VO Theory atomic and molecular data/databases

- Scientific Use cases
    - Identification of lines in observed spectra (ISO, Herschel, Alma, Spitzer, etc...) : spectroscopic data
    - Analysis of spectra for non-ETL media : spectroscopic+collisional data
    - Simulation of Interstellar Medium, circumstellar/planetary/cometary atmospheres : models + spectroscopic data + chemistry (collision, reaction, etc..)
    - Etc ....

Problems

- Uniqueness of data ??
  - Redondant data, non-existing data, data badly identified
- No or bad documentation of data (chain of errors)
- Data not always provided correctly for applications : need processing
- DB :
  - Molecular : JPL, HITRAN, NIST, GEISA, CDMS
  - Atomic : NIST, CHIANTI, VALD, Kurutz Cdrom, ...
  - Private compilations

Solutions ?

- Need to offer a ready to use solution to DB
- Offer a query service with VO output : start simple with specific applications
- UCD vocabulary:
  - Work on the logical structure of data in order to extract UCD
- Very complex problem can be simplified if some of the information is not coded

Why complex ? Ex : excitation rate coefficients

- Linked to a temperature
- Linked to a system given by 2 partners
  - Partners have identification : atom, molecules
    - Molecules or atoms have specifications
- Linked to initial and final states of partners
  - Identification of states
    - Energy levels, quantum numbers, statistical weights, ref.
- Obtained by calculations
  - Uncertainty, ref.
  - With method
  - From cross section

Suite ....

- Cross – sections
  - Uncertainty, ref.
  - With method
  - With basis set
  - With potential energy surface
    - Uncertainty, ref.
    - Basis set
    - Geometries
    - Ab initio method
    - Fitting method

WHAT LEVEL OF CODING ?
Depending on applications and constraints ?