# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet V.A2.5 MD5



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## $NO_3$ + mineral oxide (dust) surfaces

### Experimental data

| *Parameter* | Temp./K | Reference | Technique/ Comments |
|---|---|---|---|
| *Uptake coefficients: γ* | | | |
| $\gamma_{ss}$ = (6.7 ± 4.0) x$10^{-2}$ ($CaCO_3$) | 298 ± 2 | Karagulian and Rossi, 2006 | Knudsen-MS (a) |
| $\gamma_0$ = (13 ± 10) x$10^{-2}$ ($CaCO_3$) | | | |
| $\gamma_{ss}$ = (14 ± 2) x$10^{-2}$ (Kaolinite) | | | |
| $\gamma_0$ = (11 ± 8) x$10^{-2}$ (Kaolinite) | | | |
| $\gamma_{ss}$ (12 ± 8) x$10^{-2}$ (Saharan dust) | | | |
| $\gamma_0$ = (23 ± 20) x$10^{-2}$ (Saharan dust) | | | |
| $\gamma_{ss}$ = (10 ± 6) x$10^{-2}$ (Arizona dust) | | | |
| $\gamma_0$ = (20 ± 10) x$10^{-2}$ (Arizona dust) | | | |
| $\gamma$ = (12 ± 5) × $10^{-3}$ (Saharan dust, 0-70 % RH) | | Tang et al., 2010. | AFT-CRD (b) |

### Comments

(a) Continuous flow experiments using bulk samples (on a 19.6 $cm^2$ glass optical flat) prepared from a suspension in methanol or water (5-110 mg) or powder samples (up to 2000 mg) and pre-treated by drying under vacuum at 294 K until $H_2O$ desorption ceased (≈ 30 min). $NO_3$ (5 - 93 x $10^{11}$ molecule $cm^{-3}$) was generated by the thermal decomposition of $N_2O_5$. MS detection of $NO_3$ and $HNO_3$ was accompanied by REMPI detection of NO and $NO_2$ impurities / products. The uptake coefficients were calculated using the geometric surface area. A strong dependence of γ on $[NO_3]$ was observed, the values given are for $[NO_3]_0$ = 7 x $10^{11}$ molecule $cm^{-3}$.

(b) Relative rate approach in which the uptakes of $NO_3$ and $N_2O_5$ (at concentrations of ≤ $10^{10}$ molecule $cm^{-3}$) to Saharan dust aerosol were measured simultaneously. The Saharan dust sample (~1-2 mg) was supported on an inert Teflon membrane filter. No significant change in the relative uptake rate was observed when the relative humidity was varied from 0 to 70 %. The uptake coefficient ratio obtained, $\gamma(NO_3)/\gamma(N_2O_5)$ = 0.9 ± 0.4, was combined with the preferred value of $\gamma(N_2O_5)$ = 1.3 × $10^{-2}$ to give the value of $\gamma(NO_3)$ listed in the Table.

### Preferred Values

| Parameter | Value | T/K |
|---|---|---|
| γ | 1.2 × $10^{-2}$ | 298 |
| *Reliability* | | |
| Δ log (γ) | 0.5 | 298 |

*Comments on Preferred Values*

Karagulian and Rossi (2005) found efficient and irreversible uptake of $NO_3$ to various mineral dust substrates. A strong dependence of $\gamma$ on $[NO_3]$ may imply that interaction of $[NO_3]$ with the dust samples uptake is not simply defined by $\gamma$. With the exception of kaolinite, the ratio of $\gamma_0 / \gamma_{ss}$ was found to be $\approx$ a factor of two. As the uptake coefficients were based on the projected, geometric surface area of the dust sample, they represent upper limits. Tang et al. (2010), used a relative rate approach, which allowed them to derive uptake coefficients relative to $N_2O_5$ on the same substrate. This eliminated the need for absolute surface area estimation. As Tang et al. used the same dust as in their absolute AFT experiments (Wagner et al, 2008) the relative rate measurement can be reliably converted to an absolute one. The much smaller uptake coefficient for $NO_3$ + Saharan dust determined by Tang et al. compared to Karagulian et al. (despite use of the same dust sample) most probably reflects use of the geometric surface area to derive $\gamma$ in the Knudsen reactor experiments. As Tang et al point out, the two absolute studies of Karagulian et al (2005, 2006) on $N_2O_5$ and $NO_3$ uptake to Saharan dust also result on an uptake coefficient ratio close to unity, supporting the dataset of Tang et al., which provides the basis of our recommendation.

## References


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