

## Organic Functional Groups

<b>Purpose</b>	The objective of this experiment is to recognize characteristic peaks of organic functional groups in Raman spectra.																								
<b>References</b>	1 Vein, D. K.; Colthup, N. B.; Fateley, W. G.; Grasselli, J. G. <i>Infrared and Raman Characteristic Frequencies of Organic Molecules</i> . Academic Press, Inc.; San Diego, CA, 1991.																								
<b>Apparatus</b>	Delta Nu Raman Spectrometer and accessories 1 mL glass vials Pipettes																								
<b>Chemicals</b>	These are common organics found in a lab. Substitutes are possible.  <table><tr><td>Hexane</td><td>Heptane</td><td>2, 2, 4 trimethylpentane</td><td>cyclohexane</td></tr><tr><td>1-hexene</td><td>3-hexene</td><td>NN dimethylformamide</td><td>1-heptyne</td></tr><tr><td>ethyl acetate</td><td>acetone</td><td>formaldehyde</td><td>2-butanone</td></tr><tr><td>butyl ether</td><td>ethyl ether</td><td>acetaldehyde</td><td>benzonitrile</td></tr><tr><td>acetonitrile</td><td>ethanol</td><td>1, 4-butanediol</td><td>ethanol</td></tr><tr><td>2-propanol</td><td>triethylamine</td><td></td><td></td></tr></table>	Hexane	Heptane	2, 2, 4 trimethylpentane	cyclohexane	1-hexene	3-hexene	NN dimethylformamide	1-heptyne	ethyl acetate	acetone	formaldehyde	2-butanone	butyl ether	ethyl ether	acetaldehyde	benzonitrile	acetonitrile	ethanol	1, 4-butanediol	ethanol	2-propanol	triethylamine		
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<b>Theory</b>	The entire spectrum of a chemical is its fingerprint. Each peak in that spectrum, however, is characteristic of a piece of that chemical's structure. By analyzing different chemicals with similar characteristics, the peaks themselves can become fingerprints of functional groups. By using Raman spectroscopy to do this analysis, instead of IR, the need to destroy the sample by making a KBr pellet is eliminated. The nondestructive nature of Raman spectroscopy can be very useful when the amount of sample material is very limited.																								
<b>Procedure</b>	<p><b>Part 1: Analysis of Known Samples</b></p> <p>Take a Raman spectrum of each of the above chemicals integrating for 10 seconds. Print and label each spectrum.</p> <p><b>Part 2: Determination of Unknown Samples:</b></p> <p>Obtain a vial containing an unknown organic solvent and take a Raman spectrum of the sample as before.</p>																								

**Treatment** Complete the chart with the frequencies observed in the spectra and label the spectra with the same vibrational identifications shown in the chart.

Functional group	Chemical	Literature Frequencies( $\text{cm}^{-1}$ ) <sup>1</sup>	Observed Frequencies( $\text{cm}^{-1}$ )
Alkane	1. hexane	$-(\text{CH}_2)_n-$ in phase twist 1305-1295	
	2. heptane	$-(\text{CH}_2)_n-$ in phase twist 1305-1295	
Branched Alkanes	3. 2,2,4 trimethylpentane	isopropyl deformation 1170 835-795 1345 tert. butyl deformation 1250 1205 930	
	4. cyclohexane	Breathing 822 boat isomer 802 chair isomer	-----
Alkene	5. 1-hexene	C=C double bond str. 1650	
Alkyne	6. 3-hexyne	disubstituted C triple bond C str. 2250-2200	
	7. 1-heptyne	monosubstituted C triple bond C str. 2130-2100	
Amide	8. NN dimethyl formamide	C=O str. 1695-1630 NH or $\text{NH}_2$ str. 3300	-----
Ester	9. ethyl acetate	C=O str. 1750-1715	
		C—O str. 2 bands 1100-1000	
Ketone	10. acetone	C=O str. 1700	
	11. 2-butanone	C=O str. 1700	
Aldehyde	12. formaldehyde	C—H str. doublet 2870-2695 C=O str. 1740-1730	---
	13. acetaldehyde	C—H str. doublet 2870-2695 C=O str. 1740-1730	
Ether	14. butyl ether	C—O—C str. 890-820 C—O—C bend 500-400	-----
	15. ethyl ether	C—O—C str. 890-820 C—O—C bend 500-400	
Nitrile	16. benzonitrile	C triple N str. 2240-2220	
	17. acetonitrile	C triple N str. 2250-2230	
Alcohol	18. ethanol	C—C—O str. 900-800	
	19. 2-propanol	C—C—O str. 900-800	
	20. 1,4-butandiol	C—C—O str. 900-800	
Amine	21. triethylamine	C—N—C antisym. str. 1180-1130 C—N—C sym. str. 900-850	



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# Lab 2

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### Questions

- 1) Using the information in the above chart and that contained in the spectrum of the unknown sample, determine the unknown organic compounds.
- 2) Comment on the reasoning for the identification of the unknown sample.
- 3) Explain why the low wavenumber region ( $200\text{-}1000\text{ cm}^{-1}$ ) is often called fingerprint region and the higher range ( $1000\text{ - }3000\text{ cm}^{-1}$ ) is called the characteristic region.