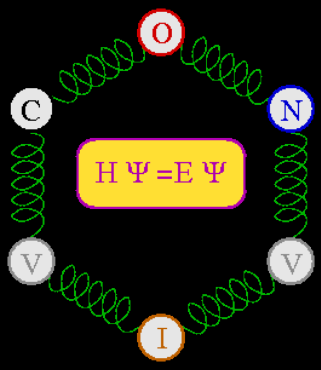
In Silico Astrochemistry



SUMMARY:
The first molecules are thought to have appeared in the Universe as early as $z \approx 2000$, and, ever since, they diversified and have populated most of astrophysical environments. They serve as probes of the physical conditions of many astrophysical objects and as tracers of their past history. They also play an active part in many processes such as cooling of collapsing clouds; accretion of grains and during a protostellar phase, heating and evaporation of ices; synthesis, locking or release of potential biogenic precursors... Our astrochemical knowledge has been build through the interplay of astronomical observations, laboratory experiments and theoretical modelling. The goal of this meteor is to present the input of the latter, in particular the contributions of quantum chemical calculations.

OBJECTIVES

- To provide the fundamentals of astrochemistry in a nutshell, with an emphasis on carbon-bearing molecules of astrobiological interest.
- To develop the ability to use a quantum chemistry computer code to predict or identify molecular spectral signatures.

PREREQUISITES

(Fundamental courses linked to this METEOR)

- General Astrophysics (in particular: The Milky way and its Interstellar Medium)
- Quantum Mechanics : Applications to Astrophysics

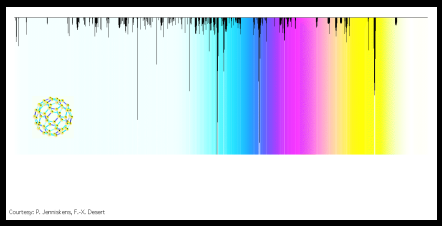
THEORY

by Patrick Cassam-Chenaï

The METEOR will introduce the basics of astrochemistry which makes it so different from the chemistry we are used to on Earth and will offer a glimpse at its diversity: astrochemistry in diffuse clouds triggered by photons versus that in dark clouds triggered by cosmic rays, chemistry in O-rich circumstellar envelopes versus that in C-rich ones, molecules occuring in shock wave regions versus those in quiescent ones, and so on. Pending astrochemical puzzles and debated questions related to the composition of carbonaceous matter in space will be presented. The hypothesis of an exogenic origin of biomolecule precursors will be discussed. Then, the specificities of molecular spectroscopy with respect to atomic spectroscopy will be emphasized. It is the main technique to identify molecules in space and probe their astrophysical environment. Finally, general methods to compute *ab initio* molecular rotation-vibration spectra will be explained.

APPLICATIONS

by Patrick Cassam-Chenaï



The practical work associated to the METEOR will consist in using a computer code implementing the methods taught in the theoretical course, to calculate *ab initio* the vibrational spectra of a molecule. The latter will be chosen in relation with spatial (JWST) or ground based (MATISSE) observations.

MAIN PROGRESSION STEPS

- First half of the period : theoretical courses (3 chapters, oral exam at the end).
- Second half of the period : numerical project, written report at the end.

EVALUATION

- Individual oral examination to assess the understanding of the theoretical part.
- Written group report in the form of a scientific article presenting the numerical results obtained during the project, to assess the practical part.
- The final mark will be half the oral examination half the written report ones.

BIBLIOGRAPHY & RESSOURCES

- Course on Interstellar chemistry
- Molecular spectroscopy in a nutshell
- The CONVIV computer code

CONTACT

☎ +33 4 8915 0524
✉ cassam@unice.fr