Lab Report: Predicting and Interpreting IR Spectra

Procedure

1. Have Your Molecule Name Here

Your Ethanol Name: _____

Your Acetone Name: _____

Your Styrene Name: _____

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2. Building the Molecule in QOOL

Describe how you constructed your molecule:
(Provide a step-by-step description in 2-3 sentences of how you built each of your molecules in QOOL.)

Optimize the Geometry:

- Before running any calculations, optimize the molecular geometry to minimize energy and achieve a realistic conformation using QOOL's optimization tool.

Submit Your Molecule Model Screen Shot Here:

Ethanol:

Acetone:

Styrene:

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3. Setting Up the IR Spectrum Calculation

- **Upload Your Set Up for Calculation Screenshot Here:**

Ethanol:

Acetone:

Styrene:

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4. Running the Calculation

Submit the Job:

- Review all settings to ensure accuracy.
- Submit the calculation and wait for it to complete.

Your Job # for each of your molecules:

Ethanol:

Acetone:

Styrene:

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5. Analyzing the IR Spectrum

Access the Results:

- Once the calculation is complete, open the IR spectrum generated by QOOL.

Identify Absorption Peaks:

- Examine the spectrum to locate key absorption peaks.
- Record the wavenumbers (in cm^{-1}) of significant peaks.

Assign Peaks to Functional Groups:

- Use IR spectroscopy reference charts to correlate observed peaks with specific bond vibrations and functional groups.

Interpret the Spectrum:

- Analyze how the peaks correspond to the molecular structure of your molecule.
- Consider factors like bond types, functional groups, and molecular symmetry.

Upload Your IR Spectrum Table Here:

Ethanol:

Acetone:

Styrene:

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6. Data Recording

Prepare a table for each compound to record the observed peaks and their assignments.

Table: IR Spectrum Key Peaks

Observed Wavenumber (cm^{-1})	Assigned Vibration	Functional Group

Observed Wavenumber (cm^{-1})	Assigned Vibration	Functional Group

Observed Wavenumber (cm^{-1})	Assigned Vibration	Functional Group

(Add or remove rows as necessary.)

Post-Lab Questions

1. Why is the O-H stretch in ethanol broad compared to other absorption peaks?

(Your answer here.)

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2. How does hydrogen bonding influence the IR spectrum of ethanol?

(Your answer here.)

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3. Explain why the C=O stretch in acetone appears as a strong, sharp peak.

(Your answer here.)

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4. What factors affect the exact position of the carbonyl stretch in the IR spectrum?

(Your answer here.)

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5. Identify the peaks associated with the aromatic C-H stretches in styrene.

(Your answer here.)

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6. Discuss how conjugation in the aromatic ring affects the absorption frequencies.

(Your answer here.)

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7. Compare the IR spectra of ethanol and acetone. How do the spectra reflect differences in their functional groups?

(Your answer here.)

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8. What challenges might you face when interpreting the IR spectrum of a molecule with multiple functional groups?

(Your answer here.)

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9. How can IR spectroscopy be used in conjunction with other analytical techniques for structural determination?

(Your answer here.)

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10. Discuss the importance of the fingerprint region (1500-500 cm^{-1}) in IR spectroscopy.

(Your answer here.)

Conclusion

(Summarize your findings and what you learned from the lab. Highlight the effectiveness of computational IR spectroscopy in identifying functional groups and understanding molecular structures.)

References

- **Textbook:** McMurry, J. "Organic Chemistry," 10th Edition, Chapters on Spectroscopy.
- **QOOL User Guides:** *(Include any tutorials or guides you used.)*
- **IR Spectroscopy Reference Charts:** *(List any charts or online resources you used for peak assignments.)*

Appendix

(Include any additional data, calculations, or images that support your lab report. For example, screenshots of your molecular models or IR spectra.)