This exam might cover any material in the textbook that we have covered this semester although the main focus will be that material that we have seen in the second half of the semester (vibrational, rotational, Raman and NMR). A review of the key things that you should have learnt from this class are listed below. There will be slightly more emphasis on the material on Raman and NMR spectroscopy. For the in-class portion of the exam you can use your notes and the textbook (Bernath) – see the last point for some extra tips. For the take-home portion of the exam you can use all your notes and text books and any other sources you wish to find.

1. Understand the factors that affect the lineshapes of spectroscopic transitions.
2. Be able to identify symmetry elements and assign point groups for a given molecule (using the flow chart from the text book). Be comfortable using character tables for the many things we have used them for this semester (including identifying the symmetry of vibrational modes (e.g. $a_{1u}$ etc) and assigning the IR and Raman activity of those modes).
3. Understand the definitions of reducible and irreducible representations and be able to break down a reducible representation into a direct sum of irreducible representations using the characters for a particular point group. We’ve used this in several instances throughout the course so be sure you can apply it to any of the problems that we have utilized it in.
4. Be able to use direct product tables (we’ve mainly used these in determining whether the transition dipole moment integral is zero or non-zero).
5. Understand the concepts of angular momentum that we introduced in the atomic spectroscopy chapter and have developed in later chapters. Understand the basis of such subjects as Russell-Saunders coupling, spin-orbit splitting, Zeeman effect, Stark effect, hyperfine splittings (in connection with atomic spectroscopy).
6. Know Hund’s rules and be able to determine the lowest energy term for an electronic configuration (an example is shown for the $d^4$ case in Figure 5.8 on page 135).
7. Understand how vibrational (and rotational structure) appears in electronic spectra. An understanding of the Franck-Condon overlap integral and its effect on intensities is very important. Note that any rotational structure discussions will be restricted to singlet-singlet electronic transitions.
8. Be familiar with the use of the Walsh correlation diagrams for figuring out whether a molecule will be linear or bent. If necessary, you will be given the Walsh correlation diagram for the specific type of system in the question so be able to use them.
9. Understand where the vibrational structure comes from in the electronic spectra of polyatomics.
10. You should have detailed understanding of electronic spectroscopy techniques like ZEKE, LIF etc. but the need to explain these techniques won’t arise on the exam.
11. Be able to identify various parameters on a potential energy curve for ground and excited electronic states (like Figure 9.27, page 333). Identify things like the dissociation energies ($D_0$, $D_e$) and so on. Know what is meant by the zero point energy and how to estimate a vibrational frequency from it.
12. Be able to classify molecules as spherical tops, asymmetric tops and so on based on relations between the moments of inertia.
13. Make sure you know the rigid rotor energy expressions for linear (6.27) and symmetric top molecules (both prolate tops (6.99) and oblate tops (6.100)). Equations (6.29) and (6.32) are very useful. Be able to use these energy expressions to derive the equation for the transition frequency (such as that for a linear molecule in (6.40)).
14. Understand what centrifugal distortion is and how it affects the spacing of the energy levels. Know how it is included in the energy expressions for the various types of rotor.

15. Understand the effect that vibrational angular momentum will have on a pure rotational spectrum. This leads to the introduction of the \( l \) quantum number. Be able to explain \( l \)-type doubling. The key equation that governs the splitting is \( \Delta v = qJ(J+1) \) – note that the splitting is expected to increase as the \( J \) level increases.

16. Understand how the energy levels of an asymmetric rotor are labeled using a symmetric top basis. Be able to identify transitions as \( a-, b- \) or \( c- \) type.

17. Understand nuclear hyperfine interactions and Stark effects as they apply to microwave spectroscopy.

18. Make sure you know the form of the harmonic oscillator wavefunctions (at least for the first few vibrational levels) and the HO energy expression (7.25). Know how an AHO differs from a HO. Know the AHO energy expression (7.34).

19. Vibration-rotation spectra for diatomics and polyatomics. The main focus involved diatomics and you should understand this fully, including the difference in the appearance of the spectra (think about \( P, Q, R \) branches and whether or not they are present). Of course, in certain circumstances, nuclear spin statistics will play an important role in governing intensity of the various transitions and can even lead to missing \( J \) levels. Be able to carry out a nuclear spin statistical analysis for a given molecule and be able to predict how the spectrum will look in terms of intensity alternation. You’ll need to be able to use the equations for determining the relative statistical weights of the symmetric and antisymmetric nuclear spin functions and to be able to put these nuclear spin functions together with the other functions (electronic, vibrational and rotational) to determine the overall appearance of the spectrum.

20. Understand the concepts behind Raman spectroscopy. Know the difference between Rayleigh, Stokes and Anti-Stokes scattered radiation.

21. Understand the various types of Raman spectra (vibration, rotation or vibration-rotation). Because of the different selection rules for this technique, this technique is complementary to other spectroscopic techniques and so you should be clear on what information might be available from Raman that we may not be able to obtain in other ways.

22. Know what is meant by the depolarization ratio and what it might tell us.

23. The spin resonance material that we covered in class will focus only on NMR. Therefore you should know the basics behind NMR. Be able to calculate the Larmor precession frequency of a particular nucleus and know what factors govern this. Obviously definitions of things like chemical shift, direct or indirect spin-spin couplings, Nuclear Overhauser effect and so on should be things you can explain.

24. Make sure you have an understanding of 2D-NMR and the information we can obtain with it.

25. Finally, make absolutely sure you know where to find various topics in your textbook. Since the final will be an open book exam you don’t want to spend hours leafing through the book to find the information you want. Because you have access to the facts in your textbook, it’s a safe bet that the exam questions will focus on you applying those facts rather than just being able to find them in the book and copy them down (bummer!). Know where the relevant things (like the selection rules, for instance) are in the book for various techniques. Also make sure that your class notes are in good shape (go back and clarify them or add details for subjects that are not clear or are not fully enough explained) otherwise they will be of little (or no) use to you in the exam. And finally, don’t blow off your studying because you feel that you will have all the information to hand in your notes and textbook – you still need to understand the material and be able to know what knowledge to apply to problems.