CHEM*3870 Molecular Spectroscopy
WINTER 2009
COURSE OUTLINE

Instructor: **Professor John D. Goddard**
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Extension: **53102** **Office: 340 MACN**

Recommended Texts:

F. A. Cotton, Chemical Applications of Group Theory. 3rd Ed. Wiley (1990).

D. C. Harris, Symmetry and Spectroscopy: An Introduction to Vibrational and Electronic Spectroscopy. Oxford University Press (1978). (Dover edition 1989).

Calendar Description:

CHEM*3870 Molecular Spectroscopy W(3-3) [0.50]: This course covers elementary group theory with applications to molecular spectroscopy and provides a continuation of the topics of rotational, vibrational, and electronic spectroscopy and their applications in chemistry from CHEM*2070.(Offered in odd-numbered years.)

Prerequisite(s): **CHEM*2070, (MATH*2150 or MATH*2160)**

Topics (Order may change.):

1. Symmetry. Symmetry Operators. Symmetry Operations. Symmetry Elements.
2. Mathematical Definition of a Group. Examples of Groups. Group Multiplication Tables. Rearrangement Theorem. Cyclic Groups. Abelian Groups. Subgroups. Classes.
3. Products of Symmetry Operations. Equivalent Symmetry Operations. Relations among Symmetry Operations.
4. Point Group Symmetry. High Symmetry Groups. Linear Molecules. Platonic Solids. Classes of Symmetry Operations. Symmetry Classification of Molecules.
5. Review of Vectors and Matrices. Definition Matrix. Rows. Columns. Vectors. Equality Two Matrices. Matrix Multiplication. Matrices and Geometric Transformations. Determinants. Adjoint. Inverse. Special Matrices. Symmetric. Diagonal. Orthogonal.
6. Matrix Multiplication. Block Factorization. Character. Conjugate Matrices. Representation Geometric Transformations by Matrices. Reflection. Inversion. Rotation. Vectors. Scalar Product. Representations of Groups. Statement Great Orthogonality Theorem. Consequences Great Orthogonality Theorem. Relation Reducible and Irreducible Representations. Character Tables. Representations Cyclic Groups.

7. Group Theory and Quantum Mechanics. Direct Product. Energy Integrals. Electric Dipole Transition Moment Integrals. Symmetry Adapted Linear Combinations.
8. Review of Rotational, Vibrational, and Vibrational-Rotational Spectra of Diatomic Molecules. Selection Rules.
9. Polyatomic Spectra. Rotational Spectra. Moments of Inertia. Selection Rules.
10. Polyatomic Vibrations. Normal Modes. Symmetry of Normal Modes. Interaction with Radiation. Selection Rules. Infrared and Raman Spectra. Force Constants, Overtones and Combinations.
11. Electronic Spectroscopy. Franck-Condon Principle. Selection Rules. Pure Electronic Transitions. Vibronic Transitions. Fate of Electronic Excitation Energy. Fluorescence. Phosphorescence.

Class Schedule:

Lectures:		**Monday Wednesday Friday**	**09:30 – 10:20**	**MACN 118**
Laboratories:	**Section 1**	**Tuesday**	**14:30 – 17:20**	**SCIE 3106**
	Section 2	**Wednesday**	**14:30 – 17:20**	**SCIE 3106**
	Section 3	**Thursday**	**14:30 – 17:20**	**SCIE 3106**

Evaluation:

Laboratory Component	**25**
Term Test (Wednesday Feb. 25, during lecture time)	**25**
Final Exam (Wednesday Apr. 08, 08:30 – 10:30)	**50**
(As Scheduled by the Registrar.)	

TOTAL	**100**

Lecture notes and other course material are available at

http://www.chemistry.uoguelph.ca/educmat/chm387/