The KInetic Database for Astrochemistry

Valentine Wakelam and the KIDA team
Laboratory astrophysics of Bordeaux
France
Compute species abundances as a function of time (non steady-state chemistry):

$$\frac{dn_i}{dt} = \sum k_{ml} n_m n_l - n_i \sum k_{ij} n_j$$

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

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

$$\frac{dn_i}{dt} = \sum k_{ml} n_m n_l - n_i \sum k_{ij} n_j$$

Production  Destruction

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

Surface processes:
- Depletion $\propto \sigma_{\text{grain}}$
- Thermal hopping $\propto e^{1/T}$
- Thermal and non thermal evaporation

Langmuir Hinshelwood mechanism
Interstellar chemical models

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

\[
\frac{dn_i}{dt} = \sum k_{ml} n_m n_l - n_i \sum k_{ij} n_j
\]

Production  
Destruction

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)
Interstellar chemical models

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)

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

\[
dn_i/dt = \sum k_{ml} n_m n_l - n_i \sum k_{ij} n_j
\]

Production \quad \text{Destruction}

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

\[
\text{depletion } \propto \sigma_{\text{grain}}
\]

\[
\text{thermal hopping } \propto e^{1/T}
\]

Surface processes

- thermal and non thermal evaporation

Langmuir hinshelwood mechanism
Improving kinetic data for ISM chemical modeling

Review of the chemistry of nitrogen bearing species

New laboratory measurements at low temperature of:
- $\text{N} + \text{NO}$ (Bergeat et al. 2009)
- $\text{N} + \text{OH}$ (Daranlot et al. 2011)
- $\text{N} + \text{CN}$ (Daranlot et al. 2012)
- $\text{N} + \text{CH}$ (Daranlot et al. 2013)
- $\text{N} + \text{C}_2$ (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$^3$yr)
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 \( \text{HNC} + \text{C} \rightarrow \text{HCN} + \text{C} \)

Cold dark cloud conditions (10K, 2×10)
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)

- Recommendations 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)

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^2Π) \rightarrow H(^2S) + O_2(X^3Σ_g^-)

Thermodynamic Data
\[ \Delta H_{298} = -68.4 \text{ kJ mol}^{-1} \]

Rate Coefficient Data

<table>
<thead>
<tr>
<th>Rate Coefficient Measurements</th>
<th>T / K</th>
<th>Reference</th>
<th>Ref</th>
</tr>
</thead>
<tbody>
<tr>
<td>( k = (3.85\pm0.13) \times 10^{-11} \times (T/298)^{-0.50} )</td>
<td>250-515K</td>
<td>Howard and Smith, 1980-81</td>
<td>(2,3)</td>
</tr>
<tr>
<td>( k = (3.0\pm1.5) \times 10^{-11} \times (T/298)^{0.36} )</td>
<td>221-499</td>
<td>Lewis and Watson, 1980</td>
<td>(4)</td>
</tr>
<tr>
<td>( (3.1\pm0.5) \times 10^{-11} )</td>
<td>158-294K</td>
<td>Brune et al, 1983</td>
<td>(5)</td>
</tr>
<tr>
<td>( f_p = 2[5 + 3 \exp(-228/T) + \exp(-326/T)] )</td>
<td>295</td>
<td>Smith and Stewart, 1994</td>
<td>(6)</td>
</tr>
<tr>
<td>( (3.17\pm0.5) \times 10^{-11} )</td>
<td>136-377</td>
<td>Robertson and Smith, 2002</td>
<td>(7)</td>
</tr>
<tr>
<td>( k = f_\text{el} \times 3.7 \times 10^{-11} \times (T/298)^{-0.24} )</td>
<td>39-142K</td>
<td>Carty et al, 2006</td>
<td>(10)</td>
</tr>
<tr>
<td>( f_\text{el} = 2/[5 + 3 \exp(-228/T) + \exp(-326/T)] )</td>
<td>150-500K</td>
<td>Atkinson et al, 2004</td>
<td>(11)</td>
</tr>
<tr>
<td>( k = 2.4 \times 10^{-11} \times \exp((110\pm50)/T) )</td>
<td>150-500K</td>
<td>Harding et al, 2000</td>
<td>(12)</td>
</tr>
<tr>
<td>( 7 \times 10^{-11} )</td>
<td>10K</td>
<td>Troe and Ushakov, 2001</td>
<td>(13)</td>
</tr>
<tr>
<td>( 0.026 \times (T/1000)^{1.47} + 1.92 \times (1000/T)^{0.46} )</td>
<td>300-5000K</td>
<td>Xu et al, 2007</td>
<td>(14)</td>
</tr>
<tr>
<td>( 5.4 \times 10^{-13} )</td>
<td>10K</td>
<td>Lin et al, 2008</td>
<td>(15)</td>
</tr>
<tr>
<td>( 7.8 \times 10^{-12} )</td>
<td>10K</td>
<td>Lique et al, 2009</td>
<td>(16)</td>
</tr>
<tr>
<td>( 4 \times 10^{-11} )</td>
<td>10K</td>
<td>Quéméner et al, 2009</td>
<td>(17)</td>
</tr>
</tbody>
</table>

Theory
No expressions are given for theoretical calculations. The range of the calculations was in general quite wide (10-5000K).

Comments
The reaction O + OH \rightarrow H + O_2 is slightly exothermic (-68.4 kJ mol^{-1}). O(^3P) + OH(X^2Π) correlates with 3^2A' + 3^2A'' + 3^4A' + 3^4A'' surfaces. Only two surfaces ("A" + 'A") correlate with the reaction products H(^2S) + O_2(X^3Σ_g^-) but the 'A" surface is purely repulsive. The 2^2A' surface, populated without barrier from O + OH, correlates only with the excited H + O_2 (a'ΔX) product channel. So it is generally assumed that reaction only occurs over the lowest "A" 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...
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)
- Recommendations for key reactions by experts
- Online interface (consulting and adding data to the database)
- Download list of reactions
- Store subsets of chemical reactions (models) for specific applications (Titan atmosphere, Hot Jupiters, ISM)
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 \((A + B \rightarrow C + D)\), ion-neutral \((A^+ + B \rightarrow C^+ + D)\), \(A^- + B \rightarrow C^- + D\), anion-cation \((A^+ + B^- \rightarrow C + D)\) reactions and dissociative neutral attachment \((A + B \rightarrow AB^+ + e^-)\)
- **Charge exchange reactions**: \(A^+ + B \rightarrow A + B^+\) and \(A^+ + B^- \rightarrow A + B\)
- **Radiative associations**: \((A + B \rightarrow AB + \text{photon})\) or \((A^+ + B \rightarrow AB^+ + \text{photon})\).
- **Associative detachment** \((A^- + B \rightarrow AB + e^-)\).
- **Electronic recombination and attachment**: Recombination of a positive ion with an electron resulting in the dissociation of the molecule \((AB^+ + e^- \rightarrow A + B)\) or the emission of a photon \((AB^+ + e^- \rightarrow AB + \text{photon})\) or the attachment of the electron \((A + e^- \rightarrow A^- + \text{photon})\)
- **Third-body assisted association**
The KIDA database

KIDA is a database of kinetic data of interest for astrochemical (interstellar medium and planetary atmospheres) studies. In addition to the available referenced data, KIDA provides recommendations over a number of important reactions.

Chemists and physicists can add their data to the database through several paths listed here. Astrophysicists can download the database through the download form. You need to log in to add or download data. Forms below allows to consult and download the data.

The website will be improved little by little so the database may not be accessible time to time. Data will also be implemented later in the database especially data for planetary atmospheres.

Search for species data

<table>
<thead>
<tr>
<th>Search by species</th>
</tr>
</thead>
<tbody>
<tr>
<td>Species*</td>
</tr>
<tr>
<td>Formula (isomers)</td>
</tr>
<tr>
<td>Exact formula</td>
</tr>
<tr>
<td>Inchi code</td>
</tr>
</tbody>
</table>

Ex: H2O, NaOH, C+, InChI=1S/O5/c1-2
Warning: Second letter of 2-letters elements have to be lowercase, eg Na

Search for reactions

<table>
<thead>
<tr>
<th>Indicate a species (ex: CH, H3O+) or a couple of species (ex: C + H2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Warning: Second letter of 2-letters elements have to be lowercase, eg Na</td>
</tr>
</tbody>
</table>

Species

Search In

- Isomers
- Exact formula (needed for l- and c- forms)
- Reactant
- Product
- Both
- Ion + neutral
- Neutral

X Find: H Next Previous Highlight all Match case
Photodissociations and photoinization by UV photons and photons induced by cosmic-rays. 
Same formalism as in the OSU database:
\[ k_{\text{CRP}} = \alpha \times \zeta \] (with \( \zeta \) the \( H_2 \) cosmic-ray ionization rate)
\[ k_{\text{phot}} = \alpha \exp(-\gamma A_v) \]
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 \( k_{\text{phot}} \) 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

- kida@obs.u-bordeaux1.fr
- News letter
- KIDA on TWITTER (@kida_database)
The KIDA database

The future of KIDA

- 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 is a database of kinetic data of interest for astrochemical (interstellar medium and planetary atmospheres) studies.

C, C+, C + H

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
Warning: Second letter of 2-letters elements have to be lowercase, eg Na

@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/j95641mkV #Namej
“Where do these data come from?”

H₂ Cosmic-ray ionization rate

\[ \text{H}_2 + \text{CRP} \rightarrow \text{H}_2^+ + e^- \quad \alpha_1 \zeta \]
\[ \text{H}_2 + \text{CRP} \rightarrow \text{H}^+ + \text{H} + e^- \quad \alpha_2 \zeta \]
\[ \text{H}_2 + \text{CRP} \rightarrow \text{H}^+ + \text{H}^- \quad \alpha_3 \zeta \]

\[ \alpha_1 + \alpha_2 + \alpha_3 = 1 \]

\( \zeta \) is total \( \text{H}_2 \) cosmic-ray ionization

Currently in osu and udfa : \( \alpha_1 = 0.93, \alpha_2 = 0.022 \) and \( \alpha_3 = 3 \times 10^{-4} \rightarrow \alpha_1 + \alpha_2 + \alpha_3 \approx 0.952 \)


Cravens & Dalgarno (1978) : \( \alpha_1 = 0.97, \alpha_2 = 0.03 \) and \( \alpha_3 = 5 \times 10^{-4} \rightarrow \alpha_1 + \alpha_2 + \alpha_3 \approx 1 \)