Summary of Evaluated Data for Atmospheric Heterogeneous Processes

IUPAC Subcommittee on Gas Kinetic Data Evaluation for Atmospheric Chemistry

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Introduction

The IUPAC Subcommittee for Data Evaluation for Atmospheric Chemistry have extended the scope of the treatment of heterogenous 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 is available on the website, prepared by the IUPAC Subcommittee, that provides background information on the models and parameters used in these evaluations, and the rational for the organisation of the material presented.

Reference numbers

The reference numbers listed in the table below refer to the numbering used 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 reactive uptake coefficient data for reactions on ice surfaces

Ref.No.	Species	α / γ_{ER}	$\Delta\alpha$	$K_{linC}(X)$ cm^{-1}	k_r cm^{2}s^{-1}	Δk_r cm^{2}s^{-1}	$\theta(Y)$ molecule cm^{-2}	Temp. K
V.A1.38	HONO + HCl	0.02	±0.01	1.0 x 10^{-5} exp(3843/T) (HONO)	7.0 x 10^{-21}	±2 x 10^{-21}	θ_{HCl} Langmuir: see HCl uptake	180-220
V.A1.39	HONO + HBr	0.02	±0.01	1.0 x 10^{-5} exp(3843/T) (HONO)	7.0 x 10^{-20}	±5 x 10^{-20}	3 x 10^{14} (HBr)	180-220
V.A1.40	HONO + HI	0.02	±0.01	1.0 x 10^{-5} exp(3843/T) (HONO)	1.6 x 10^{-20}	±1x 10^{-20}	3 x 10^{14} (HI)	180-220
V.A1.41	HOCl + HCl	0.2	±0.1	E-R mechanism			θ_{HCl} Langmuir: see HCl uptake	180-220
V.A1.42	HOCl + HBr	0.3	±0.15	See data sheet	3.3 x 10^{-15}		θ_{HBr} = 4.14 x10^{-10} [HBr]$^{0.88}$	188
V.A1.43	$ClONO_2 + H_2O$	0.5	±0.3	1.2 x 10^4 ($ClONO_2$)	5 x 10^{-17}		10^{15} (1 – 0.81θ_{HNO3})	218
				1.04 exp(2032/T)	5 x 10^{-17}		θ_{HNO3} Langmuir: see $HONO_2$ uptake	215-230
V.A1.44	$ClONO_2$ + HCl	0.24	±0.1	E-R mechanism			θ_{HCl} Langmuir: see HCl uptake	180-230
V.A1.45	$ClONO_2$ + HBr	0.56	±0.2	E-R mechanism			θ_{HBr} = 4.14 x10^{-10} [HBr]$^{0.88}$	188
V.A1.46	N_2O_5 + HCl			No recommendation			θ_{HCl} Langmuir: see HCl uptake	
V.A1.47	N_2O_5 + HBr			No recommendation				
V.A1.48	HOBr + HCl	0.24	±0.05				θ_{HCl} Langmuir: see HCl uptake	188 - 230
V.A1.49	HOBr + HBr	4.8 x 10^{-4} exp(1240/T)	0.15 (Δlog γ)					180 - 230
V.A1.50	$BrONO_2 + H_2O$	5.3x10^{-4} exp(1100/T)	$\Delta(E/R)$ = ±250 K					
V.A1.51	$BrONO_2$ + HCl	0.3	0.2 (Δlog γ)				θ_{HCl} Langmuir: see HCl uptake	190 - 200
V.A1.52	$BrONO_2$ + HBr	6.6 x 10^{-3} exp(700/T)	$\Delta(E/R)$ = ±250 K					180 - 210