



# IUPAC Subcommittee for Gas Kinetic Data Evaluation

International Union of Pure and Applied Chemistry (IUPAC)

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<http://www.iupac-kinetic.ch.cam.ac.uk/>

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## Background

The Sub-committee for Gas Kinetic Data Evaluation (I.4), which comes under IUPAC's Physical and Biophysical Chemistry Division, aims to enhance the accessibility and availability of evaluated kinetic data. The problem with data availability and consistency was noted in the 1970's, when it was recognised that a standardised data set was required for the modelling of atmospheric chemistry. Improvements to relevant physico-chemical data continue to be made and the need for reliable atmospheric chemistry modelling is as pressing as ever. Evaluation of gas kinetic data first started, under the auspices of IUPAC, in 1977. Recommendations were published in a series of nine peer-reviewed articles in *J. Phys. Chem. Ref. Data*. Huge improvements have since been made, in the dissemination of the evaluated data, with the use of the Internet.

## Website

The website, which has been operational since July 1998, currently has about 4000 accesses per week. The number of regular users of the database is also growing: currently 395 people are subscribed to the mailing list, an increase of around 10% on the previous year. From the homepage of the website, see Figure 1(a), it is possible to join the mailing list, access data sheets (as listed to the left of the figure) and download the summary tables (which are now broken into 5 sections). Supplementary information is also provided to assist users of the data evaluation. The website is currently being revised as noted in the 'Current Projects' section below.

**(a)** IUPAC Gas Kinetics homepage showing navigation links and a section for 'Evaluated Kinetic Data' with a 'Choose a category of dataset:' dropdown menu.

**(b) Drop down menu gives access to data sheets:**

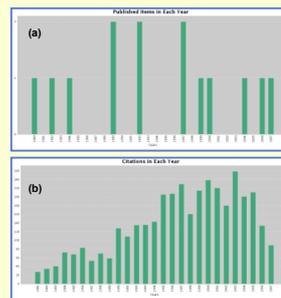
- Heterogeneous data sheets (non-reactive)
- Heterogeneous data sheets (reactive)
- Data sheets for photolysis of halogenated species
- Data sheets for gas phase O<sub>x</sub> reactions
- Data sheets for photolysis of O<sub>x</sub> species
- Data sheets for gas phase HO<sub>x</sub> reactions
- Data sheets for photolysis of HO<sub>x</sub> species
- Data sheets for gas phase NO<sub>x</sub> reactions
- Data sheets for photolysis of NO<sub>x</sub> species
- Data sheets for gas phase SO<sub>x</sub> reactions
- Data sheets for photolysis of SO<sub>x</sub> species
- Data sheets for gas-phase organic reactions: O<sub>x</sub> + VOC
- Data sheets for gas-phase organic reactions: HO<sub>x</sub> + VOC
- Data sheets for gas-phase organic reactions: NO<sub>3</sub> + VOC
- Data sheets for gas-phase organic reactions: halogens + VOC
- Data sheets for gas-phase organic reactions: organic peroxy radicals
- Data sheets for gas-phase organic reactions: organic alkoxy species
- Data sheets for gas-phase organic reactions: organic radicals + oxygen
- Data sheets for inorganic F O<sub>x</sub> reactions
- Data sheets for organic F O<sub>x</sub> reactions
- Data sheets for inorganic Cl O<sub>x</sub> reactions
- Data sheets for organic Cl O<sub>x</sub> reactions
- Data sheets for inorganic Br O<sub>x</sub> reactions
- Data sheets for organic Br O<sub>x</sub> reactions
- Data sheets for inorganic I O<sub>x</sub> reactions
- Data sheets for organic I O<sub>x</sub> reactions
- Data sheets for the photolysis of organic species

**Figure 1.** (a) IUPAC Gas Kinetics homepage and (b) drop-down menu showing different reaction categories.

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## Publications

The graphs below show (a) the number of publications which have been made by the Sub-committee in *J. Phys. Chem. Ref. Data* and, since 2004, in *Atmospheric Chemistry and Physics*, <http://www.copernicus.org/EGU/acpl/>, and (b) the total number of citations over the same period. It was decided to continue with publishing the evaluation, as well as having the web presence, in order to produce a peer-reviewed, citable and permanent archive of the data evaluation.



**Figure 2.** (a) Number of Sub-committee publications and (b) Citations of Sub-committee publications, according to the Web of Science.

## Scope

The Internet-based Gas Kinetic Data Evaluation consists of a summary table of reactions and preferred rate data, together with more detailed data sheets. Supplementary information is also included, which aims to assist individuals in their use of the data, and includes explanations of nomenclature and conventions etc. The data sheets are available in a series of categories which include:

- Gas phase and photolysis reactions of O<sub>x</sub>, HO<sub>x</sub>, NO<sub>x</sub> and SO<sub>x</sub> species.
- Gas-Phase and photolysis reactions of organic species (including reactions with HO<sub>x</sub>, NO<sub>3</sub> and halogen radicals).
- Reactions of organic peroxy radicals, organic alkoxy radicals and other organic radicals with oxygen.
- Gas Phase and photolysis reactions of inorganic FO<sub>x</sub>, ClO<sub>x</sub>, BrO<sub>x</sub> and IO<sub>x</sub> species.
- Gas Phase and photolysis reactions of organic halogen species.
- Uptake coefficients for non-reactive and reactive heterogeneous processes\*.

In carrying out its work the Sub-committee also aims to stimulate and direct further laboratory-based research, as well as encouraging consistent usage of the existing data.

## \*Current Projects

Evaluation of heterogeneous data is currently being carried out. This marks an extension to the Sub-committee's rôle. Until now the Sub-committee has only compiled homogeneous data: this new data evaluation will result in a fifth volume of the ACP series (see above). The term "heterogeneous" as applied to the atmosphere refers to multiphase chemistry that occurs on or in condensed phases, which are in contact with the gas phase. Atmospheric aerosol is greatly variable in composition, with both aqueous (water, salts (e.g. halide and sulphate), sulphuric acid, semi volatile organic) and solid (ice, acid hydrates, soot, mineral dust, salt) particles represented (a few examples are shown in Figure 3). Solid particles may also be coated with aqueous films; aqueous particles may include insoluble, solid material and may be coated with organic surface films. Heterogeneous reactions taking place at the gas-solid or gas-liquid interface are complex and are made up of several elementary physico-chemical processes such as gas phase diffusion towards the surface of interest, the mass accommodation rate, the desorption rate from the surface back to the gas phase, the chemical reaction rate at the interface, the diffusion into the bulk of the condensed phase and possible chemical reactions within the bulk condensed phase. It is clearly important for atmospheric modellers to be able to model heterogeneous processes, in order to be able to better understand atmospheric processes relevant to air quality and climate change. The publication of a data evaluation in this area will assist modellers and it will high-light areas in which laboratory research needs to be carried out.

As well as continuing the data evaluation work, members of the Subcommittee are active in pursuing additional funding for expansion of the existing website, in order to improve data access and forge links with other databases and atmospheric chemistry models. In particular, a NERC-funded project has commenced in which data from the IUPAC gas kinetics website will feed directly into a near-explicit atmospheric chemistry model (the Master Chemical Mechanism: <http://mcm.leeds.ac.uk/MCM/>), with the aim of providing a common interactive tool for atmospheric chemistry with modelling capabilities and data search and extract facilities. A data repository will also be developed, so that peer-reviewed data can be compiled at the earliest opportunity. Appropriate software and standards will be used throughout this project, in order to make the data easily accessible. For example, the search facility will make use of the InChi – the IUPAC Chemical Identifier (<http://www.iupac.org/inchi/>), which has been developed through the work of other IUPAC projects.

## Acknowledgements

A number of funding bodies, institutes and individuals have made the Gas Kinetics database possible, not least IUPAC. At this time, we would also particularly like to thank the EU ACCENT Programme and the UK's Natural Environment Research Council for funding a project, which will improve the website (as discussed above).



**Figure 3.** Images of surfaces on which heterogeneous processes may occur in the atmosphere.



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