

The Bordeaux Astrochemical Tools



Benjamin Pavone (engineer)

Pierre Gratier

Maxime Ruaud

Valentine Wakelam

**Fabrice Mendes
(engineer)**



Jean-Christophe

Loison

Bordeaux astrochemical tools

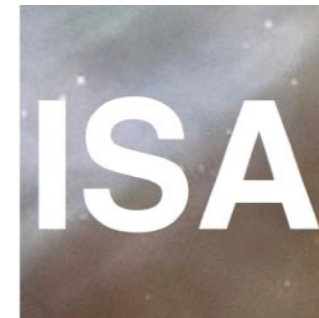
Kinetic Database for Astrochemistry

<http://kida.obs.u-bordeaux1.fr/>



InterStellar Abundance database

<http://isa.obs.u-bordeaux1.fr/>



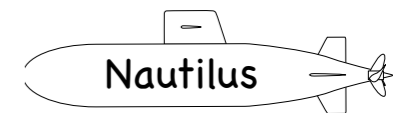
AstroChemical Newsletter

<http://acn.obs.u-bordeaux1.fr/>



Nautilus gas-grain code

(upon request)



Funding



Introduction to



KINETIC
DATABASE
FOR
ASTROCHEMISTRY

What is KIDA?

- Database of chemical reactions and associated parameters for the interstellar medium and planetary atmospheres
- Uncritical compilation of data with detailed information (uncertainties, temperature range, bibliographic reference, etc)
- Online consulting interface
- Form to download list of reactions
- You can contribute by submitting data with cvs templates
- Group of experts advising for the data to be added to the database and give recommendations on key reactions.
- Subsets of chemical reactions for specific applications (Titan atmosphere, Hot Jupiters, ISM)

What type of data?

For gas-phase reactions:

- Temperature dependent partial reaction rate coefficients for bimolecular reactions
- Photodissociation and ionisation rates (integrated over the ISRF radiation field)
- Photodissociation and ionisation rates due to UV photons induced by cosmic-ray particles (Prasad-Tarafdar mechanism)
- Direct dissociation and ionisations rates by cosmic-ray particles

For surface reactions:

- Possible pathways (with branching ratios)
- Activation energies and barrier width

For species:

- Polarizability, dipole moment and enthalpy of formation
- Diffusion and desorption energies

How can you help?

While publishing a paper on physico-chemistry: please make the abstract or the conclusion clear enough to feed the database.

Provide any missing data for species (enthalpy of formation, Inchi codes, images...):

<http://kida.obs.u-bordeaux1.fr/check-species.html>

Templates to submit data to KIDA:

<http://kida.obs.u-bordeaux1.fr/how-to-add-data.html>

demo KIDA

Bordeaux astrochemical tools

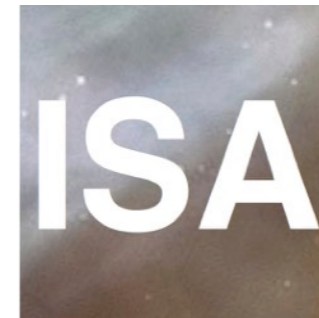
Kinetic Database for Astrochemistry

<http://kida.obs.u-bordeaux1.fr/>



InterStellar Abundance database

<http://isa.obs.u-bordeaux1.fr/>



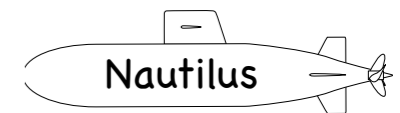
AstroChemical Newsletter

<http://acn.obs.u-bordeaux1.fr/>



Nautilus gas-grain code

(upon request)



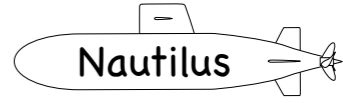
Funding



demo ISA: NH3
Showing ACN

Nautilus: grain chemistry

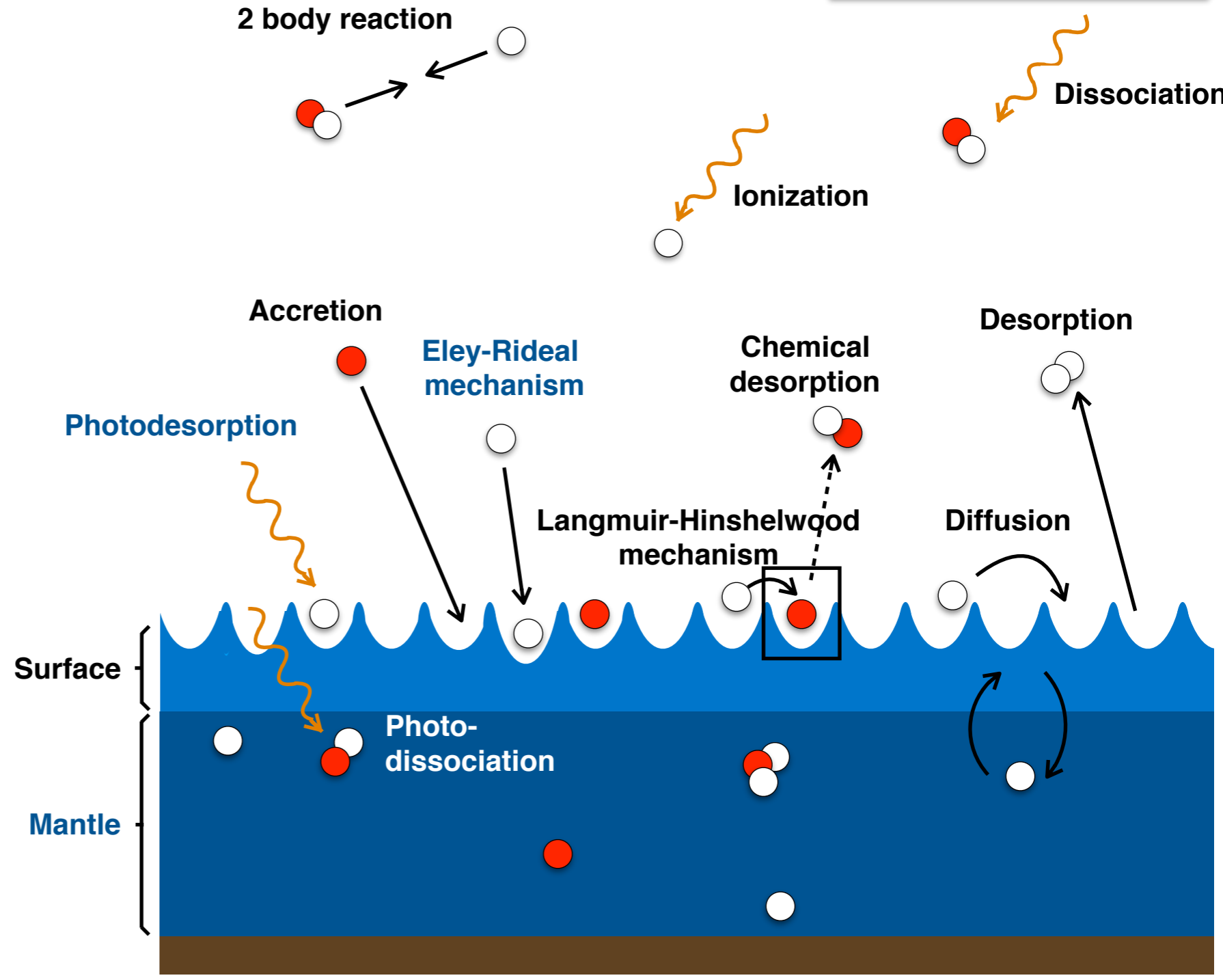
Ruaud et al. (2016)



3-phase model

Mechanisms included in the code:

- Diffusion:
 - Thermal
 - Tunneling effect
- Reaction:
 - Langmuir-Hinshelwood
 - Eley-Rideal
- Desorption:
 - Thermal
 - Chemical
 - Induced by cosmic-rays
 - Photodesorption
- Dissociation:
 - Primary photons
 - Secondary photons



The Nautilus gas-grain code

Original code from Eric Herbst's group

Many modifications over the years

Re-writing in fortran 90

Three phase version in 2016

Main reference now: Ruaud et al. (2016)

-> Version available upon request

-> keeping a list of users

-> easy to use less easy to modify

-> no guaranty and no user support (yet)

-> detailed instructions

- > Directory with the code
- > directory with the input and output files (else where in the computer)
- > python procedures to plot the results and analyse the chemistry

User cases:

- 1) 0D static -> shielded cold core
- 2) 0D time dependent -> diffuse medium evolving towards dense core
(extracted from SPH galactic dynamical model cf Maxime's talk)
- 3) 1D static -> pre-stellar core (structure from observations)