Welcome to the KIDA 2015 workshop

From May 5th to 7th in Paris

Salle de l'Espace, CNES

95 participants and 53 submissions from 13 different countries

European Research Council

Established by the European Commission

Program KIDA2015 (Salle de l'Espace, CNES, Paris)

Tuesday, 5 May

Chair: *Sébastien Le Picard*

13:00 → 13:30 (30 min) The new version of KIDA - Extension to surface reactions
Valentine Wakelam, Laboratoire d'Astrophysique de Bordeaux

13:30 → 14:00 (30 min) Some Poorly Understood Classes of Interstellar Reactions
Eric Herbst, Department of Chemistry, University of Virginia, Charlottesville

14:00 → 14:30 (30 min) Reactions Involving Nitrile Anions in the Interstellar Medium: the CRESU Laboratory Apparatus Updates
Sophie Carles, Institut de Physique de Rennes

14:30 → 14:50 (20 min) Merged Beams Studies for Astrobiology
Daniel Savin, Columbia University, New York

14:50 → 15:10 (20 min) Electron collision driven chemistry
Jonathan Tennyson, University College, London

15:10 → 15:40 (30 min) High Level Ab Initio Kinetics as a Tool for Astrochemistry
Stephen Klippenstein, Argonne National Laboratory

15:40 → 16:30 Coffee break

Chair: *Jean-Christophe Loison*

16:30 → 16:50 (20 min) Theoretical study of the Dynamics of the Si+OH → SiO+H reaction
Maurice Monnerville, Physique des Lasers, Atomes et Molécules, Lille

16:50 → 17:10 (20 min) Radiative electron attachment to molecules of astrophysical interest: Direct and indirect mechanisms
Viatcheslav Kokoouline, Department of Physics, University of Central Florida

17:10 → 17:30 (20 min) State-to-state rate constants calculations for the reaction C^++H_2 and S^++H_2
Alexandre Zanchet, Instituto de Fisica Fundamental, Madrid

17:30 → 17:50 (20 min) An updated list of photodissociation and ionisation rates in stellar and cosmic-ray induced radiation fields
Alan Heays, Leiden Observatory

17:50 → 18:20 (30 min) New insight on the metal cyanides and isocyanides abundances in the circumstellar gas
François Lique, Laboratoire Ondes et Milieux Complexes, Le Havre

Wednesday, 6 May

Chair: *Nathalie Carrasco*

09:00 → 09:20 (20 min) VUV photolysis of Hydrogenated amorphous carbons. Small hydrocarbons production in Photon Dominated Regions.
Aurélie Jallat, Institut de Physique Nucléaire d'Orsay

09:20 → 09:40 (20 min) Contribution of excited electronic states to low temperature rate constants of radical reactions
Juergen Troe, University of Goettingen

09:40 → 10:10 (30 min) High-temperature chemistry and photochemistry
Olivia Venot, Institute of Astronomy, K.U. Leuven

10:10 → 11:00 Coffee break

11:00 → 11:20 (20 min) A Fully-Consistent 1D Radiative-Convective Equilibrium Model for Planetary Atmospheres
Benjamin Drummond, University of Exeter

11:20 → 11:50 (30 min) Photochemical aerosol formation in Titan's atmosphere
Panayotis Lavvas, Groupe de spectrométrie moléculaire et atmosphérique, Reims

11:50 → 12:10 (20 min) Simulating the Density of (Iso-)Nitrile Species in the Titan Atmosphere with a Coupled Ion-Neutral Photochemical Model
Véronique Vuitton, Institut de Planétologie et d'Astrophysique de Grenoble

Gas-phase processes

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Jan Zabka, J. Heyrovský Institute of Physical Chemistry of the ASCR, v. v. i

12:30 → **14:00** Lunch

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Claire Romanzin, Synchrotron SOLEIL, Laboratoire de Chimie Physique

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Ankan Das, Indian Centre for Space Physics, Kolkata

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Jérôme Pety, Institut de RadioAstronomie Millimétrique, Grenoble

16:20 → **16:40** (20 min) Bridging the gap between ice observations and modelling: laboratory data holds the key
Helen Fraser, The Open University

16:40 → **19:00** Coffee break + Posters

Thursday, 7 May

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09:00 → **09:30** (30 min) Isotopic fractionation of deuterium, carbon and nitrogen
Evelyne Roueff, LERMA, Paris

09:30 → **09:50** (20 min) Chemistry of star forming regions including deuteration: modeling and observation
Liton Majumdar, Laboratoire d'Astrophysique de Bordeaux, Indian Centre for Space Physics

09:50 → **10:10** (20 min) Formation and recondensation of complex organics during protostellar outbursts
Vianney Taquet, Leiden Observatory

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Maryvonne Gerin, LERMA, Paris

11:30 → **12:00** Chimie des glaces interstellaires

Planetary atmospheres

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Interstellar medium

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Surface processes

11:30 → 12:00 (30 min) Chimie des glaces interstellaires
Patrice Theule, Laboratoire de Physique des Interactions Ioniques et Moleculaires, Marseille

12:00 → 12:30 (30 min) Laboratory study of thermal and non-thermal desorption processes of interstellar ices
Mathieu Bertin, LERMA, Paris

12:30 → 14:00 Lunch

Chair: *François Dulieu*

14:00 → 14:20 (20 min) Adsorption selectivity on interstellar surfaces: computational experiments. Local versus global approach.
Françoise Pauzat, Laboratoire de Chimie Théorique, Paris

14:20 → 14:50 (30 min) The lifecycle of particles on cold dust: a complete journey
Marco Minissale, LERMA, Paris

14:50 → 15:10 (20 min) Surface chemistry data for extrasolar cloud formation modelling
Christiane Helling, SUPA, School of Physics and Astronomy, University of St. Andrews

15:10 → 15:40 (30 min) Photodesorption of ice molecules
Guillermo M. Muñoz Caro, Centro de Astrobiologia, Madrid

15:40 → 16:10 (30 min) Final words and poster prize
Valentine Wakelam, Laboratoire d'Astrophysique de Bordeaux

Some practical details

- For speakers: provide pdf presentations if possible during the breaks.

- Book of abstract to download

- Long coffee breaks for discussions

- Security badges

- Lunches

- Posters

- Questionnaire

The New KIDA

KINETIC
DATABASE
FOR
ASTROCHEMISTRY

Astrochemistry: a multidisciplinary field

- **Physics of the media and evolution (interstellar medium or planetary atmospheres)**

- **Observational constraints (radiative transfer, more and more data)**

- **Atomic and molecular processes :**
    - **Large number of processes**
    - **different processes (unimolecular, bimolecular, termolecular)**
    - **methods (theory, experiment)**

The beginning of KIDA

2006 Following the updates of the OSU database -> need for something else than an ascii or excel file

2007-2009 Thinking of the datamodel (many meetings and discussions)

2009-2010 Technical development of the database (funded by 3 European contracts)

May 2010 Official opening of KIDA (only data for interstellar medium)

2011 Start feeding the database for planetary atmospheres

2013 Link to VAMDC

2014-2015 Extension to surface reactions (definition of the data model)
New web site

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 interface (consulting and adding data to the database)

•Form to download list of reactions

•Group of experts advising for the data to be added to the database and give recommendations of key reactions.

•Subsets of chemical reactions for specific applications (Titan atmosphere, Hot Jupiters, ISM)

Network for the interstellar medium: kida.uva.xxxx

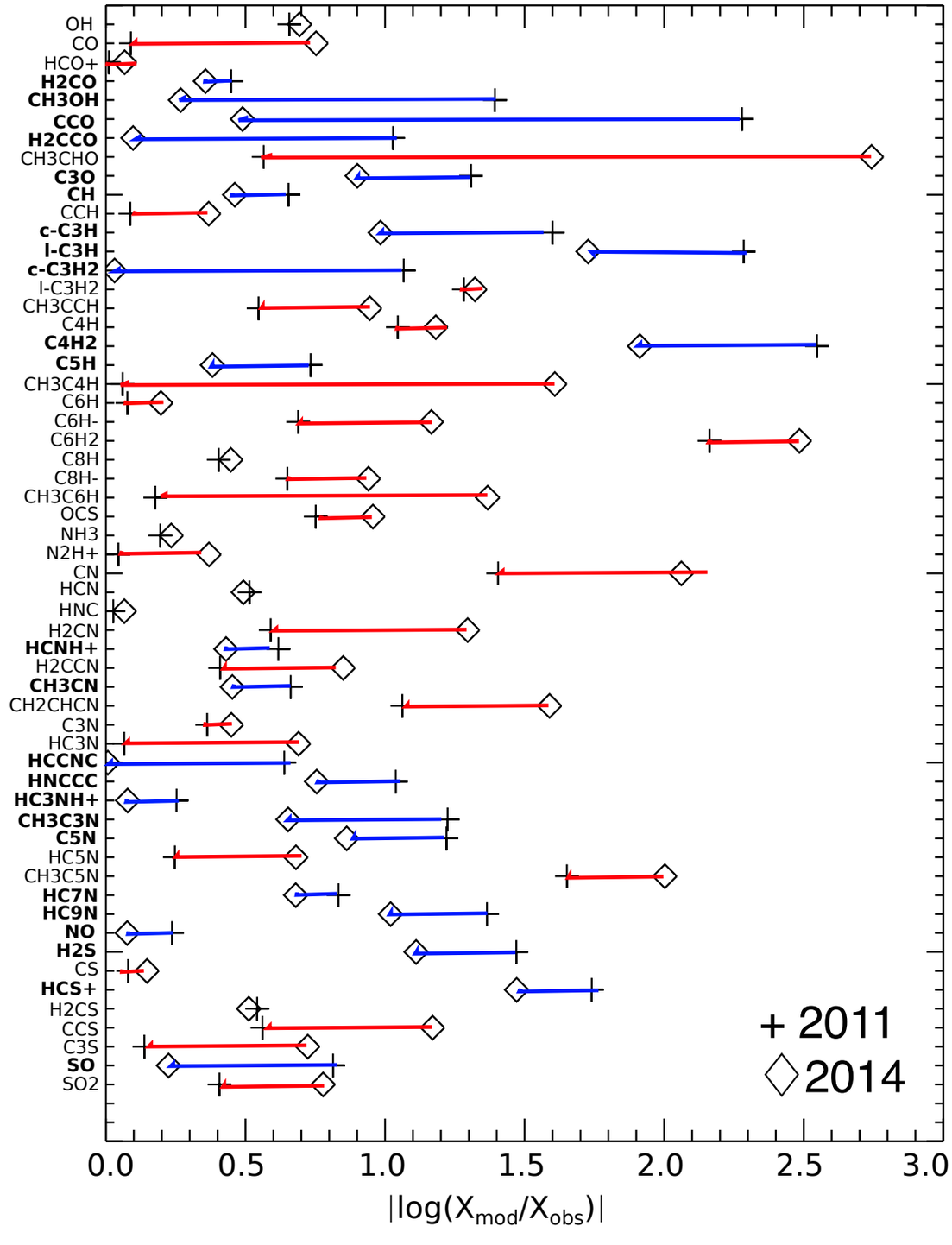
Subset of reactions downloaded from KIDA and tested

kida.uva.2011 (kida until oct. 2011):
6467 reactions and 474 species

Wakelam et al. (2012)

kida.uva.2014 (kida until oct. 2014):
7506 reactions and 489 species

Wakelam et al. (2015)



Who is in the KIDA team?

People highly involved:
Valentine Wakelam (PI)
Pierre Gratier (scientific and technical advisor)
Jean-Christophe Loison (scientific advisor)
Benjamin Pavone (lead programmer)

KIDA scientific experts 2014-2018:

Astrid Bergeat
Karine Beroff
Marin Chabot
Alexandre Faure
Wolf Dietrich Geppert
Dieter Gerlich
Eric Herbst
Kevin Michael Hickson
Pascal Honvault
Stephen Klippenstein
Sébastien Le Picard
Jean-Christophe Loison
Gunnar Nyman
Stephan Schlemmer
Ian Sims
Dahbia Talbi
Jonathan Tennyson
Roland Wester

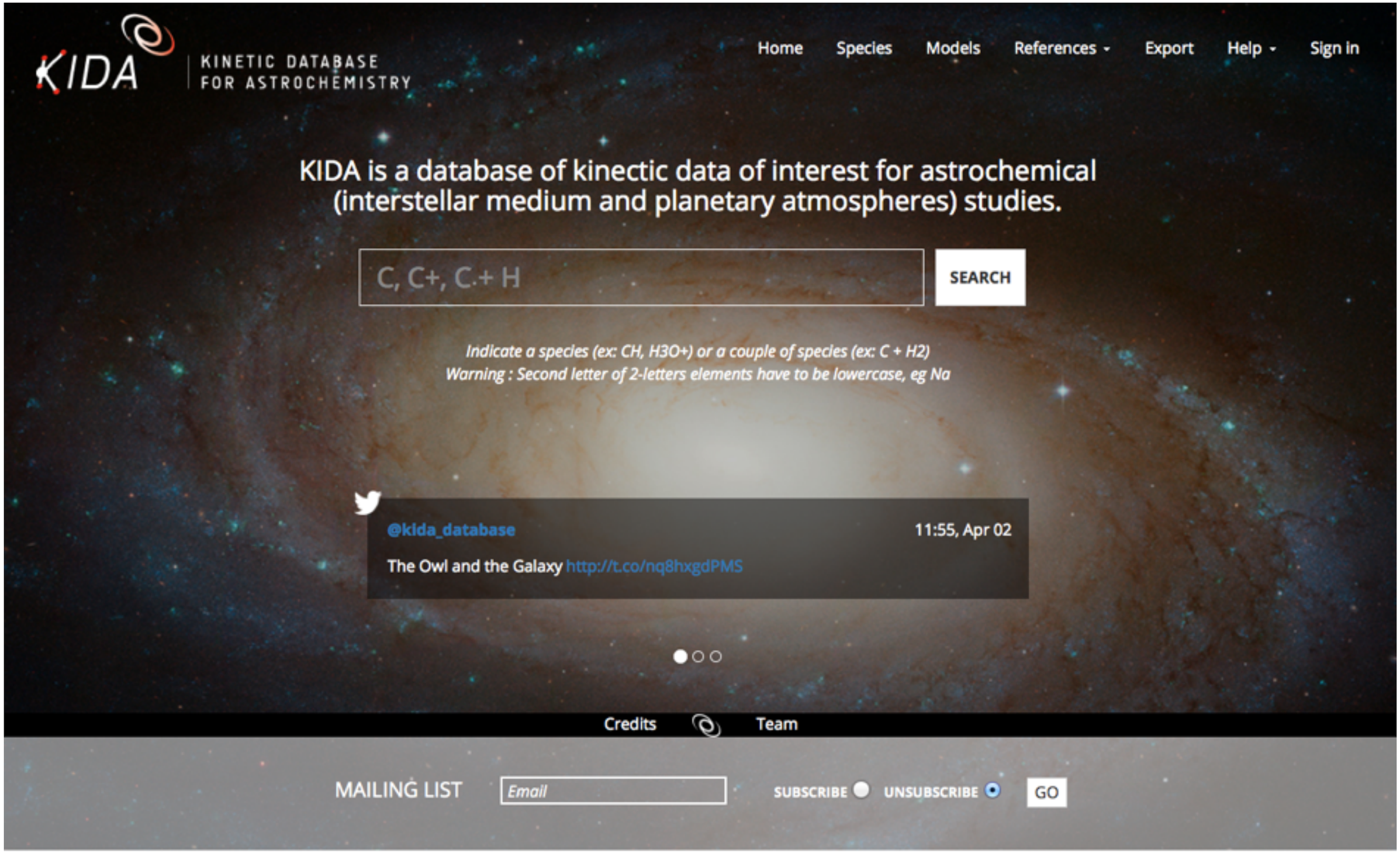
KIDA and VAMDC

VAMDC: Virtual Atomic and Molecular Data Centre
http://www.vamdc.eu/

About 30 databases and partners around the world.
Definition of standards for interoperability.
Portal for interrogating and comparing different databases still needs improvement.
UMIST and KIDA are involved.
http://portal.vamdc.eu

NEW KIDA online interface underdevelopment

http://integration-kida.obs.u-bordeaux1.fr/



Demo

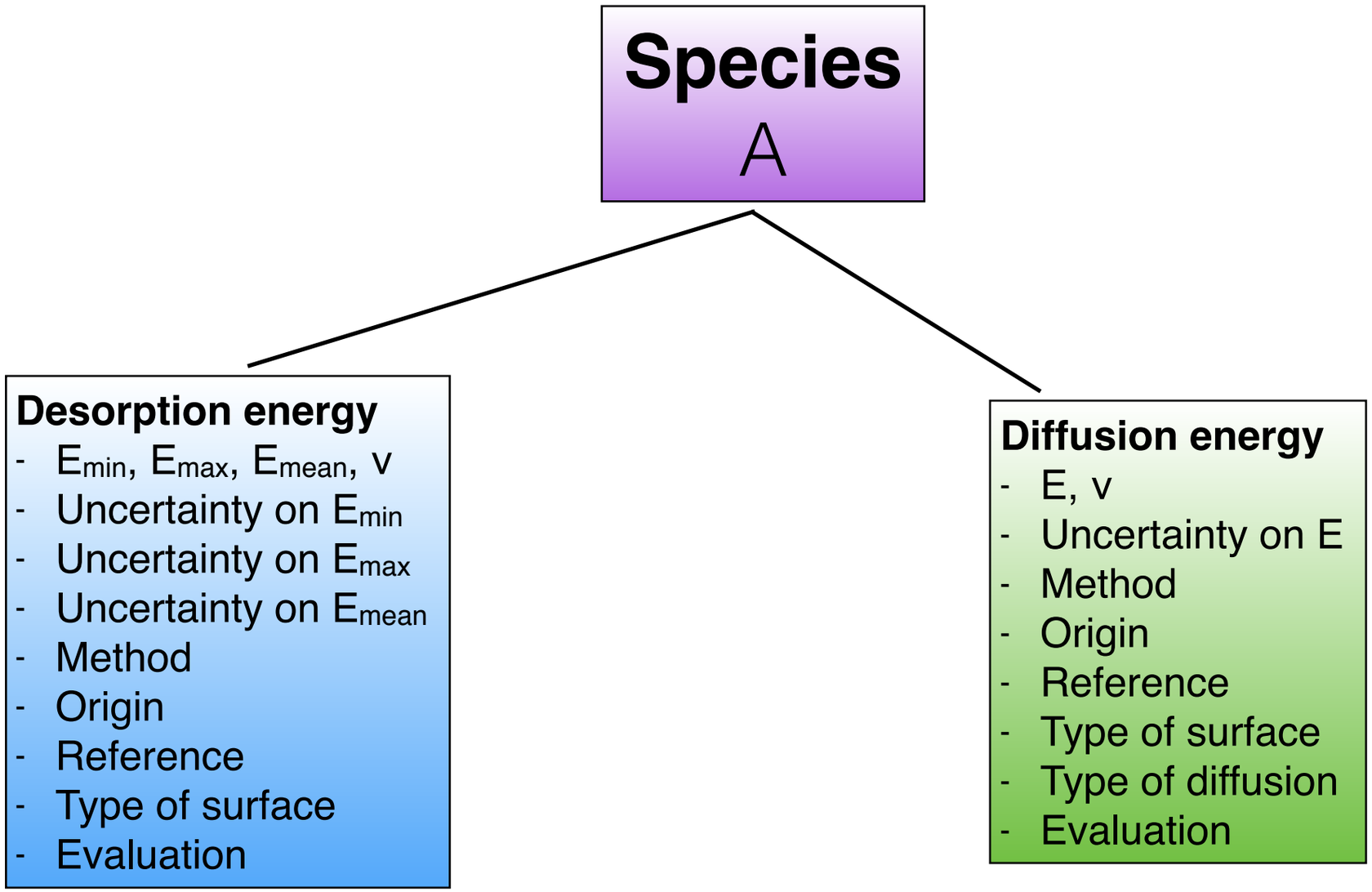
Extension to surface reactions

- Store in the database useful information to treat the surface chemistry in chemical models

- Difficulties:
  - Define which parameters and which format
  - Define the surfaces
  - Gather the data
  - Find complete data

- Definition of the datamodel with:
  - Mathieu Bertin
  - Francois Dulieu
  - Yves Ellinger
  - Jean-Hugues Fillion
  - Pierre Gratier
  - Jean-Christophe Loison
  - Françoise Pauzat
  - Patrice Theulé

Data model for surfaces reactions



Data model for surfaces reactions

Reaction

$A + B \rightarrow C + D$

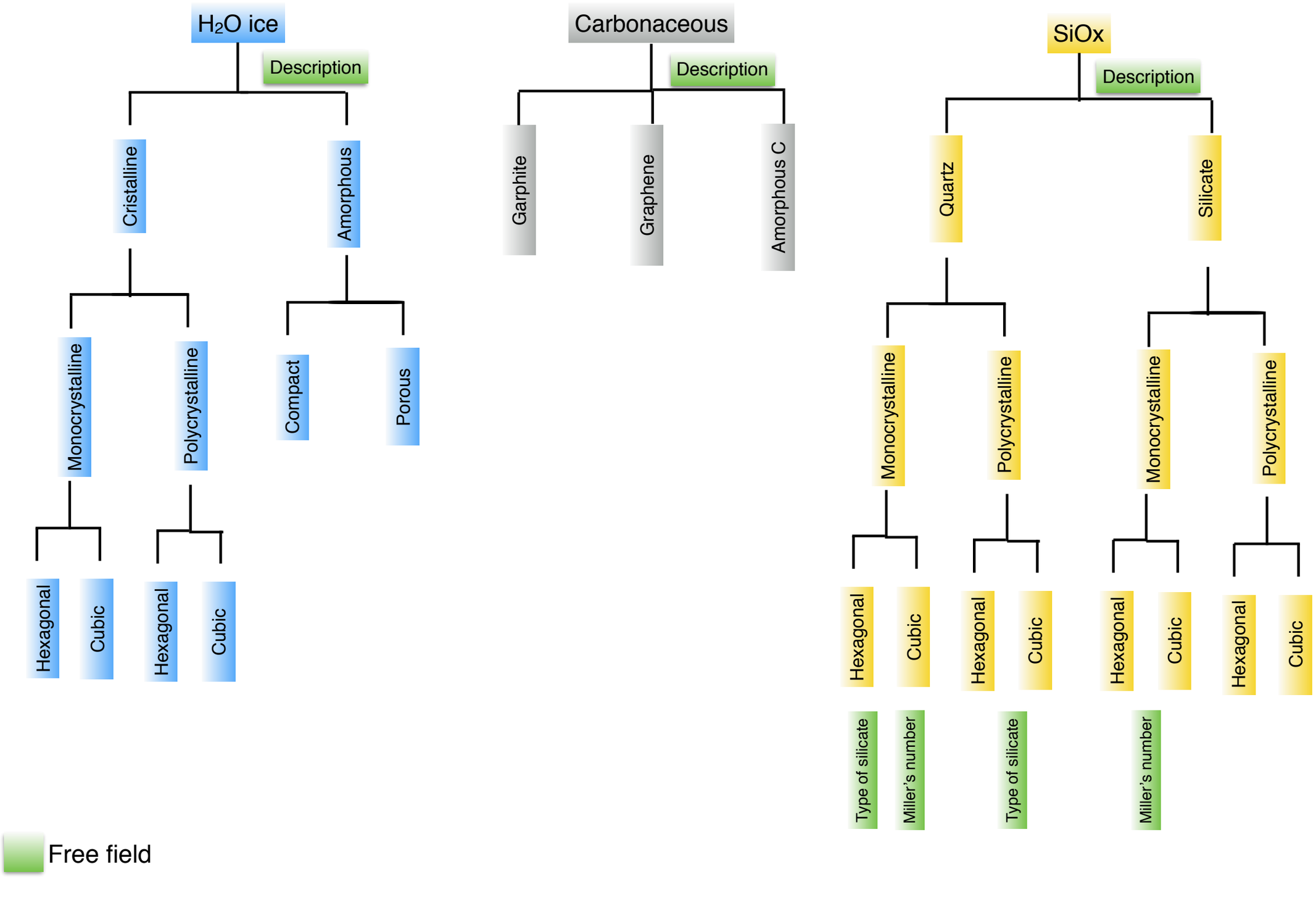
Branching ratio
- Value
- Uncertainty on BR
- Method
- Origin
- Reference
- Type of surface
- Evaluation

Activation energy
- EA
- Pre-exponantial factor
- Uncertainty on EA
- Method
- Origin
- Reference
- Type of surface
- Evaluation

Imaginary frequency for tunneling
- Value
- Uncertainty
- Method
- Origin
- Reference
- Type of surface
- Evaluation

Barrier width for tunneling
- Value
- Uncertainty
- Method
- Origin
- Reference
- Type of surface
- Form of the barrier
- Evaluation

Data model for substrate



Demo

How can you help?

For gas-phase rate coefficients:

- use the online interface to include the data (you need a partial rate coefficients with products, a bibliographic reference and an uncertainty on your value).
- or ask us for a template to make an excel table (if many reactions)

For surface reactions: any (complete) data will be useful -> there will be a call for help.

While publishing a paper on physico-chemistry: please make the abstract or the conclusion clear enough to feed the database (we will produce a guideline with keywords).

Provide any missing data (enthalpy of formation, Inchi codes, images…): http://integration-kida.obs.u-bordeaux1.fr/check-species.html

Communication

KIDA on twitter: **@kida_database**
#KIDA2015

Next KIDA workshop in 2 years (please fell in the questionnaire to help us define the format)

The **Astrochemistry Newsletter** : dissemination of recent results (papers in press or just published)

Editorial board:

Marcelino Agundez
Edith Fayolle
Mathieu Bertin
Pierre Gratier
Valentine Wakelam

Start in September 2015