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KIDA : The new kinetic database for astrochemistry

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Abstract. KIDA (KInetic Database for Astrochemistry) is a project initiated by astrochemists and physical-chemists (both theoreticians and experimentalists) in order to reinforce their mutual interaction and to simplify the work of modeling the chemistry of astrophysical environments, such as the interstellar medium and planetary atmospheres.

Keywords: astrochemistry - interstellar medium - planetary atmospheres - kinetic data

1.Introduction to KIDA

If astrochemical modeling helps our understanding of how the molecules that are observed in space are formed, it is also used as a tool to study the physical conditions prevailing in the astronomical objects where these molecules are observed. However, for astrochemical models to be successful, all the chemical processes that are important in determining the molecular abundances must be included in the model and the values of the associated rate coefficients need to be close to the correct values. Unfortunately, the fraction of chemical processes that have been studied experimentally for the physical conditions prevailing in space is small, and most of the experimentally studied reactions have their rate coefficient determined for room temperature and extrapolated to the temperatures of space, leading either to large uncertainties or to misleading values. The fraction of reactions that have been studied theoretically is even smaller and for all the processes that are unknown, rate coefficients are assigned on the basis of chemical intuition or by analogy to other reactions. In such circumstances it is obvious that a stronger interaction between modelers and physical chemists (both theoreticians and experimentalists) is the best approach to improve astrochemical models and to help prevent the use of inappropriate or obsolete data/extrapolations in chemical networks. Moreover such an interaction is the best way for modelers to publicize their most urgent data needs and for physical chemists to advertise new data. Let us point out here that since the chemical networks used to model the chemistry of the interstellar medium and of the planetary atmospheres are similar, the physical chemists who work on the determination of reaction rate coefficients for both types of environments tend to be the same individuals.

KIDA, whose logo is shown in Figure 1, is by design a collaborative project with an interface that allows users to add new data as well as information and comments. New data are validated by experts before publication. The innovative functionalities of the KIDA database are outlined in the next section.

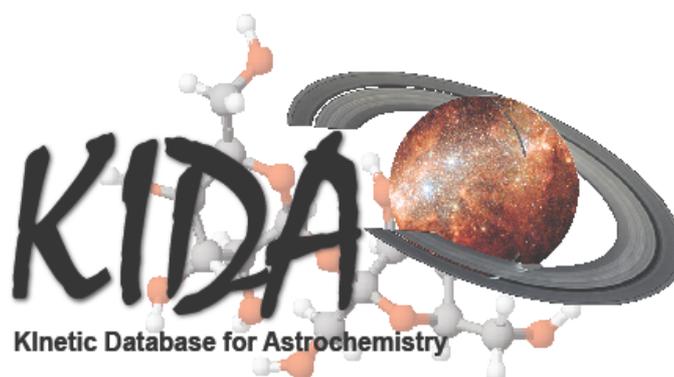


Figure 1. The logo of KIDA

2. 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. The reactions that are included in KIDA are subdivided into nine groups: direct cosmic-ray processes; photo-processes induced by cosmic-rays; photo-processes; bimolecular reactions and dissociative neutral attachment; charge exchange reactions; radiative association; associative detachment; electronic (dissociative) recombination and attachment; and third-body assisted association. The database provides the user with extensive information about the data such as references, details on the methods used to obtain the data, validity, range of temperature, etc.

2.1 User inputs

Since KIDA is by design a collaborative project, a friendly interface is provided to enable users to attach comments or new information to data already stored in KIDA, or to enrich 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 (see Figure 2).

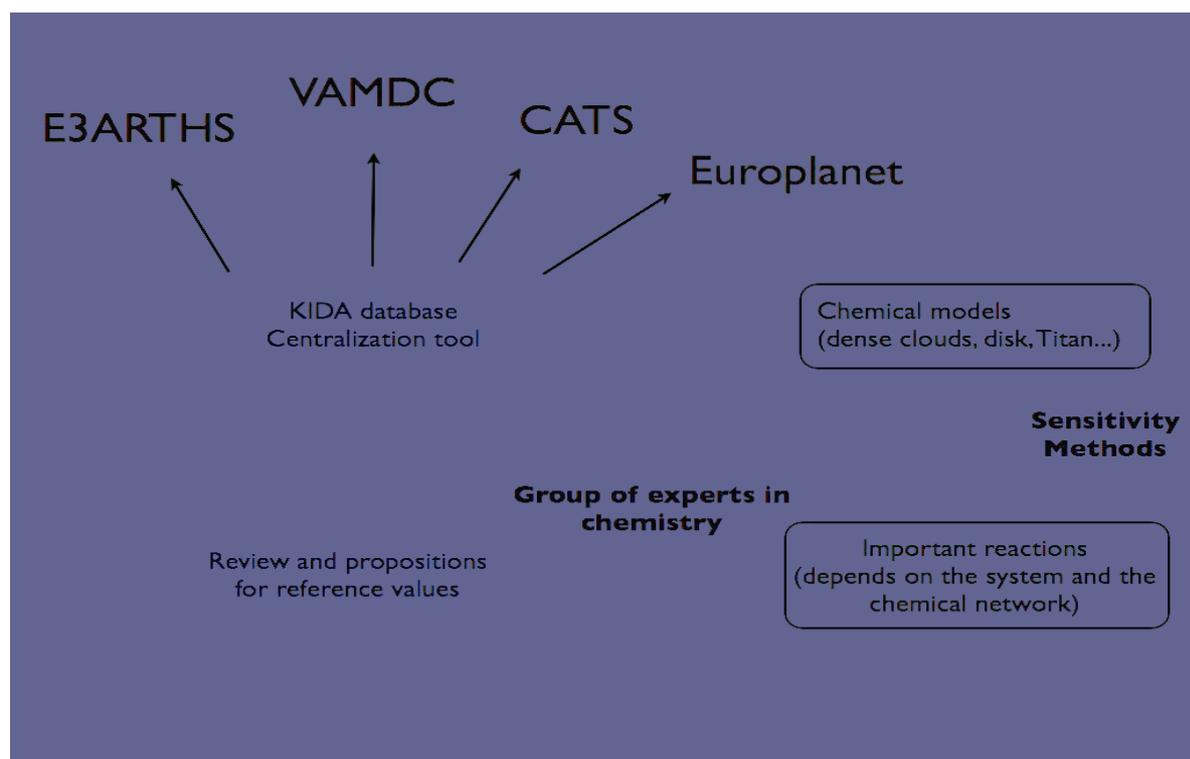


Figure 2. The specifics of KIDA: the improvement of data stored in KIDA is done by the identification of important reactions for specific objects and by the review by groups of experts on these reactions. KIDA is linked to four other projects, discussed below.

2.2 The experts

The role of the KIDA experts is to validate the addition of data from data providers, giving recommendations 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.

2.3 Data outputs

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

2.4 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.

3. Uncertainty management

Knowing the precision of input reaction rates is a basic requirement for the assessment of the precision of model outputs. These last are crucial for any comparison with observations or identification of key reactions [1, 2]. KIDA therefore puts a strong effort on uncertainty management and seeks to provide accuracy factors for all stored reaction rates, based on review by the experts. A major advantage of proper uncertainty management is to enable identification of key reactions as those having a major effect on the (im)precision of models outputs. On this basis, KIDA lists the key reactions to be studied in priority by physical chemists, as has been shown in a publication recently accepted by Space Science Reviews [3]. With such a procedure one can expect to improve optimally the accuracy of kinetic data for astrochemistry and thereby the precision of model predictions.

4. Links with other projects

KIDA is by essence an interdisciplinary project and, as shown in Figure 2, is linked to other projects, including:

Europlanet: a European network for planetary science, funded by the FP7. KIDA is part of the new databases constructed in this context.

VAMDC: a virtual Atomic and Molecular Data Center, aimed at interfacing several databases. Also funded by FP7, this project is led by M-L. Dubernet (Observatoire de Paris, France).

E3ARTHS: a project funded by the European Research Council (Starting Grant) and led by F. Selsis (Bordeaux University, France). Its goal is to build modeling tools for exo-planetary atmospheres. Simulations of the chemical composition of habitable planets will be done with KIDA.

CATS: a set of tools that are developed to optimize the analysis of future data from the giant radio telescope interferometer named ALMA. CATS is funded by Astronet and led by P. Schilke (Max Planck Institute, Bonn). KIDA will be directly interfaced with the chemical models of CATS.

5. Conclusions

KIDA was built by and for astrochemists and physical chemists. The KIDA website has been online since May 2010 (<http://kida.obs.u-bordeaux1.fr>). Anyone can register with KIDA, as well as submit

and download data. More details about the kinetic data and the spirit of KIDA can be found in the Space Science Review cited above [3], which can be downloaded from the following web site: http://kida.obs.u-bordeaux1.fr/uploads/documents/issi_database.pdf

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