# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet III.A3.64 IBrOx7



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**$Br + NO_2 + M \rightarrow BrONO + M$**

$\Delta H° = -81$ kJ·mol$^{-1}$

## Low-pressure rate coefficients

### Rate coefficient data

| $k_0$/cm$^3$ molecule$^{-1}$ s$^{-1}$ | Temp./K | Reference | Technique/ Comments |
|---|---|---|---|
| *Absolute Rate Coefficients* | | | |
| $(3.7 \pm 0.7) \times 10^{-31}$ [He] | 298 | Mellouki et al., 1989 | DF-EPR/MS (a) |
| $(2.75 \pm 0.55) \times 10^{-31}$ [He] | 298 | Kreutter, Nicovich and Wine, 1991 | PLP-RF (b) |
| $4.24 \times 10^{-31} (T/300)^{-2.4}$ [$N_2$] | 259-346 | | |

### Comments

(a) Pressure range 0.8-2.8 mbar.

(b) Pressure range 16.7-933 mbar; measurements in the bath gases He, Ar, $H_2$, $N_2$, $CO_2$, $CF_4$ and $SF_6$. Falloff curves were analyzed with $F_c = 0.59$ at 259 K, 0.55 at 298 K, and 0.50 at 346 K.

### Preferred Values

$k_0 = 4.2 \times 10^{-31} (T/300)^{-2.4}$ [$N_2$] cm$^3$ molecule$^{-1}$ s$^{-1}$ over the temperature range 250-350 K.

*Reliability*

$\Delta \log k_0 = \pm 0.3$ at 298 K.

$\Delta n = \pm 1$.

*Comments on Preferred Values*

The preferred values are based on the results of the study of Kreutter et al. (1991). The falloff curves are represented with $F_c = 0.55$. Broske and Zabel (1998) as well as Orlando and Burkholder (2000) identified BrONO to be the major product of the reaction and reevaluated the thermochemistry data from Kreutter et al. (1991).

## High-pressure rate coefficients
## Rate coefficient data

| $k_\infty$/cm$^3$ molecule$^{-1}$ s$^{-1}$ | Temp./K | Reference | Technique/ Comments |
|---|---|---|---|
| *Absolute Rate Coefficients* | | | |
| 2.66 x $10^{-1}$ | 259-346 | Kreutter, Nicovich and Wine, 1991 | PLP-RF (a) |

## Comments

(a) See comment (b) for $k_0$.

## Preferred Values

$k_\infty$ = 2.7 x $10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, independent of temperature over the range 250-350 K.

*Reliability*

$\Delta \log k_\infty = \pm 0.4$ over the range 250-350 K.

$\Delta n = \pm 1$.

*Comments on Preferred Values*

See comments on $k_0$. There is only a single determination of $k_\infty$, but the measured falloff curve appears well behaved with rate coefficients close to those of the reactions I + NO + M and I + $NO_2$ + M.

The following text-line combines the preferred values for the high and low pressure limiting rate coefficients to generate a single, cut-and-paste expression for calculation of $k$:

=((4.2e-31*(*T*/300)^-2.4)*M*(2.7e-11))/((4.2e-31*(*T*/300)^-2.4)*M+(2.7e-11))*10^(log10(0.55)/(1+(log10((4.2e-31*(*T*/300)^-2.4)*M/(2.7e-11))/(0.75-1.27*log10(0.55)))^2))

The molecular density, M = $7.243\times10^{21}$P(bar)/T(K)

## References


Broske, R. and Zabel, F.: J. Phys. Chem. A, 102, 8626, 1998.
Kreutter, K. D., Nicovich, J. M. and Wine, P. H.: J. Phys. Chem., 95, 4020, 1991.
Mellouki, A., Laverdet, G., Jourdain, J. L. and Poulet, G.: Int. J. Chem. Kinet., 21, 1161, 1989.
Orlando, J. J. and Burkholder, J. B.: J. Phys. Chem. A, 104, 2048, 2000.