The KInetic Database for Astrochemistry

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France

Interstellar chemical models

Compute species abundances as a function of time (non steady-state chemistry):

$$dn_i/dt = \underbrace{\Sigma\, k_{ml}\, n_m n_l}\; - \; \underbrace{n_i\, \Sigma\, k_{ij}\, n_j}$$

k : reaction rate coefficients ($cm^3 s^{-1}$)
n : species density (cm^{-3})

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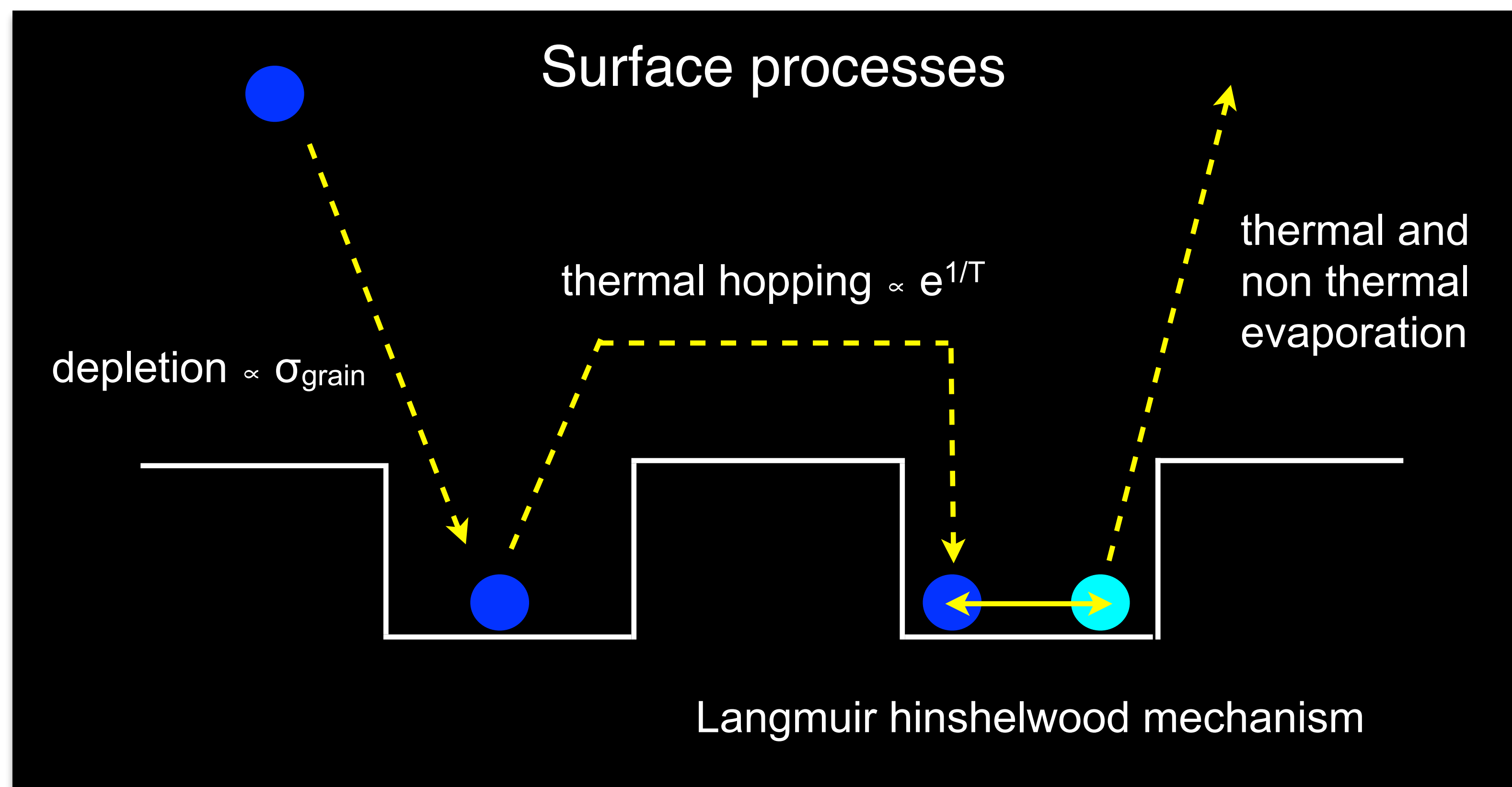

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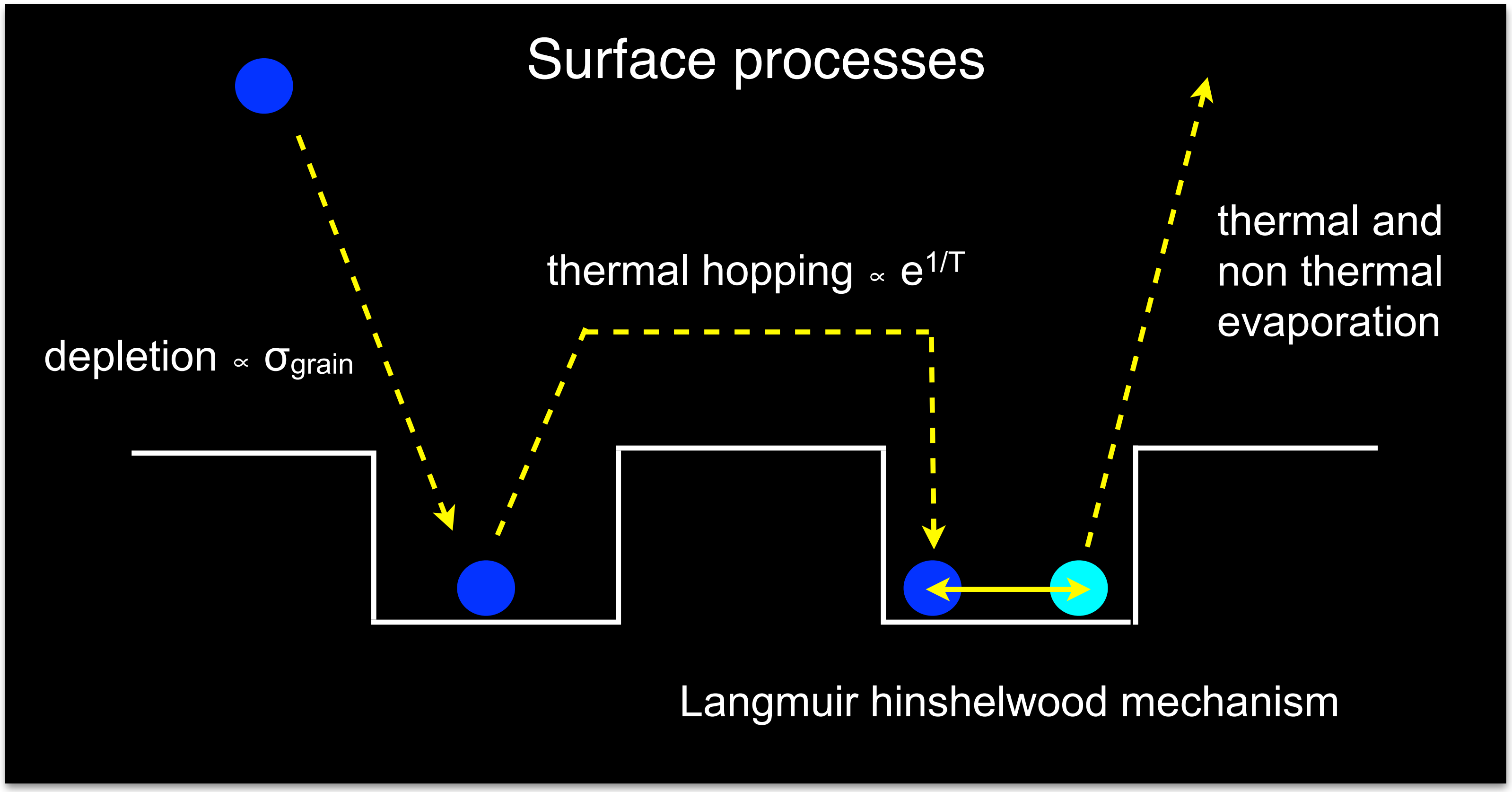
Parameters of the models:

- Gas and grain temperatures (K)
- Density (cm^{-3})
- Elemental abundances
- Conditions initiales
- UV, X-ray and Cosmic-ray fields
- Chemical networks
- Surface desorption energies
- Diffusion energies
- …



Current models follow around 600 species (400 gas-phase) through more than 6000 reactions (4500 gas-phase)

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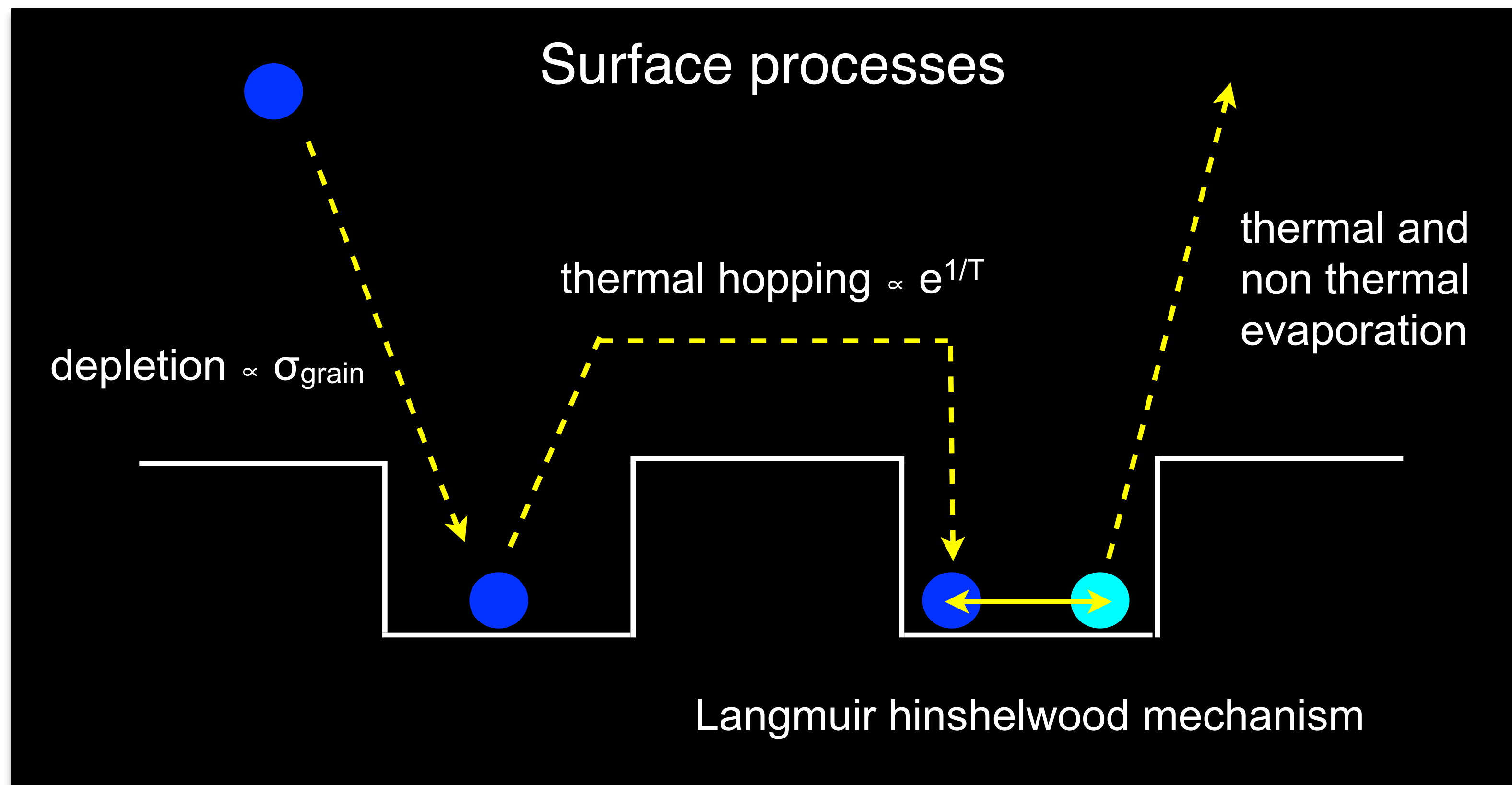

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Improving kinetic data for ISM chemical modeling

Review of the chemistry of nitrogen bearing species

New laboratory measurements at low temperature of :

- N + NO (Bergeat et al. 2009)
- N + OH (Daranlot et al. 2011)
- N + CN (Daranlot et al. 2012)
- N + CH (Daranlot et al. 2013)
- N + C_2 (Loison et al. 2014a)

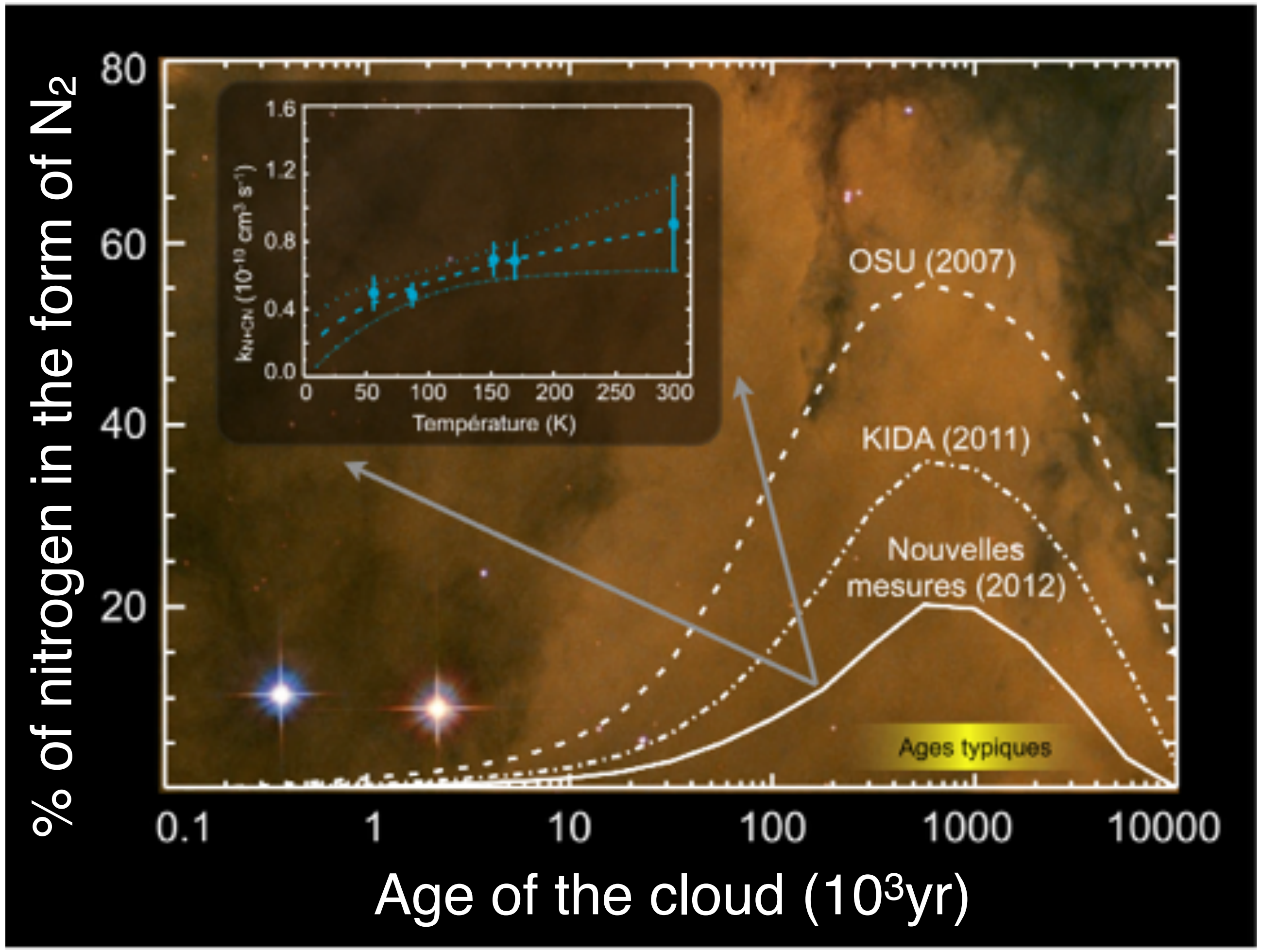
Review of rate coefficients for a number of reactions involving N-bearing species (Wakelam et al. 2010, Wakelam et al. 2013) and the HCN/HNC abundance ratio (Loison et al. 2014b).

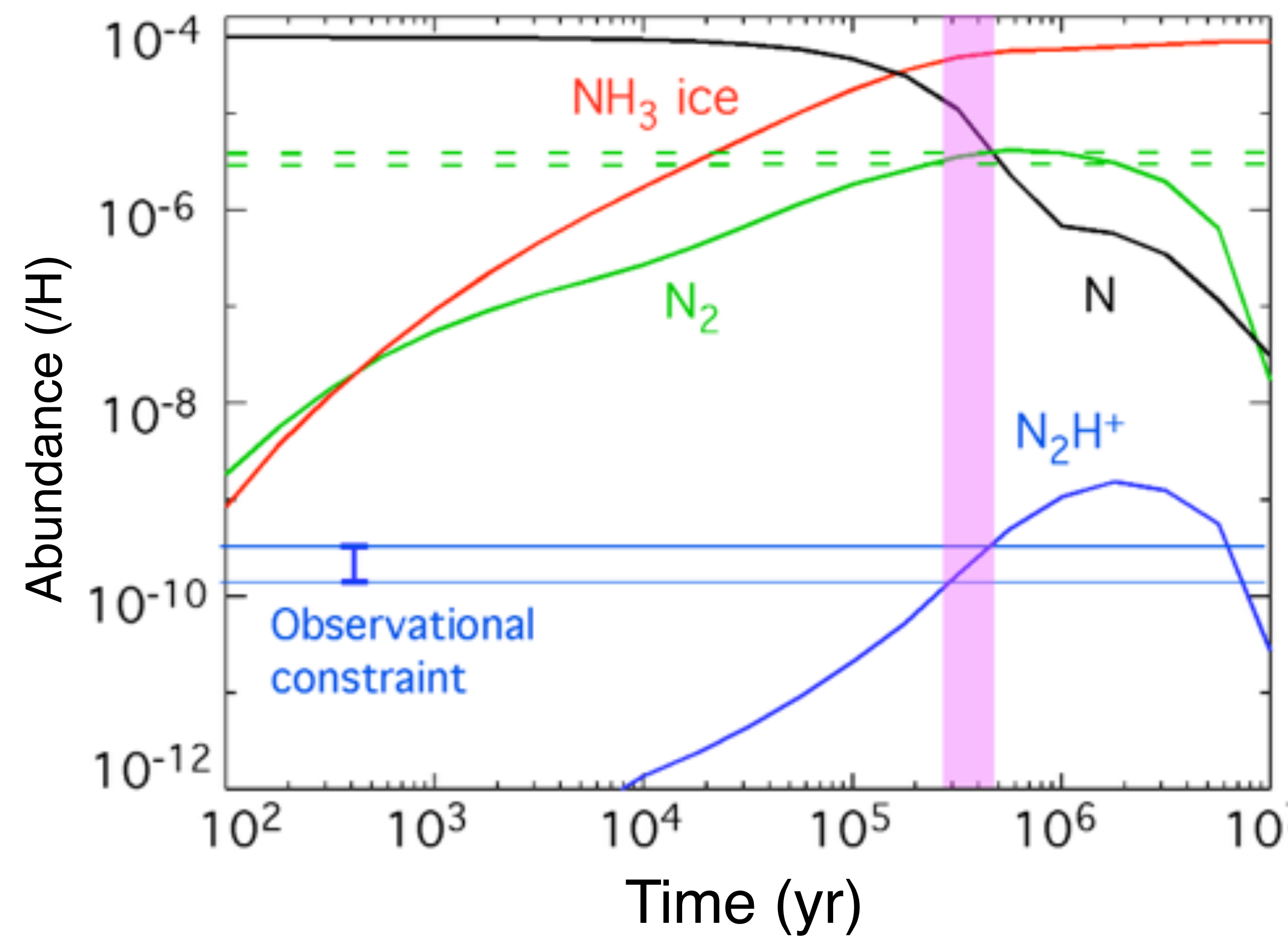
Jean-Christophe Loison
Kevin Hickson

ISSI international team from 2008

Improving kinetic data for ISM chemical modeling

Review of the chemistry of nitrogen bearing species



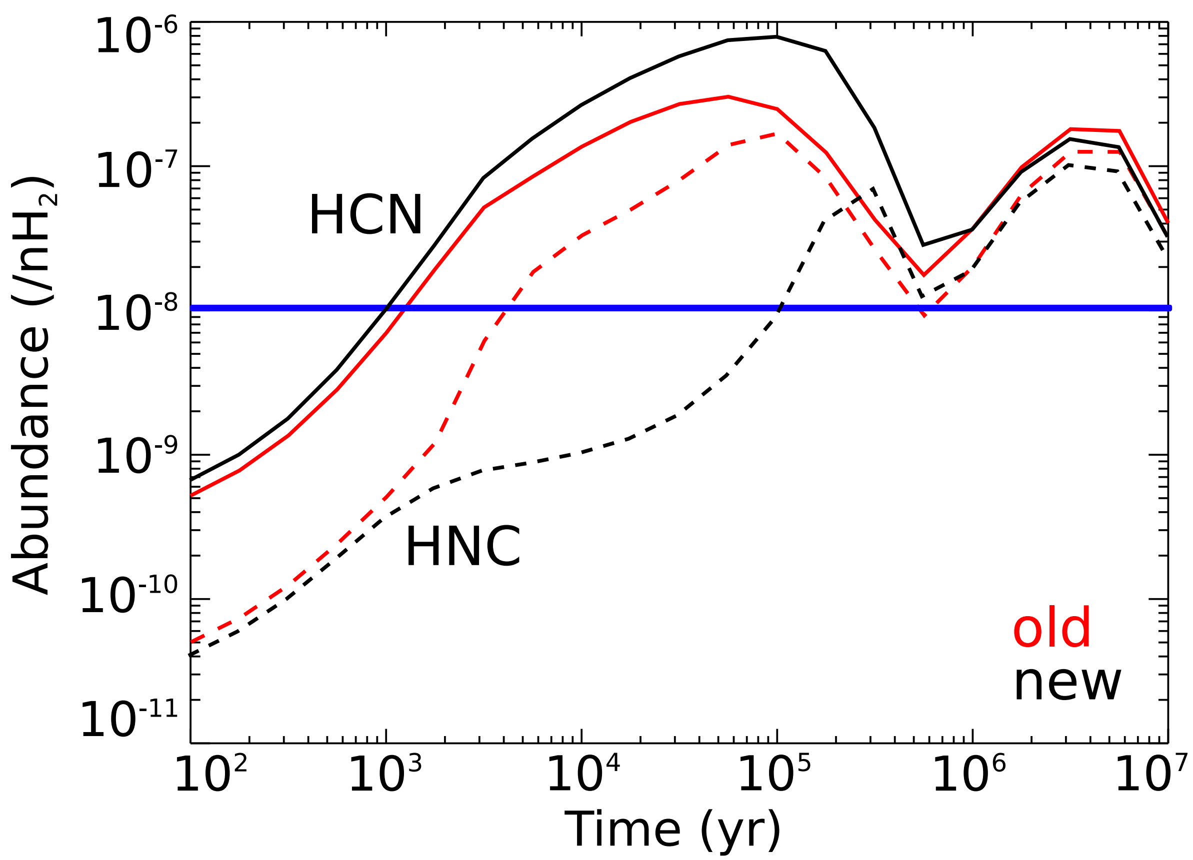


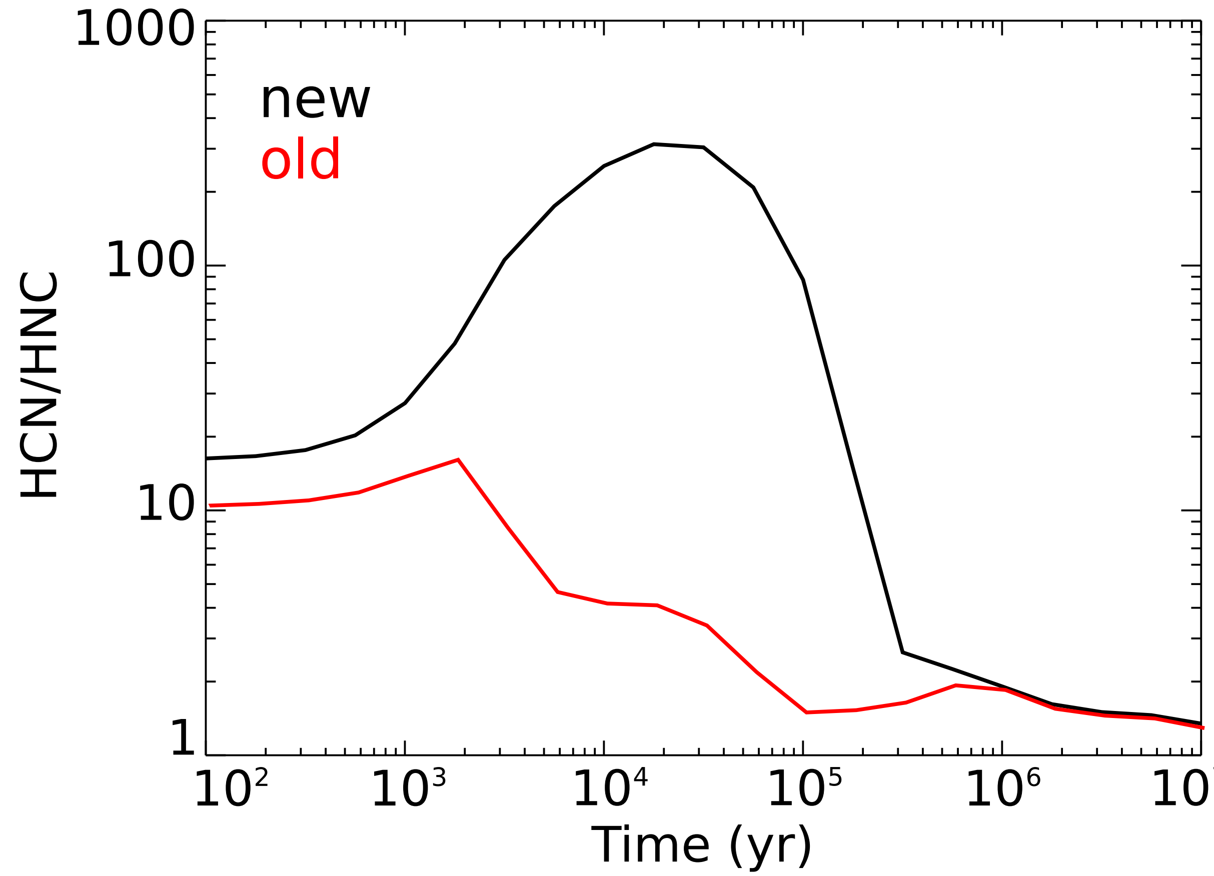
- Changing the reservoir of nitrogen in dense clouds
- reveal the importance of NH_3 formation on the surfaces.

Cold dark cloud conditions (10K, 2x10

Improving kinetic data for ISM chemical modeling

Review of the chemistry of nitrogen bearing species





- Making new predictions on HCN/HNC ratio
- reveal the importance of a new reaction of conversion HNC + C -> HCN + C

Cold dark cloud conditions
(10K, 2x10

The KIDA database

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)
- Recommandations for key reactions by experts
- Online interface (consulting and adding data to the database)
- Download list of reactions
- Group of experts advising for the data to be added to the database
- Store subsets of chemical reactions (models) for specific applications (Titan atmosphere, Hot Jupiters, ISM)
- Chemical network for ISM modeling: kida.uva.2011 (Wakelam et al. 2012), kida.uva.2014 (Wakelam et al. submitted)

Authors:

Jean-Christophe LOISON (Université de Bordeaux, France), Pascal HONVAULT (Université de Franche-Comté, France), Jürgen TROE (University of Göttingen, Germany), Ian Sims (Université de Rennes, France)

$O(^3P) + OH(X^2\Pi) \rightarrow H(^2S) + O_2(X^3\Sigma^-_g)$

Thermodynamic Data

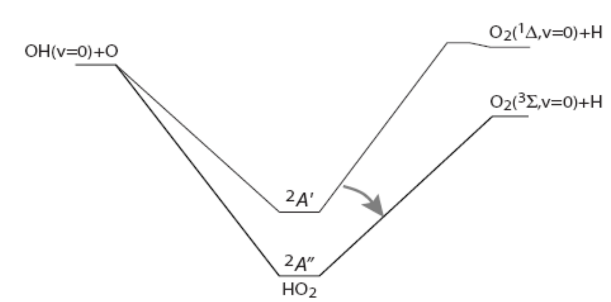
$\Delta H^o_{298} = -68.4$ kJ mol^{-1} (1)

Rate Coefficient Data *k*

k / cm^3 molecule^{-1} s^{-1}	T / K	Reference	Ref
Rate Coefficient Measurements			
$k = (3.85\pm0.13)\times10^{-11}\times(T/298)^{-(0.50\pm0.12)}$	250-515K	Howard and Smith, 1980-81	(2,3)
$k = (3.0\pm1.15)\times10^{-11}\times(T/298)^{-(0.36\pm0.07)}$	221-499	Lewis and Watson, 1980	(4)
$(3.1\pm0.5)\times10^{-11}$		Brune et al, 1983	(5)
$k = f_{el}\times3.7\times10^{-11}\times(T/298)^{-0.24}$	158-294K	Smith and Stewart, 1994	(6)
$f_{el}= 2/[\{5 + 3\exp(-228/T) + \exp(-326/T)\}\{2 + 2\exp(-205/T)\}]$			(7)
$(3.17\pm0.51)\times10^{-11}$	295	Robertson and Smith, 2002	(8)
$k = 1.8\times10^{-11}\times(T/298)^{-0.32}\exp(177/T)$	136-377	Robertson and Smith, 2006	(9)
$(3.5\pm1.0)\times10^{-11}$	39-142K	Carty et al, 2006	(10)
Review			
$k = 2.4\times10^{-11}\times\exp((110\pm50)/T)$	150-500K	Atkinson et al, 2004	(11)
Theory			
No expressions are given for theoretical calculations. The range of the calculations was in general quite wide (10-5000K).			
7×10^{-11}	10K	Harding *et al*, 2000	(12)
$0.026\times(T/1000)^{1.47} + 1.92\times(1000/T)^{0.46}$	300-5000K	Troe and Ushakov, 2001	(13)
5.4×10^{-13}	10K	Xu *et al*, 2007	(14)
7.8×10^{-12}	10K	Lin *et al*, 2008	(15)
4×10^{-11}	10K	Lique *et al*, 2009	(16)
4×10^{-11}	10K	Quéméner *et al*, 2009	(17)

Comments

The reaction $O + OH \rightarrow H + O_2$ is slightly exothermic (-68.4 kJ mol^{-1}). $O(^3P)$ + $OH(X^2\Pi)$ correlates with $3\,^2A'$ + $3\,^2A''$ + $3\,^4A'$ + $3\,^4A''$ surfaces. Only two surfaces ($^2A''$ + $^4A''$) correlate with the reaction products $H(^2S) + O_2(X^3\Sigma^-_g)$ but the $^4A''$ surface is purely repulsive. The $^2A'$ surface, populated without barrier from O + OH, correlates only with the excited $H + O_2$ ($a^1\Delta_g$) product channel. So it is generally assumed that reaction only occurs over the lowest $^2A''$ surface which corresponds to the electronic ground state of the HO_2 intermediate. Nevertheless, temporary population of excited electronic states during the reaction may take place and influence the rate. (12,18,19)



The study of this reaction has attracted considerable experimental attention (2-6,8-10), and there have also been a large number

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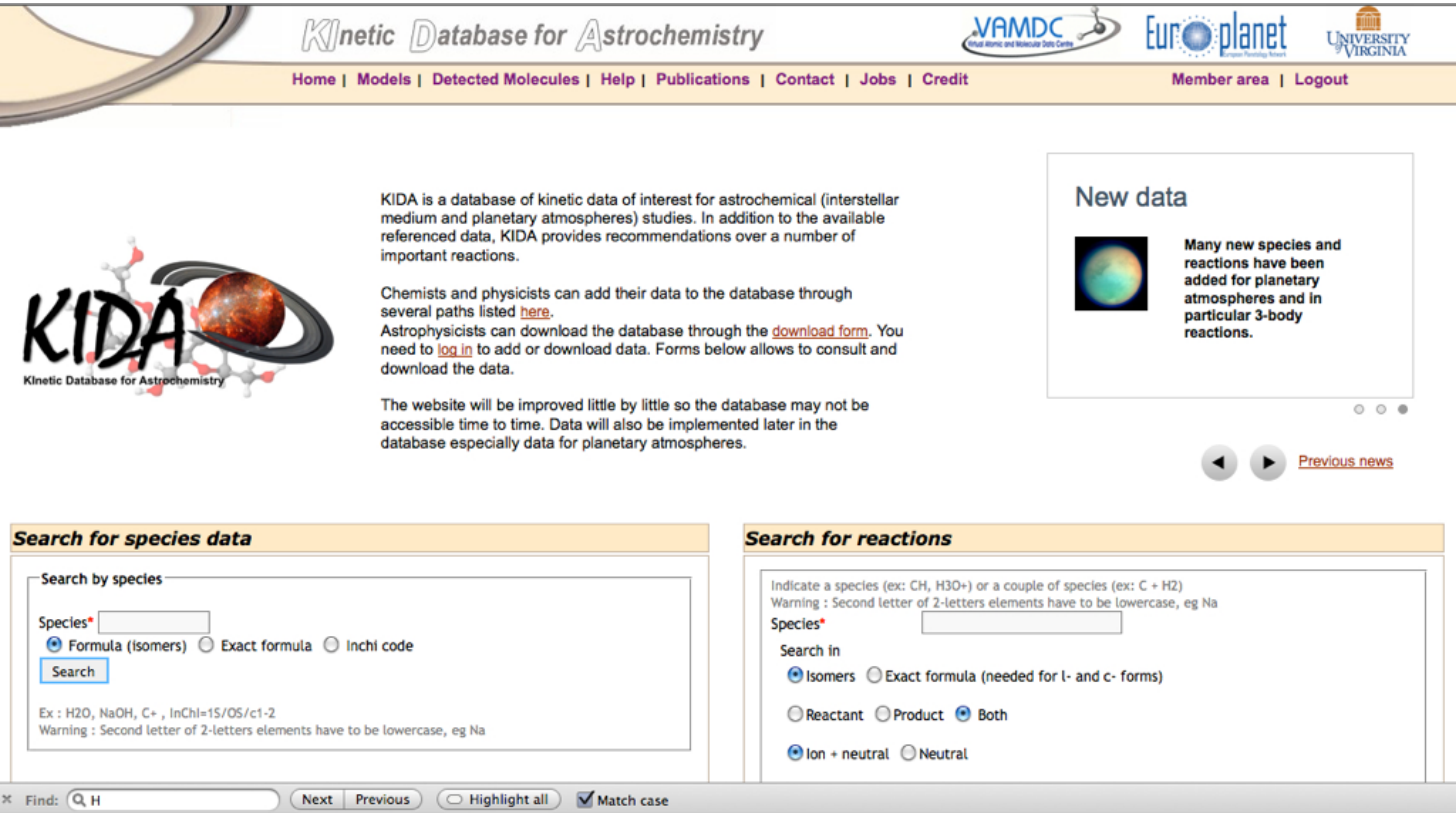
The KIDA database

What type of processes in KIDA?

- **Direct cosmic-ray processes** (dissociation or ionization of species due to direct collision with cosmic-ray particles)
- **Photo-processes induced by cosmic-rays** (secondary photons)
- **Photo-processes** (dissociation or ionization of neutral species by UV photons with a standard interstellar UV field)
- **Bimolecular reactions**: Neutral-neutral (A + B -> C + D), ion-neutral (A+ + B -> C+ +D, A- + B -> C- + D), anion-cation (A+ + B- -> C + D) reactions and dissociative neutral attachment (A + B -> AB+ + e-)
- **Charge exchange reactions**: A+ + B -> A + B+ and A+ + B- -> A + B
- **Radiative associations** (A + B -> AB + photon or A+ + B -> AB+ + photon).
- **Associative detachment** (A- + B -> AB + e-).
- **Electronic recombination and attachment**: Recombination of a positive ion with an electron resulting in the dissociation of the molecule (AB+ + e- -> A + B) or the emission of a photon (AB+ + e- -> AB + photon) or the attachment of the electron (A + e- -> A- + photon)
- **Third-body assisted association**

The KIDA database



The KIDA database

Photo-processes in KIDA

SO + Photon → O + S

Type of reaction:	Photo-processes
Enthalpy of the channel	N/A
Status:	Unknown
Number of values:	2 (0 recommended , 0 waiting for approval)

Value's number	α	β	γ	F0	g	Type of uncertainty	UV Field	Evaluation	Comments	Added By	Added On
1	3.3e-10	0e0	1.4e0	2	0	logn	Draine	?	0	V. WAKELAM	2009-03-27 09:19:02
2	4.2e-9	0e0	2.37e0	2	0	logn	Draine	✓	0	V. WAKELAM	2011-06-09 17:15:45
All									0		

Rate Coefficient | Recommendation | References | Comments

Num	Origin	Authors	Volume, Page	Year	Journal / Thesis / Book	DOI	Download ref
1	Database : OSU						
2	Bibliography	van Dishoeck, E. F. et al	133,231-243	2006	Faraday Discussions	DOI	Bibtex Ris

See full references

Photodissociations and photoinization by UV photons and photons induced by cosmic-rays.
Same formalism as in the OSU database:
$k_{CRP} = \alpha \times \zeta$ (with ζ the H_2 cosmic-ray ionization rate)
$k_{phot} = \alpha \exp(-\gamma A_v)$
Data from various bibliographic sources.

Problems with the current data:

- method and origin of the data not always easy to retrieve (in particular for CRP)
- limits of the fit for k_{phot} not necessary known by users.
- Still a lot of approximation for rate coefficients not available in the literature.

The KIDA database

PI: Valentine Wakelam
Lead programmer: Benjamin Pavone

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

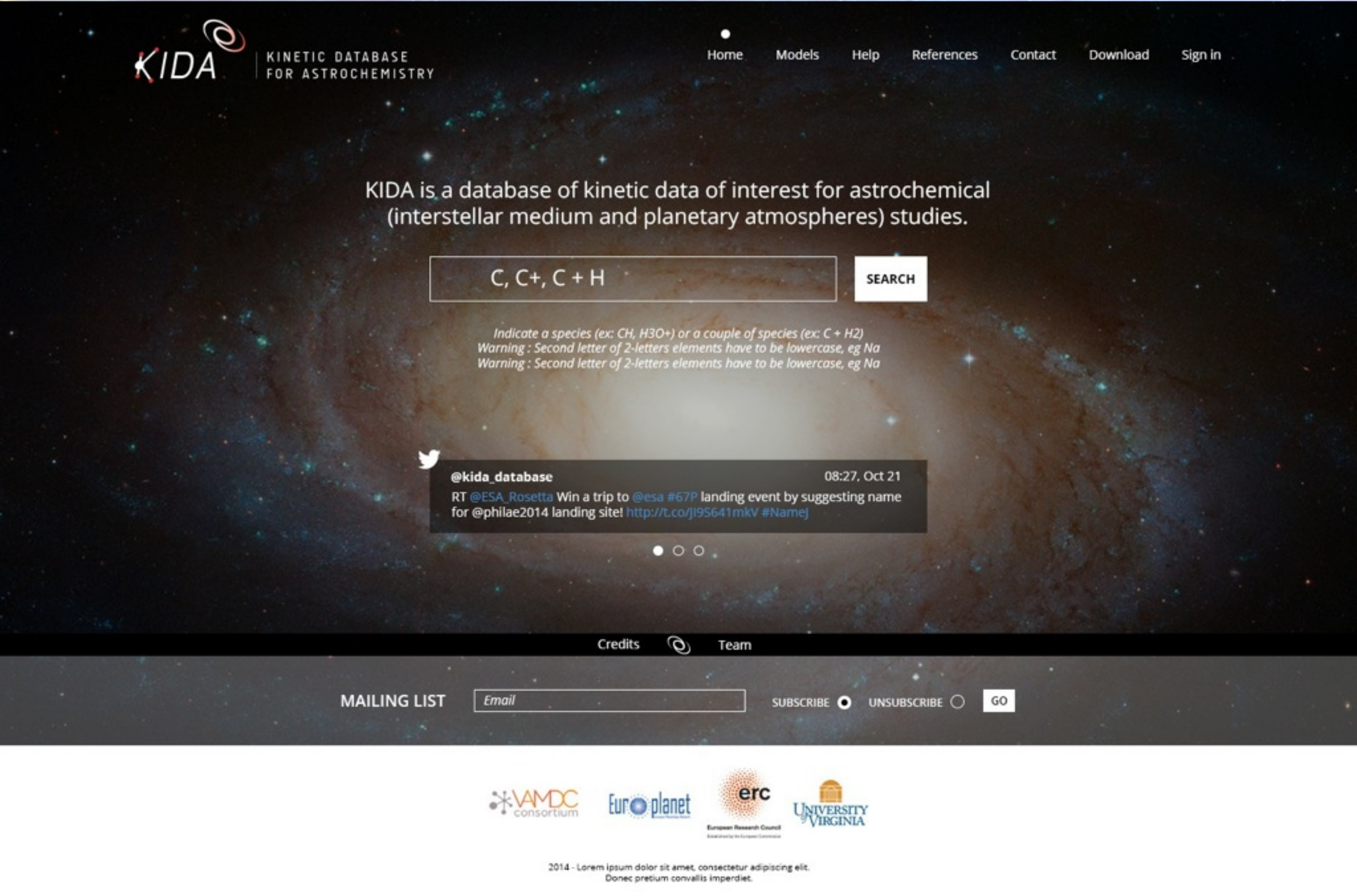
- http://kida.obs.u-bordeaux1.fr/
- kida@obs.u-bordeaux1.fr
- News letter
- KIDA on TWITTER (@kida_database)
- **The KIDA workshop from May, 5th to 7th 2015 in Paris (http://kida2015.sciencesconf.org)**

The KIDA database

The future of KIDA

KIDA
KINETIC
DATABASE
FOR
ASTROCHEMISTRY

- New KIDA website (available in 2015)
- Keep feeding the database (many updates done in 2013-2014)
- Extend the database to surface reactions (KIDA workshop in May 2012, Leiden workshop in July 2014, current discussion with a group of experts to define the data model) -> prototype in spring 2015.
- A lot of sollicitation to create a database of cross sections for photo processes


KIDA
KINETIC DATABASE FOR ASTROCHEMISTRY
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KIDA is a database of kinetic data of interest for astrochemical (interstellar medium and planetary atmospheres) studies.
C, C+, C + H
SEARCH
Indicate a species (ex: CH, H3O+) or a couple of species (ex: C + H2)
Warning : Second letter of 2-letters elements have to be lowercase, eg Na
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@kida_database
08:27, Oct 21
RT @ESA_Rosetta Win a trip to @esa #67P landing event by suggesting name for @philae2014 landing site! http://t.co/JI9S641mkV #NameJ
Credits
Team
MAILING LIST
Email
SUBSCRIBE
UNSUBSCRIBE
GO
VAMDC consortium
Europlanet
erc
European Research Council
University of Virginia
2014 - Lorem ipsum dolor sit amet, consectetur adipiscing elit.
Donec pretium convallis imperdiet.

“Where do these data come from?”

H_2 Cosmic-ray ionization rate

$H_2 + CRP \rightarrow H_2^+ + e^-$ $\alpha_1\zeta$
$H_2 + CRP \rightarrow H^+ + H + e^-$ $\alpha_2\zeta$
$H_2 + CRP \rightarrow H^+ + H^-$ $\alpha_3\zeta$

$\alpha_1 + \alpha_2 + \alpha_3 = 1$
ζ is total H_2 cosmic-ray ionization

Currently in osu and udfa : $\alpha_1 = 0.93$, $\alpha_2 = 0.022$ and $\alpha_3 = 3\times10^{-4} \rightarrow$
$\alpha_1 + \alpha_2 + \alpha_3 \approx 0.952$
From Prasad & Huntress (1984) → J. Black PhD (1974) → Cravens (1974, private communication)

Cravens & Dalgarno (1978) : $\alpha_1 = 0.97$, $\alpha_2 = 0.03$ and $\alpha_3 = 5\times10^{-4} \rightarrow$
$\alpha_1 + \alpha_2 + \alpha_3 \approx 1$