

CBC 727 - Molecular Electronic Structure and Spectroscopy

Aims and Objectives

To survey modern spectroscopy and structural theory at an advanced level.

Syllabus

Molecular mechanics; symmetry; quantum mechanics; electronic structure of atoms; electronic structure of diatomic molecules; self-consistent-field (scf) method; empirical and semiempirical methods; electron correlation methods; qualitative molecular orbital theory; comparisons of computational methods; calculation of molecular properties; molecular modeling software. Rotational spectroscopy; vibrational spectroscopy; atomic spectroscopy; electronic spectroscopy of diatomic molecules; electronic spectroscopy of polyatomic molecules; photoelectron and related spectroscopy; Auger electron and x-ray fluorescence spectroscopy; lasers and laser spectroscopy; magnetic resonance spectroscopy; excitons: theory and applications.

Assessment

Written Exam: 40%

Continuous assessment: 60%

Prerequisites

CBC 314 Physical and Biophysical Chemistry 2 or Division approval