AE1-PHY. Electronic structure and vibration-rotation spectroscopy

Person in charge: Prof. Thérèse HUET, Physics Department/PhLAM, Room P5-133

Part A. Electronic structure and ab initio methods

Chapter 1. Usual approximations and the Hartree-Fock method

1.1 Molecular Hamiltonian

1.2 Born-Oppenheimer approximation.

1.3 Hartree-Fock method.

1.4 Atomic orbitals basis sets.

Chapter 2. Treatment of the electronic correlation

2.1 The limits of the Hartree-Fock model

2.2 Definition of the electronic correlation: static and dynamic correlations

2.3 Correlated methods:

- Perturbation methods
- Configurations interaction and the problem of size-extensitivity
- « Coupled Cluster » methods
- Multiconfigurational methods
- Density functional method

Part B. Vibration-rotation spectroscopy

Chapter 1. Molecular energy levels

1.1 Eckart conditions.

1.2 Kinetic energy partition.

1.3 The rigid rotor.

1.4 The harmonic and anharmonic oscillator.

1.5 The semi-rigid rotor.

Chapter 2. Molecular spectra

2.1 Line intensities.

2.2 Selection rules.

2.3 Spectra of vibration-rotation.

2.4 Spin statistics.

Chapter 3. Spectroscopy of diatomic radicals

3.1 Angular momenta.

3.2 Relativistic Hamiltonian.

3.3 Hund cases.

3.4 Energy levels.

AE2-PHY. Radiative transfer in the atmosphere

Person in charge: Prof. Philippe DUBUISSON, Physics Department/LOA, Room P5-333

1. Principles in atmospheric radiation:
    - Radiation quantities and units
    - Atmospheric composition and structure
    - Blackbody radiation
    - Radiative transfer equation
2. Atmospheric Absorption:
    - Molecular line absorption
    - Spectroscopic databases for molecules of atmospheric interest
    - Standard methods for the calculation of gaseous absorption
3. Scattering of polarized radiation:
    - Rayleigh-Gans scattering, Mie scattering
    - Radiation scattering by spherical and non-spherical particles
    - Applications to aerosol and cloud particles
    - Polarized radiation
4. Radiative transfer equation (forward problem):
    - Analytical solutions for absorbing media
    - Radiative transfer equation in scattering and absorbing media
    - Standard numerical codes for solar and thermal radiative transfer
    - Simulation of satellite or ground-based observations
5. Examples of inverse problems in radiative transfer:
    - Lidar remote sensing of clouds and aerosols
    - Principles of solar passive remote sensing from space observations
    - Retrieval of aerosol properties from solar photometry
    - Principles of infrared passive remote sensing from space observations

AE3. Physics and chemistry of the atmosphere

Person in charge: Prof Denis PETITPREZ, Chemistry Department/PC2A, Room C11-7

Part I: Physics of the atmosphere

A – Description of the Earth's atmosphere

I - Composition

II – Vertical structure

III – Vertical distribution of gaseous constituents

B - Atmospheric motions

I - Scales. Origin of motions. Time of transport/ lifetime.

II – Atmospheric dynamics: basic equations

C – Radiative processes

I - Radiative energy

II – Radiation-Atmosphere interactions

D – Atmospheric ozone

Part II: Chemistry of the atmosphere

-I- Basics of reactivity and kinetics for the atmosphere sciences

Fundamental principles of gas-phase kinetics.

Elementary reactions and chemical mechanism.

Lifetimes

-II- Chemistry of the troposphere.

Production of OH radicals in the atmosphere.

Basic photochemical cycle of NOx and O3.

Ozone budget.

Oxidation of CO and methane.

Atmospheric Chemistry of NMVOC (nonmethane volatil organic compounds)

Atmospheric chemistry of SO2.

-III- Chemistry of the atmospheric aqueous phase.

Liquid water in the atmosphere.

Gas solubility and Henry's law.

Acidity of precipitation.

Interaction between the gas phase and the condensed phase - Mass transfert

-IV- Aerosol particles .

Knudsen number. Dynamics of a single particles.

Sources, chemical composition and size of atmospheric particles.

Size distribution. Lognormal distribution.

Interaction between the gas phase and the condensed Aerosol measurements

AE4. Advanced spectroscopic techniques for environmental analysis

Person in charge: Prof. Cristian FOCSA, Physics Department/PhLAM, Room CERLA-R01

1 Rotational Spectroscopy
- 1.1 Fourier Transform Microwave Spectroscopy
- 1.2 Supersonic beam technique
- 1.3 Millimeter wave spectroscopy: sources and detection methods
- 1.4 Application: spectra recording and analysis

2 Gas phase THz spectroscopy of atmospheric compounds
- 2.1 Electronic and optoelectronic THz sources for high resolution rotational gas phase THz spectroscopy
- 2.2 Line frequency and line profile analysis for molecules of environmental interest
- 2.3 Detection and quantification of atmospheric compounds in realistic environments
- 2.4 Low resolution rovibrational gas phase THz spectroscopy using broadband sources

3 Vibrational spectroscopy - Raman and infrared
- 3.1 Molecular vibrations
- 3.2 Instrumentation
- 3.3 Applications: sampling, gas phase analysis, aerosols analysis, in situ measurements
- 3.4 Practical work

4 Advanced absorption spectroscopy techniques
- 4.1 Basics
- 4.2 Modern techniques
  - Modulation spectroscopy
  - Background-free spectroscopic approaches
  - Advanced sensitive measurement schemes
- 4.3 Applications of photonic absorption spectroscopy:
  - UV-VIS LED-IBBCEAS
  - Infrared tunable laser absorption spectroscopy (IR-TDLAS)
  - Short-noise limited detection of reactive molecule (OH radical) by FRS
  - Modern PAS technique: QEPAS
  - Doppler-limited high resolution spectroscopy

5 Metrology of trace species by laser induced fluorescence and incandescence
- 5.1 Theoretical and experimental principles of Laser Induced Fluorescence (LIF) and Laser Induced Incandescence (LII)
- 5.2 Application to the measurement of gas and/or particulate environmental pollutants

6 Condensed phase analysis using laser-based techniques
- 6.1 Condensed phase sampling by laser ablation/desorption via electronic or vibrational energy coupling
- 6.2 Ultra-sensitive mass spectrometry detection: principles and instrumentation
- 6.3 Resonance-Enhanced Multi-Photon Ionization (REMPI) via electronic transitions (UV)
- 6.4 LIBS (Laser Induced Breakdown Spectroscopy), space- and time-resolved optical emission spectroscopy, LA/ICP/MS (laser ablation/inductively coupled plasma/mass spectrometry)
- 6.5 Applications to the analysis of complex environmental samples (lab work)

AE5. Observing systems for atmospheric composition: from satellite to in-situ scales

Person in charge: Prof. Philippe GOLOUB, Physics Department/LOA, Room P5-309

- Basis on aerosol chemical composition, microphysical (size distribution, shape), optical and radiative properties, sources and formation processes.

- Basis on radiation-matter interactions (scattering/polarization/absorption/emission) and radiative transfer in the atmosphere (single and multiple scattering).

- State of the art of ground-based and satellite remote sensing sensors dedicated to aerosol and gas characterization (optical, microphysical and chemical column integrated properties). Passive systems (sun/sky-photometer, polarimeter, spectrometer, infrared radiometer, …) mostly providing column integrated properties and active system elastic backscatter, Raman lidar, …, providing vertical distribution of aerosol/gas properties. Available aerosol/gas properties versus instrumental characteristics.

- State of the art for in situ instrumentations (online analyzers for gaseous precursors (NOx, SO2, GC-MS, PTR-MS), mass concentration analyzers and particle counters (SMPS, CPC, TEOM FDMS, beta gauges), chemical composition analyzers (aethalometers, aerosol mass spectrometers (AMS, ACSM, ATOFMS), semi-continuous analyzers (PILS, MARGA).

- Basis on inverse methods (introduction to forward and inverse problems, from simple to advanced approaches)

- Instrumental synergies. Field/Labs. Simple experiments and data analysis form available instruments operating with CaPPA consortium (sun-photometer, elastic backscatter and Raman Lidars, Wind Lidar. Links with in situ observations.

- Presentation of the main atmospheric networks (AERONET, GALION, EARLINET, EMEP, MERA) dedicated aerosol/gas monitoring (instrument, calibration, data quality, data transfer, data processing, aerosol parameters) and current National and European observating systems (ACTRIS, ORAURE, …).

- Presentation of specific field campaigns in different environments and at different scales.

- Tools for analysis (CMB, PMF models, in relation with gaseous pollutants and atmospheric dynamics), backtrajectories.