

3rd year Spectroscopy, NUIG: 2008-09, A.G. Ryder

5 CORE TOPICS:

1. General Features of Spectroscopy (~½L).
2. Pure Rotational Spectroscopy (~1L).
3. Vibrational Spectroscopy (~0.75L).
4. Vibrational-Rotational Spectroscopy (~0.75L).
5. Raman Spectroscopy (1L).

Combing all the topics should give one a good appreciation of vibrational and rotational spectroscopy.

SPECTROSCOPY TEXTS:

- *Elements of Physical Chemistry*, Atkins & DePaula, 4th ed.: Chapter 19 (All).
- *Physical Chemistry*, Atkins & DePaula, 8th ed.: Chapter 13.
- *Foundations of Spectroscopy*, Duckett & Gilbert, Oxford Chemistry Primer. Chapt. 2-3.
- *Molecular Spectroscopy*. J.M Brown, Oxford Chemistry Primer. Chapt. 1-6.
- *Fundamentals of Molecular Spectroscopy*, 4th ed. Banwell & McCash, Chapters 1-4

SPECTROSCOPY WEBSITES:

Rotational / Microwave:

- <http://hyperphysics.phy-astr.gsu.edu/HBASE/molecule/rotrig.html#c3>
- <http://dsnra.jpl.nasa.gov/IMS/>

Rotational-Vibrational spectroscopy:

- <http://www.chemistry.nmsu.edu/studntres/chem435/Lab9/intro.html>
- <http://web.mit.edu/5.33/www/lec/spec5.pdf>
- http://www.chemistrydaily.com/chemistry/Rotational_spectroscopy

Raman spectroscopy:

- <http://epsc.wustl.edu/haskin-group/raman.htm>
- <http://www.deltanu.com/dn06/tutorials.htm>
- http://www.fis.unipr.it/phevix/raman_tutorial.html
- http://www.avaloninst.com/content/raman_information/index.htm

PROBLEM SHEET:

Problem sheet handed out at 1st Quantum lecture.

<u>DETAILED COURSE OUTLINE:</u>	<u>LEARNING OUTCOMES</u>
1 <u>General Features of Spectroscopy:</u> <ul style="list-style-type: none"> ○ Introduction & review of 2nd year. ○ Transitions & probabilities. ○ Populations of energy levels & consequences. ○ Linewidths. ○ Bohr Condition. 	Be able to show an understanding of the theories behind spectroscopy. Be able to calculate populations of energy levels and spectral line widths.
1 <u>Pure Rotational Spectroscopy:</u> <ul style="list-style-type: none"> ○ Microwave spectroscopy. ○ Moments of inertia and angular momentum. ○ Rotational Energy levels & populations of E levels. ○ Degeneracy & selection rules. ○ Selection rules. ○ Centrifugal distortion. 	Understand and be able to explain rotational spectroscopy, calculate energy levels, moments of inertia, and energies of spectroscopic transitions.
1 <u>Vibrational Spectroscopy:</u> <ul style="list-style-type: none"> ○ Introduction & selection rules. ○ Potential energy level diagram. ○ Anharmonicity ○ Morse Potential Energy curve. ○ Overtones & Hot bands. 	Understand and be able to explain vibrational spectroscopy, terms and concepts. Calculate reduced masses, energy levels & transitions, force & anharmonicity constants, & number of vibrational modes.
1 <u>Vibrational-Rotational Spectroscopy :</u> <ul style="list-style-type: none"> ○ High resolution spectroscopy. ○ Selection Rules. ○ P-Q-R branches. ○ Combination Differences. ○ Calculating energies of transitions. 	Understand and be able to explain high resolution vibrational spectroscopy and the selection rules. Be able to calculate energy levels and rotational constants.
1 <u>Raman Spectroscopy:</u> <ul style="list-style-type: none"> ○ Overview and Instrumentation. ○ Selection rules & their consequences. ○ Rotational Raman. ○ Comparison between MIR and Raman. ○ Raman Microscopy. 	Understand and be able to explain Raman spectroscopy and the selection rules. Describe the instrumentation and the pros/cons of the method.