

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet VI.A4.23 HET_SL_23

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This data sheet last evaluated: June 2010; last change in preferred values: June 2010



Experimental data

Parameter	Temp./K	Reference	Technique/ Comments
<i>Uptake coefficient, γ</i>			
0.02 – 0.235 (HBr = 2 – 96 × 10 ⁻⁹ atm)	228	Abbatt and Nowak, 1997	CWFT-MS (a)

Comments

- (a) (5-20) × 10¹⁰ molecule cm⁻³ HOCl admitted into the flow tube via the movable injector. Experimental uptake coefficients for HOCl were obtained at 228 K and 69.3 wt.% H₂SO₄ with various amounts of gas-phase HBr providing an excess concentration in the H₂SO₄ film.

Preferred Values

Parameter	Value	T/K
$k_{\text{HOCl}+\text{HBr}}$ (M ⁻¹ s ⁻¹)	1 × 10 ⁻⁷	228
α_b	1	228

Reliability

$\Delta \log k_{\text{HOCl}+\text{HBr}}$	0.3
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Comments on Preferred Value

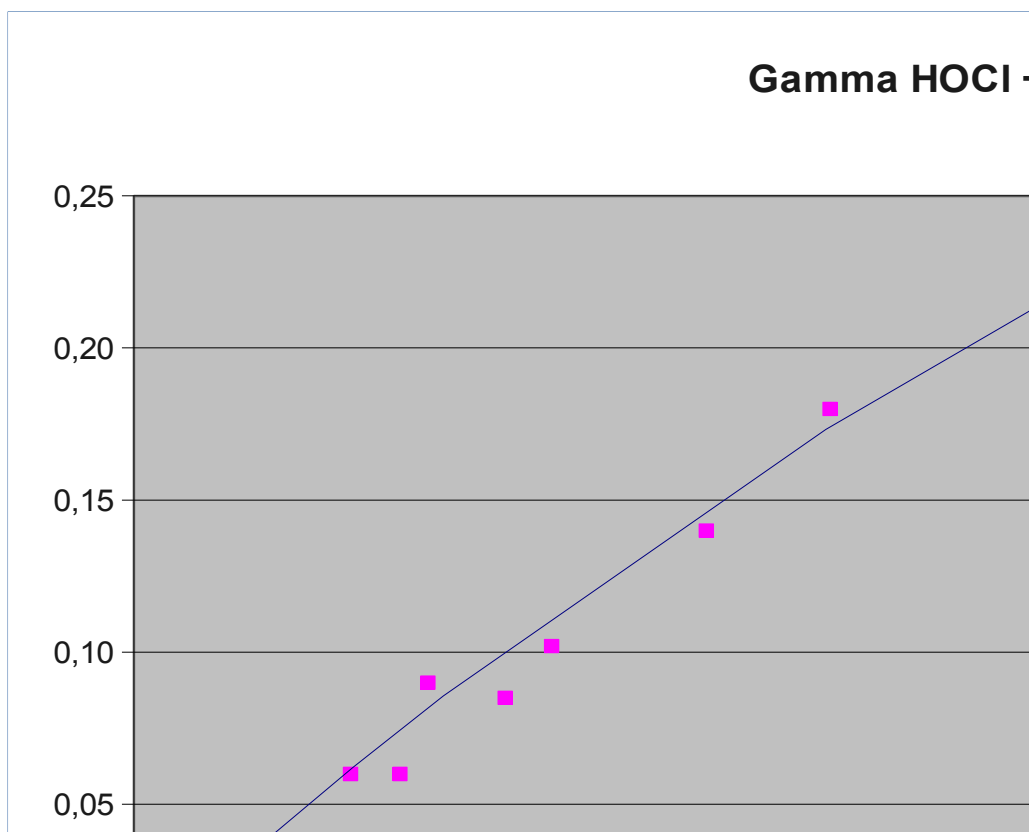
The preferred values are based on the dataset of Abbatt and Nowak, 1997. The expression:

$$\frac{1}{\gamma} = \frac{1}{\alpha_b} + \frac{1}{\Gamma_b} \quad \text{with} \quad \Gamma_b = \frac{4HRT\sqrt{D_l k_{\text{HOCl}+\text{HBr}}[\text{HBr}]}}{\bar{c}}$$

was constrained using preferred values of H and D_l for HOCl and H for HBr (IUPAC, 2010 datasheets VI.A4.17 and VI.A4.13a) with $k_{\text{HOCl}+\text{HBr}}$ varied to adjust γ to match the experimental data. α_b was assumed to be unity. The preferred value of $k_{\text{HOCl}+\text{HBr}}$ is larger than reported by Abbatt and Nowak owing to use of lower values of $H\sqrt{D_l}$. As noted by Abbatt and Nowak, the value of $k_{\text{HOCl}+\text{HBr}}$ is orders of magnitude larger than that reported for low-acidity aqueous solutions (Kumar and Margerum, 1987).

References

Abbatt, J. P. D. and Nowak, J. B.: J. Phys. Chem. A 101, 2131-2137, 1997.



Uptake coefficients for HOCl + HBr in H₂SO₄. Experimental data from Abbatt and Nowak, 1997. The solid line represents the IUPAC preferred values calculated using the parameters listed above.