate the double-bond strength for each carbonyl compound using resonance theory.
2. Calculate the (theoretical) frequencies for each carbonyl vibration using Spartan modeling program.
3. Measure the (actual) frequencies for each carbonyl compound using the FT-IR spectrophotometer.

Method

1. Draw Lewis structures for each compound; include significant resonance forms for each structure. Based on your resonance structures, predict the order of double-bond strength and list each compound from strongest to weakest.
2. Build each molecule in Spartan and use the modeling program to calculate the vibrational frequencies. Observe the calculated energy absorptions and identify the mode of vibration as a stretching or bending. Using the calculated frequencies, list each compound from strongest to weakest.
3. Use the IR spectrophotometer to collect a spectrum for each compound. Use peak picking to obtain the carbonyl frequencies then list each compound from strongest to weakest.

Mini Report

Only two sections are required for this mini report:

- I. D&O pages from your notebook.** Your notebook must have the following:
- a. All resonance structures and a summary Table that contains your prediction of bond strength.
 - b. A Table of theoretical frequencies obtained from Spartan; list each compound from highest to lowest frequency.
 - c. A Table of actual frequencies from the IR instrument; list each compound from highest to lowest frequency.
The order of frequencies may be different for each method.
 - d. Cut and paste spectra into a WORD document and attach to a notebook page(s). You may shrink the spectra to fit 3 or 4 spectra on a page.

II. A short Discussion of your Results.

Briefly compare the order of bond strength from each method (one or two paragraphs) then provide answers to the following (a-d):

- a. Which compound has the higher frequency, the acid chloride or the ketone? Explain why one is higher than the other.
- b. Which compound has the higher frequency, the amide or the ketone? Explain why one is higher than the other.
- c. Which compound has the higher frequency, the ester or the amide? Explain why one is higher than the other.

d. Which compound has the higher frequency, 4-hexen-3-one or 2-hexanone? Explain why one is higher than the other.

To help develop your answers to these questions, assume that aldehydes and ketones have a "normal" C=O frequency of about $1710 - 1715 \text{ cm}^{-1}$, the "typical" C=O frequency. Having said that, some carbonyl functional groups have C=O frequencies higher than a "typical" absorption and some functional groups have a C=O frequency that is lower than the "typical" value.

For compounds that have a higher than normal frequency, consider the presence of an electron withdrawing heteroatom bonded to the carbonyl carbon which generally increases the frequency of absorption due to the electron withdrawing effect by the heteroatom. The electron density is withdrawn from the carbonyl oxygen lone pairs and the result is to increase the electron density between the carbonyl carbon and the carbonyl oxygen, hence making this a stronger bond. This is an inductive effect.

For compounds that have a lower than normal frequency, be sure to read about resonance effects in your WADE text (pp. 523-528) for an explanation which you should use to develop your answers. Briefly, if there is a heteroatom bonded to the carbonyl carbon, the lone pairs on the heteroatom may be "pushed" towards the carbonyl carbon which will produce a resonance structure in which the C=O bond is converted into a C-O bond, which is a weaker bond. This is a resonance effect.

Your grade for this report will be based mostly on your correct answers to these questions.