Molecular Symmetry and Spectroscopy

Molecular Symmetry and Spectroscopy:	Astronomy 9701/Physics 9524
Lecturer:	Prof. Martin Houde mhoude2@uwo.ca http://www.astro.uwo.ca/~houde
Location:	PAB Chart Room (Room 213e).
Lectures:	Monday, Wednesday, and Friday, from 11:30 am to 12:30 pm
Recommended text:	**Fundamentals of Molecular Symmetry**, (Institute of Physics), by Philip R. Bunker and Per Jensen.
Useful references:	See the bibliography below.

Contact information:

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I can be reached at my office, especially after class where I will do my best to reserve time to answer your questions. I can also be reached during the week through e-mail for simple inquiries, or to make an appointment. I will try to reply to e-mails within two working days of reception.

Students should regularly check my website to find out about course material or announcements (at http://www.astro.uwo.ca/~houde/courses/astronomy_9701physics_9524.html).

Evaluation: The students will mainly be evaluated trough a series of assignments and exams, and a final project at the end of the semester. In case that were to happen, students absent on an examination day may be allowed to take a make-up exam if they present a note from a medical doctor within a reasonable amount of time. Similar consideration may be given under other exceptional circumstances.

Assignments: You will receive a few lists of suggested problems during the semester. I will indicate, for each list, which problems should be turned in for your assignments. Students will be allowed to discuss the material amongst them, *but each student will have to turn in her/his own copy of the assignment*. Assignments must be turned in at the requested date. However, a student may miss a due date *once* during the semester, and hand in the late assignment on the following lecture day without incurring any penalty. Otherwise, for *every day* for which they are late, assignments will automatically have a third of the maximum number of points subtracted from their total.

Plagiarism: Students must write their assignments on their own. Whenever students take an idea, or a passage, or a solution to a problem from another author, they must acknowledge their debt both by using quotation marks where appropriate and by proper referencing such as footnotes or citations. Plagiarism is a major academic offence (see Scholastic Offence Policy in the Western Academic Calendar)

Description

This course is intended to provide the student with a thorough introduction to molecular spectroscopy. The emphasis will be on understanding molecules and their spectra by making use of their symmetry (more precisely the symmetry of the Hamiltonian) for problem solving. The necessary tools will be developed to explain the electronic, vibrational, and rotational spectroscopy of simple molecules. We will concentrate on situations involving interactions between gas phase molecules and weak electromagnetic radiation.

Course Outline

1. Review of Quantum Mechanics.
2. Electronic states (Born-Oppenheimer approximation; spin and Pauli's exclusion principle).
3. The Rovibrational Hamiltonian (space- and molecule-fixed coordinate systems; Euler angles; Eckart conditions; principal moments of inertia)
4. Vibrational and Rotational states (harmonic vibrational and rigid rotator Hamiltonians; symmetric, spherical, and asymmetric top molecules; linear molecules).
5. Geometrical symmetry.
6. Hamiltonian symmetry.
7. Symmetry groups of rigid molecules.
8. Nuclear spin, statistical weights, and hyperfine structure.
9. Symmetry of the electronic wave functions.
10. Symmetry of the rotation-vibration wave functions.
11. Selection rules.
12. Symmetry groups of non-rigid molecules (Ammonia).

Bibliography

1. Bunker, P. R. and Jensen, P. 2005 **Fundamentals of Molecular Symmetry** (Bristol: Institute of Physics). *This is a very recent book on the subject of molecular symmetry. It is written at the student level, but uses a modern approach to the subject. The authors endeavour to explain how "symmetry" can be used to solve problems in spectroscopy and in molecular orbital theory. This will be the book used in this course.*

2. Bunker, P. R. and Jensen. P. 1998 **Molecular Symmetry and Spectroscopy** 2nd edition (Ottawa: NRC Research Press). *This book presents a very exhaustive treatment of molecular symmetry and spectroscopy at the researcher level. This is my favourite book on the subject. I will often use it to complement material presented in class.*

3. Wilson, E. B. Jr., Decius, J. C., and Cross, P. C. 1980 **Molecular Vibrations** (New York: Dover). *A true classic. Although it only deals with vibrations, it establishes a lot of the fundamentals that are needed for the more general treatment of molecular spectroscopy.*

4. Atkins, P. W. and Friedman, R. S. 1999 **Molecular Quantum Mechanics** 3rd edition (Oxford: Oxford University Press). *A fantastic book on the physics of molecules. It is written at a very accessible level, while at the same time being very thorough. Highly recommended.*

5. Cohen-Tannoudji, C., Diu, B., and Laloë, F. 1996 **Quantum Mechanics** (2 volume set) (New York: Wiley). *I guess everybody has a favourite textbook on Quantum Mechanics; this is mine (although I use the original edition in* la langue de Molière*).*