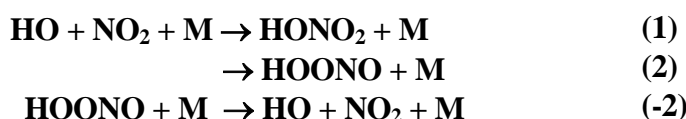


# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet I.A3.43 NOx13

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This data sheet last evaluated: Nov. 2017; last change in preferred values: Nov. 2017.



$$\Delta H^\circ(1) = -207.6 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta H^\circ(2) = -86 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta H^\circ(-2) = 86 \text{ kJ}\cdot\text{mol}^{-1}$$

## Low-pressure rate coefficients Rate coefficient data ( $k = k_1 + k_2$ )

| $k_0/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$      | Temp./K | Reference                | Technique/ Comments |
|---|---------|--------------------------|---------------------|
| <i>Absolute Rate Coefficients</i>                           |         |                          |                     |
| $2.3 \times 10^{-30} (T/295)^{-2.5} [\text{N}_2]$           | 240-450 | Anderson et al., 1974    | DF-RF (a)           |
| $2.9 \times 10^{-30} [\text{N}_2]$                          | 296     | Howard and Evenson, 1974 | DF-LMR (b)          |
| $2.6 \times 10^{-30} (T/296)^{-2.6} [\text{N}_2]$           | 220-550 | Anastasi and Smith, 1976 | FP-RA (c)           |
| $(2.6 \pm 0.4) \times 10^{-30} (T/300)^{-2.8} [\text{N}_2]$ | 247-352 | Wine et al., 1979        | RP-RF (d)           |
| $(2.7 \pm 0.2) \times 10^{-30} [\text{N}_2]$                | 295     | Burrows et al., 1983     | DF-RF (e)           |
| $(3.39 \pm 0.26) \times 10^{-30} [\text{N}_2]$              | 300     | Donahue et al., 1997     | DF-LIF (f)          |
| $2.47 \times 10^{-30} (T/300)^{-2.97} [\text{N}_2]$         | 220-250 | Brown et al., 1999       | PLP-LIF (g)         |
| $2.85 \times 10^{-30} (T/300)^{-2.67} [\text{N}_2]$         | 220-300 | Dransfield et al., 1999  | DF-LIF (h)          |
| $(2.5 \pm 0.3) \times 10^{-30} [\text{N}_2]$                | 298     | D'Ottone et al., 2001    | PLP-LIF(i)          |
| $(1.67 \pm 0.08) \times 10^{-30} [\text{N}_2]$              | 298     | Mollner et al., 2010     | PLP-LIF (j)         |

## Comments

- Measurements over the range 1-10 Torr. Evaluation assuming limiting third order behavior.
- Measurements over the range 0.4-5 Torr. Evaluation assuming limiting third order behavior.
- Measurements using bath gas concentrations of  $3.2\text{-}160 \times 10^{17} \text{ molecule cm}^{-3}$ . Falloff extrapolation using Kassel integrals towards  $k_0$  in agreement with data from Anderson et al. (1974) and Howard and Evenson (1974). Extrapolation towards  $k_\infty$  oversimplified, but data in the intermediate falloff range in agreement with later work.
- Measurements using bath gas concentrations of  $5.4\text{-}230 \times 10^{17} \text{ molecule cm}^{-3}$ . Extrapolation of the falloff data with  $F_c = 0.7$  leads to the given  $k_0$ .
- Measurements using bath gas concentrations of 1-5 Torr. Evaluation assuming limiting third order behavior.

- (f) Measurements over the range 2-600 Torr. Evaluation of the falloff curve with  $F_c = 0.3 \pm 0.03$  and  $k_\infty = 4.77 \pm 1.04 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ . Fit based on data from this work and Anderson et al.(1974), Howard and Evenson (1974), Anastasi and Smith (1976), Wine et al. (1979) and Burrows et al. (1983).
- (g) Measurements over the range 20-250 Torr. Evaluation of the falloff curve with  $F_c = 0.6$  and  $k_\infty = 1.45 \times 10^{-11} (T/300)^{-2.77} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ .
- (h) Measurements over the range 50-150 Torr. Evaluation of the falloff curve with  $F_c = \exp(-T/363)$  and  $k_\infty = 3.13 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ . Fit based on data from this work and Anderson et al.(1974), Howard and Evenson (1974), Anastasi and Smith (1976), Wine et al. (1979), Burrows et al. (1983), Donahue et al. (1997) and Brown et al. (1999).
- (i) Measurements over the range 30-700 Torr at 273 and 298 K. Data evaluated with  $F_c = 0.6$  and  $k_\infty = (2.4 \pm 1.7) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ . The use of  $F_c = 0.4$  would lead to  $k_0 = 3.7 \times 10^{-30} (T/300)^{-3.0} [\text{N}_2] \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  and  $k_\infty = 4.6 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ .
- (j) Measurements over the range 50-900 Torr. Evaluation of the falloff curve with  $F_c = 0.6$  and  $k_\infty = 1.07 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ . Measurements in air suggest  $k_0$  to be a factor of 0.94 smaller than for  $M = \text{N}_2$ .  $k_1 = (9.2 \pm 0.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 700 Torr of air and 298 K was determined. The ratio  $k_2/k_1$  at 298 K was found to increase from 0.076 at 100 Torr of  $\text{N}_2$  to 0.149 at 762 Torr. Fitting the falloff curves for  $k_1$  and  $k_2$  was done with  $F_{c,1} = F_{c,2} = 0.6$ ,  $k_{0,1} = 1.51 \times 10^{-30} [\text{air}] \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{0,2} = 6.2 \times 10^{-32} [\text{air}] \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ,  $k_{\infty,1} = 2.58 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , and  $k_{\infty,2} = 8.1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K.

### Preferred Values

$k_{0,1} = 3.2 \times 10^{-30} (T/300)^{-4.5} [\text{N}_2] \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  over the temperature range 220 -400 K.

$k_{0,2} = 1.0 \times 10^{-31} (T/300)^{-4.5} [\text{N}_2] \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  over the temperature range 220 -400 K.

### Comments on Preferred Values

The differences between the various values of  $k_0$  in part are due to different experimental results, in part they arise from different falloff expressions using either  $F_c = 0.6$  or smaller values of  $F_c$ . While the differences of the experiments are small near to the low pressure limit, they become increasingly pronounced towards the center of the falloff curve where essentially two groups of results have been obtained, those with higher rate constants (Anastasi and Smith, 1976; Wine et al. 1979; Brown et al., 1999; D'Ottone et al., 2001) and those with lower values (Donahue et al., 1997 and Dransfield et al., 1999). The most detailed measurements by Mollner et al. (2010) have clearly favored the higher values. The extrapolation towards  $k_0$  depends on the chosen values for  $F_c$  and  $k_\infty$ . While experimental information on  $k_\infty$  is available (see preferred values of  $k_\infty$ ),  $F_c$  better is obtained from modelling (Troe, 2001; Golden and Smith, 2000; Golden et al., 2003; Zhang and Donahue, 2006; Hippler et al., 2006; Troe, 2012). However, such modelling has been done on quite different levels of theory. Here, we prefer the approach from Troe (2001, 2012), which gave  $F_c = 0.41$  essentially independent of the temperature. The temperature coefficient of  $k_0$  is also taken from the analysis made by Troe (2001, 2012). A combination of the measurements by Mollner et al. (2010) and the detailed analysis by Troe (2012) has led to a reconciliation of full falloff curves for  $k_1$  and  $k_2$  over wide ranges of conditions. The derived limiting rate coefficients of the two approaches differ because Mollner et al. (2010) assumed  $F_{c,1} \approx F_{c,2}$  to be equal to 0.6 while Troe (2012) derived  $F_{c,1} \approx F_{c,2}$  from the experiments close to a value of 0.41 in agreement with the theoretical estimate from Troe (2001). The preferred values are taken from Troe (2012) on the basis of falloff curves such as expressed in the Introduction with  $F_c = 0.41$ . Slightly better results are obtained with asymmetric broadening factors (which requires slightly larger  $k_{1,\infty}$  and  $k_{2,\infty}$ , see Troe, 2012).

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

| $k_{\infty}/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ | Temp./K | Reference                  | Technique/ Comments |
|---|---------|----------------------------|---------------------|
| <i>Absolute Rate Coefficients</i>                             |         |                            |                     |
| $\geq 3.5 \times 10^{-11}$                                    | 297     | Wine et al., 1979          | FP-RF (a)           |
| $\geq 3.0 \times 10^{-11}$                                    | 295     | Robertshaw and Smith, 1982 | PLP-LIF (b)         |
| $7.5 \times 10^{-11}$   | 298     | Forster et al., 1995       | PLP-LIF (c)         |
| $(4.77 \pm 1.04) \times 10^{-11}$                             | 300     | Donahue et al., 1997       | DF-LIF (d)          |
| $(7.5 \pm 2.2) \times 10^{-11}$                               | 250-400 | Fulle et al., 1998         | PLP-LIF (e)         |
| $1.45 \times 10^{-11} (T/300)$                                | 220-250 | Brown et al., 1999         | PLP-LIF (f)         |
| $3.13 \times 10^{-11}$  | 220-300 | Dransfield et al., 1999    | DF-LIF (g)          |
| $(2.4 \pm 1.7) \times 10^{-11}$                               | 298     | D'Ottone et al., 2001      | DF-LIF (h)          |
| $(5.0 \pm 2) \times 10^{-11}$                                 | 250-600 | Hippler et al., 2002, 2006 | PLP-LIF (i)         |
| $(4.8 \pm 0.8) \times 10^{-11}$                               | 298     | Smith and Williams, 1985   | PLP-LIF (j)         |
| $(6.4 \pm 0.3) \times 10^{-11}$                               | 298     | D'Ottone et al., 2005      | PLP-LIF (k)         |
| $10.7 \times 10^{-11}$  | 298     | Mollner et al., 2010       | PLP-LIF (l)         |

**Comments**

- (a) See comment (d) for  $k_0$ . Extrapolation of the falloff curve with  $F_c = 0.7$  leads to the given lower limit of  $k_{\infty}$ .
- (b) Measurements in the bath gases Ar up to 4 bar and  $\text{CF}_4$  up to 8.6 bar.
- (c) Measurements in a static high pressure cell with the bath gas He over the range  $7.6 \times 10^{18}$ - $3.6 \times 10^{21}$  molecule  $\text{cm}^{-3}$  (1-150 bar).
- (d) See comment (f) for  $k_0$ .
- (e) See comment (c). Measurements in He at 250 K between 1.04 and 140 bar, at 300 K between 113 and 1330 bar, and at 400 K between 1.6 and 1370 bar. High pressure flow cell used below 8 bar, static cell used above 200 bar. Falloff extrapolations with  $k_0 = 1.6 \times 10^{-30} (T/300)^{-2.9}$  [He]  $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  and  $F_c = 0.45$  (268 K), 0.41 (300 K), and 0.33 (400 K).
- (f) See comment (g) for  $k_0$ .
- (g) See comment (h) for  $k_0$ .
- (h) See comment (i) for  $k_0$ .
- (i) See comment (c) and (e); repeated measurements in high pressure flow cells revealed that those measurements from Forster et al. (1995) and Fulle et al. (1998), which were done in a static high pressure cell (pressures above 200 bar), gave  $k_{\infty}$  values which are about 30 % too high. Nonexponential profiles of HO decay above 400 K at pressures around 100 bar indicate that HOONO isomers are formed besides  $\text{HNO}_3$  which become thermally unstable on a  $\mu\text{s}$ -time scale under these conditions.
- (j) Pulsed laser photolysis – LIF study of the vibrational relaxation  $\text{HO} (\nu = 1) + \text{NO}_2 \rightarrow \text{HO} (\nu = 0) + \text{NO}_2$ .
- (k) Pulsed laser photolysis-LIF study of vibrational relaxation  $\text{HO} (\nu = 1-5) + \text{NO}_2 \rightarrow \text{HO} (\nu = 0) + \text{NO}_2$ . Oxygen isotope effects were observed. Non-exponential profiles of HO decay in the recombination were obtained which are consistent with a yield of HOONO of 10( $\pm$ ) % at 500mbar of He and 400 K.
- (l) See comment (j) for  $k_0$ .

## Preferred Values

$k_{\infty,1} = 3.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  over the temperature range 220-400 K.

$k_{\infty,2} = 3.5 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  over the temperature range 220-400 K.

### Comments on Preferred Values

See comments on preferred values of  $k_0$ . The preferred values of  $k_{\infty}$  are based on the latest measurements from Hippler et al. (2006), a falloff extrapolation using the theoretical value of  $F_c = 0.41$  from Troe (2001, 2012) and the vibrational relaxation rate constant from D'Ottone et al. (2005). The preferred value of  $k(1\text{bar})$  corresponds to the present preferred values of  $k_0$  and  $k_{\infty}$  and  $F_c = 0.41$ . It agrees with the results from Anastasi and Smith (1976), D'Ottone et al. (2001), and Mollner et al. (2010).

The formation of HOONO isomers has been studied extensively (Burkholder et al., 1987; D'Ottone et al., 2005; Golden and Smith, 2000; Chakraborty et al., 1998; Matheu and Green, 2000; Dransfield et al., 2001; Sumathi and Peyerimhoff, 1997; Donahue et al., 2001; Nizkorodov and Wennberg, 2002; Bean et al., 2003; Mollner et al., 2010) and included in detailed modelling of the kinetics of the competing and linked formation of the HOONO and HONO<sub>2</sub> isomers. The ratio  $k_{\infty,1}/k_{\infty,2}$  remains relatively uncertain. The preferred values are based on a combination of the measurements by Hippler et al. (2006), Mollner et al. (2010), and the analysis by Troe (2012). Evaluation of the falloff curves with asymmetric broadening factors from Troe (2012) leads to  $k_{\infty,1} = 2.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  and  $k_{\infty,2} = 4.8 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ . The preferred values instead correspond to symmetric broadening factors. Theoretical predictions of  $k_{\infty,1}$  and  $k_{\infty,2}$  from Zhu and Lin (2003), Williams et al. (2007), and Chen et al. (2007) so far lead to controversial results. A small decrease of  $k$  (1 bar) with increasing water content in air near 298 K has been detected by Sadanaga et al. (2006).

Based on experiments by Hippler et al. (2002) at 430-475 K, the analysis of these data by Golden et al. (2003, 2004) and later theoretical work, an equilibrium constant  $K_{\text{eq}}$  for dissociation of cis,cis-HOONO decomposition (-2) of  $K_{\text{eq}} = k_2/k_{-2} = 3.5 \times 10^{-27} \exp(10135/T) \text{ cm}^3 \text{ molecule}^{-1}$  was determined, see Burkholder et al. (2015). Based on this result and the preferred values for  $k_2$  of the present evaluation, one obtains falloff curves for  $k_{-2}$  with the values for  $k_{0,-2} = 2.86 \times 10^{-5} (T/300)^{-4.5} \exp(-10135/T) [\text{N}_2] \text{ s}^{-1}$ ,  $k_{\infty,-2} = 1.0 \times 10^{16} \exp(-10135/T) \text{ s}^{-1}$ , and  $F_{c,-2} = 0.41$ .

### Preferred Values

| Parameter   | Value  | T/K     |
|---|--|---------|
| $k_{0,1} / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$                | $3.2 \times 10^{-30} (T/300)^{-4.5} [\text{N}_2]$                | 220-400 |
| $k_{\infty,1} / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$           | $3.0 \times 10^{-11}$  | 220-400 |
| $k_1(1 \text{ bar N}_2) / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ | $9.8 \times 10^{-12}$  | 298     |
| $F_{c,1}$   | 0.41   | 220-400 |
| $k_{0,2} / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$                | $1.0 \times 10^{-31} (T/300)^{-4.5} [\text{N}_2]$                | 220-400 |
| $k_{\infty,2} / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$           | $3.5 \times 10^{-11}$  | 220-400 |
| $k_2(1 \text{ bar N}_2) / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ | $1.4 \times 10^{-12}$  | 298     |
| $F_{c,2}$   | 0.41   | 220-400 |
| $k_{0,-2} / \text{s}^{-1}$  | $2.86 \times 10^{-5} (T/300)^{-4.5} \exp(-10135/T) [\text{N}_2]$ | 220-400 |
| $k_{\infty,-2} / \text{s}^{-1}$   | $1.0 \times 10^{16} \exp(-10135/T)$                              | 220-400 |
| $F_{c,-2}$  | 0.41   | 220-400 |
| $k_{-2}(1 \text{ bar N}_2) / \text{s}^{-1}$                                 | 0.7  | 298     |

|                             |            |         |
|-----------------------------|------------|---------|
| <i>Reliability</i>          |            |         |
| $\Delta \log k_{0,1}$       | $\pm 0.05$ | 298     |
| $\Delta \log k_{\infty,1}$  | $\pm 0.3$  | 298     |
| $\Delta n_{0,1}$            | $\pm 0.5$  | 220-400 |
| $\Delta n_{\infty,1}$       | $\pm 0.5$  | 220-400 |
|                             |            |         |
| $\Delta \log k_{0,2}$       | $\pm 0.1$  | 298     |
| $\Delta \log k_{\infty,2}$  | $\pm 0.3$  | 298     |
| $\Delta n_{0,2}$            | $\pm 0.5$  | 220-400 |
| $\Delta n_{\infty,2}$       | $\pm 0.5$  | 220-400 |
|                             |            |         |
| $\Delta \log k_{0,-2}$      | $\pm 0.3$  | 298     |
| $\Delta \log k_{\infty,-2}$ | $\pm 0.3$  | 298     |
| $\Delta n_{0,-2}$           | $\pm 0.5$  | 220-400 |
| $\Delta n_{\infty,-2}$      | $\pm 0.5$  | 220-400 |

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  $k_f$ :

$$= ((3.2e-30*(T/300)^{-4.5}*M*(3.0e-11))/((3.2e-30*(T/300)^{-4.5}*M+(3.0e-11))*10^{(\log_{10}(0.41)/(1+(\log_{10}((3.2e-30*(T/300)^{-4.5}*M/(3.0e-11))/(0.75-1.27*\log_{10}(0.41))))^2}))$$

$k_2$ :

$$= ((1.0e-31*(T/300)^{-4.5}*M*(3.5e-11))/((1.0e-31*(T/300)^{-4.5}*M+(3.5e-11))*10^{(\log_{10}(0.41)/(1+(\log_{10}((1.0e-31*(T/300)^{-4.5}*M/(3.5e-11))/(0.75-1.27*\log_{10}(0.41))))^2}))$$

and  $k_{-2}$ :

$$= ((2.86e-5*(T/300)^{-4.5}*\exp(-10135/T))*M*(1.0e16*\exp(-10135/T)))/((2.86e-5*(T/300)^{-4.5}*\exp(-10135/T))*M+(1.0e16*\exp(-10135/T))*10^{(\log_{10}(0.41)/(1+(\log_{10}((2.86e-5*(T/300)^{-4.5}*\exp(-10135/T))*M/(1.0e16*\exp(-10135/T))/(0.75-1.27*\log_{10}(0.41))))^2}))$$

The molecular density,  $M = 7.243 \times 10^{21} P(\text{bar})/T(\text{K})$ .

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