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KIDA (KInetic Database for Astrochemistry)

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Abstract

Modeling of chemical processes in the interstellar medium and in planetary atmospheres (hereafter referred to as *astrophysical environments*) share common difficulties, namely a lack of reference data for many processes and large uncertainty for those data which have been measured in the laboratory, in physical conditions generally not representative of the target environment.

A permanent link between modelers and physico-chemists appears therefore as a necessity for modelers to publicize their most urgent data needs and for physico-chemists to advertise new data. This is the best way to maintain prevent the use of inappropriate or obsolete data/extrapolations in chemical networks.

KIDA is a project initiated by different communities in order to i) improve the interaction between astrochemists and physico-chemists and ii) simplify the work of modeling the chemistry of astrophysical environments. The KIDA website is online since may 2010 (http://kida.obs.u-bordeaux1.fr).

We present here the main features of KIDA and it's expected benefits to the community, and we outline future evolutions.

1. Introduction to KIDA

1.1. Kinetic data

KIDA is designed to gather all the kinetic data that can be of interest for the chemical modeling of the interstellar medium and planetary atmospheres. At the moment, KIDA records nine types of reaction: direct cosmic-ray processes; photo-processes induced by cosmic-rays; photo-processes; bimolecular reactions and dissociative neutral attachment; charge exchange reactions; radiative associations; associative detachment; electronic (dissociative) recombination and attachment; third-body assisted association. The database provides the user with extensive information about the data (references, details on the methods to obtain the data, validity range of temperature, etc).

Users inputs. KIDA is by design a collaborative project. The interface enables users to attach comments or new information to data already stored in KIDA, or to populate the database with new data. The reviewing of new data by a group of experts prior to publication in the database is a strong asset of KIDA.

The experts. The role of the KIDA experts is to validate the addition of data from data providers and give recommendation about the rate coefficients to use in specific physical conditions. In most cases, when a recommendation is given, the details of the expertise can be seen in a data sheet provided on the reaction page. Recommendations can be of four types: (1) not recommended; (2) not rated; (3) valid; and (4) recommended value.

Data outputs. Modelers can extract lists of reactions from KIDA, based on different search criteria. The lists are automatically commented to alert the user on reactions that might be problematic. Output formats should enable insertion in various chemistry codes without further processing by the user.

1.2. Chemical networks

A second section of the database is an archive of chemical networks published by modelers. This feature should enable the sharing and intercomparison of models and ensure the traceability and reproducibility of models outputs.

1.3. Uncertainty management

Knowledge of the precision of input reaction rates is a basic requirement for the assessment of the precision of model outputs, be it for comparison with observations or identification of key reactions [1, 2].

KIDA puts a strong incentive on uncertainty management and provides accuracy factors for all stored reaction rates, based on review by experts. More complex uncertainty models should become available in the future, notably to enable the treatment of correlated parameters, such as branching ratios [3].

A major advantage of proper uncertainty management is to enable identification of key reactions as those having a major influence on the (im)precision of models outputs. On this basis, KIDA will publish lists of key reactions to be studied in priority by physicochemists (Fig.1). We can thus expect to improve optimally the accuracy of kinetic data for astrochemistry and thereby the precision of models predictions.

1.4. Links with other projects

As an interdisciplinary project, KIDA is linked with other projects (Fig.1):

- Europlanet is a European network for planetary science, funded by the FP7. KIDA is part of the new databases constructed in this context.
- VAMDC is a Virtual Atomic and Molecular Data Centre, which aims at interfacing several databases. This project is funded by the FP7 and lead by M-L. Dubernet (Observatoire de Paris, France).
- E3ARTHs is a project funded by the European Research Council (Starting Grant), lead by F. Selsis (Bordeaux University, France) to build modeling tools for exo-planetary atmospheres. Simulations of the chemical composition of habitable planets will be done with KIDA.
- CATS is a set of tools in development for the optimized analysis of the future ALMA data. CATS is funded by Astronet and lead by P. Schilke (Max Plank Institute, Bonn). KIDA will be directly interfaced with the chemical models of CATS.

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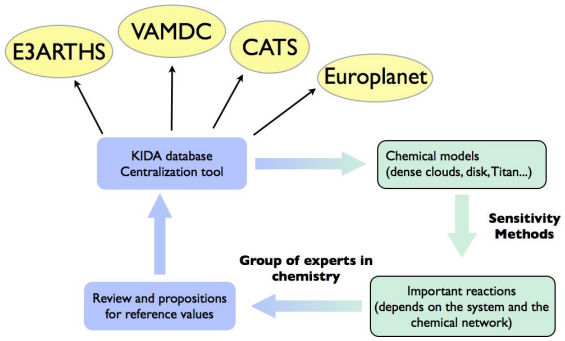

Figure 1: The context of KIDA: the improvement of the data stored in KIDA will be done by the identification of important reactions for specific objects and by the review of a group of experts on these reactions.

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