Summary of Evaluated Data for Atmospheric Heterogeneous Processes

IUPAC Subcommittee on Gas Kinetic Data Evaluation for Atmospheric Chemistry

Dr Markus Ammann
Laboratory of Radio- and Environmental Chemistry Paul Scherrer Institute, CH-5232 Villigen, Switzerland

Prof. R. Atkinson
Statewide Air Pollution Research Center and Department of Environmental Sciences, University of California, Riverside, California, USA.

Dr. R. A. Cox
Centre for Atmospheric Science, Chemistry Department, University of Cambridge, UK.

Dr. John Crowley
Department of Atmospheric Chemistry at the Max-Planck Institute for Chemistry, Mainz, Germany.

Dr Robert Hynes
CSIRO Energy Technology, Lucas Heights Science and Technology Centre, Building 2, PMB 7, Bangor, NSW 2234, Australia

Dr M. E. Jenkin
Imperial College, Department of Environmental Science and Technology, Silwood Park, Ascot, Berkshire SL5 7PY, UK

Dr. M. J. Rossi
Laboratoire de Pollution Atmosphérique et Sol (LPAS/DGR), Ecole Polytechnique Federale de Lausanne (EPFL), Lausanne, Switzerland

Prof. J. Troe
Institute of Physical Chemistry, University of Göttingen, Germany

Dr Tim Wallington
Ford Motor Company, Research and Advanced Engineering, Mail Drop RIC-2122, Dearborn, Michigan 48121-2053, USA

Prepared: January 2008.
By: R.A. Cox & G.D. Carver
Latest version available from : http://www.iupac-kinetic.ch.cam.ac.uk/

Introduction

The IUPAC Subcommittee for Data Evaluation for Atmospheric Chemistry have extended the scope of the treatment of heterogeneous reactions on this website. We are now in the process of replacing the *data tables* containing a compilation of uptake coefficient data for heterogeneous reactions of selected species with *data sheets* in which the relevant data for heterogeneous processes are evaluated and, where possible, recommendations are made for parameters describing the kinetics of these processes under atmospheric conditions. We also present *summary sheets* containing the recommended parameters. A detailed introduction to heterogeneous reactions has been prepared by the IUPAC Subcommittee and is available on the website. This provides background information on the models and definitions of the parameters used in these evaluations, and the rationale for the organisation of the material presented.

Reference numbers

The reference numbers listed in the Summary table below refer to the numbering used to reference the data sheets in the subcommittee publications in the journal Atmospheric Chemistry and Physics (ACP). The numbering scheme used is: "Volume". "Appendix". "Reaction" (e.g. V.A1.1).

Summary of preferred values of parameters for uptake on ice surfaces

Ref. No.	Species	α/γ	$\pm\Delta\alpha_s$	K_{linC} cm	N_{max} molecule cm^{-2}	$\Delta(E_{ads}/R)$ $\Delta \ln N_{max}$	Temp. K
V.A1.1	O	$7 \times 10^{-6} + 2.6 \times 10^{-24}$ exp(1370/T) [O_2]	± 0.3				110-150
V.A1.2	O_3	$<1 \times 10^{-8}$	0.7(Δlogγ)				220-260
V.A1.3	OH	0.03	± 0.02				
V.A1.4	HO_2			No recommendation			
V.A1.5	H_2O_2	0.02	0.5(Δlogγ)	1.6	3×10^{14}	±0.5 (Δlog K_{linC})	228-240
V.A1.6	H_2O			No recommendation			
V.A1.7	NO	$\leq 5 \times 10^{-6}$	1.0(Δlogγ)				
V.A1.8	NO_2			3.07×10^{-09} exp(2646/T)		±100	
V.A1.9	NO_3	$<1 \times 10^{-3}$	0.5(Δlogγ)				170-200
V.A1.10	NH_3	4×10^{-4}	0.5(Δlogγ)	No recommendation			190
V.A1.11	HONO	0.02	± 0.01	1.0×10^{-05} exp(3843/T)	3×10^{14}	±50	180-220
V.A1.12	HNO_3	> 0.2		7.5×10^{-5} exp(4585/T)	2.7×10^{14}	± 700	190-240
V.A1.13	HO_2NO_2	0.15	± 0.10	No recommendation			190-200
V.A1.14	N_2O_5	0.02	± 0.01				190-200
V.A1.15	SO_2	0.9×10^{-6}	$\pm 0.5 \times 10^{-6}$	See data sheet			210-240
V.A1.16	HCHO			0.7	2.7×10^{14}	± 0.3	198-223
V.A1.17	HCOOH			5.8×10^{-11} exp(6500/T)	2.2×10^{14}	± 300	187-221
V.A1.18	CH_3CHO			No recommendation			
V.A1.19	CH_3COOH			1.9×10^{-11} exp(6660/T)	2.4×10^{14}	± 300 0.1	195-240

V.A1.20	CH_3OH			$6.24 \times 10^{-12} \exp(6180/T)$	3.2×10^{14}	±100 0.15	
V.A1.21	C_2H_5OH			$5.0 \times 10^{-14} \exp(7500/T)$	2.8×10^{14}	±200 0.15	210-250
V.A1.22	C_3H_7OH			25.6	3.1×10^{14}	±0.2 (ΔK_{linC}) 0.15	228
V.A1.23	C_4H_9OH			$7.4 \times 10^{-16} \exp(9000/T)$	3.3×10^{14}	±1000 0.15	210-250
V.A1.24	$CH_3C(O)CH_3$			$1.0 \times 10^{-11} \exp(5850/T)$	2.7×10^{14}	±100 0.1	
V.A1.25	CH_3OOH						
V.A1.26	PAN			$1.49 \times 10^{-09} \exp(3608/T)$		±100	160-180
V.A1.27	HCl	0.3					190-210
				0.0219exp(2858/T)	3×10^{14}	± 920	208-230
V.A1.28	HOCl	0.085	0.5(Δlogγ)				180-200
				$3.06 \times 10^{-6} \exp(3841/T)$	3×10^{14}	± 1200	190-220
V.A1.29	ClO						
V.A1.30	HBr	$1 \times 10^{-5} \exp(840/T)$		4.14×10^{5}		Δ (E/R) = ± 500 K	188
						Δ log K = ± 0.3	180-200
V.A1.31	HOBr	0.35	0.3(Δlogγ)	No recommendation			180-210
		3.8×10^{-13} exp(5130/T)					210-240
V.A1.32	HI	0.2	0.3(Δlogγ)	2.29×10^{5}		Δ log K = ± 0.3	188
				0.54×10^{5}			195
V.A1.33	HOI						
V.A1.34	ICl						
V.A1.35	IBr						
V.A1.36	BrCl						