

4.089 IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation.

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Abstract:

Emissions from human activities have led to important changes in the composition of the atmosphere. Computational models are used to understand the impacts of emissions on air quality on local, regional, and global scales and the global climate system. An accurate representation of atmospheric chemistry is of critical importance in these models. The mission of the International Union of Pure & Applied Chemistry (IUPAC) Task Group on Atmospheric Chemical Kinetic Data Evaluation is to provide evaluated kinetic data for gas-phase, heterogeneous, and aqueous-phase reactions. More than 1000 datasheets are maintained on the website here <http://iupac.pole-ether.fr>. From the website, it is possible to join the mailing list, access datasheets, search the database (by species names, formula, InChI, or SMILES) and download summary tables. The Summary Tables provide kinetic data on:

- Gas-phase reactions of Ox, NOx, HOx, SOx, organic compounds, inorganic and organic halogens
- Heterogeneous reactions on solid surfaces
- Heterogeneous reactions on liquid surfaces.

The datasheets provide summaries of experimental data and procedures organized in four broad groups:

- Gas-phase reactions.
- Photolysis reactions.
- Heterogeneous reactions on solid substrates.
- Heterogeneous reactions on liquid substrates

Datasheets are being added for aqueous-phase reactions. Recommended data are published periodically in a special issue of Atmospheric Chemistry and Physics here http://www.atmos-chem-phys.net/special_issue8.html