Alan Yu

Organic Lab 309:03

Santanu Malakar

Experiment 13: Investigation of Chemical bond by IR

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Purpose:

The purpose of this experiment is to determine different bonds by IR.

Equations: NONE

Mechanisms: NONE

Amounts and Properties: NONE

Hazards and Safety:

Compounds may be harmful if inhaled or absorbed through skin. Avoid contact and inhalation. Gloves and dispose under marked containers under the hood.

Procedure:

Estimating IR:

1. Write resonance structures for all test compounds.
2. Predict based on resonance structures of the ketone bond.
3. List compounds in order of their carbonyl frequencies from high to low.
4. Model in program to estimate frequency of bond in each compound.

The purpose of writing resonance structures for all the test compounds is to give a prediction of each compound's wavenumber to rank them. The more resonance structures that can decrease the double bond character which creates a lower wavenumber for the stretch.

Obtaining IR:

1. Record IR and determine wave number of each compound's carbonyl band.
2. Calculate vibrational frequency of each compound's carbonyl group from wave number of its carbonyl group.

After acquiring the IR, the vibrational frequencies of each compound can be found and used to prove or disprove the estimated values.

Estimation:

Calculations:

Wavelength = speed of light * wavenumber

Speed of light = 3*10^10 cm/s

Dimethylformamide:

Wavelength = c * 1673.38 → 5.02*10^13 Hz

2-Heptanone:

Wavelength = c * 1715.56 → 5.15*10^13 Hz

Heptanal:

Wavelength = c * 1720.56 → 5.16*10^13 Hz

Ethyl Butyrate:

Wavelength = c * 1733.70 → 5.20*10^13 Hz

Ethyl Tricholoroacetate:

Wavelength = c * 1756.43→ 5.27*10^13 Hz

Discussions:

The prediction from lowest to highest wavenumber was: dimethylformamide → 2-Heptanone → Heptanal → Ethyl Butyrate → Ethyl Trichloroacetate. The reasoning for this was that dimethylformamide had a nitrogen group which allowed the resonance structures for that compound to create greater s character than all of the other compounds. Comparing 2-Heptanone and Heptanal, 2-Heptanone has 3 potential resonance structures while that of Heptanal only being able to produce 2 resonance structures. This allowed 2-Heptanone to have a larger s character than Heptanal. For Ethyl Butyrate, since one of the resonance structures that is able to be formed has an Oxygen group, that structure isn't as important as the other two. For the ethyl trichloroacetate since a resonance structure that is produced would be with a carbon with three withdrawing groups, the positive charge on that structure is destabilized making the resonance structure not impactful.

Conclusions:

Since there is a nitrogen group on dimethylformamide, the resonance structures that are created are all impactful. With the two seven length compounds, one creates more resonance structures than the other so the one being able to create more would be more impactful on the s character of the bond. For the other two structures, resonance structures with oxygen are ignored if there was a third one that was able to be made, but oxygen is a donating group with stabilizes the positive charge. With withdrawing groups, the charge is delocalized which mitigates the effect of a resonance structure. In conclusion, if the structures that are made are with withdrawing groups, the carbonyl bond increases in strength, and with donating groups, the carbonyl bond decreases in strength. The more s character for a bond, the lower the wavenumber.

Exercises:

4.